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THREE-DIMENSIONAL NAPL FATE AND TRANSPORT MODEL

by

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Foreword

The U. S. Environmental Protection Agency is charged by Congress with protecting the Nation's land, air, and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between activities and the ability of natural systems to support and nurture life. To meet these mandates, EPA's research program is providing data and technical support for solving environmental problems today and building a science knowledge base necessary to manage our ecological resources wisely, understand how pollutants affect our health, and prevent or reduce environmental risks in the future.

The National Risk Management Research Laboratory is the Agency's center for investigation of technological and management approaches for reducing risks from threats to human health and the environment. The focus of the Laboratory's research program is on methods for the prevention and control of pollution to air, land, water, and subsurface resources; protection of water quality in public water systems; remediation of contaminated sites and ground water; and prevention and control of indoor air pollution. The goal of this research effort is to catalyze development and implementation of innovative, cost-effective environmental technologies; develop scientific and engineering information needed by EPA to support regulatory and policy decisions; and provide technical support and information transfer to ensure effective implementation of environmental regulations and strategies.

Simulation models are needed for analyzing and predicting the fate and transport of nonaqueous phase liquids (NAPLs) in the subsurface environment and to assess the effectiveness of remedial actions at NAPL contaminated sites. There are a number of crucial questions concerning the physical, chemical, and biological processes affecting the fate and transport of NAPLs that can only be addressed by modeling the processes under realistic conditions taking into account aquifer heterogeneities, compositional phenomena, geochemistry, microbiology, and other complications. This report describes the development, testing and validation of a comprehensive flow and transport simulator (UTCHEM) that can model fate and transport of NAPLs as well as processes for their remediation. Illustrations of both surfactant remediation and bioremediation of contaminated aquifers are given.

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Abstract

We have added several new and significant capabilities to UTCHEM to make it into a general-purpose NAPL simulator. The simulator is now capable of modeling transient and steady-state three-dimensional flow and mass transport in the groundwater (saturated) and vadose (unsaturated) zones of aquifers. The model allows for: changes in fluid properties as a site is remediated; heterogeneous aquifer properties; the flow and transport of remedial fluids whose density, viscosity and temperature are variable, including surfactants, cosolvents and other enhancement agents; the dissolution and/or mobilization of NAPLs by nondilute remedial fluids; and chemical and microbiological transformations. Appropriate physical, chemical and biological process models important in describing the fate and transport of NAPLs in contaminated aquifers have been incorporated into the simulator, such as multiple organic NAPL phase, nonequilibrium interphase mass transfer, sorption, microbiological and geochemical reactions, and the temperature dependence of pertinent chemical and physical properties. The biodegradation model includes inhibition, sequential use of electron acceptors, and cometabolism and can be used to model a very general class of bioremediation processes. The model can be used to simulate the actual field operation of remediation activities such as surfactant remediation or bioremediation as well as laboratory experiments with large-scale aquifer models.

A systematic evaluation was undertaken to assess the applicability and accuracy of all physical and chemical models of the various pertinent phenomena such as capillary pressure, relative permeability, adsorption, nonequilibrium mass transfer, dispersion, and phase behavior. The microbiological model suitable for very general bioremediation simulations was added to UTCHEM and tested with data from the literature with good agreement. Comparisons to analytical solutions were made and numerical dispersion control and accuracy testing were performed. The model was tested against experimental and field data. The FORTRAN source code has been delivered to EPA along with sample input and output files.

This report contains 12 sections. Section 1 gives an overview of the project objectives and accomplishments. Sections 2 through 12 describe the formulation of UTCHEM. Appendix A contains the user's guide for UTCHEM, Appendix B contains the user's guide for UTCHEM local grid refinement. Appendix C presents the discretized flow equations.

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Section 1
Project Summary

1.1 Introduction

Pioneering research conducted at The University of Texas at Austin has provided a scientific and engineering basis for modeling the enhanced recovery of oil and the enhanced remediation of aquifers through the development and application of compositional simulators. This research has resulted in the development and application of a 3-D, multicomponent, multiphase, compositional model of chemical flooding processes, UTCHEM, which accounts for complex phase behavior, chemical and physical transformations and heterogeneous porous media properties, and uses advanced concepts in high-order numerical accuracy and dispersion control and vector and parallel processing. The simulator was originally developed by Pope and Nelson in 1978 to simulate the enhanced recovery of oil using surfactant and polymer processes. Thus, the complex phase behavior of micellar fluids as a function of surfactant, alcohol, oil, and aqueous components was developed early and has been extensively verified against enhanced oil recovery experiments. Generalizations by Bhuyan *et al.* in 1990 have extended the model to include other chemical processes and a variety of geochemical reactions between the aqueous and solid phases. The nonequilibrium dissolution of organic components from a nonaqueous phase liquid (NAPL) into a flowing aqueous or microemulsion phase is modeled using a linear mass-transfer model. In this simulator, the flow and mass-transport equations are solved for any number of user-specified chemical components (water, organic contaminants, surfactant, alcohols, polymer, chloride, calcium, other electrolytes, microbiological species, electron acceptors, etc.). These components can form up to four fluid phases (air, water, oil, microemulsion) and any number of solid minerals depending on the overall composition. The microemulsion forms only above the critical micelle concentration (CMC) of the surfactant and is a thermodynamically stable mixture of water, surfactant and one or more organic components. All of these features taken together, but especially the transport and flow of multiple phases with multiple species and multiple chemical and biological reactions make UTCHEM unique. A description of UTCHEM model formulation is given in Delshad *et al.* [1996].

The objective of this research was to develop, validate and apply a three-dimensional, multiphase, multicomponent model capable of simulating the fate and transport of NAPLs in the saturated and unsaturated zones of confined and unconfined aquifers undergoing enhanced remediation. The model is capable of simulating multiple solids and fluid phases (water/air/NAPL) under realistic aquifer conditions and transformations of both inorganic and microbiological species. The specific objectives of this research were:

- Develop a three-dimensional simulation model capable of evaluating aquifer remediation methods using enhanced dissolution and/or mobilization of NAPLs trapped at residual saturation in aquifers. The simulator is capable of modeling transient and steady-state, three-dimensional flow and mass transport in the groundwater (saturated) and vadose (unsaturated) zones of aquifers. The simulator allows for changes in fluid properties as a site is remediated; heterogeneous aquifer properties; the flow and transport of remedial fluids whose density, viscosity and temperature are variable, including surfactants, cosolvents, microbes, and other enhancement agents; the dissolution of NAPLs by nondilute remedial fluids; and chemical and microbiological transformations. Nondilute components such as surfactant can and typically do cause large changes in phase volumes, phase velocities, and phase properties that cannot be accurately modeled by assuming these components are at very low concentrations so that they follow the conventional advection-reaction-dispersion equation used in almost all groundwater models. Rather, more general mass-balance equations and constitutive equations such as those used here must be solved. The resulting set of equations are highly nonlinear and more difficult to solve than those in conventional models, but provide a vastly more general and accurate description of the processes that actually occur in aquifers undergoing remediation, the migration of NAPLs in the subsurface, and the natural attenuation processes of NAPLs in the subsurface. Many of these processes such as the migration of the NAPLs during and after a spill or disposal operation involve the flow of two or more phases, which requires the modeling of relative permeability and other effects related to multiphase flow.

- Incorporate appropriate physical, chemical, and biological process models important in describing the fate and transport of contaminants in aquifers, such as nonequilibrium interphase mass transfer, sorption, decay processes, microbiological and geochemical reactions, capillary pressure and relative permeability.

- Incorporate numerical-dispersion-minimization techniques and efficient solution algorithms into the model.

- Evaluate the model through a series of tests including comparison with analytical solutions, experimental data, and results from other models. Present a theoretical analysis and demonstration of the numerical dispersion control and minimization techniques employed in the model.

- Demonstrate the stability and robustness of the model with sensitivity analysis simulations using various aquifer conditions (surface spill conditions, initial saturation distributions) and heterogeneities (spatial variations of permeability and porosity).

- Evaluate this new model by comparison with data from actual field operations of remediation, in particular, surfactant-enhanced remediation at the Canadian Forces Borden site and other large-scale model aquifer or field operations such as the one recently completed at the Air Force Base in Utah.

- Provide copies of the UTCHEM source code and the user's guide to U.S. EPA personnel.

1.2 Model Development

During the past three years, we have added several new and significant capabilities to UTCHEM to make it into a general-purpose NAPL simulator. These new features are discussed below. The simulator is now capable of modeling transient and steady-state three-dimensional flow and mass transport in the groundwater (saturated) and vadose (unsaturated) zones of aquifers. The model allows for changes in fluid properties as a site is remediated; heterogeneous aquifer properties; the flow and transport of remedial fluids whose density, viscosity and temperature are variable, including surfactants, cosolvents and other enhancement agents; the dissolution and/or mobilization of NAPLs by nondilute remedial fluids; and chemical and microbiological transformations. Appropriate physical, chemical and biological process models important in describing the fate and transport of NAPLs in contaminated aquifers have been incorporated into the simulator, such as multiple organic NAPL phase, nonequilibrium interphase mass transfer, sorption, microbiological and geochemical reactions, and the temperature dependence of pertinent chemical and physical properties. The biodegradation model includes inhibition, sequential use of electron acceptors, and cometabolism and can be used to model a very general class of bioremediation processes. The model can be used to simulate the actual field operation of remediation activities such as surfactant remediation or bioremediation as well as laboratory experiments with large-scale aquifer models.

1.2.1 Microbiological Population Modeling

Biodegradation capabilities have been added to a three-dimensional, multiphase, multicomponent porous media flow model. The model simulates the transport and biodegradation of light nonaqueous phase liquids (LNAPLs) and dense nonaqueous phase liquids (DNAPLs). The biodegradation model describes biological transformation of the organic contaminants originating from NAPL sources and can accommodate multiple substrates, electron acceptors, and biological species.

Here we give a brief description of the model assumptions and the capabilities. For more detailed information on model formulation, method of solution, and example simulations to demonstrate its capability, please refer to de Blanc *et al*. [1996a,b]. UTCHEM simulates the biodegradation of chemical compounds that can serve as substrates (carbon and/or energy sources) for microorganisms. The model simulates the destruction of substrates, the consumption of electron acceptors (e.g., oxygen, nitrate, etc.), and the growth of biomass. Substrates can be biodegraded by free-floating microorganisms in the aqueous phase or by attached biomass present as microcolonies in the manner of Molz *et al.* [1986]. Multiple substrates, electron acceptors and biological species are accommodated by the model. Important assumptions for the biodegradation model are:

1. Biodegradation reactions occur only in the aqueous phase.
2. Microcolonies are fully penetrated; i.e., there is no internal resistance to mass transport within the attached biomass.
3. Biomass is initially uniformly distributed throughout the porous medium.
4. Biomass is prevented from decaying below a lower limit by metabolism of naturally occurring organic matter unless cometabolic reactions act to reduce the active biomass concentrations below natural levels.
5. The area available for transport of organic constituents into attached biomass is directly proportional to the quantity of biomass present.
6. The number of cells per microcolony, biomass density, and microcolony volume are constant, so that mass per microcolony is also constant.

The biodegradation model includes the following features:

- Monod, first-order, or instantaneous biodegradation kinetics.
- Formation of biodegradation by-products.

- External mass-transfer resistances to microcolonies (mass-transfer resistances can be ignored by the user if desired).
- Inhibition of biodegradation by electron acceptors and/or toxic substrates.
- Nutrient limitations to biodegradation reactions.
- First-order abiotic decay reactions.
- Enzyme competition between multiple substrates.
- Modeling of cometabolism with transformation capacities and reducing power limitations using the model of Chang and Alvarez-Cohen [1995].
- Biodegradation reactions in both the vadose and saturated zones.

The biodegradation model equations describe the transport of substrate and electron acceptor from the aqueous phase into attached biomass, the loss of substrate and electron acceptor through biodegradation reactions, and the resulting growth of the free-floating or attached biomass. The flow and biodegradation system is solved through operator splitting, in which the solution to the flow equations is used as the initial conditions for the biodegradation reactions. This approach is convenient because modifications can be made to the system of biodegradation equations without having to reformulate the partial differential equations that describe advection and dispersion.

The biodegradation equations comprise a system of ordinary differential equations that must be solved at each gridblock and each timestep after the advection and dispersion terms are calculated. Because the mass transfer terms can make the system of equations stiff, the system is solved using a Gear's method routine published by Kahaner *et al*. [1989]. The characteristics and numerical solution of this system of equations are discussed by de Blanc *et al.* [1996b].

To validate the model, one-dimensional, single-phase simulation based on the example given in Molz *et al.* [1986] has been run. The UTCHEM simulation results have been compared to biodegradation model solutions published by Molz *et al.* In this simulation, a single substrate is biodegraded by attached biomass using oxygen as the electron acceptor. The reactor is 100 cm long with initial colony density of 1.0×10^5 colonies per cm^3 of porous medium. Pore velocity is 25 cm/day. The initial substrate and oxygen concentrations are constant throughout the reactor at 5 mg/L. At the boundary $x = 0$ and time zero, the substrate concentration is increased instantaneously to 15 mg/L. At the same boundary, the oxygen concentration is maintained at 5 mg/L. Substrate profiles generated by the two models are shown in Fig. 1.1. The simulation results are very similar to the data of Molz *et al.*, indicating that the UTCHEM biodegradation model is functioning properly. The model predictions are not exactly the same because of slightly different assumptions about endogenous decay and slightly different flow conditions.

1.2.2 Numerical Enhancements to the Model

We present a summary of the local grid-refinement method and implementation in UTCHEM. The formulation and simulation examples are given in UTCHEM-LGR User's manual.

The aquifer is initially defined by a coarse grid (called a base grid) with NXCxNYCxNZC standard cells (gridblocks). Subject to memory limitations, any number and any combination of the base grid cells can be refined by a single local-level NXFxNYFxNZF that is of fixed resolution for all refined cells. The refined base grid cells are called zones. The resulting grid is comprised of coarse base cells and fine-zone regions. When a coarse base cell or a fine zone is adjacent to a refined base cell or zone, this gives rise to a coarse-fine interface or fine-fine interface, respectively. With respect to a given zone, the interfaces act as interior domain boundaries. An example is presented in Fig. 1.2, where the definition of zone and interface are illustrated in Fig. 1.2a.

The implementation strategy attempts to treat each zone as a separate domain subject to interior domain boundary conditions and is in that sense based on domain decomposition, pictorially illustrated in Fig. 1.2b. Computations in the *interior* of each local fine zone are effectively performed in isolation from other regions of the flow domain (giving rise to an inner loop) subject to appropriate interface and exterior boundary conditions that are imposed in an outer loop over the local domains and serve to connect the various local domains together.

Local grid refinement (LGR) has been implemented for the Cartesian option with a higher-order scheme or two-point upstream weighting for the concentration equations, although single-point upstream weighting is also maintained as an option. While the current code allows static (fixed) local cell refinement, where each coarse cell selected for refinement remains refined and the grid does not change throughout the computation, the implementation will allow future extension to dynamic local refinement.

Some recent examples of use of this kind of local refinement in reservoir simulation can be found in Espedal *et al.* [1990] and Deimbacher and Heinemann [1993]. However, with the exception of Edwards [1992a,b] and Edwards and Christie [1993] where a higher-order (in space and time) total-variation-diminishing type scheme is employed, all other adaptive methods in reservoir simulation to date have employed first-order upstream differencing for discretization of the advective terms in the flow equations. The new method and development reported here have led to the first simulator to include local grid refinement with a higher-order scheme and a full tensor diffusion operator in three dimensions.

Most of the current code development, in terms of new subroutines, is concerned with treatment of the domain interface conditions for the concentration equations and pressure equation, which enable the zones to link together and complete the global flow-domain solution definition. Aspects that have critical impact on this logic deal with identification of the junction type at an interface. For example, a coarse cell that has been refined can have a neighboring cell that is either refined or coarse or a physical boundary, and appropriate internal or external boundary conditions (Neumann/Dirichlet) must be imposed. In addition, the coarse-fine and/or fine-fine zone configurations that underlie the higher-order scheme for concentrations must be identified. While the pressure equation involves nearest-neighbor and nearest-interface-neighbor information, the higher-order scheme stencil support relies on neighbor and neighbor-of-neighbor information. In addition the full tensor diffusion operator relies on nearest neighbor and diagonal neighbor information, adding another level of complexity to the implementation.

Zone interior calculations can be performed in isolation and, subject to appropriate boundary interface conditions, the solution procedure can simplistically be visualized as a sequence of calls to the simulator for each domain, followed by calls to boundary-coupling routines that "seal" the isolated local zones together, forming the global domain. However, in practice, the implementation is far more involved.

In addition to the nontrivial interface routines directly concerned with solving the flow equations, further interface logic is required for the calculation of any nonlocal variable that is a function of more than a single cell. The code has to be sifted for such cases. Examples include determination of the maximum flow rate required for calculating the maximum timestep, testing for negative saturations and pressures, and material-balance calculations, and all involve tests and/or calculations over all domain cells; more complex examples arise with physical models such as capillary number, which involves further interface routines to handle the spatial derivatives. Definition of physical boundary conditions such as injection/production wells and inflow/outflow boundaries both involve summations over a range of cells, and appropriate interface tests and calculations must be built into the code to ensure that a given boundary condition extends over the desired region of the flow domain.

A cell-centered finite-volume formulation is employed in constructing discretizations of the flow equations applicable on grids with embedded local refinement. In a cell-centered formulation, the flow domain is represented by a grid of quadrilateral cells. All flow variables including saturations, concentrations and pressures are defined at the cell centers, and the flow equations are integrated over each cell using the Gauss flux theorem.

This is the first simulator to offer LGR with a higher-order scheme and full tensor diffusion in three dimensions applicable to a variety of problems of practical importance. The initial three-dimensional results were very encouraging. Successful adaptivity requires that the key coarse grid cells (containing flow variables with steep gradients) be refined. Static refinement is best suited to problems where crucial flow gradients are known *a priori* to be contained in certain regions of the domain.

1.2.3 New Relative-Permeability and Capillary-Pressure Models

A new multiphase capillary-pressure and relative-permeability function has been implemented in UTCHEM. As the result of this task, UTCHEM has now the option of either Brooks-Corey or van Genuchten capillary-pressure functions. The two-phase gas-water, water-oil, or microemulsion-oil and three-phase oil-water-gas capillary pressure-saturation functions are determined using the generalization of Parker *et al*. [1987] to the two-phase flow model of van Genuchten [1980]. The new two- and three-phase relative permeabilities are also based on the generalization of Parker and Lenhard to the two-phase flow model of van Genuchten.

Both capillary-pressure and relative-permeability functions account for hysteresis due to arbitrary changes in saturation path by incorporating an oil-phase-entrapment model. The hysteresis modeling in UTCHEM is based on the work by Kalurachchi and Parker [1992]. The assumptions made in developing and applying this model are:

- The model applies only to strongly water-wet media where the wettability in descending order is for water (or microemulsion), oil, and gas phases. Oil will be used in this report to mean any nonaqueous phase liquid (NAPL).
- The model applies to three-phase air-water-oil flow in the vadose zone and two-phase oil-water or oil-microemulsion flow in the saturated zone.
- To avoid numerical oscillations with changes from two phases (air-water) to three phases (air-water-oil), once a location is classified as a three-phase node, it will not revert back to two phases (air-water).
- Gas entrapment is neglected for the three-phase case. Therefore, oil entrapment in three-phase air-water-oil flow can be inferred directly from that in a two-phase oil-water system.
- Water relative permeability is unaffected by oil entrapment.
- There is no oil entrapment on the main drainage curve.

- There is no oil entrapment when water saturation is at its residual value in the vadose zone.

A detailed description on the formulation of the new hysteretic capillary-pressure and relative-permeability models is given in Section 2.2 of this report.

1.2.4 New Organic and Tracer Components

New organic and tracer components were added to UTCHEM. We have added multiple organic components so that we can model NAPL mixtures. Adding this capability to UTCHEM required developing a phase-behavior model for NAPL mixtures and the physical property models such as density and viscosity for each phase. We have also added additional water tracer components and gas phase tracers.

New organic components

Nonaqueous phase liquids (NAPLs) usually consist of more than one organic species that mix and form a single liquid. Common examples of such miscible species include TCE, TCA and PCE among many others. When NAPLs leak to the subsurface, they can dissolve and migrate into groundwater. To model the fate and transport of these soluble organics during remediation processes such as pump-and-treat, bioremediation and surfactant remediation, it is important to determine the migration of the individual soluble organics. The dissolution can be either a local equilibrium or a rate-limited (nonequilibrium) mass-transfer process. We have added the capability of multiple organic components to UTCHEM to model these NAPL mixtures. The multiple organic dissolution can be either local-equilibrium partitioning or a rate-limited mass transfer. We also developed and incorporated in UTCHEM a phase-behavior model for a mixture of NAPL mixtures, surfactant, and water. The physical-property models developed and implemented for a NAPL mixtures in UTCHEM were density, viscosity, and adsorption. A more detailed description of the model is given in Section 2.6 of this report.

Three recent papers by Baran *et al.* [1994a,b,c] show that the phase behavior of surfactants with both pure chlorocarbons and mixtures of chlorocarbons is similar to classical phase behavior with hydrocarbons. The phase behavior changes from microemulsion in equilibrium with excess oil (Winsor Type I or Type II(-)) to microemulsion in equilibrium with excess aqueous and organic phase (Winsor Type III), and to microemulsion in equilibrium with excess water (Winsor Type II or Type II(+)) as salinity increases. The lower and upper limits of effective salinity are the effective salinities at which three phases form or disappear. The optimal salinity is defined as the midpoint of these two salinity limits .

Hand's equation (Pope and Nelson, 1978) is used in UTCHEM to describe the phase envelope and binodal curve. For organic mixtures, the upper and lower limits of effective salinity, the height of binodal curve at lower, optimal, and upper salinities are functions of organic species concentrations. These parameters are modeled as functions of the equivalent alkane carbon number (E_{ACN}) of the mixture, which is a function of organic species concentrations. E_{ACN} for an alkane is the number of carbons in the alkane chain of the hydrocarbon; for example, it is equal to 6 for hexane. E_{ACN} for a nonalkane is obtained by measuring the optimal salinity for a binary mixture of an alkane and a nonalkane with known molar fractions. The measured optimal salinity is used to determine E_{ACN} for the binary mixture. For example, the E_{ACN} data listed in the Baran *et al.* papers are built into the UTCHEM database: PCE ($E_{ACN} = 2.90$), CCl_4 ($E_{ACN} = -0.06$), TCE ($E_{ACN} = -3.81$), p-xylene ($E_{ACN} = 2$), toluene ($E_{ACN} = 1$), 1,2-$C_6H_4Cl_2$ ($E_{ACN} = -4.89$), 1,2-$C_2H_4Cl_2$ ($E_{ACN} = -12.10$), $CHCl_3$ ($E_{ACN} = -13.67$), CH_2Cl_2 ($E_{ACN} = -13.79$), and 1,1,2,2-$C_2H_2Cl_4$ ($E_{ACN} = -22.15$).

New tracer components

The number of oil/water tracers in UTCHEM was previously limited to three. Modifications to the model have been completed to allow the simulation of any number of tracer components.

Gas tracers have been added to UTCHEM. The gas-phase tracers are either chemical nonreacting or radioactive components. The gas tracer can partition only between gas and organic phases with a constant partition coefficient. Radioactive decay is applied to radioactive tracers with a constant decay coefficient. The gas tracers can also adsorb on the soil surface using a linear adsorption model and a constant retardation factor.

Enhancements of Geochemical Option

The geochemical option in UTCHEM has been extended to allow the modeling of any aqueous and solid reactive species. In the original UTCHEM model, the component numbering in the transport calculations was fixed in the source code and each reaction option had specific geochemical components and species. Thus, the geochemical option in UTCHEM was limited only to those specific species and reactions. This restriction was removed by implementing a dynamic component-numbering scheme for geochemical components. The component numbers are increased according to the user-specified elements. Component partitioning between phases and the adsorbed and solid concentrations in the mass-balance calculations are not, however, included for all the new species.

To test and illustrate the UTCHEM capability in modeling a complex geochemical process, an application to an acid mine-tailing contamination problem was simulated. A total of 51 aqueous species and 7 solid species were simulated (Table 1.1). New components such as chromium, lead, and sulfate were included that were not available in the original UTCHEM model. The aquifer and site conditions for this example were similar to the conditions at the Nordic site near Elliot Lake, northern Ontario (Walter *et al*., 1994). The initial and injected component concentrations were similar to those used in the simulation by Walter *et al.* Initial concentrations for UTCHEM simulation were determined by equilibrating the water and mineral phases using batch equilibrium calculations. The UTCHEM results showed a very similar trend to those presented by Walter *et al*. The results were not expected to be identical since the conditions were different; i.e., species such as K, Mn, and Fe were not included in the UTCHEM simulation.

1.3 Model Evaluation

The numerical accuracy of the UTCHEM model has been evaluated through a series of tests including comparisons with analytical solutions and experimental data.

The numerical accuracy of UTCHEM model was evaluated by comparison with analytical solutions for problems such as the 1-D water tracer, 2-D tracer, and polymerflood examples given in Fig. 1.3 (Liu *et al.*, 1994) and by comparison with 2-D laboratory column data of Pennell *et al.* [1996]. The experiment involved a 2-D horizontal sandpack contaminated with tetrachloroethylene (PCE). A mixture of surfactant solution was injected under both mobilization and solubilization conditions for PCE removal from the column. The UTCHEM model with the recently added trapping number (Jin, 1995; Delshad *et al.*, 1996) was used to model this experiment.

The column was packed with 40-270 mesh Ottawa sand with a permeability of 16.3 darcies and porosity of 0.3509. Table 1.2 gives the physical properties. The surfactant solution was a 4% 1:1 mixture of sodium dihexyl sulfosuccinate and sodium dioctyl sulfosuccinate (Aerosol AY/OT) in 500 mg/L $CaCl_2$. The measured phase behavior and fluid properties such as viscosity, density, and desaturation data were used to obtain the UTCHEM input parameters. The injection rate was at 4.95 cc/min (0.0488 ft^3/day). Pennell *et al.*

observed that the injected surfactant solution appeared to preferentially flow along the top of the soil column, while mobilized PCE migrated downward through the soil column because of buoyancy forces. It took about 3 pore volumes of surfactant solution to completely displace the mobilized bank of PCE formed near the column outlet. To model the results of the laboratory data, 2-D simulations with 22 gridblocks in the horizontal direction and 10 gridblocks in the vertical direction were performed. Figure 1.4 compares the laboratory and simulated free-product PCE recovery as a function of surfactant solution throughput. This favorable comparison indicates that UTCHEM can successfully model the vertical migration and mobilization of PCE.

The model was also evaluated by comparison with data from actual field operations of remediation, in particular, surfactant enhanced aquifer remediation (SEAR) at the Canadian Forces Borden site and a field-scale tracer and SEAR tests at the Operational Unit 2 site at Hill Air Force Base in Utah. The UTCHEM simulator was used to model the surfactant-enhanced remediation of PCE in a test cell at the Borden site in Allison, Ontario (Freeze *et al.*, 1994). UTCHEM was able to closely reproduce the PCE recovery and the PCE distribution. The second sets of simulations were performed to design pre- and post-surfactant flushing partitioning interwell tracer tests and to design the surfactant flood for the Operational Unit 2 (OU2) site at Hill AFB, Utah. A multitude of simulation cases were performed to develop the recommended designs for the tests. These simulations have also allowed us to study the effect of design variables such as injection and extraction wells, number of wells, and well pattern. Figures 1.5 and 1.6 show a favorable comparison of the field and UTCHEM predictions of effluent tracer and surfactant concentrations. The field design, results, and UTCHEM predictions are given in Brown *et al*. [1996] and Brown [1999]. The stability and robustness of the simulation results were evaluated with sensitivity analysis to various aquifer conditions, for example, initial saturation distribution, permeability and porosity distributions, and injection/extraction strategies (Brown, 1999).

More examples of UTCHEM large-scale simulations are given in a report prepared by INTERA (Butler and Jin, 1996). INTERA's particular role in this project was to apply UTCHEM to typical NAPL problems that INTERA encountered during its work at various hazardous waste sites in North America. UTCHEM was used to study the distribution, volume, and remediation of DNAPL in an alluvial aquifer. The model was used to design both a partitioning interwell tracer test (PITT) and a subsequent surfactant flood at the Portsmouth Gaseous Diffusion Plant in southern Ohio. The analysis of an actual PITT conducted at Portsmouth in July 1996 is also included in the report.

1.4 Conclusions

As the result of this three-year research contract, we have developed a mathematical model capable of simulating the performance of three-dimensional, multicomponent, multiphase flow of NAPLs in subsurface environments including saturated and unsaturated conditions. A systematic evaluation was undertaken to assess the applicability and accuracy of all physical and chemical models of the various pertinent phenomena such as capillary pressure, relative permeability, adsorption, nonequilibrium mass transfer, dispersion, and phase behavior. A biological component was added to UTCHEM. Comparisons to analytical solutions were made and numerical dispersion control and accuracy testing were performed. The model was tested against experimental and field data. The model will be delivered to U.S. EPA along with user manuals and sample outputs. The model is in the form of a FORTRAN source code that has been optimized for a vector computer.

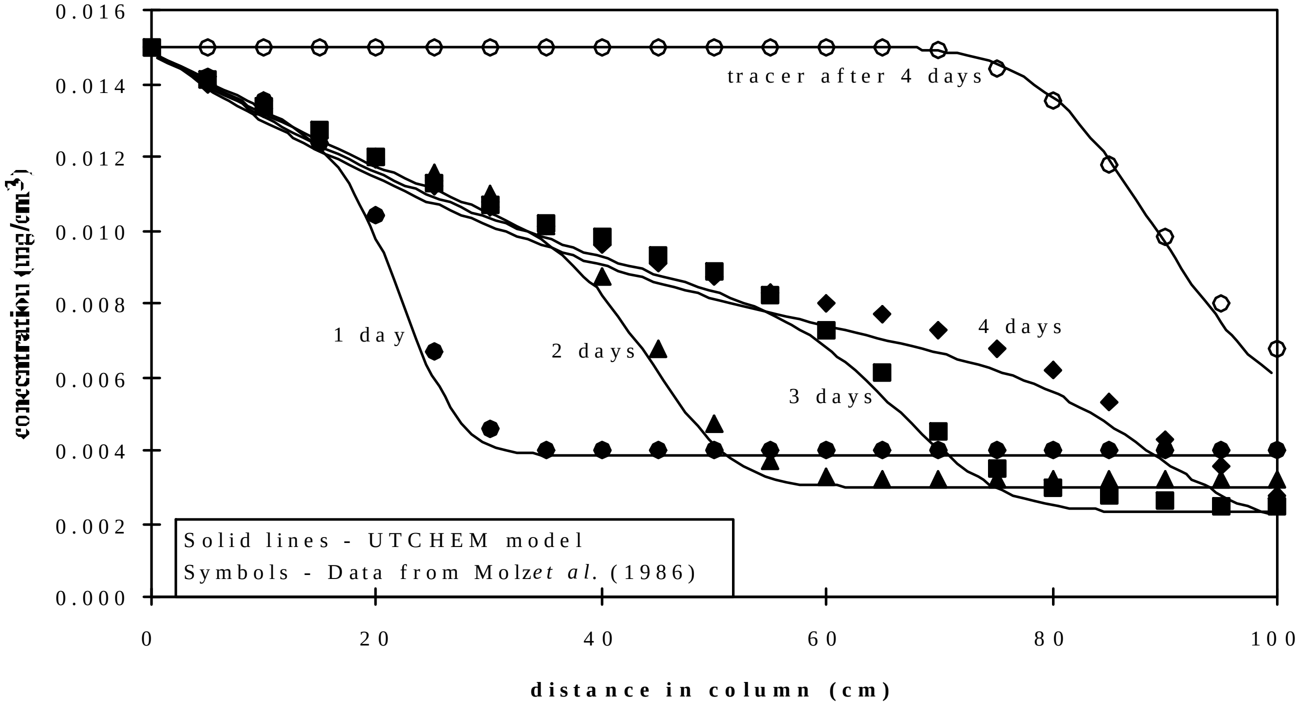

Figure 1.1. Comparison of substrate profiles calculated by UTCHEM simulator to those predicted by the model of Molz *et al.* [1986].

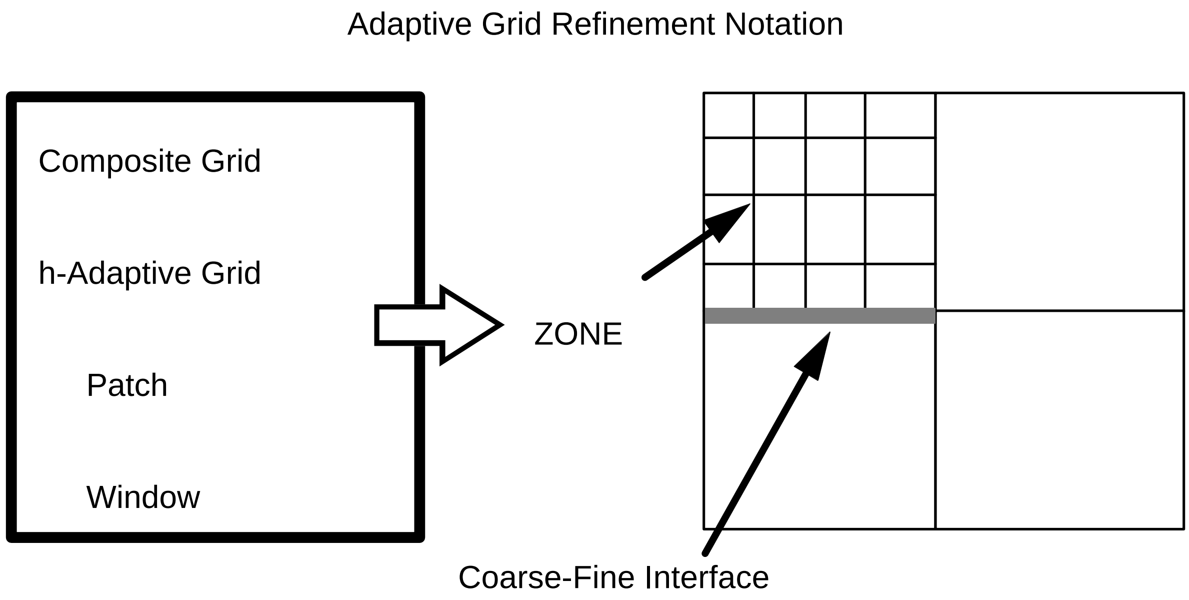
Adaptive Grid Refinement Notation

Figure 1.2a. Definition of zone and interface.

Decomposition of Domain

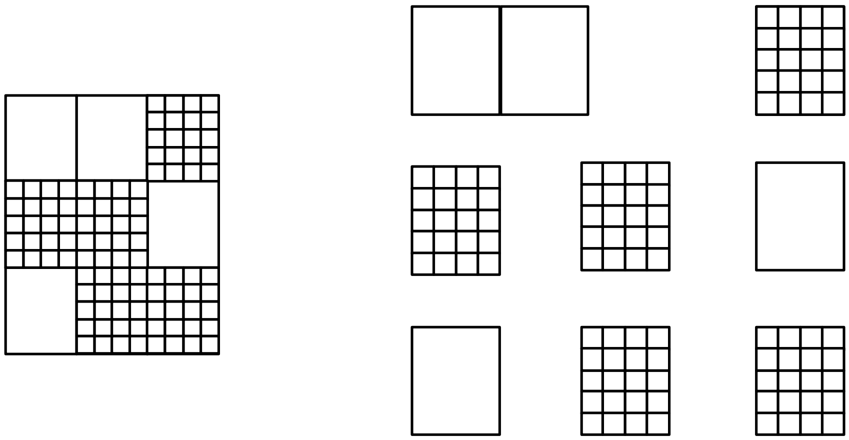

Figure 1.2b. Coarse-fine and fine-fine interfaces.

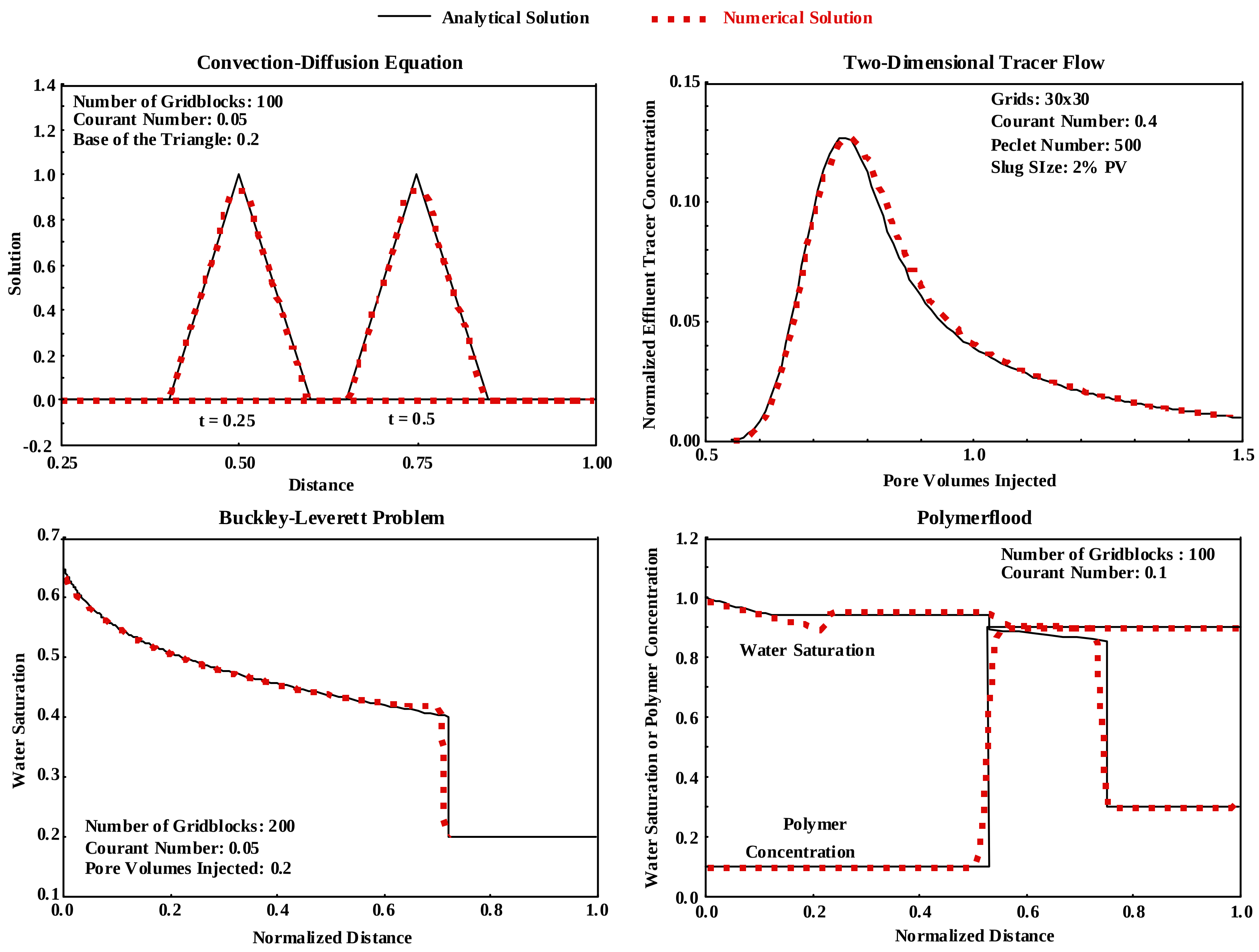

Figure 1.3. Comparison between analytical solutions and third-order finite-difference solutions in UTCHEM.

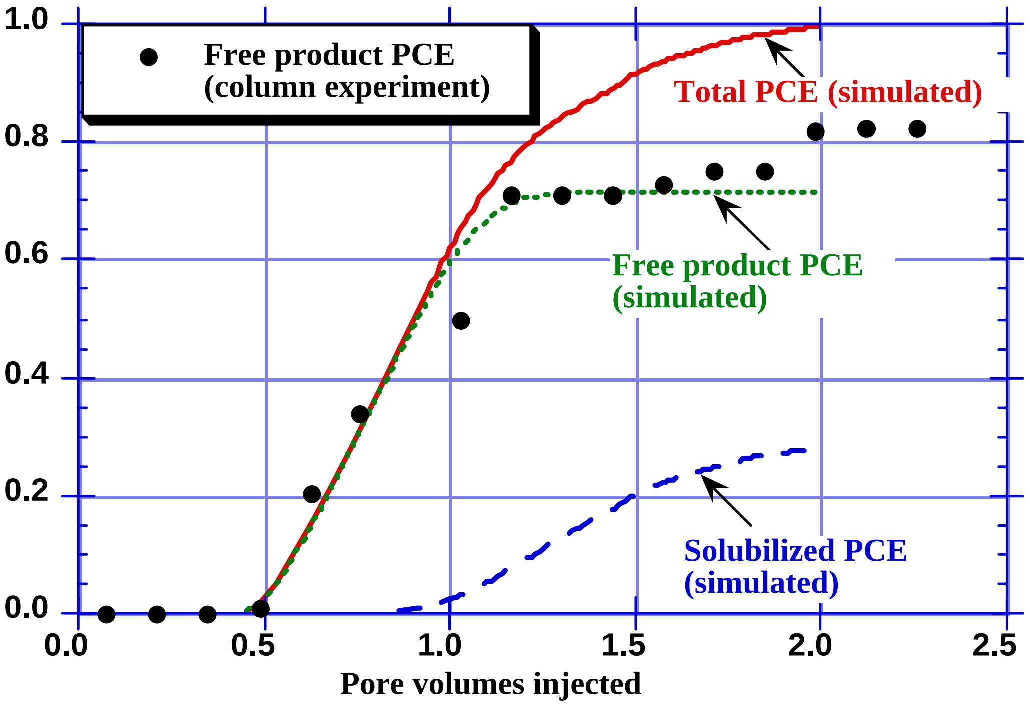

Figure 1.4. Simulated and laboratory PCE recovery from the 2-D column.

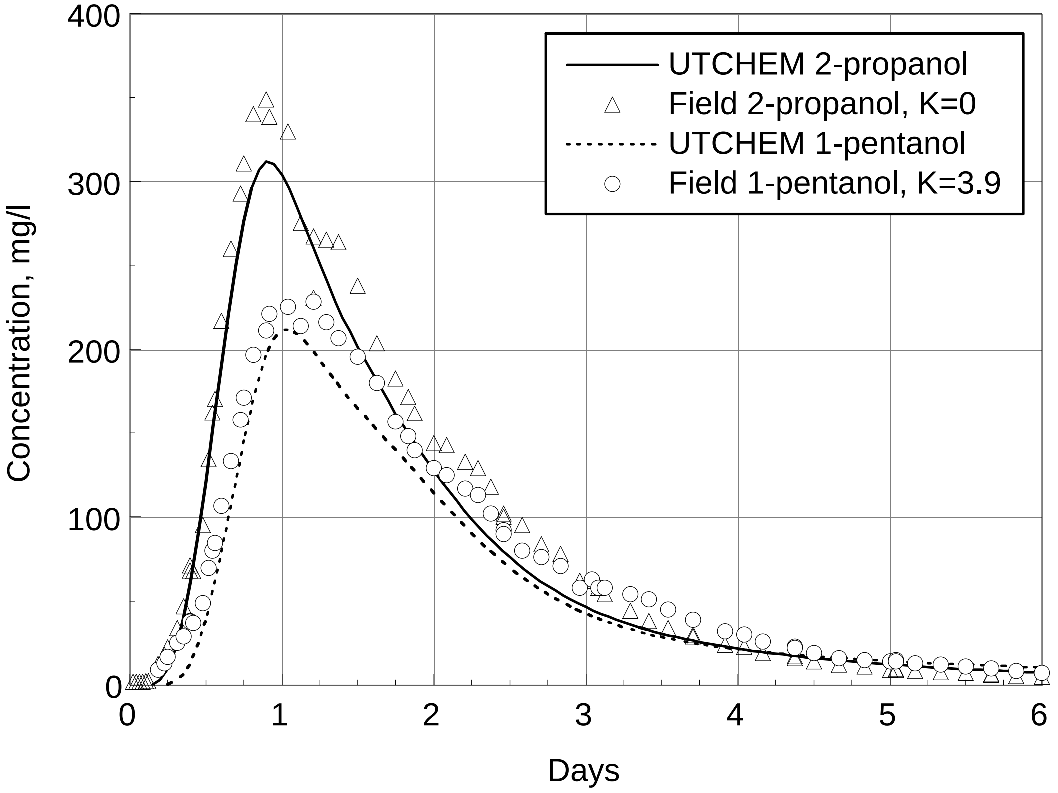

Figure 1.5. Tracer concentrations produced at extraction well SB-1 during Hill AFB Phase I test.

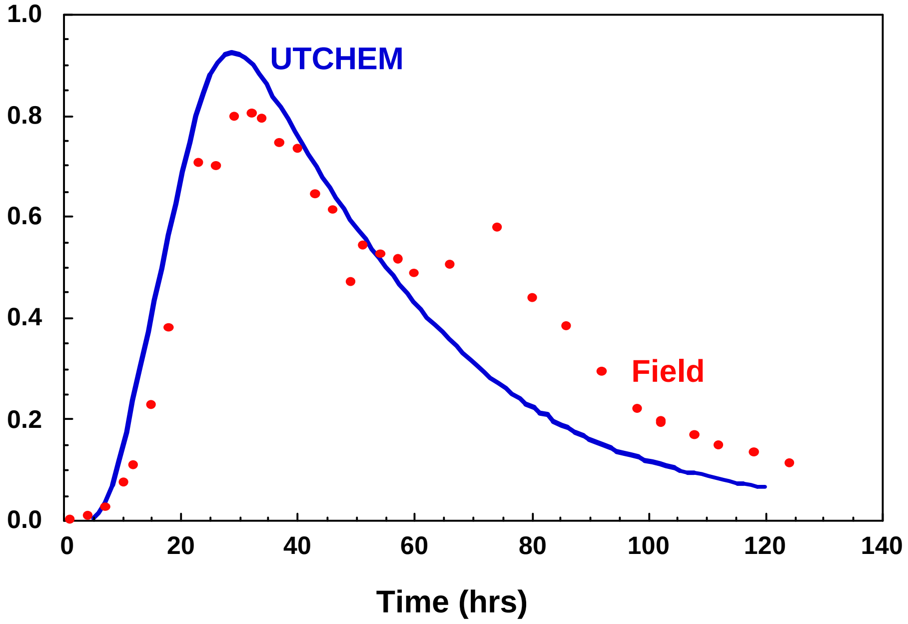

Figure 1.6. Surfactant concentrations produced at extraction well SB-1 during Hill AFB Phase I test.

Table 1.1. List of Elements and Reactive Species

ELEMENTS	AQUEOUS SPECIES	SOLID SPECIES
Cr H Pb Mg Ca Na Al Si Cl CO_3 SO_4 O	$Cr(OH)^{2+}$, H^+, Pb^{2+}, Mg^{2+}, Ca^{2+}, Na^+, Al^{3+}, H_4SiO_4, Cl^-, CO_3^{2-}, SO_4^{2-}, H_2O, OH^-, $H_3SiO_4^-$, $MgOH^+$, $MgCO_3$ (Aq.), $MgHCO_3^+$, $MgSO_4$ (Aq.), $CaOH^+$, $CaHCO_3^+$, $CaCO_3$ (Aq.), $CaSO_4$ (Aq.), $NaCO_3^-$, $NaHCO_3$ (Aq.), $NaSO_4^-$, $AlOH^{2+}$, $Al(OH)_2^+$, $AlSO_4^+$, $Al(SO_4)_2^-$, $PbCl^+$, $PbCl_2$ (Aq.), $PbCl_3^-$, $PbCl_4^{2-}$, $Pb(CO_3)_2^{2-}$, $PbOH^+$, Pb_2OH^{3+}, $PbSO_4$ (Aq.), $PbCO_3$ (Aq.), $Pb(SO_4)_2^{2-}$, $PbHCO_3^+$, HCO_3^-, H_2CO_3 (Aq.), HSO_4^-, Cr^{3+}, $Cr(OH)^{2+}$, $CrCl^{2+}$, $CrCl_2^+$, $CrSO_4^+$, $CrOHSO_4$ (Aq.), $Cr_2(OH)_2SO_4^{2+}$, $Cr_2(OH)_2(SO_4)_2$ (Aq.)	CALCITE ($CaCO_3$) GIBBSITE ($Al(OH)_3$) GYPSUM ($CaSO_4$) SiO_2 CERRUSITE ($PbCO_3$) ANGLESITE ($PbSO_4$) $Cr(OH)_3$

Table 1.2. Physical Property Data Used in the 2-D Simulations

Permeability, darcies	16.3
Porosity, fraction	0.3509
Residual water saturation	0.30
Residual PCE saturation	0.1242
Initial water saturation	0.8758
Water viscosity, cp	1.0
PCE viscosity, cp	0.89
Water density, g/cc	1.0
PCE density, g/cc	1.63
Surfactant density, g/cc	1.15
Initial/injected chloride conc., meq/L	0.009
Initial/injected calcium conc., meq/mL	0.009

Section 2
UTCHEM Model Formulation

This chapter is an expanded version of the paper by Delshad *et al.* [1996] where we describe a three-dimensional, multicomponent, multiphase compositional finite difference simulator for application to the analysis of contaminant transport and surfactant enhanced aquifer remediation (SEAR) of nonaqueous phase liquid (NAPL) pollutants. The simulator can model capillary pressures, three-phase relative permeabilities (water/gas/organic phases or water/organic/microemulsion phases), dispersion, diffusion, adsorption, chemical reactions, nonequilibrium mass transfer between phases and other related phenomena. The finite-difference method uses second- and third-order approximations for all of the time and space derivatives and a flux limiter that makes the method total variation diminishing (TVD). Mixtures of surfactant, alcohol, water and NAPL can form many types of micellar and microemulsion phases with a complex and important dependence on many variables of which the dilute aqueous solution typically assumed in SEAR models is just one example. The phase behavior model is central to our approach and allows for the full range of the commonly observed micellar and microemulsion behavior pertinent to SEAR. The other surfactant related properties such as adsorption, interfacial tension, capillary pressure, capillary number and microemulsion viscosity are all dependent on an accurate phase behavior model. This has proven to be a highly successful approach for surfactant enhanced oil recovery modeling, so it was adapted to SEAR modeling. However, there are many significant differences between petroleum and environmental applications of surfactants, so many new features have been added to model contaminant transport and remediation and these are described and illustrated for the first time here.

2.1 Introduction

Many nonaqueous phase liquids (NAPLs) are used in large quantities by many industries throughout the world. Due to their wide usage, organic liquids are among the most common type of soil and groundwater pollutants. Of the organic chemical contaminants which have been detected in groundwaters, dense nonaqueous phase liquids (DNAPLs) such as chlorinated solvents are among the most frequently and serious types encountered. DNAPLs are heavier than water, typically volatile, and only slightly soluble in water. Many conventional remediation techniques such as pump-and-treat, vapor extraction, and in-situ biorestoration have proven to be unsuccessful or of limited success in remediating soil and groundwater contaminated by DNAPL due to low solubility, high interfacial tension, and the sinking tendency below the water table of most DNAPLs. Surfactant enhanced aquifer remediation is actively under research and development as a promising technology that avoids at least some of the problems and limitations of many other remediation methods.

Surfactants have been studied and evaluated for many years in the petroleum industry for enhanced oil recovery from petroleum reservoirs (Nelson and Pope, 1978). Surfactants are injected to create low interfacial tension to reduce capillary forces and thus mobilize trapped oil. Solubilization and mobilization are the two mechanisms by which surfactants can enhance the removal of NAPLs from saturated zones. Surfactants can also be used to increase the solubility without generating ultra-low interfacial tension or mobilizing the trapped oil. Enhanced solubility is the main mechanism for recovery of entrapped organic residuals in surfactant enhanced aquifer remediation (Fountain, 1992; Fountain and Hodge, 1992; Powers *et al.*, 1991; West and Harwell, 1992; Wunderlich *et al.*, 1992; Brown *et al.*, 1994; Pennell *et al.*, 1994). For example, the solubility of perchloroethylene (PCE) is increased 300 fold by the addition of a 4% blend of sodium diamyl and dioctyl sulfosuccinates (Abriola *et al.*, 1993). SEAR can also be based on mobilization of the residual DNAPL, which has a greater potential to increase the remediation but is riskier because of the movement of free-phase DNAPL.

The objective of SEAR modeling is to aid in the scaleup and optimization of the design of SEAR, to assess the performance of the method at both the laboratory and field scales with respect to both risk and effectiveness, to improve our understanding of process mechanisms, and to explore alternative strategies and approaches to remediation. To the extent that these modeling objectives are met, risk will be reduced and fewer mistakes will be made, the performance and cost effectiveness of the method will be improved, and the number of field trials will be minimized. The model should have the capability of modeling advection, dispersion, and the mass transfer of species (surfactant, water, organic contaminants, air) in the aquifer under various pumping and injection strategies. Most multiphase compositional models reported in the environmental engineering literature (Abriola and Pinder, 1985a,b; Baehr and Corapcioglu, 1987; Faust *et al.*, 1989; Letniowski and Forsyth, 1990; Sleep and Sykes, 1990; Mayer and Miller; 1990; Kalurachchi and Parker, 1990; Sleep and Sykes, 1993) are limited in their applicability in one way or another (1-or 2-dimensional modeling, single species, equilibrium mass transfer, inadequate numerical accuracy, and lack of modeling miscibility which occurs during surfactant flooding). The only SEAR models reported in the literature are for single phase flow and are those of Wilson [1989], Wilson and Clarke [1991] and Abriola *et al*. [1993] with simplified surfactant phase behavior and properties. None of these models account for the effects of surfactant on interfacial tension (IFT), surfactant phase behavior, capillary number, or surfactant adsorption. This paper describes the formulation and application of a general purpose chemical compositional simulator, The University of Texas Chemical Flooding simulator (UTCHEM), for use in SEAR studies, that does not have these common limitations.

Enhanced oil recovery processes such as polymer flooding or surfactant/polymer flooding have utilized polymer to reduce fluid mobility to improve the sweep efficiency of the reservoir, i.e., to increase the volume of the permeable medium contacted at any given time (Lake, 1989; Sorbie, 1991). Sweep efficiency is reduced by streamline pattern effects, gravity effects, viscous fingering, channeling (caused by contrasts in the permeability) and flow barriers. Polymers could be used in the SEAR process to improve the sweep efficiency just as they have been in enhanced oil recovery and this may reduce the cost, risk and time required to remediate the aquifer. Under some conditions, polymers can also reduce the dispersion and adsorption of the surfactant and this is another potential benefit of using them. Polymer concentrations on the order of 500 mg/L are likely to be adequate for SEAR applications, so the additional cost of the polymer is small compared to the potential reduction in surfactant costs assuming that fewer pore volumes of surfactant will be needed as a result of the polymer.

UTCHEM can be used to simulate a wide range of displacement processes at both the field and laboratory scales. The model is a multiphase, multicomponent, three-dimensional finite-difference simulator. The model was originally developed to model surfactant enhanced oil recovery but modified for applications involving the use of surfactant for enhanced remediation of aquifers contaminated by NAPLs. The balance equations are the mass conservation equations, an overall balance that determines the pressure for up to four fluid phases, and an energy balance equation to determine the temperature. The number of components is variable depending on the application, but would include at least surfactant, oil and water for SEAR modeling. When electrolytes, tracers, co-solvents, polymer, and other commonly needed components are included, the number of components may be on the order of twenty or more. When the geochemical option is used, a large number of additional aqueous components and solid phases may be used.

A significant portion of the research effort on chemical flooding simulation at The University of Texas at Austin has been directed toward the development and implementation of accurate physical and chemical property models in UTCHEM. Heterogeneity and variation in relative permeability and capillary pressure are allowed throughout the porous medium, since for example each gridblock can have a different permeability and porosity.

Surfactant phase behavior modeling is based in part on the Hand representation of the ternary phase diagram (Hand, 1939). A pseudophase theory (Prouvost *et al.*, 1984b; Prouvost *et al.*, 1985) reduces the water, oil, surfactant, and co-surfactant fluid mixtures to a pseudoternary composition space. The major physical phenomena modeled are density, viscosity, velocity-dependent dispersion, molecular diffusion, adsorption, interfacial tension, relative permeability, capillary pressure, capillary trapping, cation exchange, and polymer and gel properties such as permeability reduction, inaccessible pore volume, and non-Newtonian rheology. The phase mobilization is modeled through entrapped phase saturation and relative permeability dependence on trapping number.

The reaction chemistry includes aqueous electrolyte chemistry, precipitation/dissolution of minerals, ion exchange reactions with the matrix (the geochemical option), reactions of acidic components of oil with the bases in the aqueous solution (Bhuyan, 1989; Bhuyan *et al.*, 1990 and 1991) and polymer reactions with crosslinking agents to form gel (Garver *et al.*, 1989; Kim, 1995).

Nonequilibrium mass transfer of an organic component from the oleic phase to the surfactant-rich microemulsion phase is modeled using a linear mass transfer model similar to that given by Powers *et al.* [1991]. Even in the absence of surfactant, the model allows for a small dissolution of oil in the aqueous phase. Nonequilibrium mass transfer of tracer components is modeled by a generalized Coats-Smith model (Smith *et al.*, 1988).

The model includes options for multiple wells completed either horizontally or vertically. Aquifer boundaries are modeled as constant-potential surfaces or as closed surfaces.

A dual-porosity formulation to model transport in fractured media has recently been added to the simulator (Liang, 1997). We have recently incorporated a biodegradation model in UTCHEM. Multiple organic compounds can be degraded by multiple microbial species using multiple electron acceptors (de Blanc, 1998; Delshad *et al.*, 1994).

The resulting flow equations are solved using a block-centered finite-difference scheme. The solution method is implicit in pressure and explicit in concentration (IMPES type). One- and two-point upstream and third-order spatial discretization are available as options in the code. To increase the stability and robustness of the second-and third-order methods, a flux limiter that is total-variation-diminishing (TVD) has been added (Liu, 1993; Liu *et al.*, 1994). The third-order method gives the most accurate solution.

2.2 Model Formulation

2.2.1 General Description

In this section, a brief description of the model formulation is given. Additional features needed only for enhanced oil recovery can be found in Datta Gupta *et al.*, [1986], Bhuyan *et al.*, [1990], and Saad [1989]. The balance equations are as follows:

1. The mass balance equation for each species.
2. The aqueous phase pressure is obtained by an overall mass balance on volume-occupying components (water, oil, surfactant, co-solvent, and air). The other phase pressures are computed by adding the capillary pressure between phases.
3. The energy balance equation.

Four phases are modeled. The phases are a single component gas phase (ℓ=4) and up to three liquid phases: aqueous (ℓ=1), oleic (ℓ=2), and microemulsion (ℓ=3), depending on the relative amounts and effective electrolyte concentration (salinity) of the phase environment. Any number of water, oil, or gas tracers can be modeled. The tracers can partition, adsorb, and decay if they are radioactive. UTCHEM can model partitioning interwell tracer tests (PITT) for the detection and estimation of contaminants and for the remediation performance assessment in both saturated and vadose zones (Jin *et al.*, 1995).

The flow equations allow for compressibility of soil and fluids, dispersion and molecular diffusion, chemical reactions, and phase behavior and are complemented by constitutive relations.

2.2.2 Mass Conservation Equations

The assumptions imposed when developing the flow equations are local thermodynamic equilibrium except for tracers and dissolution of organic component, immobile solid phases, slightly compressible soil and fluids, Fickian dispersion, ideal mixing, and Darcy's law. The boundary conditions are no flow and no dispersive flux across the impermeable boundaries.

The continuity of mass for component κ in association with Darcy's law is expressed in terms of overall volume of component κ per unit pore volume ($\tilde{C}_\kappa$) as

$$\frac{\partial}{\partial t}\left(\phi \tilde{C}_\kappa \rho_\kappa\right) + \vec{\nabla} \cdot \left[\sum_{\ell=1}^{n_p} \rho_\kappa \left(C_{\kappa\ell} \vec{u}_\ell - \vec{\tilde{D}}_{\kappa\ell}\right)\right] = R_\kappa \qquad (2.1)$$

where the overall volume of component κ per unit pore volume is the sum over all phases including the adsorbed phases:

$$\tilde{C}_\kappa = \left(1 - \sum_{\kappa=1}^{n_{cv}} \hat{C}_\kappa\right) \sum_{\ell=1}^{n_p} S_\ell C_{\kappa\ell} + \hat{C}_\kappa \qquad \text{for } \kappa = 1,..., n_c \qquad (2.2)$$

n_{cv} is the total number of volume-occupying components. These components are water, oil, surfactant, and air. n_p is the number of phases; $\hat{C}_\kappa$ is the adsorbed concentration of species κ; and ρ_κ is the density of pure component κ at a reference phase pressure P_R relative to its density at reference pressure P_{R0}, usually taken at the surface condition of 1 atm. We assume ideal mixing and small and constant compressibilities C_κ^o.

$$\rho_\kappa = 1 + C_\kappa^o \left(P_R \quad P_{R0}\right) \tag{2.3}$$

The dispersive flux is assumed to have a Fickian form:

$$\vec{\tilde{D}}_{\kappa\ell,x} = \phi S_\ell \vec{\vec{K}}_{\kappa\ell} \cdot \vec{\nabla} C_{\kappa\ell} \tag{2.4}$$

The dispersion tensor $\vec{\vec{K}}_{\kappa\ell}$ including molecular diffusion ($D_{k\ell}$) are calculated as follows (Bear, 1979):

$$\vec{\vec{K}}_{\kappa\ell ij} \equiv \frac{D_{\kappa\ell}}{\tau} \delta_{ij} + \frac{\alpha_{T\ell}}{\phi S_\ell} \left|\vec{u}_\ell\right| \delta_{ij} + \frac{\left(\alpha_{L\ell} - \alpha_{T\ell}\right)}{\phi S_\ell} \frac{u_{\ell i}\, u_{\ell j}}{\left|\vec{u}_\ell\right|} \tag{2.5}$$

where $\alpha_{L\ell}$ and $\alpha_{T\ell}$ are phase ℓ longitudinal and transverse dispersivities; τ is the tortuosity factor with the definition of being a value greater than one; $u_{\ell i}$ and $u_{\ell j}$ are the components of Darcy flux of phase ℓ in directions i and j; and δ_{ij} is the Kronecker delta function. The magnitude of vector flux for each phase is computed as

$$\left|\vec{u}_\ell\right| = \sqrt{\left(u_{x\ell}\right)^2 + \left(u_{y\ell}\right)^2 + \left(u_{z\ell}\right)^2} \tag{2.6}$$

The phase flux from Darcy's law is

$$\vec{u}_\ell = -\frac{k_{r\ell} \vec{\vec{k}}}{\mu_\ell} \cdot \left(\vec{\nabla} P_\ell - \gamma_\ell \vec{\nabla} h\right) \tag{2.7}$$

where $\vec{\vec{k}}$ is the intrinsic permeability tensor and h is the vertical depth. Relative permeability ($k_{r\ell}$), viscosity (μ_ℓ), and specific weight (γ_ℓ) for phase ℓ are defined in the following sections.

The source terms R_κ are a combination of all rate terms for a particular component and may be expressed as

$$R_\kappa = \phi \sum_{\ell=1}^{n_p} S_\ell \, r_{\kappa\ell} + \left(1 - \phi\right) r_{\kappa s} + Q_\kappa \tag{2.8}$$

where Q_κ is the injection/production rate for component κ per bulk volume. $r_{\kappa\ell}$ and $r_{\kappa s}$ are the reaction rates for component κ in phase ℓ and solid phase s respectively.

Analogous equations apply for the fluxes in the y- and z-directions.

2.2.3 Energy Conservation Equation

The energy balance equation is derived by assuming that energy is a function of temperature only and energy flux in the aquifer or reservoir occurs by advection and heat conduction only.

$$\frac{\partial}{\partial t}\left[\left(1 - \phi\right)\rho_s C_{vs} + \phi \sum_{\ell=1}^{n_p} \rho_\ell S_\ell C_{v\ell}\right] T + \vec{\nabla} \cdot \left(\sum_{\ell=1}^{n_p} \rho_\ell C_{p\ell} u_\ell T - \lambda_T \vec{\nabla} T\right) = q_H - Q_L \tag{2.9}$$

where T is the reservoir temperature; C_{vs} and $C_{v\ell}$ are the soil and phase ℓ heat capacities at constant volume; $C_{p\ell}$ is the phase ℓ heat capacity at constant pressure; and λ_T is the thermal conductivity (all assumed constant). q_H is the enthalpy source term per bulk volume. Q_L is the heat loss to overburden and underburden formations or soil computed using the Vinsome and Westerveld [1980] heat loss method.

2.2.4 Pressure Equation

The pressure equation is developed by summing the mass balance equations over all volume-occupying components, substituting Darcy's law for the phase flux terms, using the definition of capillary pressure, and noting that $\sum_{\kappa=1}^{n_{cv}} C_{\kappa\ell} = 1$. The pressure equation in terms of the reference phase pressure (phase 1) is

$$\phi C_t \frac{\partial P_1}{\partial t} + \vec{\nabla} \cdot \overset{\rightrightarrows}{k} \cdot \lambda_{rTc} \vec{\nabla} P_1 = -\vec{\nabla} \cdot \sum_{\ell=1}^{n_p} \overset{\rightrightarrows}{k} \cdot \lambda_{r\ell c} \vec{\nabla} h + \vec{\nabla} \sum_{\ell=1}^{n_p} \overset{\rightrightarrows}{k} \cdot \lambda_{r\ell c} \vec{\nabla} P_{c\ell 1} + \sum_{\kappa=1}^{n_{cv}} Q_\kappa \qquad (2.10)$$

where $\lambda_{r\ell c} = \frac{k_{r\ell}}{\mu_\ell} \sum_{\kappa=1}^{n_{cv}} \rho_\kappa C_{\kappa\ell}$ and total relative mobility with the correction for fluid compressibility is $\lambda_{rTc} = \sum_{\ell=1}^{n_p} \lambda_{r\ell c}$.

The total compressibility, C_t, is the volume-weighted sum of the rock or soil matrix (C_r) and component compressibilities (C_κ^o):

$$C_t = C_r + \sum_{\kappa=1}^{n_{cv}} C_\kappa^o \tilde{C}_\kappa \qquad (2.11)$$

where $\phi = \phi_R \left[1 + C_r \left(P_R - P_{R0}\right)\right]$.

2.2.5 Nonequilibrium Dissolution of Nonaqueous Phase Liquids

Mathematical models of multiphase flow in subsurface environments generally employ a local equilibrium assumption; that is, it is assumed that the concentration of water leaving a region of residual NAPL has dissolved concentrations of the organic phase at the solubility level. However, field data frequently indicate that contaminant concentrations in groundwater are lower than their corresponding equilibrium values (Mackay *et al*, 1985; Mercer and Cohen, 1990). Experimental investigations indicate that the dissolution process is mass-transfer limited when (1) NAPL is distributed nonuniformly due to aquifer heterogeneity, (2) water velocity is high and (3) NAPL saturation is low (Powers *et al.*, 1991; Guarnaccia *et al.*, 1992; Powers *et al.*, 1992). UTCHEM has the capability of modeling a nonequilibrium mass transfer relationship between NAPL and water or microemulsion phases. The NAPL dissolution rate is assumed to be represented by a linear driving force model similar to the one proposed by Abriola *et al.*, [1992], Powers *et al.*, [1991], Mayer and Miller, [1990], and Powers *et al.*, [1992]. The species mass transfer rate at the interface between the two phases ($R_{\kappa\ell}^I$) is modeled as

$$R_{\kappa\ell}^I = -M_\kappa \left(C_{\kappa\ell} - C_{\kappa\ell}^{eq}\right) \quad \text{for } \ell = 1 \text{ or } 3 \qquad (2.12)$$

where M_κ is the mass transfer coefficient for species κ across the boundary layer and $C_{\kappa\ell}$ and $C_{\kappa\ell}^{eq}$ are the mass concentrations of κ in the bulk aqueous solution and at equilibrium, respectively. Equation 2.12 can be written in terms of volumetric concentration of organic species (κ=2) as

$$\frac{\partial(S_\ell C_{2\ell}\phi)}{\partial t} = \vec{\nabla} \cdot \left(C_{2\ell}\vec{u}_\ell - \vec{\vec{D}}_{2\ell}\right) + M_2\left(C_{2\ell}^{eq} - C_{2\ell}\right) \quad \text{for } \ell = 1 \text{ or } 3 \tag{2.13}$$

where $C_{2\ell}$ is the volumetric concentration of organic species in the aqueous phase and $C_{2\ell}^{eq}$ is the equilibrium concentration. The time derivative was discretized using a backward finite difference approximation.

The equilibrium concentration for pure NAPL in water or aqueous phase with surfactant concentration below the critical micelle concentration (CMC) is an input solubility limit which is small for many of the NAPLs of interest to contaminant hydrogeologists. In the presence of surfactant, however, the equilibrium concentrations are calculated for surfactant/NAPL/water phase behavior using Hand's equation. The nonequilibrium concentration of NAPL in water and phase saturations are then computed using the previous time step saturations and concentrations and the new time step equilibrium concentrations. The mass transfer coefficient is assumed to be a constant although it may be a function of groundwater velocity, composition, saturation, and porous medium properties (Pennell *et al.*, 1993).

2.2.6 Well Models

Injection and production wells are considered source and sink terms in the flow equations. Wells can be completed vertically in several layers of the aquifer or horizontally with any length and can be controlled according to pressure or rate constraints. The well models used are based on formulations by Peaceman [1983] and Babu and Odeh [1989]. The aquifer boundaries are treated as either constant-potential or closed surfaces.

2.2.7 Fluid and Soil Properties

Geologic heterogeneities are probably the key factor which reduce the effectiveness of chemical enhanced recovery processes because their success depends on the delivery of injected chemical and water into the subsurface to contact the organic liquids. Heterogeneities result in a complex distribution of DNAPL in residual zones and pools. To capture some of the geologic features, reservoir properties such as formation permeability, porosity, residual phase saturation, phase relative permeability, and phase capillary pressure are allowed to vary spatially in UTCHEM. Phase trapping functions and adsorption of both surfactant and polymer are modeled as a function of permeability.

Many of the properties of anionic surfactants and polymers depend on the electrolyte concentrations in the water. Divalent cations such as calcium and magnesium ions are particularly important and can make significant differences in adsorption and other properties even at the low concentrations typically found in ground water. Furthermore, it cannot be assumed that these concentrations do not change since processes such as cation exchange and mineral dissolution occur during surfactant remediation. In this paper, we describe these electrolyte effects in terms of salinity or effective salinity (defined below) and these terms as used in this context refer to any electrolyte concentrations of interest, but especially to those of interest to surfactant remediation of aquifers containing ground water at low electrolyte concentrations. The same term and the same models are used to describe high salinities typical of oil reservoirs, but it should not be inferred that these electrolyte effects are only significant at high salinities. In fact, cation exchange between the water and clays and between the water and micelles (when anionic surfactant above its critical micellar concentration is present) is more important at low salinities typical of potable water than it is at high salinities such as sea water or high salinity oil reservoirs.

The description of properties in this paper assumes that alcohols, polymer/cross-linker, and components for high-pH flooding are absent. These property models are described in Saad [1989], Bhuyan *et al.* [1990], and Kim [1995].

2.2.8 Adsorption

Surfactant

Surfactant adsorption can be an important mechanism for a SEAR process since it causes retardation and consumption of surfactant. The remaining adsorbed surfactant after flushing with water at the end of the remediation process may also be important even for food grade surfactants and even though the mass concentration in the porous media at this time is likely to be very low on the order of the CMC. Some additional time will be required for this remaining surfactant to biodegrade and this will depend on the surfactant concentration among other variables. Surfactant adsorption has been the subject of extensive study for many decades and is now very well understood, especially for the types of surfactants and porous media of interest to SEAR. Rouse *et al.* [1993] and Adeel and Luthy [1994] are examples of recent studies done to compare the adsorption of different types of surfactant on soils. Somasundaran and Hanna [1977] and Scamehorn *et al.* [1982] are examples among the hundreds of studies done to evaluate the adsorption of surfactants on porous media in the context of surfactant enhanced oil recovery. These studies show that surfactant adsorption isotherms are very complex in general. This is especially true when the surfactant is not isomerically pure and the substrate is not a pure mineral. However, we and others have found that for many if not most conditions of interest to us the general tendency is for the surfactant isotherm to reach a plateau at some sufficiently large surfactant concentration. For pure surfactants, this concentration is in fact the CMC, which is often 100 times or more below the injected surfactant concentration. Thus, the complex detailed shape of the isotherm below the CMC has little practical impact on the transport and effectiveness of the surfactant and for this reason it has been found that a Langmuir-type isotherm can be used to capture the essential features of the adsorption isotherm for this purpose. Camilleri *et al.* [1987a] illustrate this by simulating an oil recovery experiment and Saad *et al.* [1989] by successfully simulating a surfactant field project using this approach. We also used a Langmuir-type adsorption isotherm for the simulation of the surfactant remediation of the Borden cell test illustrated below.

UTCHEM uses a Langmuir-type isotherm to describe the adsorption level of surfactant which takes into account the salinity, surfactant concentration, and soil permeability (Hirasaki and Pope, 1974). The adsorption is irreversible with concentration and reversible with salinity. The adsorbed concentration of surfactant ($\kappa = 3$) is given by

$$\hat{C}_\kappa = \min\left(\tilde{C}_\kappa, \frac{a_\kappa\left(\tilde{C}_\kappa - \hat{C}_\kappa\right)}{1 + b_\kappa\left(\tilde{C}_\kappa - \hat{C}_\kappa\right)}\right) \quad \kappa = 3 \text{ or } 4 \tag{2.14}$$

The concentrations are normalized by the water concentration in the adsorption calculations. The minimum is taken to guarantee that the adsorption is no greater than the total surfactant concentration. Adsorption increases linearly with effective salinity and decreases as the permeability increases as follows:

$$a_3 = \left(a_{31} + a_{32}\, C_{SE}\right) k^{-0.5} \tag{2.15}$$

where C_{SE} is the effective salinity described later. The value of a_3/b_3 represents the maximum level of adsorbed surfactant and b_3 controls the curvature of the isotherm. The adsorption model parameters a_{31}, a_{32}, and b_3 are found by matching laboratory surfactant adsorption data.

Polymer

The retention of polymer molecules in permeable media is due to both adsorption onto solid surfaces and trapping within small pores. The polymer retention similar to that of surfactant slows down the polymer velocity and depletes the polymer slug. Polymer adsorption is modeled as a function of permeability, salinity, and polymer concentration (Eq. 2.14 for $\kappa = 4$). The parameter a_4 is defined as

$$a_4 = \left(a_{41} + a_{42} C_{SEP}\right) k^{-0.5} \tag{2.16}$$

The effective salinity for polymer (C_{SEP}) is

$$C_{SEP} = \frac{C_{51} + \left(\beta_P - 1\right) C_{61}}{C_{11}} \tag{2.17}$$

where C_{51}, C_{61}, and C_{11} are the anion, calcium, and water concentrations in the aqueous phase and β_P is measured in the laboratory and is an input parameter to the model.

Organic

Organic sorption can be an important parameter in assessments of the fate and transport of DNAPLs in soils. The magnitude of sorbed organics is described in terms of a partition coefficient with respect to the organic fraction, K_{oc} (Karickhoff, 1984). The higher K_{oc}, the greater is its tendency to sorb into organic carbon in the subsurface. A linear sorption isotherm is used to model the organic sorption:

$$\hat{C}_2 = f_{oc} K_{oc} C_{21} \tag{2.18}$$

where $\hat{C}_2$ is the adsorbed organic, f_{oc} is the fraction of organic carbon in the soil, and C_{21} is the organic concentration in the water phase. K_{oc} is defined as the ratio of the amount of organic adsorbed per unit weight of organic carbon in the soil to the concentration of the organic in solution at equilibrium.

2.2.9 Cation Exchange

Cation exchange occurs when there is an incompatibility in the electrolyte composition of injected fluids and the initial fluids saturating the soil. Cation exchange affects the transport of ions in solution and therefore may have a significant effect on the optimum salinity and the surfactant phase behavior (Pope *et al.*, 1978; Fountain, 1992) and surfactant adsorption. The type and concentration of cations involved in the exchange process can also affect the hydraulic conductivity (Fetter, 1993). We use a cation exchange model based on Hirasaki's model [1982]. Cations exist in the form of free ions, adsorbed on clay surfaces, and associated with either surfactant micelles or adsorbed surfactant. The mass action equations for the exchange of calcium (κ=6) and sodium (κ=12) on clay and surfactant describe the cation exchange model as

$$\frac{\left(C_{12}^s\right)^2}{C_6^s} = \beta^s C_3^m \frac{\left(C_{12}^f\right)^2}{C_6^f} \tag{2.19}$$

$$\frac{\left(C_{12}^{c}\right)^2}{C_6^{c}} = \beta^c Q_v \frac{\left(C_{12}^{f}\right)^2}{C_6^{f}} \qquad (2.20)$$

where the superscripts f, c, and s denote free cation, adsorbed cation on clay, and adsorbed cation on micelles, respectively. The simulator input parameters are Q_v, the cation exchange capacity of the mineral, β^c and β^s, the ion exchange constants for clay and surfactant, and C_3^m, the concentration of surfactant in meq/ml. The electrical neutrality and mass balances needed to close the system of ion exchange equations are

$$C_5 = C_{12}^f + C_6^f \qquad (2.21)$$

$$C_6 = C_6^f + C_6^s + C_6^c \qquad (2.22)$$

$$C_3 = C_6^s + C_{12}^s \qquad (2.23)$$

$$Q_v = C_6^c + C_{12}^c \qquad (2.24)$$

$$C_5 - C_6 = C_{12}^f + C_{12}^s + C_{12}^c \qquad (2.25)$$

where C_κ^f is the fluid concentration for species κ normalized by water concentration All concentrations in ion exchange equations are expressed in meq/ml of water. The molar volume concentration of surfactant is computed as

$$C_3^m = \frac{1000 C_3}{C_1 M_3} \qquad (2.26)$$

where M_3 is the equivalent weight of the surfactant.

The cation exchange equations are solved for the six unknowns $C_6^c, C_{12}^c, C_6^f, C_{12}^f, C_6^s, \text{and}\, C_{12}^s$ using Newton-Raphson method.

2.2.10 Phase Behavior

The surfactant/oil/water phase behavior is based on Winsor [1954], Reed and Healy [1977], Nelson and Pope [1978], Prouvost *et al.* [1985], and others. Surfactant phase behavior considers up to five volumetric components (oil, water, surfactant, and two alcohols) which form three pseudocomponents in a solution. In the absence of alcohols (the formulation described in this paper), only three components are modeled. The volumetric concentrations of these three components are used as the coordinates on a ternary diagram. Salinity and divalent cation concentrations have a strong influence on phase behavior. At low salinity, an excess oil phase that is essentially pure oil and a microemulsion phase that contains water plus electrolytes, surfactant, and some solubilized oil exist. The tie lines (distribution curves) at low salinity have negative slope (Fig. 2.1). This type of phase environment is called Winsor Type I, or alternatively Type II(−) in some of the literature. If the surfactant concentration is below CMC, the two phases are an aqueous phase containing all the surfactant, electrolytes, and dissolved oil at the water solubility limit and a pure excess oil phase. For high salinity, an excess water phase and a microemulsion phase containing most of the surfactant and oil, and some solubilized water exist. This type of phase environment is called Winsor Type

II, or alternatively Type II(+) (Fig. 2.2). An overall composition at intermediate salinity separates into three phases. These phases are excess oil and water phases and a microemulsion phase whose composition is represented by an invariant point. This phase environment is called Winsor Type III, or just Type III (Fig. 2.3).

Other variables besides electrolyte concentrations, e.g. alcohol type and concentration, the equivalent alkane carbon number of the oil or solvent and changes in temperature or pressure also cause a phase environment shift from one type of phase behavior to another type. Three papers by Baran *et al*. [1994 a,b,c] show that the phase behavior of surfactants with both pure chlorocarbons such as trichloroethylene (TCE) and mixtures of chlorocarbons such as TCE and carbon tetrachloride is essentially identical in form to the classical behavior with hydrocarbons, so we are justified in using the same approach for these contaminants as we have used for hydrocarbons.

The surfactant/oil/water phase behavior can be represented as a function of effective salinity once the binodal curve and tie lines are described. The phase behavior model in UTCHEM uses Hand's rule (Hand, 1939) and is based on the work by Pope and Nelson [1978], Prouvost *et al.* [1984b; 1985; 1986], Satoh [1984], and Camilleri *et al.* [1987a,b,c].

Effective Salinity

The effective salinity increases with the divalent cations bound to micelles (Glover *et al.,* 1979; Hirasaki, 1982; Camilleri *et al*., 1987a,b,c) and decreases as the temperature increases for anionic surfactants and increases as the temperature increases for nonionic surfactants.

$$C_{SE} = C_{51}\left(1-\beta_6 f_6^s\right)^{-1}\left[1+\beta_T\left(T-T_{ref}\right)\right]^{-1} \tag{2.27}$$

where C_{51} is the aqueous phase anion concentration; β_6 is a positive constant; f_6^s is the fraction of the total divalent cations bound to surfactant micelles as $f_6^s = \dfrac{C_6^s}{C_3^m}$; and β_T is the temperature coefficient.

The effective salinities at which the three equilibrium phases form or disappear are called lower and upper limits of effective salinity (C_{SEL} and C_{SEU}).

Binodal Curve

The formulation of the binodal curve using Hand's rule (Hand, 1939) is assumed to be the same in all phase environments. Hand's rule is based on the empirical observation that equilibrium phase concentration ratios are straight lines on a log-log scale. Figures 2.4a and 2.4b show the ternary diagram for a Type II(−) environment with equilibrium phases numbered 2 and 3 and the corresponding Hand plot. The binodal curve is computed from

$$\frac{C_{3\ell}}{C_{2\ell}} = A\left(\frac{C_{3\ell}}{C_{1\ell}}\right)^B \qquad \ell = 1, 2, \text{ or } 3 \tag{2.28}$$

where A and B are empirical parameters. For a symmetric binodal curve where B = −1, which is the current formulation used in UTCHEM, all phase concentrations are calculated explicitly in terms of oil concentration $C_{2\ell}$ (recalling $\sum_{\kappa=1}^{3} C_{\kappa\ell} = 1$).

$$C_{3\ell} = \frac{1}{2}\left[-AC_{2\ell} + \sqrt{(AC_{2\ell})^2 + 4AC_{2\ell}(1 - C_{2\ell})}\right] \quad \text{for } \ell = 1, 2, \text{ or } 3 \tag{2.29}$$

Parameter A is related to the height of the binodal curve as follows

$$A_m = \left(\frac{2C_{3\max,m}}{1 - C_{3\max,m}}\right)^2 \quad m = 0, 1, \text{ and } 2 \tag{2.30a}$$

where m = 0, 1, and 2 are corresponding to low, optimal, and high salinities. The height of binodal curve is specified as a linear function of temperature:

$$C_{3\max,m} = H_{BNC,m} + H_{BNT,m}(T - T_{ref}) \quad m = 0, 1, \text{ and } 2 \tag{2.30b}$$

where $H_{BNC,m}$ and $H_{BNT,m}$ are input parameters. A_m is linearly interpolated as

$$\begin{aligned} A &= (A_0 - A_1)\left(1 - \frac{C_{SE}}{C_{SEOP}}\right) + A_1 \quad \text{for } C_{SE} \le C_{SEOP} \\ A &= (A_2 - A_1)\left(\frac{C_{SE}}{C_{SEOP}} - 1\right) + A_1 \quad \text{for } C_{SE} > C_{SEOP} \end{aligned} \tag{2.31}$$

where C_{SEOP} is the optimum effective salinity and the arithmetic average of C_{SEL} and C_{SEU}. The heights of the binodal curve at three reference salinities are input to the simulator and are estimated based on phase behavior laboratory experiments.

Tie lines for two-phases

For both Type II(–) and Type II(+) phase behavior, there are only two phases below the binodal curve. Tie lines are the lines joining the composition of the equilibrium phases and are given by

$$\frac{C_{3\ell}}{C_{2\ell}} = E\left(\frac{C_{33}}{C_{13}}\right)^F \tag{2.32}$$

where ℓ=1 for Type II(+) and ℓ=2 for Type II(–). In the absence of available data for tie lines, F is calculated from $F = -1/B$. For a symmetric binodal curve (B=–1), F is equal to 1. Since the plait point is on both the binodal curve and tie line, we have

$$E = \frac{C_{1P}}{C_{2P}} = \frac{1 - C_{2P} - C_{3P}}{C_{2P}} \tag{2.33}$$

Applying the binodal curve equation to the plait point and substituting C_{3P} (Eq. 2.29) in Eq. 2.33, we have

$$E = \frac{1 - C_{2P} - \frac{1}{2}\left[-AC_{2P} + \sqrt{(AC_{2P})^2 + 4AC_{2P}(1 - C_{2P})}\right]}{C_{2P}} \tag{2.34}$$

where C_{2P} is the oil concentration at the plait point and is an input parameter for Type II(–) and Type II(+) phase environments.

Tie lines for Type III

The phase composition calculation for the three-phase region of Type III is simple due to the assumption that the excess oleic and aqueous phases are pure. The microemulsion phase composition is defined by the coordinates of the invariant point. The coordinates of the invariant point (M) are calculated as a function of effective salinity:

$$C_{2M} = \frac{C_{SE} - C_{CSEL}}{C_{SEU} - C_{CSEL}} \tag{2.35}$$

C_{3M} is computed by substituting C_{2M} in Eq. 2.29 and noting that $C_{1M} = 1 - C_{2M} - C_{3M}$.

The phase composition calculations for lobes II(–) and II(+) are analogous. The plait point must vary from zero to the II(+) value, C^*_{2PL} or zero to II(–) value, C^*_{2PR}. Here, we only consider the II(–) lobe. The plait point is calculated by interpolation on effective salinity:

$$C_{2PR} = C^*_{2PR} + \frac{C_{SE} - C_{SEL}}{C_{SEU} - C_{SEL}} \left(1 - C^*_{2PR}\right) \tag{2.36}$$

In order to apply Hand's equation, we transform the concentrations as shown in Fig. 2.5. The transformed concentrations are

$$\begin{aligned} C'_{1\ell} &= C_{1\ell} \sec\theta \\ C'_{3\ell} &= C_{3\ell} - C_{2\ell} \tan\theta \qquad \text{for } \ell = 2 \text{ or } 3 \\ C'_{2\ell} &= 1 - C'_{1\ell} - C'_{3\ell} \end{aligned} \tag{2.37}$$

The angle θ is

$$\begin{aligned} \tan\theta &= \frac{C_{3M}}{C_{1M}} \\ \sec\theta &= \frac{\sqrt{C^2_{1M} + C^2_{3M}}}{C_{1M}} \end{aligned} \tag{2.38}$$

Parameter E of the tie line equation is now calculated in terms of untransformed coordinates of the plait point as

$$E = \frac{C'_{1P}}{C'_{2P}} = \frac{1 - (\sec\theta - \tan\theta) C_{2PR} - C_{3PR}}{C_{2PR} \sec\theta} \tag{2.39}$$

where C_{3PR} is given by Eq. 2.29 and $C_{1PR} = 1 - C_{2PR} - C_{3PR}$.

2.2.11 Phase Saturations

The phase saturations in the saturated zone in the presence of surfactant are calculated from the phase concentrations, overall component concentration, and saturation constraints once the phase environment and phase compositions are known. The overall component concentration and saturation constraints are

$$C_{\kappa} = \sum_{\kappa=1}^{3} S_{\ell} C_{\kappa\ell} \qquad \ell = 1, 2, \text{or } 3 \tag{2.40}$$

$$\sum_{\ell=1}^{3} S_{\ell} = 1 \tag{2.41}$$

The phase saturations in the vadose zone (phase 3 is absent) are computed from the overall component concentration and the saturation constraint by

$$S_2 = \frac{C_2 - C_{21}}{1 - C_{21}}, S_1 = \frac{C_1}{1 - C_{11}}, S_4 = 1 - S_1 - S_2 \tag{2.42}$$

where C_{21} is the concentration of dissolved organic species in the water phase.

2.2.12 Interfacial Tension

The two models for calculating microemulsion/oil (σ_{23}) and microemulsion/water (σ_{13}) interfacial tension (IFT) are based on Healy and Reed [1974] and Huh [1979]. The IFTs for water and oil (σ_{ow}) and water and air (σ_{aw}) are assumed to be known constants.

Healy *et al.*

The first IFT model is based on Hirasaki's modification (Hirasaki, 1981) of the model of Healy and Reed [1974]. Once the phase compositions have been determined, the interfacial tensions between microemulsion and the excess phases (σ_{13}, σ_{23}) are calculated as functions of solubilization parameters:

$$\begin{cases} \log_{10} \sigma_{\ell 3} = \log_{10} F_{\ell} + G_{\ell 2} + \dfrac{G_{\ell 1}}{1 + G_{\ell 3} R_{\ell 3}} & \text{for } R_{\ell 3} \ge 1 \\ \log_{10} \sigma_{\ell 3} = \log_{10} F_{\ell} + (1 - R_{\ell 3}) \log_{10} \sigma_{ow} + R_{\ell 3} \left(G_{\ell 2} + \dfrac{G_{\ell 1}}{1 + G_{\ell 3}} \right) & \text{for } R_{\ell 3} < 1 \end{cases} \qquad \text{for } \ell = 1,2 \tag{2.43}$$

where $G_{\ell 1}$, $G_{\ell 2}$, and $G_{\ell 3}$ are input parameters. $R_{\ell 3}$ is the solubilization ratio ($\frac{C_{\ell 3}}{C_{33}}$). The correction factor introduced by Hirasaki, F_{ℓ}, ensures that the IFT at the plait point is zero and is

$$F_{\ell} = \frac{1 - e^{-\sqrt{\text{con}_{\ell}}}}{1 - e^{-\sqrt{2}}} \qquad \text{for } \ell = 1, 2 \tag{2.44}$$

where

$$\text{con}_{\ell} = \sum_{\kappa=1}^{3} (C_{\kappa\ell} - C_{\kappa 3})^2 \tag{2.45}$$

and in the absence of surfactant or the surfactant concentration below CMC, the IFTs equal σ_{ow}.

Chun-Huh

The interfacial tension is related to solubilization ratio in Chun-Huh's equation as

$$\sigma_{\ell 3} = \frac{c}{R_{\ell 3}^2} \quad \text{for } \ell = 1 \text{ or } 2 \tag{2.46}$$

where c is typically equal to about 0.3. We introduced Hirasaki's correction factor F_ℓ (Eq. 2.44) and modified Huh's equation so that it reduces to the water-oil IFT (σ_{ow}) as the surfactant concentration approaches zero.

$$\sigma_{\ell 3} = \sigma_{ow}\, e^{-a R_{\ell 3}} + \frac{c F_\ell}{R_{\ell 3}^2}\left(1 - e^{-a R_{\ell 3}^3}\right) \quad \text{for } \ell = 1 \text{ or } 2 \tag{2.47}$$

where a is a constant equal to about 10.

2.2.13 Density

Phase specific weights ($\gamma_\ell = g\rho_\ell$) are modeled as a function of pressure and composition as follows:

$$\gamma_\ell = C_{1\ell}\gamma_{1\ell} + C_{2\ell}\gamma_{2\ell} + C_{3\ell}\gamma_{3\ell} + 0.02533 C_{5\ell} - 0.001299 C_{6\ell} + C_{8\ell}\gamma_{8\ell} \quad \text{for } \ell = 1,\ldots, n_p \tag{2.48}$$

where $\gamma_{k\ell} = \gamma_{kR}\left[1 + C_k^o\left(P_\ell - P_{R0}\right)\right]$. γ_{kR} is the component κ specific weight at a reference pressure and is an input parameter. The numerical constants account for the weight of dissolved ions and have units of psi/ft per meq/ml of ions.

We have recently modified the density calculation for the microemulsion phase ($\ell = 3$) to use an apparent oil component specific weight in the microemulsion phase (γ_{23R}) instead of the oil component specific weight (γ_{2R}).

2.2.14 Capillary Pressure

Both the Parker *et al.* [1987] generalization of the van Genuchten [1980] model and the Brooks and Corey [1966] model are options used to calculate the capillary pressure. Hysteresis in capillary pressure is taken into account in a very simplistic fashion discussed below, but a full hysteretic and trapping number dependent model that is more complete is also available (Delshad *et al.*, 1994).

Brooks-Corey

Capillary pressure in Brooks and Corey capillary pressure-saturation relationship (Brooks and Corey, 1966) is scaled for interfacial tension, permeability, and porosity (Leverett, 1941). The organic spill event in the unsaturated (vadose) zone is assumed to be in the imbibition direction (total liquid saturation increasing). The organic spill event in the saturated zone is taken to be in the first drainage direction (wetting phase, water, saturation decreasing) for the entire spill process. The water flushing or surfactant injection process is assumed to be in the imbibition direction for the entire injection period.

Vadose Zone

Implicit assumptions in the capillary pressure formulation in the vadose zone where up to three phases exist are that the direction of descending wettability is water, organic, and air and that the water phase is always present.

$$\left(\frac{P_b}{P_{c1\ell}}\right)^{\lambda_i} = 1 - S_{n1} \quad \text{for } \ell = 2 \text{ or } 4 \tag{2.49}$$

where the maximum capillary pressure P_b is scaled by soil permeability and porosity and is equal to $C_{pci} \frac{\sigma_{1\ell}}{\sigma_{12}} \sqrt{\frac{\phi}{k}}$, which then gives

$$P_{c1\ell} = C_{pci} \sqrt{\frac{\phi}{k}} \frac{\sigma_{1\ell}}{\sigma_{12}} \left(1 - S_{n1}\right)^{-1/\lambda_i} \quad \text{for } \ell = 2 \text{ or } 4 \tag{2.50}$$

where C_{pci} and $EPC_i = -1/\lambda_i$ are positive input parameters. The normalized saturations are defined as

$$S_{n\ell} = \frac{S_\ell - S_{\ell r}}{1 - S_{1r} - S_{2r} - S_{4r}} \tag{2.51}$$

The entrapped organic saturation for three-phase (air/organic/water) flow (S_{2r}) is based on a function by Fayers and Matthews [1982] which uses the two-phase entrapped saturation values:

$$S_{2r} = S_{2r1}\left(1 - \frac{S_4}{1 - S_{1r} - S_{2r4}}\right) + S_{2r4}\left(\frac{S_4}{1 - S_{1r} - S_{2r4}}\right) \tag{2.52}$$

where S_{2r1} and S_{2r4} are the entrapped organic saturations to flowing water and air phases, respectively.

Saturated Zone

The capillary pressure in the saturated zone where up to three phases (water, organic, microemulsion) exist according to the surfactant phase behavior is calculated as follows.

Two-phase organic-water

The drainage capillary pressure is modeled using the Brooks-Corey function:

$$\left(\frac{P_b}{P_{c12}}\right)^{\lambda_d} = S_{n1} \tag{2.53}$$

where λ_d is a measure of pore size distribution of the medium, the entry pressure P_b equals $C_{pcd} \sqrt{\frac{\phi}{k}}$ and the normalized water saturation is defined as

$$S_{n1} = \frac{S_1 - S_{1r}}{1 - S_{1r}} \tag{2.54}$$

where C_{pcd} and $EPC_d = -1/\lambda_d$ are input parameters. The UTCHEM input parameter EPC_d must be a negative value.

Two-phase water/microemulsion or organic/microemulsion

The imbibition capillary pressure using a Corey-type function is

$$\left(\frac{P_{b\ell}}{P_{c\ell 3}}\right)^{\lambda_i} = 1 - S_{n\ell'} \tag{2.55}$$

For $\ell = 1$, $\ell' = 1$ while for $\ell = 2$, $\ell' = 3$. $P_{b\ell}$ equals $C_{pci}\frac{\sigma_{\ell 3}}{\sigma_{12}}\sqrt{\frac{\phi}{k}}$. The normalized saturations are defined as

$$S_{n1} = \frac{S_1 - S_{1r}}{1 - S_{1r} - S_{3r}} \tag{2.56}$$

$$S_{n3} = \frac{S_3 - S_{3r}}{1 - S_{2r} - S_{3r}} \tag{2.57}$$

Three-phase water/organic/microemulsion

$$\left(\frac{P_{b1}}{P_{c13}}\right)^{\lambda_i} = 1 - S_{n1} \tag{2.58}$$

$$\left(\frac{P_{b2}}{P_{c23}}\right)^{\lambda_i} = 1 - \frac{S_2 - S_{2r}}{\left(S_1 - S_{1r}\right) + \left(S_3 - S_{3r}\right)} \tag{2.59}$$

where $S_{n1} = \frac{S_1 - S_{1r}}{1 - S_{1r} - S_{2r} - S_{3r}}$ and $P_{b\ell}$ equals $C_{pci}\frac{\sigma_{\ell 3}}{\sigma_{12}}\sqrt{\frac{\phi}{k}}$.

The residual saturations ($S_{\ell r}$) in Brooks and Corey's model are either a constant and input to the simulator or computed as a function of trapping number discussed later.

van Genuchten

The three-phase capillary pressure-saturation function determined using the generalization of Parker *et al.* [1987] to the two-phase flow model of van Genuchten [1980] is represented by

$$\begin{aligned} \bar{S}_\ell &= \left[1 + \left(\alpha\, h^*\right)^n\right]^{-m} && h^* > 0 \\ \bar{S}_\ell &= 1 && h^* \le 0 \end{aligned} \tag{2.60}$$

where $\bar{S}_\ell = \frac{S_\ell - S_{1r}}{1 - S_{1r}}$ is the effective saturation, $h^* = \beta_{\ell\ell'} P_{C\ell\ell'}$ is the scaled capillary pressure; $\beta_{\ell\ell'}$ is the scaling coefficient for fluid pair of ℓ and ℓ'; α (UTCHEM parameter of CPC) and n (UTCHEM parameter of EPC) are the model parameters, and m = 1–1/n. A significant difference between the van Genuchten and Brooks Corey models is the discontinuity in the slope of the capillary pressure curve at the entry pressure in the latter model whereas Eq. 2.60 is both continuous and has a continuous slope. The implementation of this model in the simulator includes scaling α with soil permeability and porosity similar to that described in Brooks-Corey model.

2.2.15 Relative Permeability

Multiphase relative permeabilities are modeled based on either Corey-type functions (Brooks and Corey, 1966; Delshad and Pope, 1989) or Parker *et al.* [1987] extension of van Genuchten two-phase flow equation to three-phase flow. Hysteresis in the Corey-type relative permeability model discussed below is accounted for by assuming the flow in the saturated zone is on the drainage curve for the spill event and the remediation of the saturated zone is an imbibition process. However, a full hysteretic relative permeability model that is trapping number dependent is also available (Delshad *et al.*, 1994).

Corey-Type

Multiphase imbibition and drainage relative permeabilities in both the vadose and saturated zones are modeled using Corey-type functions that are a function of trapping number.

Vadose Zone

The organic phase movement in a three-phase porous medium consisting of water/organic/air is assumed to be in the imbibition direction during the organic spill in the vadose zone. We also assume that water and air relative permeabilities are unique functions of their respective saturations only. Organic phase relative permeability, however, is assumed to be a function of two saturations (Delshad and Pope, 1989). These assumptions are consistent with relative permeability measurements (Corey *et al.*, 1956; Saraf and Fatt, 1967; Schneider and Owens, 1970; Saraf *et al.*, 1982; Fayers and Matthews, 1982; Oak, 1990; Oak, *et al.*, 1990).

$$k_{r\ell} = k^{o}_{r\ell}\left(S_{n\ell}\right)^{n_\ell} \quad \text{for } \ell = 1, 2, \text{ or } 4 \tag{2.61}$$

where the normalized saturations are defined as

$$S_{n\ell} = \frac{S_\ell - S_{\ell r}}{1 - S_{1r} - S_{2r\ell} - S_{4r}} \quad \text{for } \ell = 1, \text{ or } 4 \tag{2.62}$$

$$S_{n2} = \frac{S_2 - S_{2r}}{1 - S_{1r} - S_{2r} - S_{4r}} \tag{2.63}$$

where $k^{o}_{r\ell}$, n_ℓ, and $S_{\ell r}$ are the relative permeability endpoint, exponent, and entrapped saturation for phase ℓ. The trapped organic saturation for three-phase flow (S_{2r}) is calculated from Eq. 2.52. These equations reduce to two-phase flow relative permeabilities in the absence of the third phase.

Saturated Zone

The organic phase movement during the spill event in the saturated zone where up to two fluid phases (water and organic) exist is assumed to be in the drainage direction. The organic movement during the remediation process, e.g., water flushing or surfactant injection, however, is assumed to be in the imbibition direction for the entire injection period.

Organic spill process

The relative permeabilities for water and organic fluid phases are

$$k_{r1} = k^{o}_{r1}\left(S_{n1}\right)^{n_1} \tag{2.64}$$

$$k_{r2} = k^{o}_{r2}\left(1 - S_{n1}\right)^{n_2} \tag{2.65}$$

where the normalized water saturation is $S_{n1} = \dfrac{S_1 - S_{1r}}{1 - S_{1r}}$.

Remediation process

There are up to three liquid phases present according to the surfactant/water/ organic phase behavior during a SEAR process in the saturated zone. The relative permeabilities are assumed to be unique functions of their respective saturations only. The latter assumption is supported by experimental data measured at The University of Texas at Austin for a mixture of petroleum sulfonate, n-decane, isobutyl alcohol, and water (Delshad *et al.*, 1987; Delshad, 1990). The relative permeability is defined by

$$k_{r\ell} = k^o_{r\ell}\left(S_{n\ell}\right)^{n\ell} \quad \text{for } \ell = 1, 2, \text{ or } 3 \tag{2.66}$$

where the normalized saturations are defined as

$$S_{n\ell} = \frac{S_\ell - S_{\ell r}}{1 - \sum_{\ell=1}^{3} S_{\ell r}} \quad \text{for } \ell = 1, 2, \text{ or } 3 \tag{2.67}$$

The relative permeabilities reduce to water/organic, water/microemulsion, or organic/microemulsion two phase flow functions. The residual saturations, relative permeability endpoints, and exponents are either constants and input parameters or functions of trapping number as discussed in the next section.

Parker *et al.*

Parker *et al*. [1987] extended the two-phase relative permeability-saturation expression derived by van Genuchten to three-phase water/oil/air flow using scaled variables as follows:

$$k_{r1} = \bar{S}_1^{1/2}\left[1 - \left(1 - \bar{S}_1^{1/m}\right)^m\right]^2 \tag{2.68}$$

$$k_{r2} = \left(\bar{S}_t - \bar{S}_1\right)^{1/2}\left[\left(1 - \bar{S}_1^{1/m}\right)^m - \left(1 - \bar{S}_t^{1/m}\right)^m\right]^2 \tag{2.69}$$

$$k_{r4} = \left(\bar{S}_4\right)^{1/2}\left(1 - \bar{S}_t^{1/m}\right)^{2m} \tag{2.70}$$

where S_t is the total liquid saturation. The assumptions in deriving the above relative permeability functions are that water or gas relative permeability is a function of its own saturation only whereas oil relative permeability is a function of both water and oil saturations.

2.2.16 Trapping Number

One of the possible mechanisms for SEAR is the mobilization of trapped organic phase due to reduced interfacial tension resulting from the injection of surfactants into the aquifer (Tuck *et al.*, 1988; Cherry *et al.*, 1990; Pennell *et al.*, 1994; Brown *et al.*, 1994). Buoyancy forces can also affect the mobilization of a trapped organic phase and can be expressed by the Bond number (Morrow and Songkran, 1982). The Bond and capillary numbers for the trapping and mobilization of a nonwetting phase are usually treated as two separate dimensionless groups, one to represent gravity/capillary forces (Bond number) and the other to represent viscous/capillary forces (capillary number). One of several classical definitions of capillary number (Brownell and Katz, 1949; Stegemeier, 1977; Chatzis and Morrow, 1981; Lake, 1989) is as follows

$$N_{c_\ell} = \frac{\left|\vec{\vec{k}}\cdot\vec{\nabla}\Phi_{\ell'}\right|}{\sigma_{\ell\ell'}} \qquad \text{for } \ell = 1,\ldots, n_p \tag{2.71}$$

where ℓ and ℓ' are the displaced and displacing fluids and the gradient of the flow potential is given by $\nabla\Phi_{\ell'} = \nabla P_{\ell'} - g\rho_{\ell'}\nabla h$.

Bond number can be defined as

$$N_{B_\ell} = \frac{k\, g\left(\rho_\ell - \rho_{\ell'}\right)}{\sigma_{\ell\ell'}} \qquad \text{for } \ell = 1,\ldots, n_p \tag{2.72}$$

where k is the permeability and g is the gravitational force constant.

We have recently developed a new dimensionless number called the trapping number which includes both gravity and viscous forces. The dependence of residual saturations on interfacial tension is modeled in UTCHEM as a function of the trapping number. This is a new formulation that we found necessary to adequately model the combined effect of viscous and buoyancy forces in three dimensions. Buoyancy forces are much less important under enhanced oil recovery conditions than under typical SEAR conditions and so had not until now been carefully considered under three-dimensional surfactant flooding field conditions as a result.

The trapping number is derived by applying a force balance on the trapped NAPL globule. The forces controlling the movement of the blob are the viscous force due to the hydraulic gradient, the trapping force due to capillary pressure and the gravity force, which can act as either a driving or trapping force depending on the direction of the flow. The condition for mobilizing a trapped blob of length L is as follows

Hydraulic force + Buoyancy force • Capillary force (2.72a)

Substituting the definition for each of these forces we have

$$\Delta L\left|\nabla\Phi_w - g\Delta\rho\right| \geq \Delta P_c \tag{2.72b}$$

The trapping number is defined by the left-hand side of Eq. 2.72b as

$$N_{T\ell} = \frac{\left|-\vec{\vec{k}}\cdot\vec{\nabla}\Phi_{\ell'} - \vec{\vec{k}}\cdot\left[g\left(\rho_{\ell'} - \rho_\ell\right)\vec{\nabla}h\right]\right|}{\sigma_{\ell\ell'}} \tag{2.72c}$$

For one-dimensional vertical flow, the viscous and buoyancy forces add directly and a trapping number can be defined as $N_{T_\ell} = \left|N_{c_\ell} + N_{B_\ell}\right|$. For two-dimensional flow a trapping number is defined as

$$N_{T_\ell} = \sqrt{N_{c\ell}^2 + 2\, N_{c\ell}\, N_{B\ell}\sin\theta + N_{B\ell}^2} \qquad \text{for } \ell = 1,\ldots, n_p \tag{2.73}$$

where θ is the angle between the local flow vector and the horizontal (counter clockwise). The derivation of trapping number for three-dimensional heterogeneous, anisotropic porous media is given by Jin [1995].

Residual saturations are then computed as a function of trapping number as

$$S_{\ell r} = \min\left(S_\ell \, , \, S_{\ell r}^{high} + \frac{S_{\ell r}^{low} - S_{\ell r}^{high}}{1 + T_\ell \, N_{T_\ell}} \right) \quad \text{for } \ell = 1,..., n_p \tag{2.74}$$

where T_ℓ is a positive input parameter based on the experimental observation of the relation between residual saturations and trapping number. $S_{\ell r}^{low}$ and $S_{\ell r}^{high}$ are the input residual saturations for phase ℓ at low and high trapping numbers. This correlation was derived based on the experimental data for n-decane (Delshad, 1990) and have recently been successfully applied to residual PCE as a function of trapping number measured by Abriola *et al.* [1994; 1995].

The endpoints and exponents of both the relative permeability curves and capillary pressure curves change as the residual saturations change at high trapping numbers because of detrapping (Morrow and Chatzis, 1981; Morrow *et al.*, 1985; Fulcher *et al.*, 1985; Delshad *et al.*, 1986). The endpoints and exponents in relative permeability functions are computed as a linear interpolation (Delshad *et al.*, 1986) between the given input values at low and high trapping numbers $\left(k_{r\ell}^{o\,low}, k_{r\ell}^{o\,high}, n_\ell^{low}, n_\ell^{high} \right)$:

$$k_{r\ell}^{o} = k_{r\ell}^{o\,low} + \frac{S_{\ell' r}^{low} - S_{\ell' r}}{S_{\ell' r}^{low} - S_{\ell' r}^{high}} \left(k_{r\ell}^{o\,high} - k_{r\ell}^{o\,low} \right) \quad \text{for } \ell = 1,..., n_p \tag{2.75}$$

$$n_\ell = n_\ell^{low} + \frac{S_{\ell' r}^{low} - S_{\ell' r}}{S_{\ell' r}^{low} - S_{\ell' r}^{high}} \left(n_\ell^{high} - n_\ell^{low} \right) \text{for } \ell = 1,..., n_p \tag{2.76}$$

The above correlations have successfully been tested against experimental data (Delshad *et al.*, 1986).

2.2.17 Viscosity

Liquid phase viscosities are modeled in terms of pure component viscosities and the phase concentrations of the organic, water and surfactant:

$$\mu_\ell = C_{1\ell} \mu_w e^{\alpha_1 (C_{2\ell} + C_{3\ell})} + C_{2\ell} \mu_o \, e^{\alpha_2 (C_{1\ell} + C_{3\ell})} + C_{3\ell} \alpha_3 \, e^{(\alpha_4 C_{1\ell} + \alpha_5 C_{2\ell})} \quad \text{for } \ell = 1, 2, \text{ or } 3 \tag{2.77}$$

where the α parameters are determined by matching laboratory microemulsion viscosities at several compositions. In the absence of surfactant and polymer, water and oil phase viscosities reduce to pure water and oil viscosities (μ_w, μ_o). When polymer is present, μ_w is replaced by μ_p defined below.

The following exponential relationship is used to compute viscosities as a function of temperature (T).

$$\mu_\kappa = \mu_{\kappa,ref} \exp\left[b_\kappa \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right] \quad \text{for } \kappa = \text{ water, oil, or air} \tag{2.78}$$

where $\mu_{\kappa,ref}$ is the viscosity at a reference temperature of T_{ref} and b_κ is an input parameter.

Air viscosity is computed as a linear function of pressure by

$$\mu_4 = \mu_{a0} + \mu_{aS} \left(P_R - P_{R0} \right) \tag{2.79}$$

where μ_{a0}, the air viscosity at a reference pressure of P_{R0} and μ_{aS}, the slope of air viscosity vs. pressure, are input parameters.

The viscosity of a polymer solution depends on the concentration of polymer and on salinity. The Flory-Huggins equation (Flory, 1953) was modified to account for variation in salinity as

$$\mu_p^0 = \mu_w \left(1 + \left(A_{p1} C_{4\ell} + A_{p2} C_{4\ell}^2 + A_{p3} C_{4\ell}^3\right) C_{SEP}^{S_p}\right) \quad \text{for } \ell = 1 \text{ or } 3 \tag{2.80}$$

where $C_{4\ell}$ is the polymer concentration in the water or microemulsion phase, μ_w is the water viscosity, A_{P1}, A_{P2}, and A_{P3} are constants. The factor $C_{SEP}^{S_p}$ allows for dependence of polymer viscosity on salinity and hardness. The effective salinity for polymer is given by Eq. 2.17 and S_p is the slope of $\left(\frac{\mu_p^0 - \mu_w}{\mu_w}\right)$ vs. C_{SEP} on a log-log plot.

The reduction in polymer solution viscosity as a function of shear rate ($\dot{\gamma}$) is modeled by Meter's equation (Meter and Bird, 1964):

$$\mu_p = \mu_w + \frac{\mu_p^0 - \mu_w}{1 + \left(\frac{\dot{\gamma}}{\dot{\gamma}_{1/2}}\right)^{P_\alpha - 1}} \tag{2.81}$$

where $\dot{\gamma}_{1/2}$ is the shear rate at which viscosity is the average of μ_p^0 and μ_w and P_α is an empirical coefficient. When the above equation is applied to flow in permeable media, μ_p is usually called apparent viscosity and the shear rate is an equivalent shear rate $\dot{\gamma}_{eq}$. The in-situ shear rate for phase ℓ is modeled by the modified Blake-Kozeny capillary bundle equation for multiphase flow (Lin, 1981; Sorbie, 1991) as

$$\dot{\gamma}_{eq} = \frac{\dot{\gamma}_c \left|u_\ell\right|}{\sqrt{\bar{k}\, k_{r\ell}\, \phi S_\ell}} \tag{2.82}$$

where $\dot{\gamma}_c$ is equal to 3.97C sec^{-1} and C is the shear rate coefficient used to account for non-ideal effects such as slip at the pore walls (Wreath *et al.*, 1990; Sorbie, 1991). The appropriate average permeability $\bar{k}$ is given by

$$\bar{k} = \left[\frac{1}{k_x}\left(\frac{u_{x\ell}}{u_\ell}\right)^2 + \frac{1}{k_y}\left(\frac{u_{y\ell}}{u_\ell}\right)^2 + \frac{1}{k_z}\left(\frac{u_{z\ell}}{u_\ell}\right)^2\right]^{-1} \tag{2.83}$$

2.2.18 Polymer Permeability Reduction

Polymer solutions reduce both the mobility of the displacing fluid and the effective permeability of the porous medium. The permeability reduction is measured by a permeability reduction factor, R_k, defined as

$$R_k = \frac{\text{effective permeability of water}}{\text{effective permeability of polymer}} \tag{2.84}$$

The change in mobility due to the combined effect of increased viscosity and reduced permeability is called resistance factor, R_F, calculated by

$$R_F = R_k \frac{\mu_p}{\mu_w} \tag{2.85}$$

The effect of permeability reduction lasts even after the polymer solution has passed through the porous medium and is called the residual resistance factor, R_{RF}, defined as

$$R_{RF} = \frac{\text{mobility before polymer solution}}{\text{mobility after polymer solutio}} \tag{2.86}$$

The permeability reduction factor in UTCHEM is modeled as

$$R_k = 1 + \frac{\left(R_{k\,max} - 1\right) b_{rk} C_{4\ell}}{1 + b_{rk} C_{4\ell}}$$

where

$$R_{k\,max} = \left[1 - \frac{c_{rk} \left(A_{p1} C_{SEP}^{S_p} \right)^{1/3}}{\left(\dfrac{\sqrt{k_x k_y}}{\phi} \right)^{1/2}} \right]^{-4} \tag{2.87}$$

and ℓ refers to the phase with the highest polymer concentration, b_{rk} and C_{rk} are the input parameters.

The effect of permeability reduction is assumed to be irreversible i.e., it does not decrease as polymer concentration decreases and thus $R_{RF} = R_k$. The viscosity of the phase that contains the polymer is multiplied by the value of the R_k to account for the mobility reduction in the simulator.

2.2.19 Polymer Inaccessible Pore Volume

The reduction in porosity due to inaccessible or excluded pores to the large size polymer molecules is called inaccessible pore volume. The resulting effect is a faster polymer velocity than the velocity of water. This effect is modeled by multiplying the porosity in the conservation equation for polymer by the input parameter of effective pore volume.

2.3 Numerical Methods

The pressure equation and species conservation equations are discretized spatially and temporally as described below. The discretized equations are given in Appendix C.

2.3.1 Temporal Discretization

The temporal discretization in UTCHEM is implicit in pressure, explicit in concentration (IMPES-like). The solution of the pressure equation using the Jacobi conjugate gradient method is then followed by a back substitution into the explicit mass conservation equation for each component. The temporal accuracy for the conservation equation is increased by using a time-correction technique that is second-order in time (Liu, 1993; Liu *et al.*, 1994).

2.3.2 Spatial Discretization

Either one-point upstream, two-point upstream, or a third-order spatial discretization of the advective terms is used (see Appendix C). It is well-known that lower-order upwind schemes cause smearing of the saturation and concentration profiles by increasing numerical dispersion. There have been a number of discretization methods developed to minimize these effects associated with multiphase flow and transport simulation (Todd *et al.*, 1972; Leonard, 1979; Taggart and Pinczewski, 1987; Bell *et al.*, 1989; Le Veque, 1990; Datta Gupta *et al.*, 1991; Blunt and Rubin, 1992; Dawson, 1993; Arbogast and Wheeler, 1995). We use a scheme that is approximately third-order in space to minimize numerical dispersion and grid-orientation effects. In order to obtain oscillation-free, high-resolution, high-order results, Harten [1983] developed the total-variation-diminishing scheme (TVD) that includes a limiting procedure. The limiter is a flux limiter with constraints on the gradient of the flux function (Sweby, 1984; Datta Gupta *et al*., 1991; Liu *et al*., 1994). The limiter function developed by Liu [1993], which varies as a function of timestep and gridblock size, was implemented in the simulator.

2.4 Model Verification and Validation

UTCHEM has extensively been verified by comparing problems such as one-dimensional two-phase flow with the Buckley-Leverett solution (Buckley and Leverett, 1942), one-dimensional miscible water/tracer flow against the analytical solution of the convection-diffusion equation, two-dimensional ideal tracer flow with the analytical solution given by Abbaszadeh-Dehghani and Brigham [1984], and two-dimensional nonlinear Burgers equation (Schiesser, 1991) by Liu [1993]. Excellent agreement between the numerical and analytical solutions were obtained when the TVD third-order scheme was used. The model has also been validated by comparisons with laboratory surfactant floods (Camilleri *et al.*, 1987a), field data from the Big Muddy surfactant pilot (Saad *et al.*, 1989), and a multiwell waterflood tracer field project (Allison *et al.*, 1991). Pickens *et al.* [1993] have compared UTCHEM results with a tetrachloroethylene (PCE) infiltration experiment in a sandpack with four types of sands performed by Kueper [1989] and Kueper and Frind [1991]. They concluded that the simulator can accurately predict the vertical and lateral distribution of DNAPL in a heterogeneous medium.

The model has recently been used to model the surfactant-enhanced remediation of PCE in a test cell at Canadian Forces Base Borden in Allison, Ontario (Freeze *et al.*, 1994). The model was 3 m by 3 m by 4 m deep test cell described as layered with soil properties estimated from the field data. The detailed description of the test cell is given by Kueper *et al.* [1993]. PCE in the amount of 231 L was first injected to the center of the test cell. The remediation process involved the following steps:

1. Direct pumping of free-phase for about two weeks where 47 L of PCE was recovered,

2. Pump and treat for about two months where additional 12 L of free-phase and dissolved PCE was removed, and

3. Surfactant flushing to solubilize additional PCE for about seven months. The surfactant solution was 1 wt% nonyl phenol ethoxylate (NP 100) and 1 wt% phosphate ester of the nonyl phenol

ethoxylate (Rexophos 25-97). A total of 130,000 L of surfactant solution was recirculated through the test cell. Additional 62 L of PCE was recovered as a result of enhanced solubility by the surfactant solution. The surfactant-enhanced solubility of PCE was measured to be about 11,700 mg/L as compared to an aqueous solubility of about 200 mg/L.

The measured and simulated vertical distributions of PCE before and after the surfactant injection are shown in Figs. 2.6 and 2.7 and show good agreement. Here we discuss the features of UTCHEM model that were used in this application and the input parameters for the physical property models since Freeze *et al*. did not discuss these in their paper. The assumptions made based on the test cell conditions were 1) isothermal simulations, 2) insignificant electrolyte concentration, incompressible fluids and soil, equilibrium PCE dissolution, and no mobilization of PCE. The species considered in the simulation were water, PCE, and surfactant and the resulting phases were water, PCE, and microemulsion. The phase behavior parameters were chosen such that either residual PCE/microemulsion, residual PCE/water, or single phase microemulsion are present. Due to lack of any phase behavior measurements for this surfactant mixture, the phase behavior parameters (C_{2P}, H_{bnc70} in Eq. 2.30b) were adjusted such that the simulated solubility is similar to the measured value of 11700 mg/L. Table 2.1 gives the input parameters for the physical properties. The test cell was simulated using 12 and 9 gridblocks in the x and y directions and 14 vertical layers. The porosity was constant equal to 0.39 and the hydraulic conductivity in the range of 0.003 to 0.01 cm/s. The ratio of vertical to horizontal permeability was 1. Longitudinal and transverse dispersivities for all three phases were assumed to be 0.03 and 0.01 m, respectively. The 201-day simulation of surfactant flooding took 22 minutes on a DEC 3000/500 alpha workstation.

UTCHEM was able to closely reproduce both the PCE recovery and the vertical distribution of PCE over the period of 201 days. The favorable comparison of UTCHEM results with the field test results demonstrates the utility of the model in predicting SEAR processes at the field scale.

2.5 Summary and Conclusions

We have presented the description of a three-dimensional, multicomponent, multiphase compositional model, UTCHEM, for simulating the contamination of aquifers by organic species and the remediation of aquifers by surfactant injection. UTCHEM has the capability of simulating both enhanced dissolution and separate phase removal of NAPLs from both saturated and vadose zones. The simulator has been verified with several analytical solutions and validated by comparisons with both laboratory and field experiments.

The model uses a block-centered finite-difference discretization. The solution method is analogous to the implicit in pressure and explicit in concentration method. Either one-, two-point upstream, or third-order spatial weighting schemes is used. A flux limiter that is total-variation-diminishing has also been added to the third-order scheme to increase stability and robustness.

UTCHEM accounts for effects of surfactants on interfacial tension, surfactant phase behavior, capillary trapping, and surfactant adsorption. Multiphase capillary pressures, relative permeabilities, physical dispersion, molecular diffusion, cation exchange, and partitioning of NAPLs to the aqueous phase which accounts for nonequilibrium effects are some of the important physical properties features in the simulator.

UTCHEM can be used to design the most efficient surfactant remediation strategies taking into account realistic soil and fluid properties. Due to its capability, several important variables that can significantly affect the outcome of any SEAR program such as mobilization vs. solubilization, mobility control by adding polymer, nonequilibrium interphase mass transfer, temperature gradient, and electrolyte concentrations where the soil/water interactions are important; e.g., fresh water in the presence of clay can be studied before implementing a field project.

2.6 Nomenclature

a_3	Surfactant adsorption parameter
a_{31}	Surfactant adsorption parameter, $(L^2)^{0.5}$
a_{32}	Surfactant adsorption parameter, $(L^2)^{0.5}$ $(Eq/L^3)^{-1}$
b_3	Surfactant adsorption parameter
a_4	Polymer adsorption parameter
a_{41}	Polymer adsorption parameter, $(L^2)^{0.5}$
a_{42}	Polymer adsorption parameter, $(L^2)^{0.5}$ $(Eq/L^3)^{-1}$
b_4	Polymer adsorption parameter, L^3/wt% polymer
b_{rk}	Permeability reduction factor parameter, L^3/wt% polymer
$C_{i,\kappa}$	Total concentration of species κ in gridblock i, L^3/L^3 PV
C_{SE}	Effective salinity for phase behavior and surfactant adsorption, Eq/L^3
C_{SEL}	Salinity for Type II(–)/III phase boundary or lower effective salinity limit, Eq/L^3
C_{SEP}	Effective salinity for polymer, Eq/L^3
C_{SEU}	Salinity for Type III/II(+) phase boundary or upper effective salinity limit, Eq/L^3
C_6^o	Concentration of free calcium cations, L^3/L^3
C_9^o	Concentration of free sodium cations, L^3/L^3
C_κ	Overall concentration of species κ in the mobile phases, L^3/L^3
C_κ^{eq}	Equilibrium concentration of species κ, L^3/L^3
C_κ^o	Compressibility of species κ, $(mL^{-1}t^{-2})^{-1}$
$\hat{C}_\kappa$	Adsorbed concentration of species κ, L^3/L^3 PV
$\tilde{C}_\kappa$	Overall concentration of species κ in the mobile and stationary phases, L^3/L^3 PV
$C_{\kappa\ell}$	Concentration of species κ in phase ℓ, L^3/L^3
$C_{p\ell}$	Constant pressure heat capacity of phase ℓ, $QT^{-1}m^{-1}$
C_r	Rock compressibility, $(mL^{-1}t^{-2})^{-1}$
C_T	Total compressibility, $(mL^{-1}t^{-2})^{-1}$
$C_{v\ell}$	Volumetric heat capacity of phase ℓ, $QT^{-1}m^{-1}$
C_{vs}	Volumetric heat capacity of soil, $QT^{-1}m^{-1}$
c_{rk}	Permeability reduction factor parameter, $L(wt\%)^{1/3}$
D_a	Damkohler number
$D_{\kappa\ell}$	Diffusion coefficient of species κ in phase ℓ, L^2t^{-1}
f_{oc}	Organic carbon fraction in soil
f_κ^s	Amount of species κ associated with surfactant, L^3/L^3
g	Gravitational constant, Lt^{-2}
h	Depth, L
K	Dispersion coefficient, L^2t^{-1}
k	Average permeability, L^2

$\vec{K}$	Permeability tensor, L^2
k	Soil permeability, L^2
k_a	Apparent permeability used in capillary pressure calculations, L^2
K_{oc}	Amount of organic adsorbed per unit weight of organic carbon in soil, $(mL^{-3})^{-1}$
$k_{r\ell}$	Relative permeability of phase ℓ
$k_{r\ell}^{o}$	Endpoint relative permeability of phase ℓ
$k_{r\ell}^{o^{high}}$, $k_{r\ell}^{o^{low}}$	Endpoint relative permeability of phase ℓ at high and low capillary numbers
k_x, k_y, k_z	Absolute permeability in the x, y and z directions, L^2
L	Length of the core, or reservoir length, L
M_κ	Mass transfer coefficient for species κ, t^{-1}
n_{pc}	Capillary pressure exponent
n_ℓ	Relative permeability exponent for phase ℓ (dimensionless)
n_ℓ^{high}, n_ℓ^{low}	Relative permeability exponent for phase ℓ at high and low capillary numbers
$N_{B\ell}$	Bond number of phase ℓ
$N_{c\ell}$	Capillary number of phase ℓ
$N_{T\ell}$	Trapping number of phase ℓ
$P_{C\ell\ell'}$	Capillary pressure between phases ℓ and ℓ', $mL^{-1}t^{-2}$
P_ℓ	Pressure of phase ℓ, $mL^{-1}t^{-2}$
P_R	Reference pressure, $mL^{-1}t^{-2}$
Q_κ	Source/sink for species κ, L^3/T
Q_L	Heat loss, $Qt^{-1}L^{-2}$
Q_v	Cation exchange capacity of clay, Eq./L^3
q_H	Enthalpy source per bulk volume, $Qt^{-1}L^{-3}$
R_F	Polymer resistance factor
R_k	Polymer permeability reduction factor
R_{RF}	Polymer residual resistance factor
$R_{\ell 3}$	Solubilization ratio for phase ℓ, L^3/L^3
R_κ	Total source/sink for species κ, $mL^{-3}t^{-1}$
$R_{\kappa\ell}^{I}$	Mass exchange rate at interface for species κ in phase ℓ, $mL^{-3}t^{-1}$
$r_{\kappa\,\ell}$	Reaction rate for species κ in phase ℓ, $mL^{-3}t^{-1}$
$r_{\kappa\,s}$	Reaction rate for species κ in solid phase, $mL^{-3}t^{-1}$
$S_{n\ell}$	Normalized mobile saturation of phase ℓ used in relative permeability and capillary pressure calculations
S_ℓ	Saturation of phase ℓ, L^3/L^3 PV
$S_{\ell r}$	Residual saturation of phase ℓ, L^3/L^3 PV
$S_{\ell r}^{high}$, $S_{\ell r}^{low}$	Residual saturation of phase ℓ at high and low capillary numbers L^3/L^3 PV
t	Time, t

Δt^n, Δt^{n+1}	Time-step size at n^{th} and $n+1^{th}$ time level, t
T	Temperature, T
T_ℓ	Trapping parameter for phase ℓ
$\vec{u}_\ell$	Darcy flux, Lt^{-1}
$\bullet x_i$, $\bullet y_i$, $\bullet z_i$	Size of gridblock i in the x, y, and z directions, L

Greek Symbols

α_1-α_5	Microemulsion phase viscosity parameters
α_L, α_T	Longitudinal and Transverse dispersivity, L
β^C	Cation exchange constant for clay
β^S	Cation exchange constant for surfactant
β_6	Effective salinity parameter for calcium
γ_κ	Specific weight of species κ, $mL^{-2}t^{-2}$
$\dot{\gamma}$	Shear rate, t^{-1}
$\gamma_{\kappa R}$	Specific weight of species κ at reference pressure, $mL^{-2}t^{-2}$
μ_o	Oil viscosity, $ML^{-1}T^{-1}$
μ_P	Polymer viscosity, $ML^{-1}T^{-1}$
μ_p^0	Polymer viscosity at zero shear rate, $mL^{-1}t^{-1}$
μ_w	Water viscosity, $mL^{-1}t^{-1}$
μ_ℓ	Viscosity of phase ℓ, $mL^{-1}t^{-1}$
$\mu_{a,ref}$	Viscosity of air at reference pressure, $mL^{-1}t^{-1}$
$\mu_{a,s}$	Slope of air viscosity function
λ_d	Drainage Capillary pressure exponent
λ_i	Imbibition Capillary pressure exponent
λ_ℓ	Relative mobility of phase ℓ, $(mL^{-1}t^{-1})^{-1}$
λ_{rT}	Total relative mobility, $(mL^{-1}t^{-1})^{-1}$
λ_T	Thermal conductivity, $Qt^{-1}T^{-1}L$
ρ_g	Rock density, m/L^3
ρ_s	Soil density, m/L^3
ρ_ℓ	Density of phase ℓ, m/L^3
σ_{aw}	Interfacial tension between air and water, mt^2
σ_{wo}	Interfacial tension between oil and water, mt^2
$\sigma_{\ell\ell'}$	Interfacial tension between phases ℓ and ℓ', mt^2
ϕ	Porosity, fraction
ϕ_i	Porosity of gridblock i, fraction
Φ	Potential, $mL^{-1}t^{-2}$
τ	Tortuosity factor

Subscripts

κ	species number 1 - Water 2 - Oil 3 - Surfactant 4 - Polymer 5 - Chloride 6 - Calcium 7 - Alcohol 8 - air 9-κ - Tracer components
ℓ	Phase number 1 - Aqueous 2 - Oleic 3 - Microemulsion 4 - Air
r	Residual
s	solid

Superscripts

C	Cation
f	Free
S	Surfactant

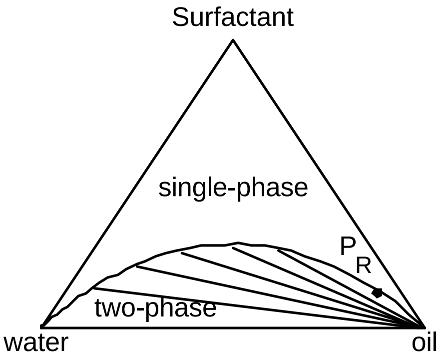

Figure 2.1. Schematic representation of Type II (-).

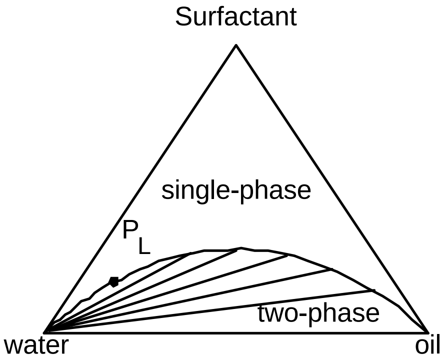

Figure 2.2. Schematic representation of high-salinity Type II (+).

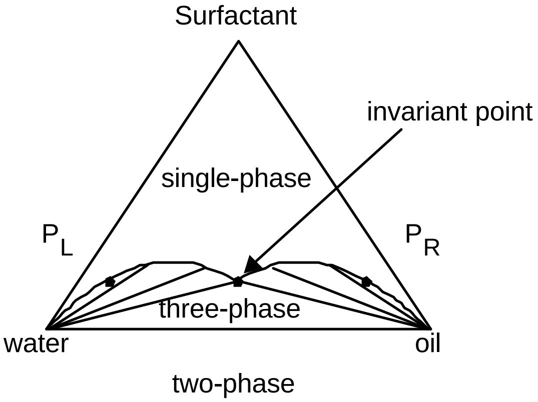

Figure 2.3. Schematic representation of Type III.

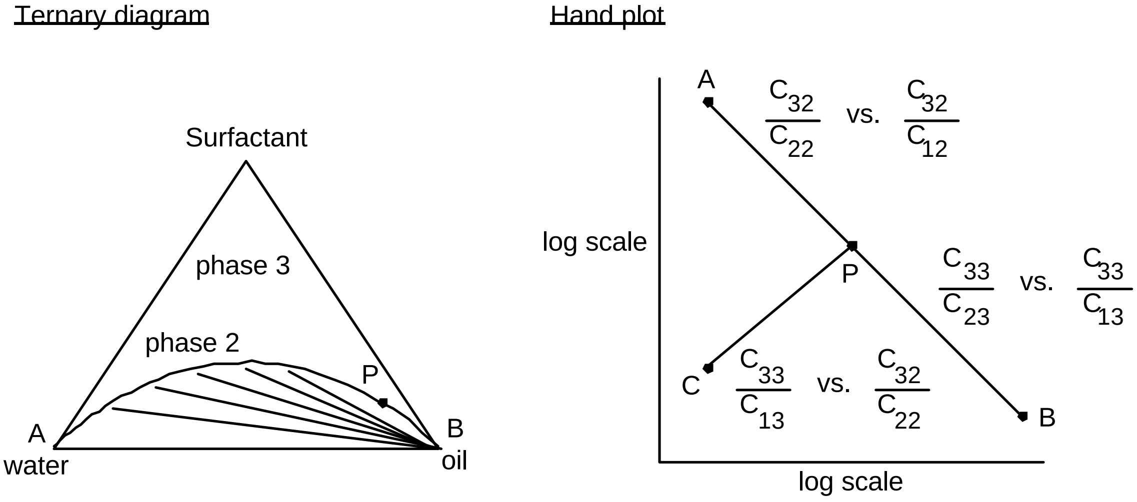

Figure 2.4. Correspondence between (a) ternary diagram and (b) Hand plot.

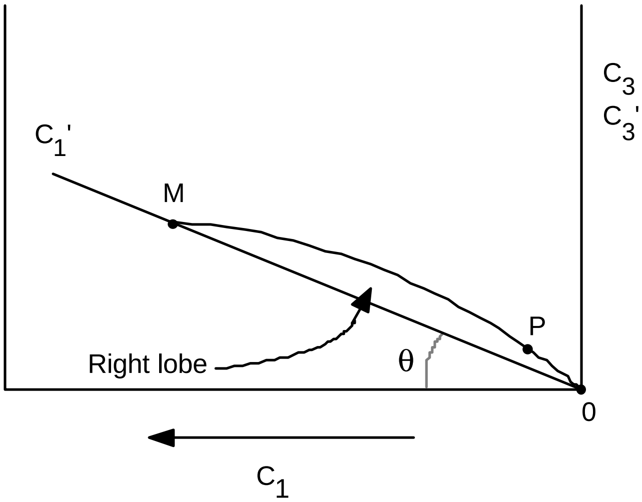

Figure 2.5. Coordinate transformation for the two-phase calculations in Type III.

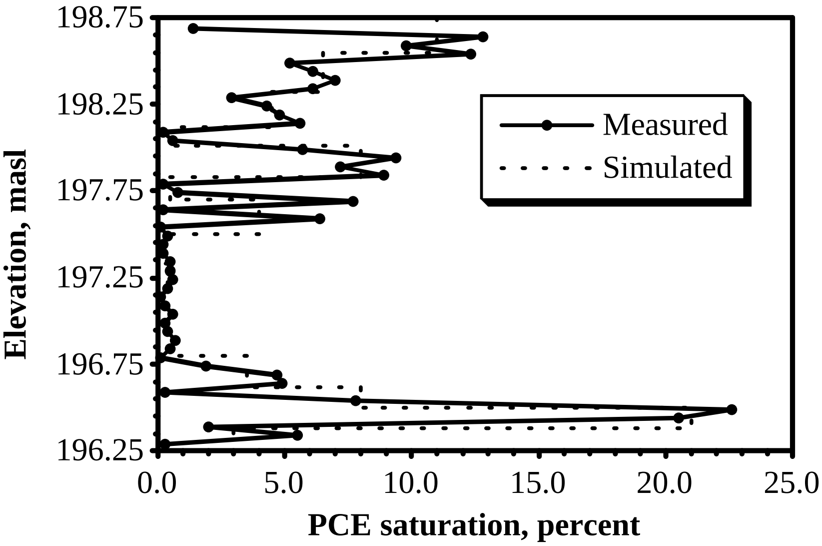

Figure 2.6. Measured and simulated PCE saturation at the location of Core 3 prior to surfactant flooding (after Freeze *et al.*, 1994).

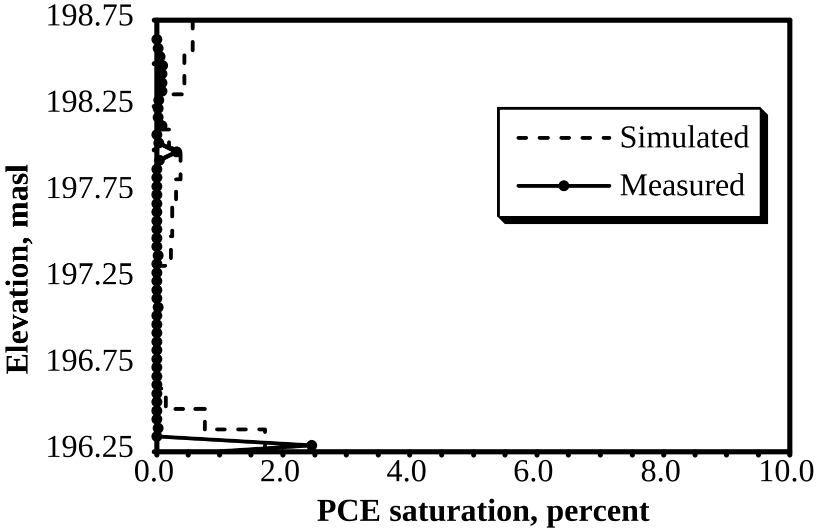

Figure 2.7. Measured and simulated PCE saturation at the location of Core 6 at the end of surfactant flooding (after Freeze *et al.*, 1994).

Table 2.1. Physical Property Input Parameters for the Test Cell Simulation

Property	Value	References and Comments
Density Pure water, g/cc Pure PCE, g/cc Surfactant, g/cc	 1 1.6249 1.15	
Viscosity Pure water (μ_w), cp Pure PCE (μ_o), cp Microemulsion (max. value) α_1 - α_5 parameter values	 1 0.89 4 3.4, 1.0, 3.0, 1.0, 1.0	Eq. 2.77; Parameters were estimated based on the measured data for a different surfactant mixture (Pennell *et al.*, 1994)
Interfacial tension PCE/water (σ_{ow}), dyne/cm PCE/microemulsion (minimum value), dyne/cm G_{21}, G_{22}, G_{23} (Healy and Reed 1974)	 45 0.02 13, -14.5, 0.01	Eq. 2.43; parameters are based on the measured data for a different surfactant mixture (Pennell *et al.*, 1994)
PCE solubility Max. in water, mg/L Max. in surfactant, mg/L	 200 11,700	 West and Harwell [1992] Fountain [1992]
Surfactant adsorption Max. value, mg/g soil Parameter values: a_{31}, a_{32}, b_3	 0.311 1.1, 0.0, 1000	Eq. 2.15; but assuming surfactant adsorption is independent of permeability
Capillary pressure (Corey function) Imbibition: C_{pci}, λ_i	 2.7, -0.454	Eq. 2.55; based on Kueper [1989]
Relative permeability (Corey function) Water (Imbibition): S_{1r}, n_1, k_{r1}^o PCE: S_{2r}, n_2, k_{r2}^o Microemulsion: S_{3r}, n_3, k_{r3}^o	 0.306, 2.2, 0.556 0.0, 2.2, 0.309 0.306, 2.2, 0.556	Eq. 2.66; based on Kueper [1989]

Section 3
Hysteretic Relative Permeability and Capillary Pressure Models

3.1 Introduction

A new multiphase capillary pressure and relative permeability function has been implemented in UTCHEM. Both capillary pressure and relative permeability functions account for hysteresis due to arbitrary changes in saturation path by incorporating an oil phase entrapment model. The hysteresis modeling in UTCHEM is based on the work by Kalurachchi and Parker [1992]. The assumptions made in developing and applying this model are

- The model applies only to strongly water-wet media where the wettability in descending order is for water (or microemulsion), oil, and gas phases. Oil will be used in this report to mean any non-aqueous phase liquid (NAPL).
- The model applies to three-phase air-water-oil flow in the vadose zone and two-phase oil-water or oil-microemulsion flow in the saturated zone
- To avoid numerical oscillations with changes from two phases (air-water) to three phases (air-water-oil), once a location is classified as a three-phase node, it will not revert back to two phases (air-water).
- Gas entrapment is neglected for the three-phase case. Therefore, oil entrapment in a three-phase air-water-oil can be inferred directly from that in a two-phase oil-water system.
- Water relative permeability is unaffected by oil entrapment e.g. $k_{rw} = f(S_w)$.
- There is no oil entrapment on the main drainage curve.
- There is no oil entrapment when water saturation is at its residual value in the vadose zone.

We use the notation adapted from Parker *et al*. [1987] shown in Table 3.1.

3.2 Oil Phase Entrapment

On any scanning curve (e.g. point A on Fig. 3.1), effective residual oil saturation is estimated from Land's equation (Land, 1968), where the residual nonwetting phase saturation after imbibition is related empirically to the initial nonwetting saturation $(1 - \overline{S}_w^{min})$ as

$$\bar{S}_{or}^{A} = \frac{1-\bar{S}_{w}^{min}}{1+R\left(1-\bar{S}_{w}^{min}\right)} \qquad (3.1)$$

$$\text{where } R = \frac{1}{\bar{S}_{or}^{max}} - 1$$

The trapped oil saturation at nonzero capillary pressure is calculated from the following relationships.

3.2.1 Kalurachchi and Parker

To estimate trapped oil saturation at nonzero capillary pressure, Kalurachchi and Parker estimated the trapped oil saturation as the difference between residual oil saturation for the actual scanning curve and that for a curve with a reversal point equal to the free (continuous) oil saturation on the actual path. This is exactly the same idea as proposed by Stegemeier in 1977 and described in Lake [1989]. For example, consider point B on the scanning curve on Fig. 3.1 with apparent water saturation of $\bar{\bar{S}}_w = \bar{S}_w + \bar{S}_{ot}$. Points B and C have the same capillary pressure, therefore the difference between the x coordinates of points B and C is the disconnected nonwetting phase saturation ($\bar{S}_{ot}$). Using Land's relation for the residual oil saturation for the scanning path starting from point A ($\bar{S}_{or}^{A}$) and that starting from point C ($\bar{S}_{or}^{C}$) we have

$$\bar{S}_{or}^{A} = \frac{1-\bar{S}_{w}^{min}}{1+R\left(1-\bar{S}_{w}^{min}\right)} \qquad (3.2)$$

$$\bar{S}_{or}^{C} = \frac{1-\bar{\bar{S}}_{w}}{1+R\left(1-\bar{\bar{S}}_{w}\right)} \qquad (3.3)$$

and

$$\bar{S}_{ot} = \bar{S}_{or}^{A} - \bar{S}_{or}^{C}$$

$$\bar{S}_{ot} = \begin{cases} \left[\min\left(\dfrac{1-\bar{S}_{w}^{min}}{1+R\left(1-\bar{S}_{w}^{min}\right)} - \dfrac{1-\bar{\bar{S}}_{w}}{1+R\left(1-\bar{\bar{S}}_{w}\right)}\right), \bar{S}_o\right] & \text{when } \bar{S}_w > \bar{S}_{w}^{min} \\ 0.0 & \text{otherwise} \end{cases} \qquad (3.4)$$

Equation 3.4 is a conditional quadratic equation that can be solved for $\bar{S}_{ot}$ since $\bar{\bar{S}}_w = \bar{S}_w + \bar{S}_{ot}$. Once $\bar{S}_{ot}$ is computed, capillary pressures and relative permeabilities are computed from the equations discussed below.

3.2.2 Parker and Lenhard

The trapped oil saturation is calculated by linear interpolation since the effective trapped oil saturation along any scanning curve (e.g., the curve with reversal point of A in Fig. 3.1) varies from zero at the reversal point of $\bar{S}_{w}^{min}$ to $\bar{S}_{or}^{A}$ at $\bar{\bar{S}}_w = 1$ as

$$\bar{S}_{ot} = \min\left(\bar{S}_{or}^{A}\left(\frac{\bar{\bar{S}}_{w} - \bar{S}_{w}^{min}}{1 - \bar{S}_{w}^{min}}\right), \bar{S}_{o} \right) \tag{3.5}$$

where $\bar{S}_{or}^{A}$ is calculated from Eq. 3.2.

3.3 Capillary Pressure

The two-phase air-water, water-oil or microemulsion-oil and three-phase oil-water-air capillary pressure-saturation function determined using the generalization of Parker *et al.* [1987] to the two-phase flow model of van Genuchten [1980] is represented as follows.

3.3.1 Two-Phase Flow

$$\bar{\bar{S}}_{w} = \left[1 + \left(\alpha\beta_{\ell\ell'}\, P_{c\ell\ell'}\right)^{n}\right]^{-m} \tag{3.6}$$

where $\beta_{\ell\ell'}$ is the scaling coefficient for fluid pair ℓ and ℓ'; α and n are the adjustable parameters, and m = 1–1/n. The implementation of this model in the simulator includes scaling with intrinsic permeability (k) and porosity (ϕ) where α is replaced by $\alpha\sqrt{\frac{k}{\phi}}$. β is approximated by the ratio of water-air interfacial tension (σ_{aw}) to the interfacial tension of the fluid pair. Here and elsewhere the subscript w applies to either water or microemulsion for the case of two-phase flow with oil.

$$\beta_{\ell\ell'} = \sigma_{aw} / \sigma_{\ell\ell'}$$

3.3.2 Three-Phase Oil/Water/Air Flow

$$\bar{\bar{S}}_{w} = \left[1 + \left(\alpha\beta_{ow}\, P_{cow}\right)^{n}\right]^{-m} \tag{3.7}$$

$$\bar{S}_{t} = \left[1 + \left(\alpha\beta_{ao}\, P_{cao}\right)^{n}\right]^{-m} \tag{3.8}$$

3.4 Relative Permeability

The two- and three-phase relative permeabilities are based on the generalization of Parker and Lenhard to the two-phase flow model of van Genuchten.

$$k_{rw} = \bar{S}_{w}^{1/2}\left[1 - \left(1 - \bar{S}_{w}^{1/m}\right)^{m}\right]^{2} \tag{3.9}$$

$$k_{ro} = \left(\bar{S}_{t} - \bar{\bar{S}}_{w}\right)^{1/2}\left[\left(1 - \bar{\bar{S}}_{w}^{1/m}\right)^{m} - \left(1 - \bar{S}_{t}^{1/m}\right)^{m}\right]^{2} \tag{3.10}$$

$$k_{ra} = \left(1 - \bar{S}_{t}\right)^{1/2}\left(1 - \bar{S}_{t}^{1/m}\right)^{2m} \tag{3.11}$$

3.5 Capillary Number Dependent Hysteretic Model

An important new extension of these models is the inclusion of their dependence on interfacial tension via the trapping number. The capillary number traditionally used by both the groundwater and oil reservoir literatures has been generalized by Jin [1995] and is now called the trapping number. We assume that 1) the capillary pressure parameters n and m are independent of trapping number and 2) the residual oil saturation (S_{or}^{max}) and residual water (or microemulsion) saturation (S_{wr}) are functions of trapping number. We compute the residual water and residual oil saturations as a function of trapping number as follows:

$$S_{\ell r} = \min\left(S_{\ell} \,,\; S_{\ell r}^{high} + \frac{S_{\ell r}^{low} - S_{\ell r}^{high}}{1 + T_{\ell}\, N_{T\ell}} \right) \qquad \text{where } \ell = \text{w (or microemulsion), oil} \tag{3.12}$$

where the $S_{\ell r}^{high}$ and $S_{\ell r}^{low}$ are the phase ℓ residual saturations at high and low trapping numbers, T_{ℓ} is the adjustable parameter. This correlation was derived based on the experimental data for n-decane (Delshad, 1990) and have recently been successfully applied to residual PCE as a function of trapping number measured by Pennell *et al.* [1996]. The trapping number $N_{T\ell}$ is computed as

$$N_{T\ell} = \frac{\left| -\vec{\vec{k}} \cdot \vec{\nabla}\Phi_{\ell'} - \vec{\vec{k}} \cdot \left[g\,(\rho_{\ell'} - \rho_{\ell})\vec{\nabla} h \right] \right|}{\sigma_{\ell\ell'}} \tag{3.13}$$

where h is the vertical depth (positive downward), ρ_{ℓ} and $\rho_{\ell'}$ are the displaced and displacing fluid densities, and the gradient of the flow potential is given by $\vec{\nabla}\Phi_{\ell'} = \vec{\nabla}P_{\ell'} - g\,\rho_{\ell'}\,\vec{\nabla}h$.

We then substitute the water (or microemulsion) and oil residual saturations calculated from Eq. 3.13 for S_{wr} and S_{or}^{max} in the calculations of entrapped oil phase saturations (S_{ot}), capillary pressure, and relative permeabilities described above. This extension makes the hysteretic model suitable for remediation processes that involve changes in interfacial tension; e.g., co-solvent, surfactant, etc. (Delshad *et al.*, 1996). The reduction in interfacial tension due to the presence of surfactant or co-solvent in the above equations is calculated from a modified Huh's equation (Huh, 1979) where the interfacial tension is related to the solubilization ratio (Delshad *et al.*, 1996). The interfacial tension for oil-water in the absence of surfactant or co-solvent or water-air fluid pairs is assumed to be a constant.

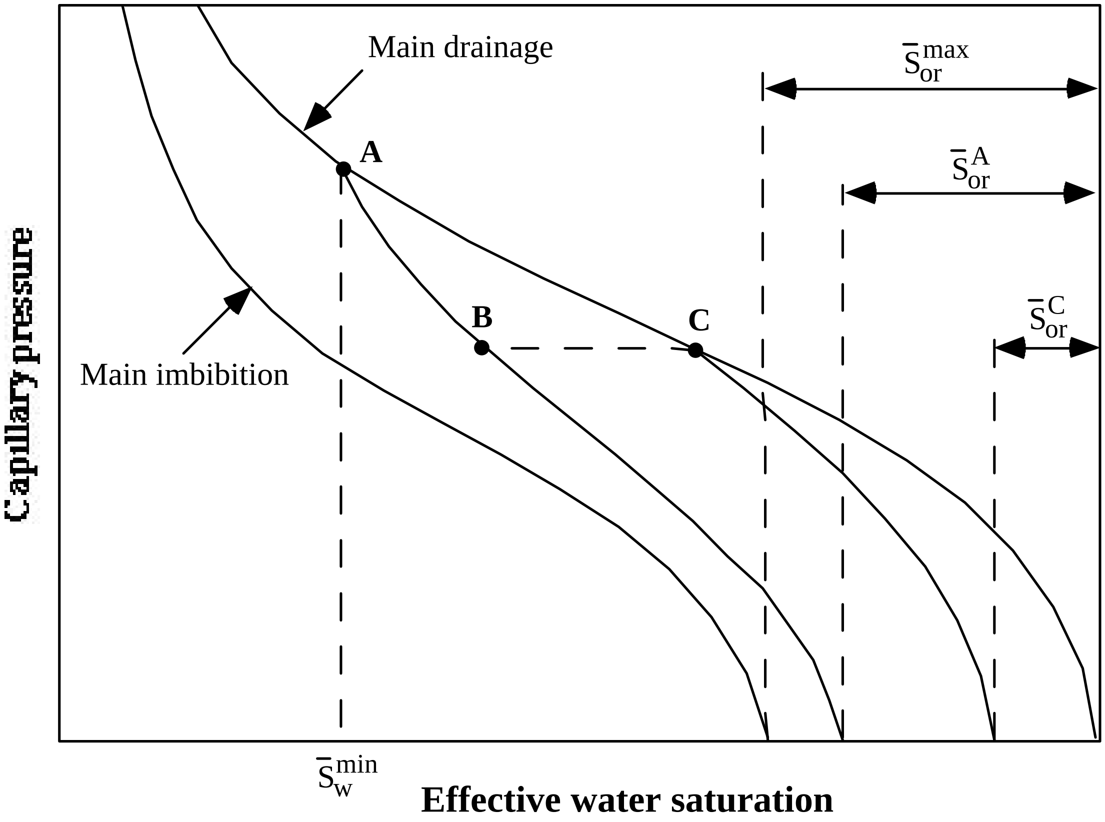

Figure 3.1. Capillary pressure curves as a function of effective water saturation.

Table 3.1. Notation Used in Section 3

Water and oil saturations:	S_w, S_o
Residual water saturation:	S_{wr}
Effective water saturation :	$\bar{S}_w = \dfrac{S_w - S_{wr}}{1 - S_{wr}}$
Effective total liquid saturation:	$\bar{S}_t = \dfrac{S_w + S_o - S_{wr}}{1 - S_{wr}}$
Effective oil saturation:	$\bar{S}_o = \dfrac{S_o}{1 - S_{wr}}$
Apparent water saturation:	$\bar{\bar{S}}_w = \bar{S}_w + \bar{S}_{ot}$
Residual and trapped oil saturation:	Residual oil saturation corresponds to the trapped oil saturation at zero capillary pressure, $\bar{S}_{or} = \bar{S}_{ot}(@ P_c = 0.0)$
Minimum effective water saturation (corresponds to the reversal from drainage to imbibition):	$\bar{S}_w^{min}$
Maximum effective residual oil saturation (corresponds to main imbibition curve):	$\bar{S}_{or}^{max} = \dfrac{S_{or}^{max}}{1 - S_{wr}}$

Section 4
UTCHEM Tracer Options

4.1 Introduction

Any number of tracers can be modeled in UTCHEM. These tracers can be water tracer, oil tracer, partitioning oil/water tracer, gas tracer, and partitioning gas/oil tracer. There are up to two reacting tracers allowed. Reacting tracers are considered only for water/oil tracers and tracer components 2 and 3 are reacting and product tracers for the first reacting tracer. Tracer components 4 and 5 are reacting and product tracers for the second reacting tracer. The assumptions made in the modeling of tracers are:

1. Tracers do not occupy volume
2. Tracers have no effect on the physical properties

The overall tracer concentrations are computed from the species conservation equations which include a reaction term for the reacting tracer. The tracer phase concentrations are calculated according to the tracer type: water, oil, gas, or partitioning.

UTCHEM can model single-well tracer test (Descant, 1989), partitioning interwell tracer tests (Allison *et al.*, 1991; Jin *et al.*, 1995), and single-well wettability tracer test (Ferreira *et al.*, 1992).

4.2 Non-Partitioning Tracer

The tracer phase composition for a non-partitioning tracer is proportional to the ratio of the total tracer concentration to the total concentration of water, oil, or gas depending on the tracer type as

$$C_{T_\ell} = C_{\kappa\ell} \frac{C_T}{C_\kappa} \qquad T = \text{water, oil, or gas tracer} \tag{4.1}$$

4.3 Partitioning Tracer

4.3.1 Water/Oil

The tracer partitioning coefficient for a water/oil tracer is defined on the basis of water or oil pseudocomponent concentration as

$$K_T = \frac{C_{T_2}}{C_{T_1}} \tag{4.2}$$

where C_{T_1} and C_{T_2} are the tracer concentrations in the water and oil pseudocomponents. The tracer phase compositions are then computed from the tracer material balance equation as

$$C_{T_\ell} = C_{1\ell} C_{T_1} + C_{2\ell} C_{T_2}$$

where

$$C_{T_1} = \frac{C_T}{C_1 + C_2 K_T} \tag{4.3}$$

$$C_{T_2} = K_T \frac{C_T}{C_1 + C_2 K_T}$$

where C_1, C_2 are the overall concentrations for water and oil species.

The partitioning coefficient of tracer i as a function of reservoir salinity is modeled using a linear relationship as

$$K_{T_i} = K_{T_{i,Sref}} \left(1 + TKS_i \left(C_{51} - C_{51,ref}\right)\right) \tag{4.4}$$

where C_{51} is the concentration of anions in aqueous phase and $C_{51,ref}$ is the electrolytes concentration in chloride equivalent (eq/l) at a reference condition (initial electrolyte concentrations). TKS_i is a constant input parameter in $(eq/l)^{-1}$ and $K_{Ti,Sref}$ is the partitioning coefficient at the reference salinity of $C_{51,ref}$ in eq/l.

UTCHEM also has the capability of modeling tracer partitioning coefficients as a function of reservoir temperature. Partitioning coefficient for tracer i as a function of temperature is given by a linear function as:

$$K_{T_i} = K_{T_{i,Tref}} \left(1 + TK_i \left(T - T_{ref}\right)\right) \quad \text{for tracer i} \tag{4.5}$$

where the temperatures are in •F and $K_{Ti,Tref}$ is the partitioning coefficient of tracer i at reference temperature, T_{ref}. TK_i is a constant input parameter in $(^\circ F)^{-1}$.

4.3.2 Gas/Oil

The partitioning coefficient for a gas/oil tracer is defined as

$$K_T = \frac{C_{T_2}}{C_{T_8}} \tag{4.6}$$

and the phase concentration for the tracer is computed using the tracer material balance equation as

$$C_{T_\ell} = C_{8\ell} C_{T_8} + C_{2\ell} C_{T_2}$$

where

$$C_{T_8} = \frac{C_T}{C_8 + C_2 K_T} \qquad \ell = 2 \text{ and } 4 \tag{4.7}$$

$$C_{T_2} = K_T \frac{C_T}{C_8 + C_2 K_T}$$

where C_8, C_2 are the overall concentrations for gas and oil species.

UTCHEM has the capability of modeling gas/oil tracer partitioning coefficients as a function of reservoir temperature. Partitioning coefficient for tracers as a function of temperature is given by a linear function as:

$$K_{T_i} = K_{T_i,\mathrm{ref}}\left[1 + TK_i\left(T - T_{\mathrm{ref}}\right)\right] \quad \text{for tracer i} \tag{4.8}$$

where the temperatures are in •F and $K_{T_i,\mathrm{ref}}$ is the partitioning coefficient of tracer i at reference temperature (T_{ref}) and TK_i is a constant input parameter in $(\bullet F)^{-1}$.

4.4 Radioactive Decay

Radioactive decay can be used for any type of tracer (oil, water, gas) as

$$\frac{dC_T}{dt} = -\lambda C_T \tag{4.9}$$

where λ is a constant input radioactive decay coefficient in $(\mathrm{days})^{-1}$. The above equation is solved for decayed tracer concentration once the overall tracer concentration (C_T) is solved for as

$$\left(C_T\right)_{\mathrm{decay}} = C_T\left(1 - \lambda\Delta t\right) \tag{4.10}$$

where Δt is the time step size in days.

4.5 Adsorption

The tracer adsorption for any type of tracer is assumed to be linear and can be modeled using an input retardation factor parameter (D_s) as

$$D_s = \frac{\overline{C}_T}{C_{T\ell}} = \frac{(1-\phi)\rho_r a_T}{\phi\rho_\ell C_{T\ell}} \qquad \ell = 1 \text{ or } 4 \tag{4.11}$$

where a_T is the mass of adsorbed tracer divided by the mass of rock. ρ_r and ρ_ℓ are the rock and water (ℓ = 1) or gas phase (ℓ = 4) densities. $\overline{C}_T$ is the adsorbed tracer concentration. The adsorption is applied to total tracer flux (convective and dispersive) and modeled as

$$\left(V_t\right)_{\mathrm{ret.}} = \frac{u}{\phi S_\ell}\left(\frac{1}{1 + D_s}\right) \tag{4.12}$$

where u is the Darcy flux in ft/d and ϕ is the porosity.

4.6 Reaction

Hydrolysis of an ester to form an alcohol is assumed to be irreversible and of first order. The reaction of an acetate as an example is:

$$\underset{\text{Acetate}}{\mathbf{1}\ CH_3COO[C_nH_{2n+1}]} \quad + \quad \underset{\text{Water}}{\mathbf{1}\ H_2O} \quad \text{-------->} \quad \underset{\text{Alcohol}}{\mathbf{1}\ C_nH_{2n+1}[OH]} \quad + \quad \underset{\text{Acetic Acid}}{\mathbf{1}\ C_2H_4O_2}$$

where 1 mole of acetate (e.g., component 10) generates one mole of product alcohol (e.g. . component 11). The reaction is modeled as

$$\frac{\partial C_{10}}{\partial t} = -K_h C_{10}$$

and (4.13)

$$\frac{\partial C_{11}}{\partial t} = K_h C_{10}$$

where K_h is an input reaction rate in day^{-1}. UTCHEM has the capability of modeling the tracer reaction rate as a function of reservoir temperature. The rate of hydrolysis of tracer as a function of reservoir temperature is given by:

$$K_{h_i} = K_{h_i,\mathrm{ref}} \exp\left[HK_i \left(\frac{1}{T} - \frac{1}{T_{\mathrm{ref}}} \right) \right] \quad \text{for tracer i} \tag{4.14}$$

where the temperature is in •K and $K_{h_i,\mathrm{ref}}$ is the rate of tracer hydrolysis at reference temperature (T_{ref}) and HK_i is a constant input parameter in (•K)$^{-1}$.

4.7 Capacitance

The capacitance model is based on a generalized Coats-Smith model (Smith *et al.*, 1988) and is applied to water/oil tracer components and gas tracer components (κ). The model is unsteady state, therefore the flowing and dendritic saturations can change in each time step. The phase saturations and phase composition from the overall species concentration and phase flash are the flowing saturation (S_ℓ^f) and phase concentrations ($C_{\kappa\ell}^f$) in the capacitance model in UTCHEM. The mass transfer between the flowing and dendritic fraction is given by

$$\frac{\partial}{\partial t}\left(S_\ell^d C_{\kappa\ell}^d\right) = M_{\kappa\ell}\left(C_{\kappa\ell}^f - C_{\kappa\ell}^d\right) \tag{4.15}$$

The dendritic saturation is calculated from:

$$S_\ell^d = \left(1 - F_\ell\right) S_\ell \tag{4.16}$$

where F_ℓ is the flowing fraction for phase ℓ defined as

$$F_\ell = \frac{S_\ell^f}{S_\ell} = F_{\ell 0} + \left(F_{\ell 1} - F_{\ell 0}\right) f_\ell \tag{4.17}$$

where the flowing fraction (F_ℓ) is assumed to be a linear function of fractional flow (f_ℓ). The intercepts of the flowing fraction line versus fractional flow at the residual saturation of nonwetting phase ($f_1 = 0.0$) and wetting phase ($f_1 = 1.0$) are $F_{\ell 0}$ and $F_{\ell 1}$ and are input parameters. The product of dendritic saturation (S_ℓ^d) and dendritic phase composition ($C_{\kappa\ell}^d$) is

$$\left(C_{\kappa\ell}^{d} S_{\ell}^{d}\right)^{n+1} = \left(C_{\kappa\ell}^{d} S_{\ell}\right)^{n} + \Delta t M_{\kappa} \left(C_{\kappa\ell}^{f} - C_{\kappa\ell}^{d}\right)^{n} \qquad (4.18)$$

where M_{κ} is the input mass transfer coefficient in $(\text{day})^{-1}$ and the dendritic phase composition ($C_{\kappa\ell}^{d}$) is calculated from

$$C_{\kappa\ell}^{d} = \frac{C_{\kappa\ell}^{d} S_{\ell}^{d}}{S_{\ell}^{d}} \qquad (4.19)$$

The flowing phase saturations are then determined from

$$S_{\ell}^{f} = F_{\ell} S_{\ell} \qquad (4.20)$$

and the total flowing tracer concentrations are computed as

$$C_{\kappa}^{f} \quad \sum_{\ell=1}^{n_p} \left(C_{\kappa}^{f} \ \ S^{f}\right) = C_{\kappa} - \sum_{\ell=1}^{n_p} \left(C_{\kappa\ell}^{d} S_{\ell}^{d}\right) \qquad (4.21)$$

Section 5
Dual Porosity Model

5.1 Introduction

In most naturally fractured reservoirs, fractures tend to be developed in a way that makes the fractures interconnected and the bulk reservoir rock isolated into blocks. Fractured reservoirs can thus be considered as blocks of porous rock matrix surrounded by a network of communicating channels (fractures). The rock matrix generally has high bulk volume and high porosity, but very low permeability. In contrast, the fractures occupy very small volume, but have high permeability. The dual porosity model assumes that there are two flow systems coexisting in a fractured reservoir – an interconnected fracture system and a disjoint matrix system. In the dual porosity model, continuity equations are solved for the two systems using conventional methods, while the mass transfer between the two systems is calculated by so-called transfer functions that characterize flow between matrix blocks and fractures. By dividing the matrix system into subgrids at each fracture node, transient flow of fluid in the matrix and between matrix and fractures can be studied. For simplicity, matrix blocks are often assumed to be regularly shaped. In this implementation, we use parallelepiped matrix blocks to handle vertical fractures and slabs for horizontal fractures.

This section presents results of a project to implement dual porosity behavior for tracer studies in UTCHEM, a chemical flood simulator developed at the University of Texas at Austin. Two approaches were implemented. In the first, a capacitance model already existing in UTCHEM was made to mimic dual porosity behavior by setting capacitance parameters to equivalent dual porosity parameters. This approach is equivalent to a dual porosity model with no subgridding. The second approach involved adapting a subgridding approach developed by J. Chen [1993] for counter current imbibition in fractured reservoirs. Test runs and comparisons with the SWIFT II simulator (Reeves *et al.*, 1986) are also made.

5.2 Capacitance Model

Dispersion into matrix blocks from surrounding fractures is typically calculated by assuming that the tracer concentration in the fractures is uniform within a given volume of reservoir rock. This assumption results in the following equation for diffusion of a single tracer in a single fluid phase:

$$\frac{\partial\left(\phi^m \overline{C}^m\right)}{\partial t} = \phi^m K^m S_A \left[\frac{\partial C^m}{\partial n}\right]_f \tag{5.1}$$

where

ϕ^m = matrix porosity, fraction

$\overline{C}^m$ = average tracer concentration in matrix block, m/L^3

K^m = tracer diffusion coefficient in matrix, L^2/t

S_A = matrix block surface area per unit bulk volume of reservoir, L^{-1}

$\left[\frac{\partial C^m}{\partial n}\right]_f$ = tracer concentration gradient normal to matrix block surface, m/L^4

If transient behavior is ignored, Eq. 5.1 may be approximated by

$$\frac{\partial\left(\overline{C}^m\right)}{\partial t} = \sigma K^m \left(C^f - \overline{C}^m\right) \tag{5.2}$$

where *s* is a shape factor to account for matrix block geometry and number of matrix blocks per unit reservoir volume, and C^f is the tracer concentration in the fracture. Note that the shape factor has units of L^{-2}. Kazemi *et al.* [1976] recommended a shape factor for cubic matrix blocks of

$$\sigma = \frac{4nN}{L^2} \tag{5.3}$$

where n is the number of matrix blocks per unit bulk volume of reservoir and N is the "dimensionality" of the fracture set. A good discussion of shape factors can be found in M. M. Chen [1993].

UTCHEM includes a "capacitance" model that treats diffusive transfer in a similar manner. In the capacitance model a fluid phase is divided into two fractions: a flowing fraction (which is analogous to the fracture system in a dual porosity model) and a dendritic fraction (which is analogous to the matrix system). Since matrix and fracture porosities are both based on total reservoir bulk volume, the flowing fraction, F, and the dendritic fraction, 1–F, are equivalent to:

$$F = \frac{\phi^f}{\phi^m + \phi^f} = \frac{S^f}{S} \tag{5.4}$$

$$1 - F = \frac{\phi^m}{\phi^m + \phi^f} = \frac{S^d}{S} \tag{5.5}$$

For single phase flow, of course, S = 1. Total porosity is simply

$$\phi = \phi^m + \phi^f \tag{5.6}$$

In the capacitance model, mass transfer from the flowing to dendritic fractions is calculated by

$$\frac{\partial\left[(1-F)C^d\right]}{\partial t} = M\left(C^f - C^d\right) \tag{5.7}$$

or for a fixed dendritic fraction:

$$\frac{\partial\left(C^d\right)}{\partial t}=\frac{M}{1-F}\left(C^f-C^d\right) \tag{5.8}$$

where C^d is the tracer concentration in the dendritic fraction, C^f is the tracer concentration in the flowing fraction, and M is the capacitance mass transfer coefficient. The capacitance model can thus be made to calculate dual porosity behavior using the equivalents given in Table 5.1.

Figure 5.1 shows comparisons of capacitance runs in UTCHEM compared to UTDUAL, a dual porosity simulator developed at the University of Texas at Austin. Although UTDUAL has the capability of subgridding matrix blocks (which would yield more accurate results), these comparisons were made with no subgridding. For these comparisons, UTDUAL was modified slightly to account for tracer diffusion in a manner similar to counter current water imbibition. Data used to generate Fig. 5.1 are given in Table 5.2. Note the high degree of agreement. In fact, for a mass transfer coefficient of 10^{-5} sec^{-1}, the two curves are indistinguishable on the graph.

5.3 Subgridding

Due to the relatively low permeability in matrix blocks, viscous convection of phases is very slow and is ignored in this formulation. Molecular diffusion of tracer becomes the dominant process flow within the matrix. The equation for tracer diffusion into the matrix can be simplified into the following equation:

$$\frac{\partial}{\partial t}\left(\phi^m C^m\right)=\nabla\cdot\left(\phi^m\vec{K}^m\cdot\nabla C^m\right)-\lambda\phi^m C^m \tag{5.9}$$

where λ is the radioactive decay constant of the tracer.

Parallelepiped matrix blocks are assumed for the subgridding. In the horizontal direction (j-index) the matrix is subdivided into N_{sub} concentric grids. In the vertical direction (k-index), the matrix is sliced into M_{sub} slabs. Figure 5.2 shows the discretization of a single matrix block. The advantage of subgridding the matrix this way is that many types of fracture systems can be described. By setting $M_{sub}=1$ and the vertical diffusion coefficient to zero, a vertical fracture network can be simulated. If $N_{sub}=1$ and the horizontal diffusion coefficient is equal to zero, then horizontal fractures can be simulated. A combination of subgridding in these two directions can be used to simulate a 3D fracture system. When $M_{sub}=1$ and $N_{sub}=1$, the system reduces to the capacitance (no subgridding) model.

The volume fraction of each subgrid is an input value with the property:

$$\sum_{j=1}^{N_{sub}} f_{jk}=1 \qquad k=1,\ldots,M_{sub} \tag{5.10}$$

The volume fraction of the jth ring and kth layer subgrid is:

$$f_{jk}=\frac{\left(L_{xjk}L_{yjk}-L_{xj-1k}L_{yj-1k}\right)h_k}{V_{bk}^m} \tag{5.11}$$

where V_{bk}^{m} is the bulk volume of the kth layer of the matrix, L_{xjk} and L_{yjk} are the outer dimensions of the subgrid, h_k is the thickness of the kth layer, and N_{sub} is the number of the subgrids in the horizontal direction (Fig. 5.2).

From Eqs. 5.10 and 5.11, the outer dimensions for each subgrid are calculated by:

$$L_{xjk} = L_x \left[\sum_{i=1}^{j} f_{ik} \right]^{\frac{1}{2}} \qquad j = 1,...,N_{sub};\ k = 1,...,M_{sub} \tag{5.12}$$

$$L_{yjk} = L_y \left[\sum_{i=1}^{j} f_{ik} \right]^{\frac{1}{2}} \qquad j = 1,...,N_{sub};\ k = 1,...,M_{sub} \tag{5.13}$$

where L_x and L_y are the dimensions of the matrix block.

The dimensions of a matrix block can be different than the dimensions of a gridblock. The mass transfer rate is simply calculated by multiplying the mass transfer rate of one representative matrix block by the number of matrix blocks per gridblock.

Using one-point upstream weighting, the finite-difference form of Eq. 5.9 becomes

$$\begin{aligned} \phi^m\left[\left(C^m\right)^{n+1} - \left(C^m\right)^{n}\right] = \frac{\Delta t}{\Delta V_{jk}^{m}} \Big[& TV_{jk-\frac{1}{2}}\left(C^m\right)_{jk-1}^{n} + TH_{j-\frac{1}{2}k}\left(C^m\right)_{j-1k}^{n} + TC_{jk}\left(C^m\right)_{jk}^{n} \\ & + TH_{j+\frac{1}{2}k}\left(C^m\right)_{j+1k}^{n} + TV_{jk+\frac{1}{2}}\left(C^m\right)_{jk+1}^{n} - \Delta V_{jk}^{m}\lambda\phi^m\left(C^m\right)_{jk}^{n} \Big] \end{aligned} \tag{5.14}$$

where ΔV_{jk}^{m} is the volume of the jth ring and the kth layer, and TV and TH are the transmissibilities in the vertical and horizontal directions, respectively:

$$TH_{j+\frac{1}{2}k} = \frac{L_{yjk} h_k K_{xy}^{m}}{L_{x\,j+1k} - L_{x\,jk}} + \frac{L_{xjk} h_k K_{xy}^{m}}{L_{y\,j+1k} - L_{y\,jk}} \tag{5.15}$$

$$TV_{jk+\frac{1}{2}} = \frac{f_{jk} L_x L_y K_z^{m}}{h_{jk+1} + h_{jk}} \tag{5.16}$$

and TC is calculated by:

$$TC_{jk} = -(TV_{jk-\frac{1}{2}} + TH_{j-\frac{1}{2}k} + TH_{j+\frac{1}{2}k} + TV_{jk+\frac{1}{2}}) \tag{5.17}$$

The boundary condition is

$$C_{jk}^{m} = C^{f} \qquad \begin{aligned} & j = N_{sub};\ k = 1,...,M_{sub}\ \text{(sides)} \\ & j = 1,...,N_{sub};\ k = 1 \text{ and } k = M_{sub}\ \text{(top and bottom)} \end{aligned} \tag{5.18}$$

5.4 Implementation

In this implementation the original 3D compositional code, UTCHEM, solves the pressure distributions and tracer concentrations in the fracture system. After solving the fracture system equations, the tracer concentration at each node is used as the boundary condition for the matrix at the same node. Only a single tracer in single phase flow is handled.

An additional subroutine, TDIFFU, is added to UTCHEM to do the matrix calculations. The methodology used for this implementation is described by J. Chen [1993] and Chen *et al*. [1994]. In this routine, the equations developed above are used to solve the tracer concentration distribution in the subgridded matrix system. Concentrations in the fracture are modified to account for mass transfer between the matrix and fracture.

Several other subroutines are also modified. Subroutine INOUT is extended to read in the parameters used to describe the subgridding system. The initial values of the matrix tracer concentration are also read in this routine. Subroutine TIME0 is modified to set the initial tracer concentrations in the matrix system. Calculations of the horizontal and vertical transmissibilities of the subgrids are added to the TRAN1 routine. Some output commands are added to subroutine OUTDT1. And, of course, the MAIN program is also modified to handle the new calculations. The distribution of tracer concentrations within the matrix are written to output file CAPP.

In order to minimize the code changes to the whole system, the control flag for the dual porosity option is the variable ICAP, which is also used to flag use of the capacitance model. A value of 2 is used to represent that the dual porosity model with subgridding is used.

5.5 Results

Several test runs were made with this implementation. The first test is a comparison of the capacitance model with the case of only one subgrid. A 1D linear reservoir 1000 ft long with 10 ft width and depth is simulated. Gridblock size is 10x10x10 ft^3. Matrix blocks are also 10x10x10 ft^3. There are thus 100 gridblocks in the x–direction. Fracture and matrix porosities are 0.01 and 0.19, respectively. Permeability in the fractures is 1000 md and longitudinal dispersivity is 1.0 ft. Fluid injection rate is 0.5 ft^3/day. Figure 5.3 shows results for mass transfer coefficients of 10^{-5}, 10^{-8} and 10^{-9} sec^{-1}. Results show that the dual porosity model reduces to the capacitance model when there is no subgridding.

The second comparison is between UTCHEM and UTDUAL (J. Chen, 1993). The reservoir and fluid conditions are the same as the first set of runs, except that a diffusion coefficient (K^m) of 4.32×10^{-3} ft^2/day was used. The subgrid numbers compared are 1, 2, 4, and 8. One more run with 16 subgrids was run on UTDUAL which showed that the curve converges with only 8 subgrids. Figure 5.4 shows the results. Figure 5.5 shows agreement between UTCHEM and UTDUAL. The pore volumes reported in these figures refer to the total (fracture + matrix) pore volumes. The UTCHEM output files, however, give the fracture pore volumes only.

The third case run was a 2D case. The reservoir is 100x100x10 ft^3 and with grid number of 10x10x1. Each grid size is 10x10x10 ft^3. Fluid is injected in one corner and produced from an opposite corner, simulating a quarter of a five-spot pattern. All other properties are the same as the second set of runs. The number of matrix subgrids ranges from 1 to 8. Figure 5.6 shows the result. Note that the solid line is the overlap of the two curves of the capacitance model and the dual porosity model with one subgrid.

It is expected that increasing the number of subgrids will increase computing time. However, the amount of additional time required for additional subgridding is very small in this implementation. Figures 5.7 and 5.8 show CPU times for the runs made above. Note that only slightly more time was needed, even with 8 subgrids.

The last comparison is with SWIFT II (Reeves *et al.*, 1986), a code developed for contaminant transport studies. The case simulated is the transport of a decaying radionuclide in a fractured porous medium. A thin fracture is situated within a saturated porous rock matrix. Both the fracture and matrix are semi-infinite in extent. The radionuclide is convected and dispersed through the fracture with constant velocity and is diffused into the rock matrix. The fracture aperture is 10^{-4} m, matrix porosity is 0.01, matrix tortuosity is 0.1, fracture dispersivity is 0.5 m, molecular diffusion coefficient in water is 1.6×10^{-5} cm^2/sec, radionuclide decay constant is 0.0561 yr^{-1}, and fracture velocity is 0.01 m/day. Note that the value of the dispersivity in UTCHEM (K^m) is equivalent to the product of tortuosity times the molecular diffusion coefficient in water used by SWIFT II. A constant tracer concentration boundary condition on the source side of the system is required to match an analytical solution to this problem (Tang *et al.*, 1981). UTCHEM was modified slightly to handle this boundary condition. Variable gridblocks are used in both fracture and matrix. A 10,000-day period was simulated. Figure 5.9 shows the radionuclide concentration in the fracture. Note that the simulated results and the analytical solution by Tang *et al*. match very well. Figure 5.10 shows the radionuclide concentration in the matrix 1.5 m from the injection point at 10,000 days. The result also matches the analytical solution. This problem is described in detail in the SWIFT II manual (Reeves *et al.*, 1986).

5.6 Conclusions

From the above test runs and comparisons with other simulators, the following conclusions are made:

1. A dual porosity formulation to model tracer flow in fractured reservoirs has been implemented in the UTCHEM chemical flooding simulator. Good matches are obtained compared with other simulators.
2. Different fracture systems can be modeled by the simulator. These include vertical fractures, horizontal fractures, and combinations of the two.
3. Computer time required to refine the matrix system does not appreciably increase for reasonable numbers of subgrids.
4. The dual porosity model reduces to the capacitance model when the number of subgrids is equal to one.

5.7 Nomenclature

C^d = tracer concentration in dendritic fraction, m/L^3

C^f = tracer concentration in flowing fraction or fracture system, m/L^3

C^m = matrix block tracer concentration, m/L^3

$\overline{C}^m$ = average tracer concentration in matrix block, m/L^3

f_{jk} = volume fraction of subgrid j, k, dimensionless

F = flowing fraction $\left(\frac{S^f}{S}\right)$, dimensionless

$1-F$ = dendritic fraction $\left(\frac{S^d}{S}\right)$, dimensionless

h_k = thickness of k^{th} layer, L

K^m = tracer diffusion coefficient in matrix, L^2/t

K_{xy}^m = tracer diffusion coefficient in matrix in horizontal direction, L^2/t

K_z^m = tracer diffusion coefficient in matrix in vertical direction, L^2/t

L_x, L_y = matrix dimensions, L

L_{xjk}, L_{yjk} = subgrid dimensions in x and y directions, L

M = capacitance mass transfer coefficient, t^{-1}

M_{sub} = number of subgrids in vertical direction (layers)

n = number of matrix blocks per unit bulk volume of reservoir

N = dimensionality of fracture set

N_{sub} = number of subgrids in horizontal direction (rings)

S_A = matrix block surface area per unit bulk volume of reservoir, L^{-1}

S^d = dendritic saturation, dimensionless

S^f = flowing saturation, dimensionless

TC = sum of transmissibilities in the vertical and horizontal directions, L^3/t

TH = transmissibility in the horizontal direction, L^3/t

TV = transmissibility in the vertical direction, L^3/t

t = time, t

V_{bk}^m = bulk volume of layer k of the matrix, L^{-3}

ΔV_{jk}^m = volume of the j^{th} ring and the k^{th} layer of matrix subgrids, L^{-3}

ϕ = total porosity, fraction

ϕ^f = fracture porosity, fraction

ϕ^m = matrix porosity, fraction

λ = radioactive decay constant, t^{-1}

σ = shape factor, L^{-2}

$\left[\frac{\partial C^m}{\partial n}\right]_f$ = tracer concentration gradient normal to matrix block surface, m/L^4

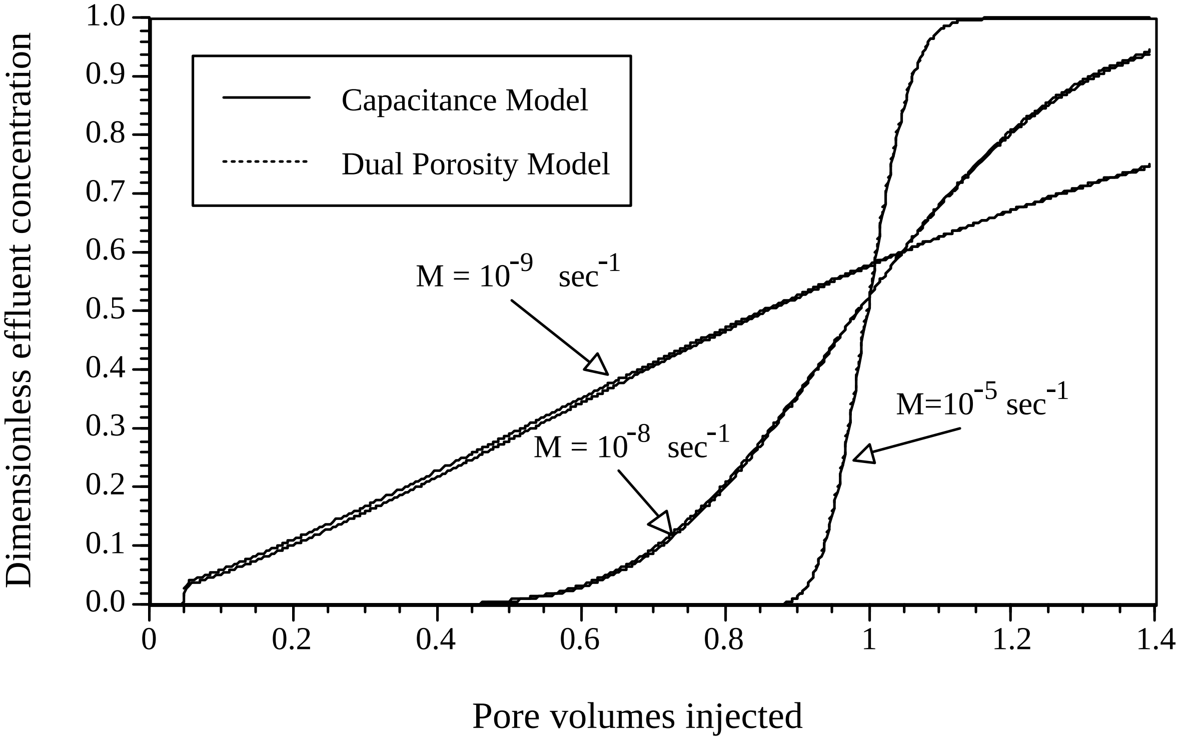

Figure 5.1. Comparison of capacitance model (UTCHEM) to equivalent dual porosity model (UTDUAL) results.

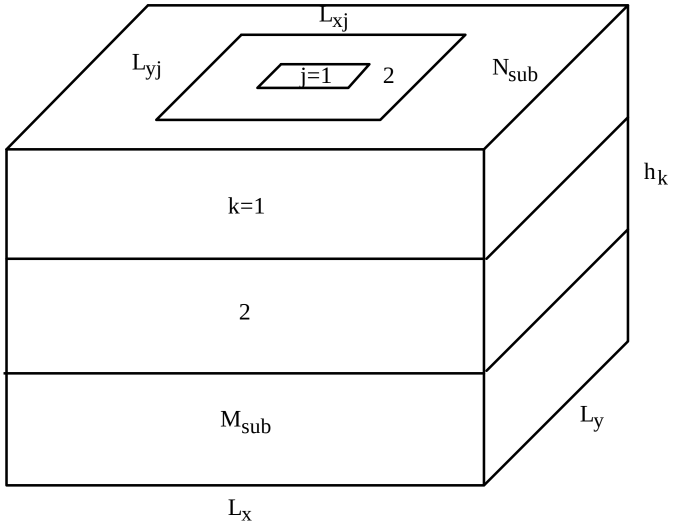

Figure 5.2. Schematic of matrix block subgrids.

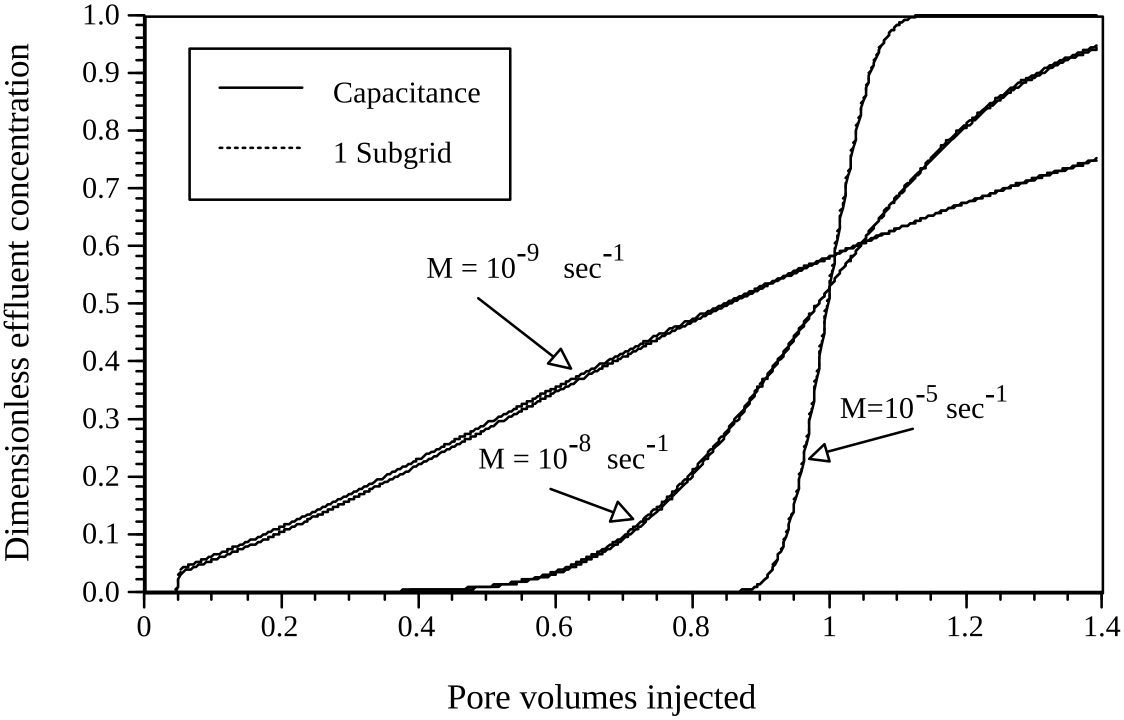

Figure 5.3. Comparison of capacitance model vs. subgrid model in UTCHEM.

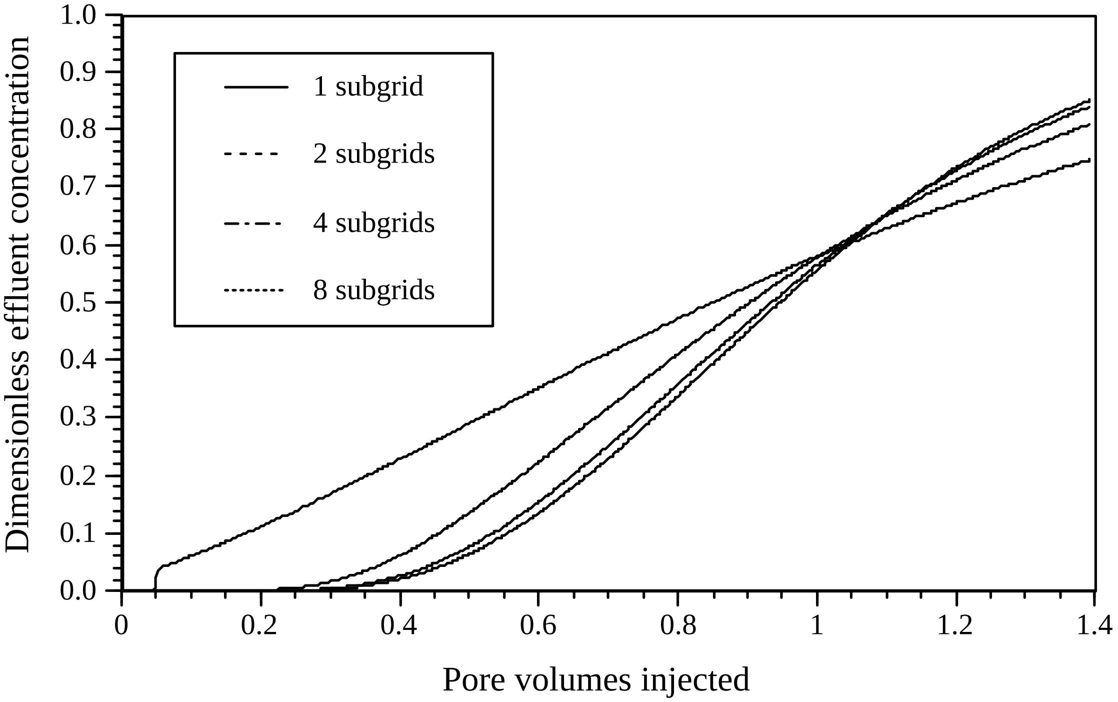

Figure 5.4. Subgrid refinement studies with UTCHEM, $K^m = 3.243 \times 10^{-2}$ ft^2/day.

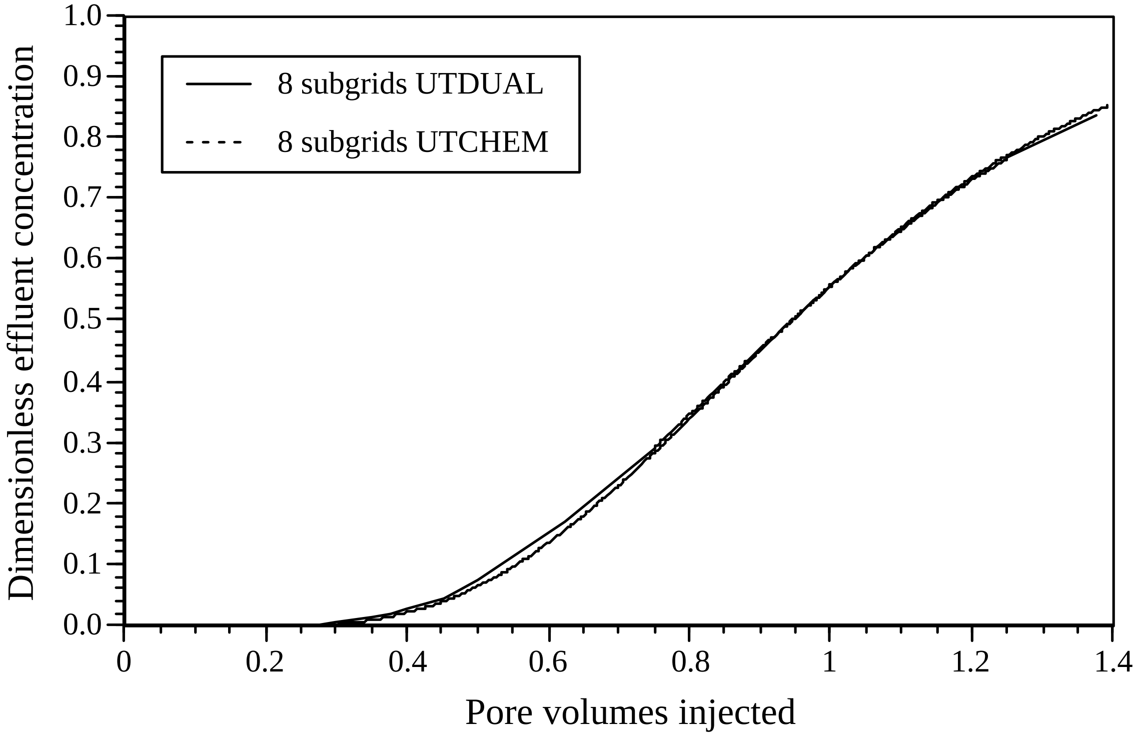

Figure 5.5. Comparison of UTCHEM and UTDUAL subgridding.

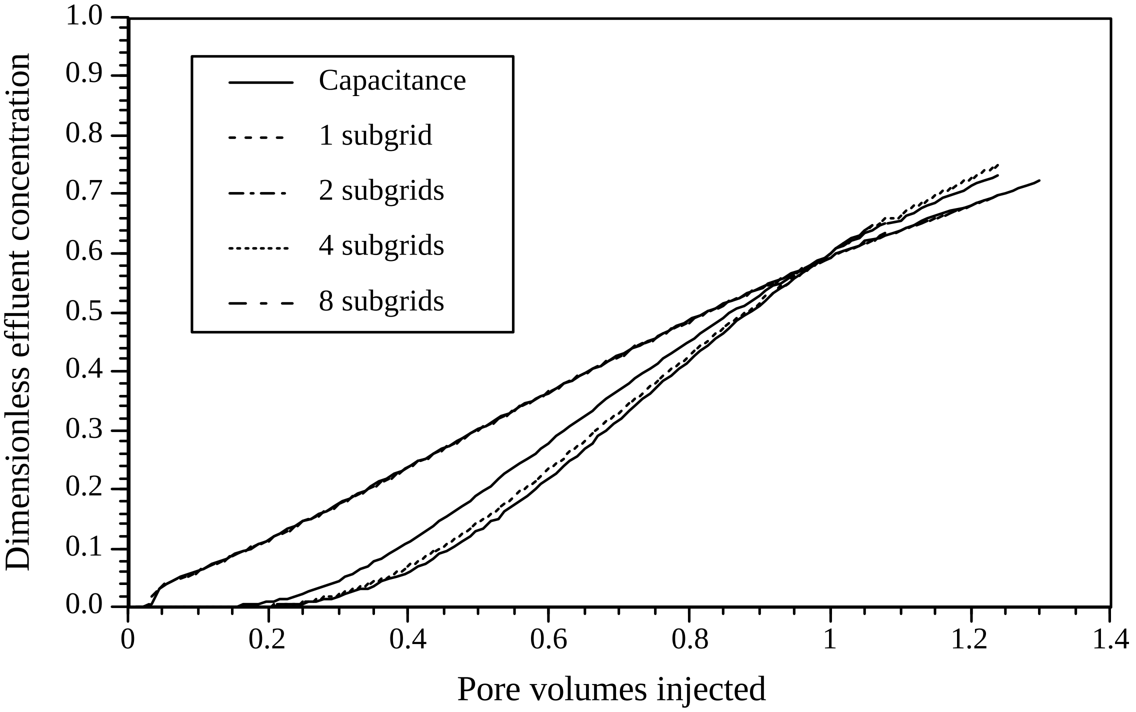

Figure 5.6. 2D subgrid refinement studies with UTCHEM.

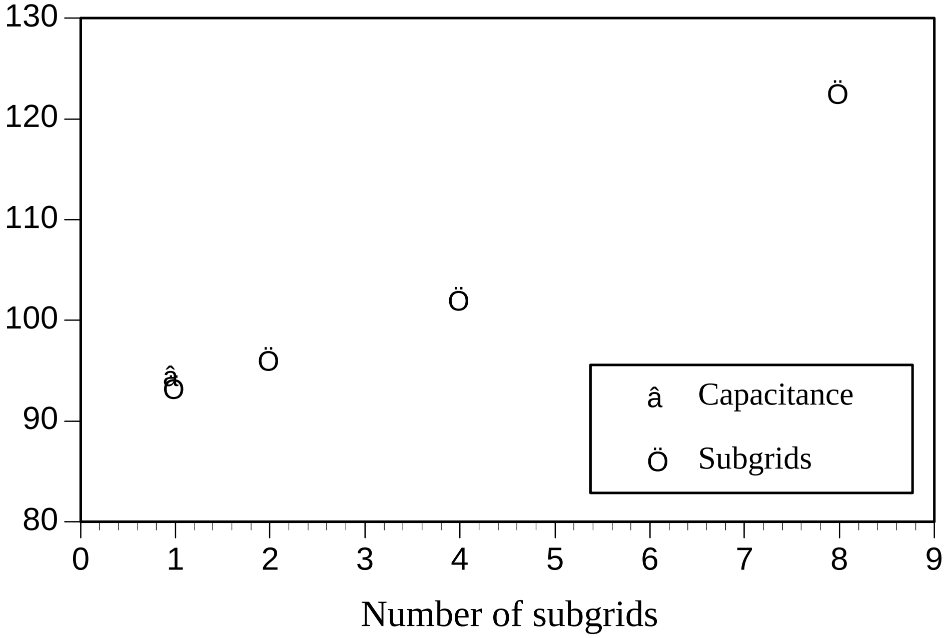

Figure 5.7. Comparison of execution time with different numbers of subgrids, 1D case.

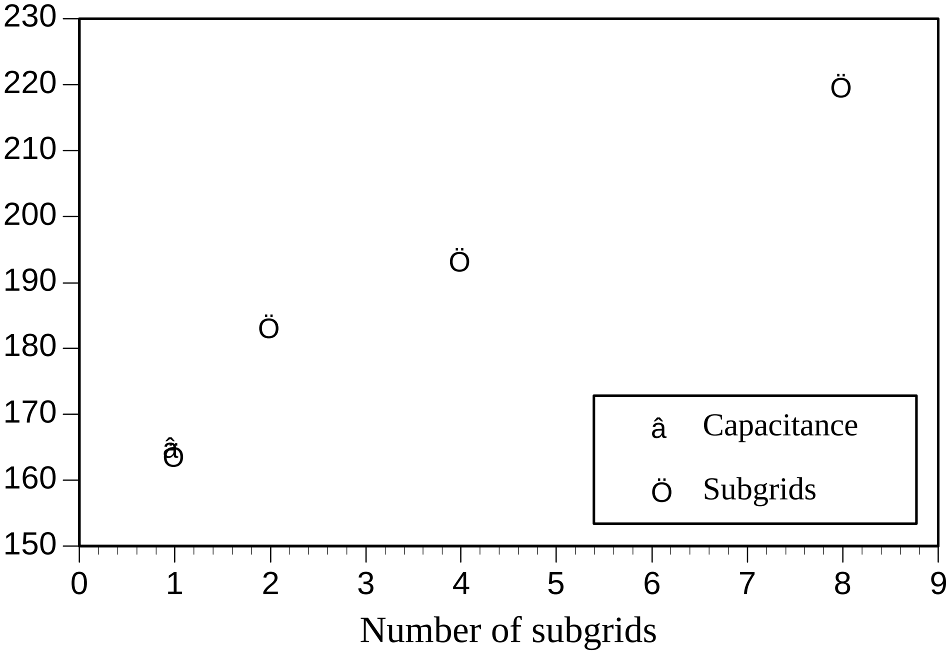

Figure 5.8. Comparison of execution time with different numbers of subgrids, 2D case.

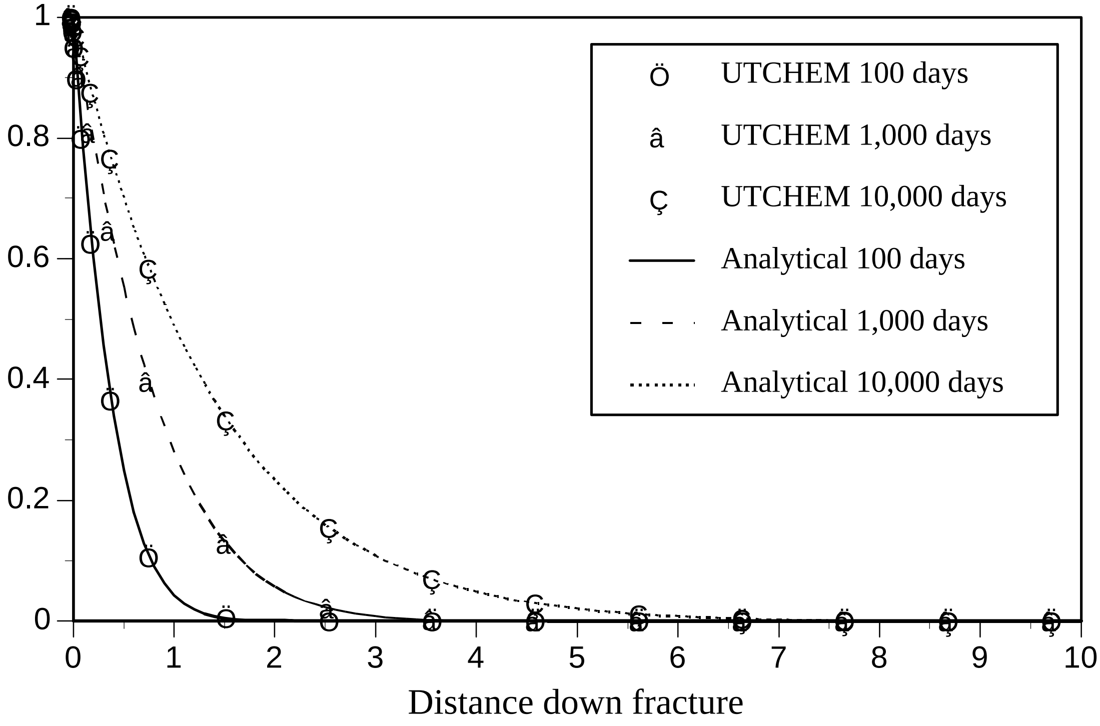

Figure 5.9. Comparison of simulated results vs. analytical solution (Tang *et al.*, 1981) for radionuclide concentration in the fracture.

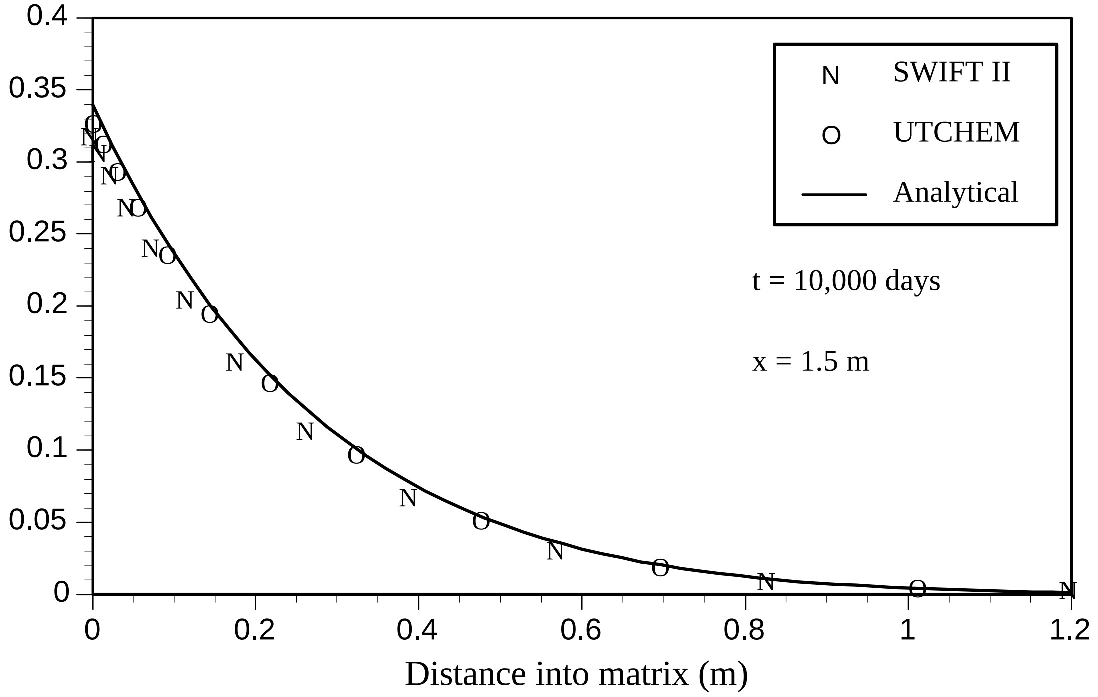

Figure 5.10. Comparison of simulated results vs. analytical solution (Tang *et al.*, 1981) and SWIFT II (Reeves *et al.*, 1986) for radionuclide concentration in the matrix.

Table 5.1. Equivalence Between Capacitance and Dual Porosity Models

Capacitance Model	Dual Porosity Model
Porosity (ϕ)	$\phi^m + \phi^f$
Flowing fraction (F)	$\frac{\phi^f}{\phi^m + \phi^f}$
Dendritic fraction ($1-F$)	$\frac{\phi^m}{\phi^m + \phi^f}$
Flowing fraction tracer concentration (C^f)	C^f
Dendritic fraction tracer concentration (C^d)	$\overline{C}^m$
Mass transfer coefficient (M)	$\sigma K^m \frac{\phi^m}{\phi^m + \phi^f}$

Table 5.2. Input Data for the Comparisons of Capacitance Model in UTCHEM to Dual Porosity Model in UTDUAL

System size	100x10x10	ft
Fluid injection rate	0.5	ft^3/day
Capacitance Model		
Total porosity	0.20	
Flowing fraction	0.05	
Dendritic fraction	0.95	
Mass transfer coefficient	10^{-5} 10^{-8} 10^{-9}	sec^{-1} sec^{-1} sec^{-1}
Dual Porosity Model		
Fracture porosity	0.01	
Matrix porosity	0.19	
Shape factor	0.08	ft^{-2}
Matrix block size	10x10x10	ft
Diffusion coefficient	10.8 1.08×10^{-2} 1.08×10^{-3}	ft^2/day ft^2/day ft^2/day

Section 6
UTCHEM Model of Gel Treatment

6.1 Introduction

This section is based on the dissertation entitled "A Simulation Study of Gel Conformance Treatments" by H. Kim, The University of Texas at Austin, Ph.D., May 1995.

6.2 Gel Conformance Treatments

The operational aspect of a gel treatment includes the following :

- Zonal isolation
- Types of gel treatments
- Shut-in time
- Gel injection rate
- Amount of gelant

The types of gel treatments are 1) simultaneous injection of polymer and crosslinker into the reservoir, 2) alternate injection of polymer and crosslinker slugs, and 3) injection of pre-gelled fluid into the reservoir. The type of gel treatment selected influences the placement of the gel in the reservoir. In this study, the simultaneous mode of injection of polymer and crosslinker was modeled.

The shut-in time allowed after injection, before the well is put back on production, is critical to the success of a gel job. If the gel does not reach most of its strength, its efficacy in plugging the high-permeability layer will suffer.

The injection rate determines the rate of shearing of the polymer and gel as well as the injection pressure. The injection rate should be such that the wellbore pressure does not exceed the fracture pressure of the rock matrix.

The amount of gelants injected determines the depth of penetration of the gel into the formation. The amount injected must ensure adequate plugging of the high-permeability, watered-out zone.

Zonal isolation is used to selectively treat the problem zone. In some wells, improper well completion or casing damage may lead to mechanical difficulties in achieving zonal isolation. In this work, gel treatments were simulated with and without zonal isolation to demonstrate the effectiveness of zonal isolation.

The polymer-gel system chosen for a particular treatment will depend on its compatibility with the reservoir and operational conditions. The properties considered when choosing a particular system are

- Viscosity
- Gelation time
- Permeability reduction
- Thermal and mechanical stability
- Mechanical strength
- Safety

Viscosity of the gel and polymer determines the wellbore pressure during injection. Very high viscosities may cause the wellbore pressure to exceed the fracture pressure of the reservoir.

Gelation time depends on the kinetics of gel formation and influences the injection rate and shut-in time used during the treatment. Ideally, the gelation time should allow proper placement of the gel before full gel strength develops.

The permeability reduction caused by the gel in the porous medium is an indicator of its ability to modify the flow patterns in the reservoir. In near-wellbore treatments, the gel should be able to plug the high water-cut zones.

The ultimate mechanical strength developed by a gel is a measure of the pressure it can withstand before breaking down. The gel should have enough mechanical strength to remain in place when subjected to normal drawdown during production.

Safety of the gel, polymer and crosslinker may ultimately determine its usage. Gel components need to be safe for handling and storage and should pose no risk to the environment. The application of some toxic gels may be limited or restricted by the environmental concerns in certain locations. Studies of environmentally benign gels that do not use any toxic materials as a gel component are active.

It is important to characterize the reservoir in which the gel is ultimately going to be placed. Some reservoir characteristics that have a significant impact on gel treatment success are

- Permeability contrast
- Vertical communication
- Rock properties such as clay content
- Salinity
- Temperature

The permeability contrast between the layers influences the relative depth of penetration in the layers. A high permeability contrast mitigates the damage done to the oil-producing low-permeability zone.

Crossflow between the layers leads to mixing of fluids between the layers. This can cause some penetration of low-permeability layers even during selective treatments. During post-gel treatment production, crossflow may cause the water to bypass the plugged zone and be produced.

The clay content and the cation exchange capacity of the clays can have a significant impact on crosslinker propagation. Experiments indicate that a significant portion of injected cations like chromium may be retained on the clays and hence are not available for gelation. Salinity influences polymer and gel viscosities, while the temperature of the reservoir affects the rate of gelation and the stability of the gel for an extended period of time.

The gel properties modeled in UTCHEM include

- effect of gel on aqueous-phase viscosity,
- gel retention on matrix, and
- aqueous phase permeability reduction.

6.3 Gel Viscosity

The viscosity of an aqueous solution containing gel is modeled using the Flory-Huggins equation with additional terms for gel (Thurston *et al.*, 1987).

$$\mu_1 = \mu_w \left[1 + \left(A_{p1} C_{4,1} + A_{p2} C_{4,1}^{\,2} + A_{p3} C_{4,1}^{\,3} \right) C_{SEP}^{S_P} + A_{g1} C_{15,1} + A_{g2} C_{15,1}^{\,2} \right] \tag{6.1}$$

6.4 Gel Adsorption

Gel retention modeling is done using a "Langmuir-type" isotherm to correlate adsorbed concentration with the aqueous-phase concentrations.

$$\hat{C}_{15} = \frac{a_{15} C_{15,1}}{1 + b_{15} C_{15,1}} \tag{6.2}$$

6.5 Gel Permeability Reduction

The effect of gel on aqueous-phase permeability reduction is taken into account through a residual resistance factor commonly used for polymer flooding.

$$R_{RF} = 1 + \frac{(R_{RF\,max} - 1)\, A_{gk}\, C_{15,1}}{1 + B_{gk}\, C_{15,1}} \tag{6.3a}$$

where the maximum residual resistance factor is calculated by

$$R_{RF\,max} = \left[1 - \frac{c_{rg} \left(A_{p1} C_{SEP}^{S_p} \right)^{1/3}}{\left(\frac{\sqrt{k_x k_y}}{\phi} \right)^{1/2}} \right]^{-4} \tag{6.3b}$$

The parameter c_{rg} is an input parameter which depends on the gel type. The permeability reduction for silicate gel (KGOPT=3) is independent of the silicate viscosity and the maximum residual resistance factor (R_{RFmax}) is equal to 10.

6.5.1 Chromium Retention

The following equilibria have been implemented in UTCHEM to simulate the exchange between chromium, sodium and hydrogen on the clays.

6.5.2 Cation Exchange

6.5.2.1 Chromium-Sodium Exchange

$$3\,\widehat{Na^+} + Cr^{3+} = 3\,Na^+ + \widehat{Cr^{3+}}$$

$$K_{14,9} = \frac{\hat{C}_{14}\,C_{9,1}{}^3}{\hat{C}_9{}^3 C_{14,1}} \tag{6.4}$$

6.5.2.2 Hydrogen-Sodium Exchange

$$\widehat{Na^+} + H^+ = Na^+ + \widehat{H^+}$$

$$K_{16,9} = \frac{\hat{C}_{16}\,C_{9,1}}{\hat{C}_9\,C_{16,1}} \tag{6.5}$$

6.5.3 Adsorption

As an alternative to cation exchange, the retention of chromium has also been modeled as a "Langmuir-type" isotherm in UTCHEM.

$$\hat{C}_{14} = \frac{a_{14}C_{14,1}}{1 + b_{14}C_{14,1}} \tag{6.6}$$

6.5.4 Precipitation

Chromium precipitation is modeled using geochemical reaction equilibria in UTCHEM. Cr(III) precipitates in the form of chromium hydroxide complex.

$$Cr^{3+} + H_2O = Cr(OH)^{2+} + H^+ \tag{6.7}$$

$$Cr^{3+} + 2\,H_2O = Cr(OH)_2^+ + 2\,H^+ \tag{6.8}$$

$$Cr(OH)_3 \downarrow = Cr^{3+} + 3\,OH^- \tag{6.9}$$

Gel reactions are implemented in the source term as gel kinetic equations and the mass-conservation equation is solved with reacted amount of each gel component.

Polymer molecules are crosslinked by Cr(III), which is known to be one of the most widely used crosslinkers. Three types of gel reactions and kinetics are implemented in UTCHEM. The kinetics of polymer/chromium chloride gel were modified, and gel reactions of polymer/chromium malonate gel and silicate were modeled.

6.5.5 Polymer/Chromium Chloride Gel

Two sets of reactions and kinetics for polymer/chromium chloride gel are implemented in UTCHEM. The first is in-situ gelation of polymer with sodium dichromate with reducing agent thiourea, and the second is the gelation of Cr(III) with polymer to form gel.

The kinetics for the reaction between polymer and chromium have been generalized to allow for any exponent (Hunt, 1987). The gel is formed by fast reaction of trivalent chromium (Cr(III)) and polymer. There is an option for the slow delaying reaction between Cr(VI) and thiourea. The sodium dichromate ($Na_2Cr_2O_7$) and thiourea ($(CS(NH_2))_2$) are treated like tracers in the sense that they do not occupy any volume. The Cr(III) for the gelation process can be generated in situ by redox reaction between Cr(VI) and thiourea.

$$Cr_2O_7^{2-} + 6CS(NH_2)_2 + 8H^+ \xrightarrow{k_1} 2Cr^{3+} + 3\left[CS(NH_2)_2\right]_2 + 7H_2O$$

The gel reaction is highly dependent on pH (Lockhart, 1992; Seright and Martin, 1991). For more realistic simulations of gel reactions, pH was implemented in the gel kinetic equation as hydrogen ion concentration.

6.5.6 Polymer/Chromium Malonate Gel

The components of polymer/chromium chloride gel are as follows:

1. Polymer – Hydrolyzed polyacrylamide (HPAM) and HE-100 (acrylamido-3-propane sulfonic acid co-polymer) were used. HE-100/chromium malonate is reported to have a longer gelation time than HPAM/chromium malonate (Lockhart, 1992).
2. Crosslinker – Chromium malonate, $Cr(HOOC - CH_2 - COOH)_3$. Among various complexes of chromium, chromium malonate has the longest gelation time and stability at high temperature (Lockhart, 1992).
3. Ligand (delaying) – Malonate ion (uncomplexed), $(HOOC - CH - COOH)^-$. The uncomplexed malonate ion as a delaying ligand is an optional component that gives a longer gelation time.

6.5.6.1 Kinetics

Case I (polymer and crosslinker only)

The kinetics for this gel are the same as the kinetics of chromium chloride gel except with different exponents:

$$[\text{polymer}] + n\,[\text{Cr(III)}] = [\text{gel}] ,$$

$$\frac{d\,[\text{Cr (III)}]}{dt} = -\,k\,\frac{[\text{Cr (III)}]^{X14}\,[\text{polymer}]^{X4}}{\left[H^+\right]^{X16}} ,$$

$$\frac{d\,[\text{gel}]}{dt} = -\,\frac{1}{n}\,\frac{d\,[\text{Cr (III)}]}{dt} ,$$

where the possible values for exponents from Lockhart [1992] are

X4 2.6

X14	0.6
X16	1.0

Case II (polymer, crosslinker, and malonate ion)

When the malonate ion is used as a delaying ligand, the gelation kinetics are different, with zero-order reaction for chromium :

$$\frac{d\,[\,Cr\,(III)\,]}{dt} = -\,k\,\frac{[\,polymer\,]^{X4}}{[\,malonate\,]^{X13}\left[H^{+}\right]^{X16}} \quad ,$$

$$\frac{d\,[\,gel\,]}{dt} = -\,\frac{1}{n}\,\frac{d\,[\,Cr\,(III)\,]}{dt}$$

where some possible values for exponents from Lockhart [19912] are

X4	2.6
X13	0.3
X16	1.0

The uncomplexed malonate ion slowly decomposes to acetate and carbon dioxide, and this is a first-order reaction:

$$(\,HOOC - CH - COOH\,)^{-} \quad ----> \quad CH_3COO^{-} + CO_2$$

First-order reaction :

$$\frac{d\,[\,malonate\,]}{dt} = -\,0.037347\;[\,malonate\,]$$

6.5.7 Silicate Gel

UTCHEM was modified to simulate the gel reaction of the silicate gel. Polymer and chromium were replaced with silicate (SiO_2) and hydroxyl ion (OH^-), respectively. The gelation was limited to occur only for pH > 7 (Bennett *et al.*, 1988; Iler, 1979) to eliminate complex behavior of gel reaction rate at pH < 7, and the aqueous-phase permeability-reduction factor was independent of silicate viscosity.

Silicate gel is formed by polymerization when appropriate conditions are established. The exact mechanism of gelation is not clear yet; several authors (Iler, 1979; Jurinak *et al.*, 1989) explain the general mechanism of gelations of various types of gels.

The general process of gelation is as follows (Jurinak *et al.*, 1989):

- condensation of monomer and dimer silicate species to form higher-order oligomers,
- intramolecular condensation of silanol groups within polymers leading to ring closure and eventual particle formation, and
- aggregation of individual particles to form chains and microgel.

The rate of gelation (Kristensen *et al.*, 1993) is a function of

- silicate concentration
- pH
- ionic strength
- temperature

The basic equations that govern polymerization of silicate (Iler, 1979) are as follows:

$$SiO_2 + 2\,H_2O = Si(OH)_4 \tag{6.10}$$

$$-\,SiOH + HOSi\,- = -\,SiOSi\,- + H_2O \tag{6.11}$$

In general form,

$$n\,SiO_2 + z\,OH^- = Si_nO_y(OH)^{z-}_{(nx-z)} + (y-2)\,H_2O\ , \tag{6.12}$$

where

n = degree of polymerization

x = ratio of OH:Si

$x = 4.85\,n^{-1/3} - 7.8\,n^{-2/3} + 4.2\,n^{-1}$

$y = \dfrac{4n - nx}{2} + z$

z = number of charges on polymer

Equation 6.12 can be written in simplified form as

$$[SiO_2] + m\,[OH^-] = [\text{silicate gel}]\ , \tag{6.13}$$

where m is the stoichiometric ratio.

From Eq. 6.13, the gelation kinetics equation can be derived.

$$\frac{d[SiO_2]}{dt} = -k[SiO_2]^{X4}\left[OH^-\right]^{X14} \tag{6.14}$$

where

X4 = gelation kinetics exponent for silicate

X14 = gelation kinetics exponent for hydroxyl ion

$$\frac{d\,[\,gel\,]}{dt} = -\frac{d\,[\,SiO_2\,]}{dt}$$

where some possible values for exponents (Kristensen *et al.*, 1993) are

X4	3.8
X14	-2.5

6.6 Temperature Effects

The reaction constants for gel (k) and the delaying reaction of sodium dichromate and thiourea (k_1) are calculated as a function of temperature if the temperature variation is modeled in the simulations as below.

$$k_1 = k_{1ref} \exp\left[k_{T1} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right]$$

where the temperature T and T_{ref} are in ^{0}R. The input parameters are T_{ref} , K_{T1}, and k_{1ref} for the dichromate reaction.

$$k = k_{ref} \exp\left[k_{T2} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right]$$

where the input parameters are T_{ref} , K_{T2}, and k_{ref} for the gel reaction.

Section 7
Multiple Organic Components

We have added multiple organic components so that we can model NAPL mixtures. Adding this capability to UTCHEM required developing a phase behavior model for NAPL mixtures and the physical property models such as density and viscosity for each phase.

7.1 Introduction

Nonaqueous phase liquids (NAPLs) usually consist of more than one organic species that mix and form a single liquid. Common examples of such miscible species include TCE, TCA and PCE among many others. When NAPLs leak to the subsurface, they can dissolve and migrate into groundwater. To model the fate and transport of these soluble organics during remediation processes such as pump-and-treat, bioremediation and surfactant remediation, it is important to determine the migration of the individual soluble organics. The dissolution can be either a local equilibrium or a rate-limited (non-equilibrium) mass transfer process. We have added the capability of multiple organic components to UTCHEM to model these NAPL mixtures. The multiple organic dissolution can be either at local equilibrium partitioning or a rate-limited mass transfer. We also present the phase behavior model developed for a mixture of NAPL mixtures, surfactant, and water. The physical property models to calculate the density, viscosity, and adsorption of the organic species and NAPL mixtures are also included.

7.2 Mass Transfer for Nonaqueous Phase Liquid

When a NAPL component dissolves in water, its concentration in ground water can reach its solubility (equilibrium mass transfer) but often is much lower than the solubility due to a rate-limited mass transfer. UTCHEM allows for both equilibrium and nonequilibrium mass transfer for a multiple organic NAPL. The mass transfer is modeled for the cases with or without surfactant.

7.2.1 No Surfactant or Surfactant Concentration Below CMC

7.2.1.1 Equilibrium Mass Transfer

For the equilibrium case, a constant partition coefficient between water and NAPL is assumed for each organic species:

$$K_k^o = \frac{C_{k1}^o}{C_{k2}^o} \quad k=1,2,3,...,n_o \qquad (7.1)$$

The overall fluid concentrations for water (C_1), surfactant (C_3), and each organic components (C_k^o) are solved from the species mass conservation equation. The overall fluid phase concentration is the summation of phase concentrations over all the phases:

$$C_k = C_{k1}S_1 \quad k=1,3 \tag{7.2}$$

and

$$C^o_k = C^o_{k1}S_1 + C^o_{k2}S_2 \quad k=1,2,3,...,n_o \tag{7.3}$$

The definitions of overall phase concentrations (Eqs. 7.2 and 7.3), the constraints that phase concentrations sum up to one ($C_{31} + \sum_{k=1}^{n_o} C^o_{k1} + C_{11} = 1$ and $\sum_{k=1}^{n_o} C^o_{k2} = 1$), and the known partition coefficients for organic components (Eq. 7.1) are used to solve the phase concentrations and saturations. These equations are solved by reformulating C_{31} and C^o_k in terms of C_{11} and using Newton's method to solve $f(C_{11}) = C_{31} + \sum_{k=1}^{n_o} C^0_{k1} + C_{11} - 1 = 0$. A phase stability rule is used to determine the number of phases. If $\sum_{k=1}^{n_o} \frac{C^o_k}{K^o_k} > 1$, the fluid is two phases. Otherwise, it is a single phase.

7.2.1.2 Nonequilibrium Mass Transfer

For nonequilibrium mass transfer, a linear driving force rate, as proposed by Powers *et al.* [1992] is used. The mass transfer rate between NAPL and water interface for each NAPL component is a mass transfer coefficient times the driving force that is the difference between the equilibrium and phase concentrations. The mass transfer coefficient is currently modeled as a constant. The computational procedure for non-equilibrium mass transfer requires the calculation of the equilibrium organic concentrations, C^{oeq}_{k1}, first. Then we solve for the phase concentrations and saturations for the nonequilibrium case. It is similar to the equilibrium case, except that the mass balance equation for the organic in the water phase is used instead of constant partition coefficient of the equilibrium case. The organic species mass balance equations in the water phase are given by:

$$\frac{\partial \phi \left[1 - \sum_{n=1}^{n_c} \hat{C}_n\right]\left[1 + c^a_k (P_1 - P_{Ra})\right] S_1 C^o_{k1}}{\partial t} + \vec{\nabla} \cdot \left[1 + c^a_k (P_1 - P_{Ra})\right]\left(C^o_{k1}\vec{u}_1 \bar{\bar{D}}^o_{k1}\right) \tag{7.4}$$

$$= R^o_{k1} + Q^o_{k1} + M^o_k \left(C^{oeq}_{k1} - C^o_{k1}\right) \quad k = 1, 2, 3, ..., n_o$$

7.2.2 Surfactant Concentration Above CMC

7.2.2.1 Equilibrium Mass Transfer

When the surfactant concentration is greater than the CMC, micelles form. When organic species are solubilized into these micelles under certain conditions, a microemulsion forms. Organic species dissolve by two mechanisms: (1) organic components dissolve into water according to their equilibrium solubilities in water and (2) the organic mixture solubilized by the micelles has the same composition as the NAPL. To model both mechanisms, each organic component is divided into two parts, one associated with water, C^{ow}_k, and the other associated with the micelles, C^{oo}_k.

The organic dispersed into water follows the constant partition coefficient as described above. The remainder of the organic is assumed to follow the same microemulsion as used for a single component (as given in Appendix C and based upon Hand's equation). The calculations of phase compositions are divided into two parts. First, assume the surfactant is not present and calculate phase equilibrium concentrations as before. This calculation gives the overall concentration of each organic components associated with water,

$$C_k^{ow} = C_1 \frac{C_{k1}^{ow}}{1 - \sum_{k=1}^{n_o} C_{k1}^{ow}} .$$

Hand's equation is then used to calculate the phase concentrations and saturations using the normalized total concentrations as

$$C_{1N} = \frac{C_1}{1 - \sum_{k=1}^{n_o} C_k^{ow} - CMC} \tag{7.5}$$

$$C_{2N} = \frac{\sum_{k=1}^{n_o} C_k^o - \sum_{k=1}^{n_o} C_k^{ow}}{1 - \sum_{k=1}^{n_o} C_k^{ow} - CMC} \tag{7.6}$$

$$C_{3N} = \frac{C_3 - CMC}{1 - \sum_{k=1}^{n_o} C_k^{ow} - CMC} \tag{7.7}$$

The phase concentrations and saturations for the normalized concentrations are calculated from Hand's equations.

$$C_{kN} = \sum_{\ell=1}^{3} C_{k\ell N} S_{\ell N} \qquad k=1,2,3 \tag{7.8}$$

For the Type II(-) phase environment with corner plait point, $C_{12N}=0$, $C_{22N}=1$, $C_{32N}=0$, and $S_{1N}=0$. The phase concentrations in terms of the original concentrations are calculated from the following equations:

$$C_{1\ell} = C_{1\ell N}\left(1 - \sum_{k=1}^{n_o} C_k^{ow} - CMC\right) \tag{7.9}$$

$$C_{k\ell}^{o} = C_{k2}^{oo} C_{2\ell N}\left(1 - \sum_{k=1}^{n_o} C_k^{ow} - CMC\right) + C_k^{ow} \qquad k = 1,2,...,n_o \tag{7.10}$$

$$C_{3\ell} = C_{3\ell N}\left(1 - \sum_{k=1}^{n_o} C_k^{ow} - CMC\right) + CMC \tag{7.11}$$

and the saturation is unaffected by the normalization.

7.2.2.2 Nonequilibrium Mass Transfer

Once the equilibrium saturations and concentrations are known, the organic species mass balance equations in the aqueous phase (Eq. 7.12) are used to calculate the nonequilibrium saturations and concentrations. A single mass transfer coefficient is assumed for all organic components.

$$\frac{\partial \phi \left[1 - \sum_{n=1}^{n_c} \hat{C}_n\right] \left[1 + c_k^a \left(P_1 - P_{Ra}\right)\right] S_1 C_{k1}^o}{\partial t} + \vec{\nabla} \cdot \left[1 + c_k^a \left(P_1 - P_{Ra}\right)\right] \left(C_{k1}^o \vec{u}_1 \vec{\vec{D}}_{k1}^o\right) \tag{7.12}$$

$$= R_{k1}^o + Q_{k1}^o + M_2 \left(C_{k1}^{oeq} - C_{k1}^o\right) \quad k = 1, 2, 3, \ldots, n_o$$

where the equilibrium concentrations and saturations are already known from the phase behavior calculations.

7.3 Physical Properties for NAPL Mixture

Phase behavior, adsorption, viscosity, and density are the physical property relations modeled for the NAPL mixtures.

7.3.1 Phase behavior

Three recent papers by Baran *et al.* [1994a,b,c] show that the phase behavior of surfactants with both pure chlorocarbons and mixtures of chlorocarbons is similar to classical phase behavior with hydrocarbons. The phase behavior changes from microemulsion in equilibrium with excess oil (Winsor Type I or Type II(-)) to microemulsion in equilibrium with excess aqueous and organic phase (Winsor Type III), and to microemulsion in equilibrium with excess water (Winsor Type II or Type II(+)) as salinity increases. The lower (C_{SEL}) and upper (C_{SEU}) limits of effective salinity are the effective salinity which three phases form or disappear. The optimal salinity (C_{SEOP}) is defined as the midpoint of these two salinity limits (Salager *et al.* 1979).

Hand's equation (Pope and Nelson, 1978) is used in UTCHEM to describe the phase envelope, binodal curve. The concentrations at binodal curve are described by the following equation:

$$\frac{C_{3\ell}}{C_{2\ell}} = A\left(\frac{C_{3\ell}}{C_{1\ell}}\right)^B \quad \ell = 1, 2, 3 \tag{7.13}$$

where parameter A and B are empirical parameters. Parameter A is related to the height of the binodal curve and B is assumed to be -1 in UTCHEM for a symmetric binodal curve. Parameter A is a function of salinity and is linearly interpolated with the values of A at low (m=0), optimal (m=1) and high (m=2) salinities as following:

$$A = \left(A_0 - A_1\right)\left(1 - \frac{C_{SE}}{C_{SEOP}}\right) + A_1 \quad C_{SE} \bullet C_{SEOP} \tag{7.14}$$

and

$$A = \left(A_2 - A_1\right)\left(\frac{C_{SE}}{C_{SEOP}} - 1\right) + A_1 \quad C_{SE} > C_{SEOP} \tag{7.15}$$

Parameter A in terms of the height of binodal curve is described as

$$A_m = \left(\frac{2C_{3\max,m}}{1 - C_{3\max,m}}\right)^2 \quad m=0,1,2 \tag{7.16}$$

For organic mixtures, the upper and lower limits of effective salinity for Type III region, the height of binodal curve at lower, optimal, and upper salinities are functions of organic species concentrations. These parameters are modeled as functions of the equivalent alkane carbon number (E_{ACN}) of the mixture, which is a function of organic species concentrations.

$$E_{ACN} = \sum_{k=1}^{n_o} E^o_{ACN,k} x^o_k \tag{7.17}$$

where x^o_k is the molar fraction for organic components only, $\sum_{k=1}^{n_o} x^o_k = 1$. E_{ACN} for an alkane is the number of carbons in the alkane chain of the hydrocarbon, for example it is equal to 6 for hexane. E_{ACN} for a nonalkane is obtained by measuring the optimal salinity for a binary mixture of an alkane and a nonalkane with known molar fractions. The measured optimal salinity is used to determine E_{ACN} for the binary mixture from Salager's equation. Then E_{ACN} for the nonalkane is calculated from Equation (7.17). The E_{ACN} data listed in the Baran *et al.* papers are built into the UTCHEM database: C_2Cl_4 (PCE, $E_{ACN} = 2.90$), CCl_4 ($E_{ACN} = -0.06$), C_2HCl_3 (TCE, $E_{ACN} = -3.81$), p-xylene ($E_{ACN} = 2$), toluene ($E_{ACN} = 1$), 1,2-$C_6H_4Cl_2$ (DCB, $E_{ACN} = -4.89$), 1,2-$C_2H_4Cl_2$ ($E_{ACN} = -12.10$), $CHCl_3$ ($E_{ACN} = -13.67$), CH_2Cl_2 (DCE, $E_{ACN} = -13.79$), and 1,1,2,2-$C_2H_2Cl_4$ ($E_{ACN} = -22.15$).

The natural log of the optimal salinity is a linear function of E_{ACN} (Salager *et al.*, 1979; Baran *et al.*, 1994a,b.c)

$$\ln C_{SEOP} = s_{se}(E_{ACN} - E_{min}) \tag{7.18}$$

The slope s_{se} is about 0.16 for the optimal salinity with the unit of wt.% per liter. The difference of the upper and lower effective salinities for the three-phase region is assumed as a linear function of E_{ACN}

$$\frac{C_{SEU} - C_{SEL}}{C_{SEOP}} = s_{ds} E_{ACN} + b_{ds} \tag{7.19}$$

where

$$C_{SEOP} = \frac{C_{SEU} + C_{SEL}}{2} \tag{7.20}$$

C_{SEOP}, C_{SEL}, and C_{SEU} can be solved using Eqs. 7.18-7.20.

The solubilization parameter is usually reported by experimentalists doing surfactant phase behavior measurements rather than the height of the binodal curve. The solubilization parameter is defined as the oil concentration divided by the surfactant concentration in the microemulsion phase as $\sigma = \frac{C_{2,\max}}{C_{3,\max}}$. Thus, parameter A can be expressed in terms of the solubilization parameter:

$$A_m = (\sigma_m)^{-2} \quad m = 0,1,2 \tag{7.21}$$

The solubilization parameter is a linear function of E_{ACN} as

$$\sigma_m = s_{\sigma,m} E_{ACN} + b_{\sigma,m} \quad m = 0,1,2 \tag{7.22}$$

In UTCHEM, coefficients s_{se}, E_{min}, s_{ds}, b_{ds}, $s_{\sigma,m}$, and $b_{\sigma,m}$ are not input data. Instead, data for two measured samples including concentrations and component names, the optimal salinity, the difference of the lower and upper salinity limits, and the solubilization parameters at three salinities are specified since these are what are typically measured and reported (see Baran *et al.*, 1994a,b.c for examples). UTCHEM calculates the coefficients based on the input values for the two specified compositions and $E^o_{ACN,k}$ values in the UTCHEM database, or those entered by the user as needed.

7.4 NAPL Mixture Viscosity

Microemulsion viscosities are modeled as:

$$\mu_\ell = C_{1\ell}\mu_1 e^{\alpha_1(C_{2\ell}+C_{3\ell})} + C_{2\ell}\mu_{2\ell} e^{\alpha_2(C_{1\ell}+C_{3\ell})} + C_{3\ell}\alpha_3 e^{\alpha_4(C_{1\ell}+\alpha_5 C_{3\ell})} \tag{7.23}$$

where $C_{2\ell}$ is the total organic concentration, $C_{2\ell} = \sum_{k=1}^{n_o} C^o_{k\ell}$, and $\mu_{2\ell}$ is the organic mixture viscosity. Grumberg and Nissan’s correlation is used to calculate the NAPL viscosity as a function of organic species concentration.

$$\ln \mu_{2\ell} = \sum_{k=1}^{n_o} x^o_{k\ell} \ln \mu^o_k \tag{7.24}$$

7.5 Density of NAPL Mixtures

Hydrostatic pressure gradients for the microemulsion ($\gamma=\rho g$) are calculated as:

$$\gamma_\ell = C_{1\ell}\gamma_{1\ell} + C_{2\ell}\gamma_{2\ell} + C_{3\ell}\gamma_{3\ell} + 0.02535 C_{5\ell} - 0.001299 C_{6\ell} + C_{8\ell}\gamma_{8\ell} \tag{7.25}$$

For a NAPL mixture, the overall organic hydrostatic pressure gradient is obtained by assuming ideal mixing

$$C_{2\ell}\gamma_{2\ell} = \sum_{k=1}^{n_o} C^o_k \gamma^o_{k\ell} \tag{7.26}$$

UTCHEM allows two different hydrostatic pressure gradients for the organic species, one for the microemulsion phase and the other for the organic phase.

7.6 Adsorption of Organic Species

The organic adsorption is modeled as a linear adsorption isotherm. A constant partition coefficient with respect to the organic fraction is used for each organic component as

$$\hat{C}_k^o = f_{oc} K_{oc,k}^o C_{k\ell}^o \quad \ell \text{ is the water-rich phase} \tag{7.27}$$

7.7 Nomenclature

c_k = Compressibility of species k

C_k, C_k^o = Overall fluid concentration of species k and organic species k

$C_{k\ell l}$, $C_{k\ell l}^o$ = Concentration of species k and organic species k in phase ℓ

$\hat{C}_k$, $\hat{C}_k^o$ = Adsorbed concentration of species k and organic species k

C_{SE} = Effective salinity

C_{SEL} = Lower effective salinity

C_{SEOP} = Optimal effective salinity

C_{SEU} = Upper effective salinity

$\vec{\vec{D}}_{k\ell}$ = Dispersion flux of species k in phase ℓ

f_{oc} = Organic carbon fraction in soil

$K_{oc,k}^o$ = Adsorption of organic species k per unit weight of organic carbon in soil

n_o = Total number of organic species

P_R = Reference pressure

Q_k, Q_k^o = Source/sink term for species k and organic species k

R_k = Reaction rates for species

t = Time

$\vec{u}_\ell$ = Darcy flux of phase ℓ

ϕ = Porosity

Section 8
EQBATCH Program Description

8.1 Introduction

EQBATCH is a preprocessor batch program to calculate the equilibrium concentrations for all the flow and solid species based on the chemical reactions considered in UTCHEM simulations. In this program, it is assumed that all the flow species dissolve in a single phase, water. The initial pH of the formation or makeup water can be matched by using EQBATCH with suitable input data. Also, the output of EQBATCH can be used as the input data of UTCHEM for the geochemical options (IREACT = 2-4). In this section, a detailed description for preparation of input data for EQBATCH is presented. To specify the reactions considered in the simulations, elements and chemical species need to be identified. Based on the information of the formation and makeup water analyses and the rock constituents, the key elements and chemical species can be decided. The example shown in this section is based on the water analysis results listed in Table 8.1. The elements such as hydrogen, sodium, calcium, magnesium, carbonate, and chlorine, are considered since these chemicals are the primary ions contained in the formation and makeup water. The pseudo-element (oleic acid, A) is taken into account as an element when the mechanism of *in situ* generated surfactant is considered. From these elements, the expected chemical species involved in fluid reactions, clay adsorptions, cation exchange, and solid dissolution/precipitation reactions can be specified (Table 8.2). There are 7 elements, 18 fluid species, 4 solid species, 4 clay adsorbed cations, and 3 surfactant cation exchangers considered in this example. To represent the interactions among these chemical species, the reaction equilibrium relations are required (Table 8.3). Tables 8.4-8.19 give the example input data for different sections of the input file. A sample input file for EQBATCH is given in Table 8.20 and the output file for this example is given in Table 8.21. The EQBATCH program also writes the output data in a format similar to the geochemistry input data of UTCHEM (Section 3.5 of the UTCHEM user's guide, lines 3.5.4 through 3.5.41) so it can be directly pasted into the UTCHEM input file (Table 8.22).

8.2 User's Guide

A detailed user's guide for the EQBATCH program is presented as follows:

1. **TITLE**
   A title line is required.

2. **IREACT, ICHARGE, IMG**
   IREACT - Flag indicating the components to be considered
      Possible values:
         2 - Without acidic crude
         3 - With acidic crude (insitu surfactant generation)

4- Gel option without acidic crude

ICHRGE - Flag indicating whether an oxygen mass balance or a charge balance will be used.

Possible Values:

0 - Oxygen balance used

1 - Charge balance in solution used

Note: If solid SiO_2 is considered, the oxygen balance must be used

IMG - Flag indicating whether magnesium ions participate in cation exchange reactions or not.

Possible Values:

0 - Magnesium ions are considered.

1 - Magnesium ions are not considered.

3. **NELET, NFLD, NSLD, NSORB, NACAT**

NELET - Total number of elements less non reacting element.
NFLD - Total number of fluid species.
NSLD - Total number of solid species.
NSORB - Total number of sorbed species.
NACAT - Total number of surfactant associated cations.

4. **NIAQ, NEX, NSLEL, NSURF1** (This line is read only if IMODE > 2)

NIAQ - Total number of independent fluid species.
NEX - Total number of insoluble exchangers.
NSLEL - Total number of elements comprising the solid species.
NSURF1 - Position number corresponding to the *in situ* generated surfactant anion in the fluid species array FLDSPS.

Note: NSURF1 is automatically set to 0 by the program if IMODE = 2 or 4.

5. **NH, NNA, NCA, NMG, NCARB**

NH - Position number corresponding to the hydrogen element in the element array ELEMNT.
NNA - Position number corresponding to the sodium element in the element array ELEMNT.
NCA - Position number corresponding to the calcium element in the element array ELEMNT.
NMG - Position number corresponding to the magnesium element in the element array ELEMNT.
NCARB - Position number corresponding to the carbonate pseudo-element in the element array ELEMNT.

Note: If any of these elements is not considered, the position no. must be set equal to 0.

6. **NALU, NSILI, NOXY**

NALU - Position number corresponding to the aluminum element in the element array ELEMNT.
NSILI - Position number corresponding to the silicon element in the element array ELEMNT.
NOXY - Position number corresponding to the oxygen element in the element array ELEMNT.

7. **NACD** (This line is read only if IREACT = 3)

NACD - Position number corresponding to the petroleum acid pseudo-element in the element array ELEMNT.

8a. **NCR, NHFD, NCRFD** (This line is read only if IREACT = 4)

NCR - Position number corresponding to the chromium in the element array ELEMNT.

NHFD - Position number corresponding to the hydrogen ion element in the fluid species array FLDSPS.
NCRFD - Position number corresponding to CR(III) ion in the fluid species array FLDSPS.

8b. **ELEMNT(I), ELCRG(I), for I = 1, NELET**
ELEMNT(I) - Name of the Ith element.
ELCRG(I) - Charge for the Ith element.
Note: The name of each element may not exceed 32 characters and each name must be on a separate line of the input file.

9. **FLDSPS(I), for I = 1, NFLD**
FLDSPS(I) - Name of the Ith fluid species.
Note: The name of each fluid species may not exceed 32 characters and each name must be on a separate line of the input file. If IREACT=3, the last fluid species must be HA_w (petroleum acid in water).

10. **SLDSPS(I), for I = 1, NSLD** (This line is read only if NSLD > 0)
SLDSPS(I) - Name of the Ith solid species.
Note: The name of each solid may not exceed 32 characters and each name must be on a separate line of the input file.

11. **SORBSP(I), for I = 1, NSORB** (This line is read only if NSORB > 0)
SORBSP(I) - Name of the Ith adsorbed cation.
Note: The name of each adsorbed cation may not exceed 32 characters and each name must be on a separate line of the input file.

12. **ACATSP(I), for I = 1, NACAT** (This line is read only if NACAT > 0)
ACATSP(I) - Name of the Ith surfactant adsorbed cation.
Note: The name of each surfactant adsorbed cation may not exceed 32 characters and each name must be on a separate line of the input file.

13. **NSORBX(I), for I = 1, NEX** (This line is read only if NSORB > 0)
NSORBX(I) - Number of cations for Ith exchanger.

14. **AR(I,J), for J = 1, NFLD, for I = 1, NELET** << or >>
AR(I,J), for J = 1, NFLD, for I = 1, NELET-1
AR(I,J) - Stoichiometric coefficient of Ith element in Jth fluid species.
Note: If ICHRGE = 0, then NFLD × NELET values are required by the program. If ICHRGE = 1, then NFLD × (NELET-1) values are required by the program.

15. **BR(I,J), for J = 1, NSLD, for I = 1, NELET** << or >>
BR(I,J), for J = 1, NSLD, for I = 1, NELET-1 (This line is read only if NSLD > 0)
BR(I,J) - Stoichiometric coefficient of Ith element in Jth solid species.
Note:If ICHRGE = 0, then NSLD × NELET values are required by the program. If ICHRGE = 1, then NSLD × (NELET-1) values are required by the program.

16. **DR(I,J), for J = 1, NSORB, for I = 1, NELET** << or >>

DR(I,J), for J = 1, NSORB, for I = 1, NELET-1 (This line is read only if NSORB > 1)
DR(I,J) - Stoichiometric coefficient of Ith element in Jth sorbed species.
Note: If ICHRGE = 0, then NSORB × NELET values are required by the program. If ICHRGE = 1, then NSORB × (NELET-1) values are required by the program.

17. **ER(I,J), for J = 1, NACAT, for I = 1, NELET** << or >>
ER(I,J), for J = 1, NACAT, for I = 1, NELET-1 (This line is read only if NACAT > 1)
ER(I,J) - Stoichiometric coefficient of Ith element in Jth surfactant associated cation.
Note: If ICHRGE = 0, then NACAT × NELET values are required by the program. If ICHRGE = 1, then NACAT × (NELET-1) values are required by the program.

18. **BB(I,J), for J = 1, NIAQ+NSORB+NACAT, for I = 1, NFLD+NSORB+NACAT**
BB(I,J) - Exponent of the Jth independent fluid species concentration when the Ith fluid species is expressed in terms of independent species concentrations.

19. **EXSLD(I,J), for J = 1, NIAQ, for I = 1, NSLD** (This line is read only if NSLD > 0)
EXSLD(I,J) - Exponent of the Jth independent fluid species concentration in the solubility product definition of the Ith solid.

20. **CHARGE(I), for I = 1, NFLD**
CHARGE(I) - Charge of the Ith fluid species.

21. **EQK(I), for I = 1, NFLD**
EQK(I) - Equilibrium constant for Ith fluid species when expressed in independent species concentrations only.

22. **SCHARG(I,J), for J = 1, NSORBX(I), for I = 1, NEX** (This line is read only if NSORB > 0)
SCHARG(I,J) - Charge of the Jth sorbed species on the Ith exchanger.

23. **EXK(I,J), for J = 1, NSORBX(I)-1, for I = 1, NEX** (This line is read only if NEX > 0)
EXK(I,J) - Exchange equilibrium constant for Jth exchange equilibrium of the Ith insoluble exchanger.

24. **EXEX(I,J,K), for K = 1, NIAQ+NSORB+NACAT, for J = 1, NSORBX(I)-1, for I = 1, NEX** (This line is read only if and NEX > 0)
EXEX(I,J,K) - Exponent of Kth independent species in Jth equilibrium relation of the Ith exchanger

25. **REDUC(I,J), for J = 1, NSORBX(I)-1, for I = 1, NEX** (This line is read only if NEX > 0)
REDUC(I,J) - Valence difference of the two cations involved in the exchange reaction J on exchanger I.
Note: This value is positive if the higher valence cation bulk concentration has a positive exponent in EXEX(I,J) definition and is negative otherwise.

26. **EXCAI(I), for I = 1, NEX** (This line is read only if NEX >0)
EXCAI(I) - Exchange capacity of Ith insoluble exchanger.
Units: meq/ml pore volume

27. **SPK(I), for I = 1, NSLD** (This line is read only if NSLD > 0)
SPK(I) - Solubility product of Ith solid defined in terms of independent fluid species concentrations only.

28. **CHACAT(I), for I = 1, NACAT** (This line is read only if NACAT > 0)
CHACAT(I) - Charge of Ith surfactant associated cation.

29. **ACATK(I), for I = 1, NACAT-1** (This line is read only if NACAT > 0)
ACATK(I) - Equilibrium constant for Ith exchange equilibrium for cation exchanges on surfactant.

30. **EXACAT(I,J) for J = 1, NIAQ+NSORB+NACAT, for I = 1, NACAT-1** (This line is read only if NACAT > 0)
EXACAT(I,J) - Exponent of Jth independent species in Ith equilibrium for cation exchange on surfactant.

31. **C5I, CSURF**
C5I - Initial concentration of chloride ion.
Units: meq/ml
CSURF- Initial concentration of surfactant.
Units: vol. fraction

32. **CELAQI(J), for J = 1, NELET-1**
CELAQI(J) - Initial concentrations of NELET-1 elements.
Units: equivalents/liter

33. **CSLDI(I), for I = 1, NSLD** (This line is read only if NSLD > 0)
CSLDI(I) - Initial concentration of Ith solid.
Units: moles/liter pore volume

34. **CSORBI(I), for I = 1, NSORB** (This line is read only if NSORB > 0)
CSORBI(I) - Initial concentration of Ith adsorbed cation.
Units: moles/liter pore volume

35. **CAQI(J), for J = 1, NIND**
CAQI(J) - Initial guesses for Jth independent species concentration, adsorbed species, and surfactant associated species.
Units: moles/liter water

36. **S**
S - Initial water saturation in core flooding or reservoir condition.
Units: fraction

37. **EQWPS** (This line is read only if IREACT= 3)
EQWPS - Equivalent weight of petroleum acid.

Table 8.1. Water Analysis for Makeup and Formation Water

Ions	Formation water	Makeup water
Na^{+}, mg/l	2,398.90	52.9
Mg^{2+}, mg/l	36.46	11.54
Ca^{2+}, mg/l	54.2	67.13
Cl^{-}, mg/l	2091	39.00
HCO_3^{-}, mg/l	2623	152.55
CO_3^{2-}, mg/l	240	6.00
SO_4^{2-}, mg/l	—	134.56
pH	8.1	7.95

Table 8.2. Example List of Elements and Reactive Species

Elements or pseudo-element:	Hydrogen (reactive), Sodium, Calcium, Magnesium, Carbonate, A (from acid HA), Chlorine,
Independent aqueous or oleic species:	H^{+}, Na^{+},Ca^{2+}, Mg^{2+},CO_3^{2-}, HA_o, H_2O
Dependent aqueous or oleic species:	$Ca(OH)^{+}$, $Mg(OH)^{+}$, $Ca(HCO_3)^{+}$, HA_w, $Mg(HCO_3)^{+}$, OH^{-}, HCO_3^{-}, A^{-}, H_2CO_3, $CaCO_3^{o}$, $MgCO_3^{o}$
Solid species:	$CaCO_3$ (Calcite), $Ca(OH)_2$ (Calcium hydroxide), $MgCO_3$ (Magnesite), $Mg(OH)_2$ (Magnesium hydroxide)
Adsorbed cations:	$\overline{H}^{+}$, $\overline{Na}^{+}$, $\overline{Ca}^{2+}$, $\overline{Mg}^{2+}$
Adsorbed cations on micelles:	$\overline{\overline{Na}}^{+}$, $\overline{\overline{Ca}}^{2+}$, $\overline{\overline{Mg}}^{2+}$

Table 8.3. List of Reactions for the Example Run

Partitioning of HA	**Partition Coefficient**
$HA_o \overset{K_D}{\rightleftharpoons} HA_w$	$K_D = \dfrac{[HA_w]\,\text{water}}{[HA_o]\,\text{oil}}$
Aqueous Reactions	**Equilibrium Constant**
$H_2O \overset{K_1^{eq}}{\rightleftharpoons} H^+ + OH^-$	$K_1^{eq} = [H^+]\,[OH^-]$
$HA_w + OH^- \overset{K_2^{eq}}{\rightleftharpoons} A^- + H_2O$	$K_2^{eq} = \dfrac{[A^-]\,[H^+]}{[HA_w]}$
$H^+ + CO_3^{2-} \overset{K_3^{eq}}{\rightleftharpoons} HCO_3^-$	$K_3^{eq} = \dfrac{\left[HCO_3^-\right]}{[H^+]\left[CO_3^{2-}\right]}$
$Ca^{2+} + H_2O \overset{K_4^{eq}}{\rightleftharpoons} Ca(OH)^+ + H^+$	$K_4^{eq} = \dfrac{[Ca(OH)^+]\,[H^+]}{[Ca^{2+}]}$
$Mg^{2+} + H_2O \overset{K_5^{eq}}{\rightleftharpoons} Mg(OH)^+ + H^+$	$K_5^{eq} = \dfrac{[Mg(OH)^+]\,[H^+]}{[Mg^{2+}]}$
$Ca^{2+} + H^+ + CO_3^{2-} \overset{K_6^{eq}}{\rightleftharpoons} Ca(HCO_3)^+$	$K_6^{eq} = \dfrac{\left[Ca(HCO_3)^+\right]}{[Ca^{2+}]\left[CO_3^{2-}\right][H^+]}$
$Mg^{2+} + H^+ + CO_3^{2-} \overset{K_7^{eq}}{\rightleftharpoons} Mg(HCO_3)^+$	$K_7^{eq} = \dfrac{\left[Mg(HCO_3)^+\right]}{[Mg^{2+}]\left[CO_3^{2-}\right][H^+]}$
$2H^+ + CO_3^{2-} \overset{K_8^{eq}}{\rightleftharpoons} H_2CO_3$	$K_8^{eq} = \dfrac{[H_2CO_3]}{\left[CO_3^{2-}\right][H^+]^2}$
$Ca^{2+} + CO_3^{2-} \overset{K_9^{eq}}{\rightleftharpoons} CaCO_3^o$	$K_9^{eq} = \dfrac{\left[CaCO_3^o\right]}{[Ca^{2+}]\left[CO_3^{2-}\right]}$
$Mg^{2+} + CO_3^{2-} \overset{K_{10}^{eq}}{\rightleftharpoons} MgCO_3^o$	$K_{10}^{eq} = \dfrac{\left[MgCO_3^o\right]}{[Mg^{2+}]\left[CO_3^{2-}\right]}$

Table 8.3. List of Reactions for the Example Run (cont.)

Dissolution Reactions	**Solubility Product**
$CaCO_3 \overset{K_1^{sp}}{\rightleftharpoons} Ca^{2+} + CO_3^{2-}$	$K_1^{sp} = [Ca^{2+}]\left[CO_3^{2-}\right]$
$MgCO_3 \overset{K_2^{sp}}{\rightleftharpoons} Mg^{2+} + CO_3^{2-}$	$K_2^{sp} = [Mg^{2+}]\left[CO_3^{2-}\right]$
$Ca(OH)_2 \overset{K_3^{sp}}{\rightleftharpoons} Ca^{2+} + 2OH^-$	$K_3^{sp} = [Ca^{2+}][H^+]^{-2}$
$Mg(OH)_2 \overset{K_4^{sp}}{\rightleftharpoons} Mg^{2+} + 2OH^-$	$K_4^{sp} = [Mg^{2+}][H^+]^{-2}$
Exchange Reactions (On Matrix)	**Exchange Equilibrium Constant**
$2\overline{Na}^+ + Ca^{2+} \overset{K_1^{ex}}{\rightleftharpoons} 2Na^+ + \overline{Ca}^{2+}$	$K_1^{ex} = \dfrac{\left[\overline{Ca}^{2+}\right][Na^+]^2}{[Ca^{2+}]\left[\overline{Na}^+\right]^2}$
$2\overline{Na}^+ + Mg^{2+} \overset{K_2^{ex}}{\rightleftharpoons} 2Na^+ + \overline{Mg}^{2+}$	$K_2^{ex} = \dfrac{\left[\overline{Mg}^{2+}\right][Na^+]^2}{[Mg^{2+}]\left[\overline{Na}^+\right]^2}$
$\overline{H}^+ + Na^+ + OH^- \overset{K_3^{ex}}{\rightleftharpoons} \overline{Na}^+ + H_2O$	$K_3^{ex} = \dfrac{[Na^+]\left[\overline{H}^+\right]}{\left[\overline{Na}^+\right][H^+]}$
Exchange Reactions (On Micelle)	**Exchange Equilibrium Constant**
$2\overline{\overline{Na}}^+ + Ca^{2+} \overset{K_1^{exm}}{\rightleftharpoons} 2Na^+ + \overline{\overline{Ca}}^{2+}$	$K_1^{exm} = \dfrac{\left[\overline{\overline{Ca}}^{2+}\right][Na^+]^2}{\left[\overline{\overline{Na}}^+\right]^2[Ca^{2+}]}$ where $K_1^{exm} = \beta_1^{exm}\{[A^-]+[S^-]\}$
$2\overline{\overline{Na}}^+ + Mg^{2+} \overset{K_2^{exm}}{\rightleftharpoons} 2Na^+ + \overline{\overline{Mg}}^{2+}$	$K_2^{exm} = \dfrac{\left[\overline{\overline{Mg}}^{2+}\right][Na^+]^2}{\left[\overline{\overline{Na}}^+\right]^2[Mg^{2+}]}$ where $K_2^{exm} = \beta_2^{exm}\{[A^-]+[S^-]\}$

Table 8.4. Stoichiometric Coefficient of Ith Element in Jth Fluid Species (for the AR Array)

		Ca	Mg	CO_3	Na	H	A
1	H^+	0	0	0	0	1	0
2	Na^+	0	0	0	1	0	0
3	Ca^{2+}	1	0	0	0	0	0
4	Mg^{2+}	0	1	0	0	0	0
5	CO_3^{2-}	0	0	1	0	0	0
6	HA_o	0	0	0	0	1	1
7	H_2O	0	0	0	0	2	0
8	$Ca(OH)^+$	1	0	0	0	1	0
9	$Mg(OH)^+$	0	1	0	0	1	0
10	$Ca(HCO_3)^+$	1	0	1	0	1	0
11	$Mg(HCO_3)^+$	0	1	1	0	1	0
12	A^-	0	0	0	0	0	1
13	OH^-	0	0	0	0	1	0
14	HCO_3^-	0	0	1	0	1	0
15	H_2CO_3	0	0	1	0	2	0
16	$CaCO_3$	1	0	1	0	0	0
17	$MgCO_3$	0	1	1	0	0	0
18	HA_w	0	0	0	0	1	1

Note: The transposition of this table is the form required for EQBATCH Program

Table 8.5. Stoichiometric Coefficient of Ith Element in Jth Solid Species (for the BR Array)

	$CaCO_3$	$MgCO_3$	$Ca(OH)_2$	$Mg(OH)_2$
Ca	1	0	1	0
Mg	0	1	0	1
CO_3	1	1	0	0
Na	0	0	0	0
H	0	0	2	2
A	0	0	0	0

Table 8.6. Stoichiometric Coefficient of Ith Element in Jth Sorbed Species (for the DR Array)

	H^+	Na^+	Ca^{2+}	Mg^{2+}
Ca	0	0	1	0
Mg	0	0	0	1
CO_3	0	0	0	0
Na	0	1	0	0
H	1	0	0	0
A	0	0	0	0

Table. 8.7. Stoichiometric Coefficient of Ith Element in Jth Surfactant Associated Cation (for the ER Array)

	Na^+	Ca^{2+}	Mg^{2+}
Ca	0	1	0
Mg	0	0	1
CO_3	0	0	0
Na	1	0	0
H	0	0	0
A	0	0	0

Table 8.8. Exponent of Jth Independent Fluid Species (for BB Array)

		H^+	Na^+	Ca^{2+}	Mg^{2+}	CO_3^{2-}	HA_o	H_2O	H^+	Na^+	Ca^{2+}	Mg^{2+}	Na^+	Ca^{2+}	Mg^{2+}
1	H^+	1													
2	Na^+		1												
3	Ca^{2+}			1											
4	Mg^{2+}				1										
5	CO_3^{2-}					1									
6	HA_o						1								
7	H_2O							1							
8	$Ca(OH)^+$	-1		1											
9	$Mg(OH)^+$	-1			1										
10	$Ca(HCO_3)^+$	1		1		1									
11	$Mg(HCO_3)^+$	1			1	1									
12	A^-	-1					1								
13	OH^-	-1													
14	HCO_3^-	1				1									
15	H_2CO_3	2				1									
16	$CaCO_3$			1		1									
17	$MgCO_3$				1	1									
18	HA_w						1								
19	H^+s								1						
20	Na^+s									1					
21	$Ca^{2+}s$										1				
22	$Mg^{2+}s$											1			
23	Na^+												1		
24	Ca^{2+}													1	
25	$Mg^{2+}sa$														1
										Sorbed Species			Surfactant Assoc. Cation		

Note: The blank cells in the above table need to be filled with zero for the input data for EQBATCH program.

Table 8.9. Exponent of Jth Independent Species in the Ith Solid (for EXSLD Array)

	H^+	Na^+	Ca^{2+}	Mg^{2+}	CO_3^{2-}	HA_o	H_2O
$CaCO_3$	0	0	1	0	1	0	0
$MgCO_3$	0	0	0	1	1	0	0
$Ca(OH)_2$	-2	0	1	0	0	0	0
$Mg(OH)_2$	-2	0	0	1	0	0	0

Table 8.10. Charge of Ith Fluid Species (for CHARGE Array)

	Fluid species	Charge
1	H^+	1
2	Na^+	1
3	Ca^{2+}	2
4	Mg^{2+}	2
5	CO_3^{2-}	-2
6	HA_o	0
7	H_2O	0
8	$Ca(OH)^+$	1
9	$Mg(OH)^+$	1
10	$Ca(HCO_3)^+$	1
11	$Mg(HCO_3)^+$	1
12	A^-	-1
13	OH^-	-1
14	HCO_3^-	-1
15	H_2CO_3	0
16	$CaCO_3$	0
17	$MgCO_3$	0
18	HA_w	0

Table 8.11. Equilibrium Constants for Ith Fluid Species (for EQK Array)

	Fluid species	Equilibrium Constants
1	H^+	1
2	Na^+	1
3	Ca^{2+}	1
4	Mg^{2+}	1
5	CO_3^{2-}	1
6	HA_o	1
7	H_2O	1
8	$Ca(OH)^+$	0.12050E-12
9	$Mg(OH)^+$	0.38871E-11
10	$Ca(HCO_3)^+$	0.14124E+12
11	$Mg(HCO_3)^+$	0.58345E+12
12	A^-	0.85480E-14
13	OH^-	0.10093E-13
14	HCO_3^-	0.21380E+11
15	H_2CO_3	0.39811E+17
16	$CaCO_3$	0.15849E+04
17	$MgCO_3$	0.47863E+04
18	HA_w	0.85480E-04

Table 8.12. Charge of Jth Sorbed Species (for SCHARG Array)

Adsorbed species	Charge
H^+(sorbed)	1
Na^+(sorbed)	1
Ca^{2+}(sorbed)	2
Mg^{2+}(sorbed)	2

Table 8.13. Exchange Equilibrium Constants for Jth Exchange (for EXK Array)

Adsorbed	Equilibrium Constants
K_{ex1}	0.2623E+03
K_{ex2}	0.1509E+03
K_{ex3}	0.1460E+08

Table8.14. Exponent of Kth Independent Species in Jth Equilibrium Relation (for EXEX Array)

H^+	Na^+	Ca^{2+}	Mg^{2+}	CO_3^{2-}	HA_o	H_2O	H^+	Na^+	Ca^{2+}	Mg^{2+}	Na^+	Ca^{2+}	Mg^{2+}
0	2	-1	0	0	0	0	0	-2	1	0	0	0	0
0	2	0	-1	0	0	0	0	-2	0	1	0	0	0
-1	1	0	0	0	0	0	1	-1	0	0	0	0	0
							Sorbed Species				Surfactant Assoc. Cation		

Table 8.15. Valence Difference Between Cation Involved In Exchange (for REDU Array)

	Ca^{2+}	Mg^{2+}	Na^+
Na^+	-1		
Na^+		-1	
H^+			0

Table 8.16. Solubility Product of Ith Solid (for SPK Array)

$CaCO_3$	$MgCO_3$	$Ca(OH)_2$	$Mg(OH)$
0.4953E-09	0.00007	4.7315E+22	5.6104E+16

Table 8.17. Charge of Ith Surfactant Associated Cation (for CHACAT Array)

Na^+	Ca^{2+}	Mg^{2+}
1	2	2

Table 8.18. Equilibrium Constant for Ith Exchange (for ACATK Array)

Na^+	Ca^{2+}
2.5	2.94

Table 8.19. Exponent of Jth Independent Species in Ith Cation Exchange on Surfactant (for EXACAT Array)

H^+	Na^+	Ca^{2+}	Mg^{2+}	CO_3^{2-}	HA_o	H_2O	H^+	Na^+	Ca^{2+}	Mg^{2+}	Na^+	Ca^{2+}	Mg^{2+}
0	2	-1	0	0	0	0	0	0	0	0	-2	1	0
0	2	0	-1	0	0	0	0	0	0	0	-2	0	1
							Sorbed Species				Surfactant Assoc. Cation		

Table 8.20. Sample Input Data for EQBATCH Program

```
R1                                                                      (* TITLE *)
3   1   1                                                  (* IREACT ICHARGE IMG *)
7  18  4  4  3                                   (* NNELET NFLD NSLD NSORB NACAT *)
7  1  4  12                                             (* NIAQ NEX NSLWL NSURF1 *)
5  4  1  2  3                                            (* NH NNA NCA NMG NCARB *)
0   0  0                                                     (* NALU NSILI NOXYG *)
6                                                                        (* NACD *)
CALCIUM                         2
MAGNESIUM                       2
CARBON (AS CARBOBATES)          -2
SODIUM                          1
HYDROGEN (REACTIVE)             1
ACID (PETROLEUM)                -1
CHLORINE                        -1
HYDROGEN ION
SODIUM ION
CALCIUM ION
MAGENSIUM ION
CARBONATE ION
PETROLEUM ACID IN OIL
WATER
CALCIUM MONOHYDROXIDE ION
MAGNESIUM MONOHYROXIDE ION
CA (HC03) +
MG (HCO3) +
PETRLEUM ACID ANION
HYDROXIDE ION
BICARBONATE ION
DISSOLVED CARBON MONOHYDROXIDE
AQUEOUS CALCIUM CARBONATE
AQUEOUS MAGNESIUM CARBONATE
PETROLEUM ACID IN OIL                                                 (* FLDSPS *)
CALCIUM CARBONATE(SOLID)
MAGNESIUM CARBONATE (SOLID)
CALCIUM HYDROXIDE (SOLID)
MAGNESIUM HYDROXIDE(SOLID)                                             (* SLDSPS *)
SORBED HYDROGEN ION
SORBED SODIUM ION
SORBED CALCIUM ION
SORBED MAGNESIUM ION                                                  (* SORBSPS *)
SURF. ASSOCIATED SODIUM ION
SURF. ASSOCIATED CALCIUM ION
SURF. ASSOCIATED MAGNESIUM ION                                        (* ACATSPC *)
4                                                                      (* NSORBX *)
0.  0.  1.  0.  0.  0.  0.  1.  0.  1.  0.  0.  0.  0. 0. 1. 0. 0.
0.  0.  0.  1.  0.  0.  0.  0.  1.  0.  1.  0.  0.  0. 0. 0. 1. 0.
0.  0.  0.  0.  1.  0.  0.  0.  0.  1.  1.  0.  0.  1. 1. 1. 1. 0.
0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0. 0. 0. 0. 0.
1.  0.  0.  0.  0.  1.  2.  1.  1.  1.  1.  0.  1.  1. 2. 0. 0. 1.
0.  0.  0.  0.  0.  1.  0.  0.  0.  0.  0.  1.  0.  0. 0. 0. 0. 1.         (* AR *)
1.0  0.0  1.0  0.0
0.0  1.0  0.0  1.0
1.0  1.0  0.0  0.0
0.0  0.0  0.0  0.0
0.0  0.0  2.0  2.0
0.0  0.0  0.0  0.0                                                         (* BR *)
0.0  0.0  1.0  0.0
0.0  0.0  0.0  1.0
0.0  0.0  0.0  0.0
0.0  1.0  0.0  0.0
1.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0                                                         (* DR *)
0.0  1.0  0.0
0.0  0.0  1.0
0.0  0.0  0.0
```

```
1.0  0.0  0.0
0.0  0.0  0.0
0.0  0.0  0.0                                                              (* ER *)
1.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
```

Table 8.20. Sample Input Data for EQBATCH Program (cont.)

```
0.  0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
0.  0.  0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
0.  0.  0.  0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.
0.  0.  0.  0.  0.  1.  0.  0.  0.  0.  0.  0.  0.  0.
0.  0.  0.  0.  0.  0.  1.  0.  0.  0.  0.  0.  0.  0.
-1. 0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
-1. 0.  0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
1.  0.  1.  0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.
1.  0.  0.  1.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.
-1. 0.  0.  0.  0.  1.  0.  0.  0.  0.  0.  0.  0.  0.
-1. 0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
1.  0.  0.  0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.
2.  0.  0.  0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.
0.  0.  1.  0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.
0.  0.  0.  1.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.
0.  0.  0.  0.  0.  1.  0.  0.  0.  0.  0.  0.  0.  0.
0.  0.  0.  0.  0.  0.  0.  1.  0.  0.  0.  0.  0.  0.
0.  0.  0.  0.  0.  0.  0.  0.  1.  0.  0.  0.  0.  0.
0.  0.  0.  0.  0.  0.  0.  0.  0.  1.  0.  0.  0.  0.
0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  1.  0.  0.  0.
0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  1.  0.  0.
0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  1.  0.
0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  1.                     (* BB *)
0.  0.  1.  0.  1.  0.  0.
0.  0.  0.  1.  1.  0.  0.
-2. 0.  1.  0.  0.  0.  0.
-2. 0.  0.  1.  0.  0.  0.                                              (* EXSLD *)
1.  1.  2.  2. -2.  0.  0. 1. 1. 1. 1. -1. -1. -1. 0. 0. 0. 0.         (* CHAEGE *)
1.  1.  1.  1.  1.  1. 1.  0.1205e-12 0.38871e-11 0.14125e+12
0.58345e+12  0.959e-12 0.10093e-13 0.2138e+11 0.3981e+17
0.15849e+04  0.47863e+04  0.959-04                                        (* KEQ *)
1.  1.  2.  2.                                                        (* SCHARGE *)
0.793+01  0.52+01 0.27+07                                                 (* KEX *)
0.  2.  -1.  0.  0.  0.  0.  0.  -2.  1.  0.  0.  0.  0.
0.  2.  0.  -1.  0.  0.  0.  0.  -2.  0.  1.  0.  0.  0.
-1. 1.   0.  0.  0.  0.  0.  1.  -1.  0.  0.  0.  0.  0.                 (* EXEX *)
-1.  -1.  0.                                                            (* REDUC *)
0.3403                                                                  (* EXCAI *)
0.474851e-09  0.00007 0.47315e+23 0.56045e+17                             (* KSP *)
1.  2.   2.                                                            (* CHACAT *)
2.5   2.94                                                              (* KACAT *)
0.  2.  -1.  0.  0.  0.  0.  0.  0.  0.  0.  -2.  1.  0.0
0.  2.  0.  -1.  0.  0.  0.  0.  0.  0.  0.  -2.  0.  1.               (* EXACAT *)
0.059   0.0                                                          (*C50, Csurf*)
0.00135  0.0015  0.047 0.1043  111.043  0.019               (*CELFLT 1,NELEMENT-1*)
2.00  0.0   0.0000  0.0                                       (*CSLD(I), I=1,NSLD*)
 0.05 0.25  0.01  0.002                                                (* CSORBI *)
0.1200077231590e-05 0.01 0.1e-04
0.4616423363603e-05 0.3092684582095e-08 0.5399766653843e-03
55.49999314650  1.0e-06  1.0e-02   1.0e-03  1.0e-04
1.0e-06   1.0e-08   1.0e-08                                                (*CIND*)
0.602                                                                        (*S1*)
500                                                                         (*EQW*)
```

Table 8.21. Sample Output of EQBATCH Program

```
R1

     REACTIVE SYSTEM DESCRIPTION

     TOTAL NO. OF ELEMENTS LESS ONE  =  7
     TOTAL NO. OF FLUID SPECIES      = 18
     TOTAL NO. OF SOLID SPECIES      =  4
     TOTAL NO. OF ADSORBED SPECIES   =  4
     NO. OF CATIONS ASSOC. WITH SURF.=  3
     TOTAL NO. OF IND. FLUID SPECIES =  7
     TOTAL NO. OF EXCHANGER          =  1

     ELEMENT NO.          NAME                                    CHARGE

          1               CALCIUM                                    2
          2               MAGNESIUM                                  2
          3               CARBON (AS CARBOBATES)                    -2
          4               SODIUM                                     1
          5               HYDROGEN (REACTIVE)                        1
          6               ACID (PETROLEUM)                          -1
          7               CHLORINE                                  -1

     FLUID SPECIES NO.    NAME

     (INDEPENDENT)

          1               HYDROGEN ION
          2               SODIUM ION
          3               CALCIUM ION
          4               MAGENSIUM ION
          5               CARBONATE ION
          6               PETROLEUM ACID IN OIL
          7               WATER

     (DEPENDENT)

          8               CALCIUM MONOHYDROXIDE ION
          9               MAGNESIUM MONOHYROXIDE ION
         10               CA (HC03) +
         11               MG (HCO3) +
         12               PETRLEUM ACID ANION
         13               HYDROXIDE ION
         14               BICARBONATE ION
         15               DISSOLVED CARBON MONOHYDROXIDE
         16               AQUEOUS CALCIUM CARBONATE
         17               AQUEOUS MAGNESIUM CARBONATE
         18               PETROLEUM ACID IN OIL

     SOLID SPECIES NO.    NAME

          1               CALCIUM CARBONATE(SOLID)
          2               MAGNESIUM CARBONATE (SOLID)
          3               CALCIUM HYDROXIDE (SOLID)
          4               MAGNESIUM HYDROXIDE(SOLID)

     SORBED SPECIES NO.   NAME

          1               SORBED HYDROGEN ION
          2               SORBED SODIUM ION
          3               SORBED CALCIUM ION
          4               SORBED MAGNESIUM ION

     ASSOC. CATION NO.    NAME

          1               SURF. ASSOCIATED SODIUM ION
```

```
          2                SURF. ASSOCIATED CALCIUM ION
          3                SURF. ASSOCIATED MAGNESIUM ION
```

Table 8.21. Sample Output of EQBATCH Program (cont.)

```
     NO. OF MOLES OF ELEMENT I IN ONE MOLE OF
     FLUID SPECIES J

 J=      1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20  21
22  23  24  25

 I= 1   0.  0.  1.  0.  0.  0.  0.  1.  0.  1.  0.  0.  0.  0.  0.  1.  0.  0.
 I= 2   0.  0.  0.  1.  0.  0.  0.  0.  1.  0.  1.  0.  0.  0.  0.  0.  1.  0.
 I= 3   0.  0.  0.  0.  1.  0.  0.  0.  0.  1.  1.  0.  0.  1.  1.  1.  1.  0.
 I= 4   0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
 I= 5   1.  0.  0.  0.  0.  1.  2.  1.  1.  1.  1.  0.  1.  1.  2.  0.  0.  1.
 I= 6   0.  0.  0.  0.  0.  1.  0.  0.  0.  0.  0.  1.  0.  0.  0.  0.  0.  1.


     NO. OF MOLES OF ELEMENT I IN ONE MOLE OF
     SOLID SPECIES K
 K=      1    2    3    4    5    6    7    8    9   10

 I= 1   1.   0.   1.   0.
 I= 2   0.   1.   0.   1.
 I= 3   1.   1.   0.   0.
 I= 4   0.   0.   0.   0.
 I= 5   0.   0.   2.   2.
 I= 6   0.   0.   0.   0.


     NO. OF MOLES OF ELEMENT I IN ONE MOLE OF
     ADSORBED SPECIES K

 K=      1    2    3    4    5

 I= 1   0.   0.   1.   0.
 I= 2   0.   0.   0.   1.
 I= 3   0.   0.   0.   0.
 I= 4   0.   1.   0.   0.
 I= 5   1.   0.   0.   0.
 I= 6   0.   0.   0.   0.


     NO. OF MOLES OF ELEMENT I IN ONE MOLE OF
     SURF. ASS. SPECIES K

 K=      1    2    3    4    5

 I= 1   0.   1.   0.
 I= 2   0.   0.   1.
 I= 3   0.   0.   0.
 I= 4   1.   0.   0.
 I= 5   0.   0.   0.
 I= 6   0.   0.   0.


     EXPONENT OF THE IND. SPECIES CONC. J
     FOR FLUID SPECIES I

 J=        1    2    3    4    5    6    7    8    9   10

 I= 1     1.   0.   0.   0.   0.   0.   0.
 I= 2     0.   1.   0.   0.   0.   0.   0.
 I= 3     0.   0.   1.   0.   0.   0.   0.
 I= 4     0.   0.   0.   1.   0.   0.   0.
```

```
    I= 5     0.   0.   0.   0.   1.   0.   0.
    I= 6     0.   0.   0.   0.   0.   1.   0.
    I= 7     0.   0.   0.   0.   0.   0.   1.
    I= 8    -1.   0.   1.   0.   0.   0.   0.
    I= 9    -1.   0.   0.   1.   0.   0.   0.
    I=10     1.   0.   1.   0.   1.   0.   0.
    I=11     1.   0.   0.   1.   1.   0.   0.
    I=12    -1.   0.   0.   0.   0.   1.   0.
    I=13    -1.   0.   0.   0.   0.   0.   0.
    I=14     1.   0.   0.   0.   1.   0.   0.
```

Table 8.21. Sample Output of EQBATCH Program (cont.)

```
    I=15     2.   0.   0.   0.   1.   0.   0.
    I=16     0.   0.   1.   0.   1.   0.   0.
    I=17     0.   0.   0.   1.   1.   0.   0.
    I=18     0.   0.   0.   0.   0.   1.   0.


   FLUID SPECIES NO.                CHARGE

             1                       1.0
             2                       1.0
             3                       2.0
             4                       2.0
             5                      -2.0
             6                       0.0
             7                       0.0
             8                       0.0
             9                       1.0
            10                       1.0
            11                       1.0
            12                      -1.0
            13                      -1.0
            14                      -1.0
            15                       0.0
            16                       0.0
            17                       0.0
            18                       0.0


        ADSORBED SPECIES NO. CHARGE

             1                 1.0
             2                 1.0
             3                 2.0
             4                 2.0


        ASSOC. CATION(SURF)  CHARGE

             1                 1.0
             2                 2.0
             3                 2.0


        EXPONENT OF IND. FLUID SPECIES J IN THE
        SOLUBILITY PRODUCT DEFINITION OF SOLID I

    J=        1    2    3    4    5    6    7    8    9   10   11   12   13   14   15

    I= 1     0.   0.   1.   0.   1.   0.   0.
    I= 2     0.   0.   0.   1.   1.   0.   0.
    I= 3    -2.   0.   1.   0.   0.   0.   0.
    I= 4    -2.   0.   0.   1.   0.   0.   0.


        FLUID SPECIES NO.   EQUILM. CONSATNT
```

```
           1                0.10000E+01
           2                0.10000E+01
           3                0.10000E+01
           4                0.10000E+01
           5                0.10000E+01
           6                0.10000E+01
           7                0.10000E+01
           8                0.12050E-12
           9                0.38871E-11
          10                0.14125E+12
          11                0.58345E+12
          12                0.95900E-12
          13                0.10093E-13
          14                0.21380E+11
          15                0.39810E+17
```

Table 8.21. Sample Output of EQBATCH Program (cont.)

```
          16                0.15849E+04
          17                0.47863E+04
          18                0.95900E-04


     EXCHANGE EQUILIBRIUM CONSTANT FOR EQUILM. J
     OF THE EXCHANGER I

 J=           1         2         3         4         5

 I= 1   0.7930E+01   0.5200E+01   0.2700E+07


       EXCHANGER NO.      EXCHANGE CAPACITY

           1                             0.34030E+00

     EXPONENT OF THE IND. SPECIES CONC. K IN
     THE EXCHANGE EQUILIBRIUM J ON EXCHANGER I

     I= 1

 K=     1     2     3     4     5     6     7     8     9    10    11    12    13    14
15    16   17   18

 J=1   0.0   2.0  -1.0   0.0   0.0   0.0   0.0   0.0  -2.0   1.0   0.0   0.0   0.0   0.0
 J=2   0.0   2.0   0.0  -1.0   0.0   0.0   0.0   0.0  -2.0   0.0   1.0   0.0   0.0   0.0
 J=3  -1.0   1.0   0.0   0.0   0.0   0.0   0.0   1.0  -1.0   0.0   0.0   0.0   0.0   0.0

     SOLID NUMBER        SOLUBILITY PRODUCT

           1                0.47485E-09
           2                0.70000E-04
           3                0.47315E+23
           4                0.56045E+17

EXCHANGE EQLM. (I) ON SURF.  BETAS(I)

                1                 0.25000E+01
                2                 0.29400E+01

     EXPONENT OF THE IND. SPECIES CONC. K IN
     THE EXCHANGE EQUILIBRIUM J ON SURFACTANT

 K=     1     2     3     4     5     6     7     8     9    10    11    12    13    14
15    16   17   18

 J=1   0.0   2.0  -1.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0  -2.0   1.0   0.0
 J=2   0.0   2.0   0.0  -1.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0  -2.0   0.0   1.0
```

```
          INITIAL AQ. ELEMENTAL CONCS.(MOLES/L)

     1           2           3           4           5           6           7           8
9          10

 .13500E-02  .15000E-02  .47000E-01  .10430E+00  .11104E+03  .19000E-01

          INITIAL CHLORIDE CONC.(EQ/LITER)   =    0.5900E-01
          INITIAL SURFACTANT CONC.(EQ/LITER) =    0.0000E+00

          INITIAL SOLID CONCS.(MOLES/LITRE PV)

     1           2           3           4           5           6           7           8
9          10

 .20000E+01  .00000E+00  .00000E+00  .00000E+00

          INITIAL ADSORED IONS(MOLES/LITRE PV)

     1           2           3           4           5           6           7           8
9          10
```

Table 8.21. Sample Output of EQBATCH Program (cont.)

```
 .50000E-01  .25000E+00  .10000E-01  .20000E-02

          INITIAL GUESSES OF INDEPENDENT CONCENTRATIONS

  1.200077231590000E-006  1.000000000000000E-002  1.000000000000000E-005
  4.616423363603000E-006  3.092684582095000E-009  5.399766653843000E-004
   55.4999931465000       1.000000000000000E-006  1.000000000000000E-002
  1.000000000000000E-003  1.000000000000000E-004  1.000000000000000E-006
  1.000000000000000E-008  1.000000000000000E-008

          END OF REACTION MODULE INPUT DATA

          RESIDUALS AT THE END OF 18 ITERATIONS IDAMP =  1

0.000E+00 0.000E+00 -.555E-16 0.142E-13 0.000E+00 0.000E+00 0.000E+00 0.999E-15
0.666E-15 0.000E+00 0.000E+00 -.486E-16 -.245E-12 0.000E+00

FLUID SPECIES CONCENTRATIONS

0.7849769316806E-08 0.7529549105585E-01 0.2274287723632E-05 0.5387616767727E-04
0.2087910843759E-03 0.1899585758862E-01 0.5548234868752E+02 0.3491206679296E-10
0.2667875232078E-07 0.5265052518920E-06 0.5151920872179E-04 0.2320708633881E-05
0.1285770268228E-05 0.3504100430504E-01 0.5121744571970E-03 0.7525913499000E-06
0.5384043523296E-04 0.1821702742749E-05

          SOLID SPECIES CONCENTRATIONS

0.2011131391413E+01 0.0000000000000E+00 0.0000000000000E+00 0.0000000000000E+00

          SORBED SPECIES CONCENTRATIONS

0.7318622640939E-01 0.2600025853849E+00 0.2150482869699E-03 0.3340545815905E-02

          SURF. ASSOCIATED CATION CONCS.

0.1900192355929E-01 0.6880963477427E-08 0.1916937102421E-06

          ELEMENT NO.       OLD TOTAL          NEW TOTAL              ERROR

               1        0.2011350000000E+01   0.2011350000000E+01   0.0000000000000E+00
               2        0.3500000000000E-02   0.3500000000000E-02   0.0000000000000E+00
               3        0.2047000000000E+01   0.2047000000000E+01   0.0000000000000E+00
               4        0.3543000000000E+00   0.3543000000000E+00   0.2220446049250E-15
```

```
              5        0.1110930000000E+03   0.1110930000000E+03  -0.1110223024625E-15
              6        0.1900000000000E-01   0.1900000000000E-01   0.0000000000000E+00

         ISOLN=  14

         COMPUTATION TIME=  0.00000E+00

         INITIAL CONDITIONS FOR UTCHEM

C1I,C2I,C50,C60,C12I,C13I,C14I,C15I
 0.999997928798602       0.985633815850358       5.900000000000000E-002
 7.120600401936443E-006  9.429741461513917E-002   111.019813773591
 3.189083681891565E-004  7.173721717434252E-002
A- + HA(WATER) =   4.142411376630453E-006  HA(OIL) =   2.915115922082504E-002
VOLUMES FRACTIONS OF WATER,OIL AND ACID
 0.601998753136758       0.392282258708443       5.718988154799202E-003
EQUIV. OF ACID/LITRE TOTAL VOL  1.143797630959840E-002
EQK(          12)  EQK(          18)    6.249160552927827E-013
 6.249160552927826E-005
CSLDI(I),I=1,NSLD UNIT=MOLES/LITER PV
  1.21069859002472       0.000000000000000E+000  0.000000000000000E+000
 0.000000000000000E+000
CSORBI(I),I=1,NSORB UNIT=MOLES/LITER PV
 4.405801704523635E-002  0.156521232214020       1.294588006200680E-004
 2.011004415971278E-003
EXCHANGE CAPACITY(MEQ/ML PV)=   0.204860175692439
```

Table 8.22. Sample UTCHEM Input File Generated From EQBATCH Program

```
        FOLLOWING LINES OF DATA FORMATED FOR UTCHEM

    7 18  4  4  3  1
    7  1  4 12
    5  4  1  2  3
    6
    CALCIUM                         2
    MAGNESIUM                       2
    CARBON (AS CARBOBATES)          -2
    SODIUM                          1
    HYDROGEN (REACTIVE)             -1
    ACID (PETROLEUM)                -1
    CHLORINE
    HYDROGEN ION
    SODIUM ION
    CALCIUM ION
    MAGENSIUM ION
    CARBONATE ION
    PETROLEUM ACID IN OIL
    WATER
    CALCIUM MONOHYDROXIDE ION
    MAGNESIUM MONOHYROXIDE ION
    CA (HC03) +
    MG (HCO3) +
    PETRLEUM ACID ANION
    HYDROXIDE ION
    BICARBONATE ION
    DISSOLVED CARBON MONOHYDROXIDE
    AQUEOUS CALCIUM CARBONATE
    AQUEOUS MAGNESIUM CARBONATE
    PETROLEUM ACID IN OIL
    CALCIUM CARBONATE(SOLID)
    MAGNESIUM CARBONATE (SOLID)
    CALCIUM HYDROXIDE (SOLID)
    MAGNESIUM HYDROXIDE(SOLID)   (*
    SORBED HYDROGEN ION
    SORBED SODIUM ION
    SORBED CALCIUM ION
    SORBED MAGNESIUM ION         (*
    SURF. ASSOCIATED SODIUM ION
    SURF. ASSOCIATED CALCIUM ION
    SURF. ASSOCIATED MAGNESIUM ION
    4
    0.  0.  1.  0.  0.  0.  0.  1.  0.  1.  0.  0.  0.  0.  0.
    1.  0.  0.
    0.  0.  0.  1.  0.  0.  0.  0.  1.  0.  1.  0.  0.  0.  0.
    0.  1.  0.
    0.  0.  0.  0.  1.  0.  0.  0.  0.  1.  1.  0.  0.  1.  1.
    1.  1.  0.
   0.  1.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
    0.  0.  0.
    1.  0.  0.  0.  0.  1.  2.  1.  1.  1.  1.  0.  1.  1.  2.
    0.  0.  1.
    0.  0.  0.  0.  0.  1.  0.  0.  0.  0.  0.  1.  0.  0.  0.
    0.  0.  1.
    1.  0.  1.  0.
    0.  1.  0.  1.
    1.  1.  0.  0.
    0.  0.  0.  0.
    0.  0.  2.  2.
    0.  0.  0.  0.
    0.  0.  1.  0.
    0.  0.  0.  1.
    0.  0.  0.  0.
    0.  1.  0.  0.
```

```
 1.  0.  0.  0.
 0.  0.  0.  0.
 0.  1.  0.
 0.  0.  1.
 0.  0.  0.
```

Table 8.22. Sample UTCHEM Input File Generated From EQBATCH Program (cont.)

```
 1.  0.  0.
 0.  0.  0.
 0.  0.  0.
 1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
-1.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
-1.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 1.0  0.0  1.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 1.0  0.0  0.0  1.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
-1.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
-1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0
1.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 2.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
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 0.0  0.0  1.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 0.0  0.0  0.0  1.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0
 0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0
 0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0
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 0.0  0.0
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 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 1.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  1.0
 0.0  0.0  1.0  0.0  1.0  0.0  0.0
 0.0  0.0  0.0  1.0  1.0  0.0  0.0
-2.0  0.0  1.0  0.0  0.0  0.0  0.0
-2.0  0.0  0.0  1.0  0.0  0.0  0.0
 1.0  1.0  2.0  2.0 -2.0  0.0  0.0  1.0  1.0  1.0  1.0 -1.0
-1.0 -1.0  0.0  0.0  0.0  0.0
 1.0  1.0  2.0  2.0
```

```
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0.1000000000000E+01 0.1000000000000E+01 0.1000000000000E+01
0.1000000000000E+01 0.1205000000000E-12 0.3887100000000E-11
0.1412500000000E+12 0.5834500000000E+12 0.6249160552928E-12
0.1009300000000E-13 0.2138000000000E+11 0.3981000000000E+17
0.1584900000000E+04 0.4786300000000E+04 0.6249160552928E-04
0.7930000000000E+01 0.5200000000000E+01 0.2700000000000E+07
 0.0  2.0 -1.0  0.0  0.0  0.0  0.0  0.0 -2.0  1.0  0.0  0.0
 0.0  0.0
 0.0  2.0  0.0 -1.0  0.0  0.0  0.0  0.0 -2.0  0.0  1.0  0.0
 0.0  0.0
```

Table 8.22. Sample UTCHEM Input File Generated From EQBATCH Program (cont.)

```
-1.0  1.0  0.0  0.0  0.0  0.0  0.0  1.0 -1.0  0.0  0.0  0.0
 0.0  0.0
-1.0 -1.0  0.0
0.2048601756924E+00
0.4748510000000E-09 0.7000000000000E-04 0.4731500000000E+23
0.5604500000000E+17
1.0  2.0  2.0
0.2500000000000E+01 0.2940000000000E+01
 0.0  2.0 -1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0 -2.0
 1.0  0.0
 0.0  2.0  0.0 -1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0 -2.0
 0.0  1.0
0.1900192355929E-01 0.6880963477427E-08 0.1916937102421E-06
0.5900000000000E-01 0.7120600401936E-05
0.9429741461514E-01 0.1110198137736E+03 0.3189083681892E-03
0.7173721717434E-01 0.4142411376630E-05
0.2915115922083E-01
0.7849769316806E-08 0.7529549105585E-01 0.2274287723632E-05
0.5387616767727E-04 0.2087910843759E-03 0.1899585758862E-01
0.5548234868752E+02
0.1210698590025E+01 0.0000000000000E+00 0.0000000000000E+00
0.0000000000000E+00
0.4405801704524E-01 0.1565212322140E+00 0.1294588006201E-03
0.2011004415971E-02
0.9999979287986E+00 0.9856338158504E+00
0.1000000000000E-07 0.5000000000000E+03
```

Section 9
A 3-D NAPL Flow and Biodegradation Model

Biodegradation capabilities have been added to a three-dimensional, multi-phase, multi-component porous media flow model. The model simulates the transport and biodegradation of lighter-than-water nonaqueous phase liquids (LNAPLs) and denser-than-water nonaqueous phase liquids (DNAPLs). The biodegradation model describes biological transformation of the organic contaminants originating from NAPL sources, and can accommodate multiple substrates, electron acceptors, and biological species. The biodegradation model includes inhibition, sequential use of electron acceptors, and cometabolism. Example simulations illustrate the model capabilities.

9.1 Introduction

The University of Texas is completing improvements to a multi-phase flow simulator called UTCHEM. Advanced biodegradation capabilities have recently been incorporated into UTCHEM that allow both the flow of nonaqueous phase liquids (NAPLs) and the fate of organic NAPL constituents to be described within the same model. This paper describes the biodegradation model components, discusses the biodegradation model equations and features, and provides two example UTCHEM simulations that demonstrate some of the capabilities of the combined NAPL flow and biodegradation model.

9.2 Model Description and Features

UTCHEM is a multi-phase, multi-component, three-dimensional, numerical model that simulates the fate and transport of both dissolved and nonaqueous phase organic contaminants in porous media. The model describes flow of the NAPL resulting from capillary, gravity and pressure forces. Dispersion of organic constituents in each phase is also modeled. The model can be used to simulate spills of either lighter-than-water NAPLs (LNAPLs) or denser-than-water NAPLs (DNAPLs). The transfer of organic contaminants from the NAPL to the aqueous phase is described through either equilibrium partitioning or a linear driving force nonequilibrium mass transfer model. Adsorption of organic constituents is modeled through equilibrium partitioning. An arbitrary number of injection and pumping wells can be specified so that bioremediation schemes can be modeled and optimized. The full development of the UTCHEM flow model is described in detail by Delshad *et al*. [1996] and Datta Gupta *et al*. [1986].

UTCHEM simulates the biodegradation of chemical compounds that can serve as substrates (carbon and/or energy sources) for microorganisms. The model simulates the destruction of substrates, the consumption of electron acceptors (e.g., oxygen, nitrate, etc.), and the growth of biomass. Substrates can be biodegraded by free-floating microorganisms in the aqueous phase or by attached biomass present as microcolonies in the manner of Molz *et al.* (1986). Multiple substrates, electron acceptors and biological species are accommodated by the model. Important assumptions for the biodegradation model are:

1. Biodegradation reactions occur only in the aqueous phase.
2. Microcolonies are fully penetrated; i.e., there is no internal resistance to mass transport within the attached biomass.
3. Biomass is initially uniformly distributed throughout the porous medium.
4. Biomass is prevented from decaying below a lower limit by metabolism of naturally occurring organic matter unless cometabolic reactions act to reduce the active biomass concentrations below natural levels.
5. The area available for transport of organic constituents into attached biomass is directly proportional to the quantity of biomass present.
6. The number of cells per microcolony, biomass density, and microcolony volume are constant, so that mass per microcolony is also constant.

The biodegradation model includes the following features:

- Monod, first-order, or instantaneous biodegradation kinetics.
- Formation of biodegradation by-products.
- External mass transfer resistances to microcolonies (mass transfer resistances can be ignored by the user if desired).
- Inhibition of biodegradation by electron acceptors and/or toxic substrates.
- Nutrient limitations to biodegradation reactions.
- First-order abiotic decay reactions.
- Enzyme competition between multiple substrates.
- Modeling of cometabolism with transformation capacities and reducing power limitations using the model of Chang and Alvarez-Cohen [1995].
- Biodegradation reactions in both the vadose and saturated zones.

9.3 Biodegradation Equations and Solution Procedure

The biodegradation model equations describe the transport of substrate and electron acceptor from the aqueous phase into attached biomass, the loss of substrate and electron acceptor through biodegradation reactions, and the resulting growth of the free-floating or attached biomass. The flow and biodegradation system is solved through operator splitting, in which the solution to the flow equations is used as the initial conditions for the biodegradation reactions. This approach is convenient because modifications can be made to the system of biodegradation equations without having to reformulate the partial differential equations that describe advection and dispersion.

The biodegradation equations comprise a system of ordinary differential equations that must be solved at each gridblock and each time step after the advection and dispersion terms are calculated. Because the mass transfer terms can make the system of equations stiff, the system is solved using a Gear's method routine published by Kahaner *et al*. [1989]. The characteristics and numerical solution of this system of equations is discussed by de Blanc *et al.* [1996b].

For a simple system of a single substrate, electron acceptor and biological species, the system of biodegradation equations is:

$$\frac{dS}{dt} = -\frac{\beta\kappa\overline{X}}{m_c}\left(S-\overline{S}\right) - \frac{\mu_{max}X}{Y}\left(\frac{S}{K_s+S}\right)\left(\frac{A}{K_a+A}\right) - k_{abio}S \tag{9.1}$$

$$\frac{d\overline{S}}{dt} = -\frac{\beta\kappa}{V_c}\left(S-\overline{S}\right) - \frac{\mu_{max}\rho_x}{Y}\left(\frac{\overline{S}}{K_s+\overline{S}}\right)\left(\frac{\overline{A}}{K_a+\overline{A}}\right) - k_{abio}\overline{S} \tag{9.2}$$

$$\frac{dA}{dt} = -\frac{\beta\kappa\overline{X}}{m_c}\left(A-\overline{A}\right) - \frac{\mu_{max}XE}{Y}\left(\frac{S}{K_s+S}\right)\left(\frac{A}{K_a+A}\right) \tag{9.3}$$

$$\frac{d\overline{A}}{dt} = -\frac{\beta\kappa}{V_c}\left(A-\overline{A}\right) - \frac{\mu_{max}\rho_x E}{Y}\left(\frac{\overline{S}}{K_s+\overline{S}}\right)\left(\frac{\overline{A}}{K_a+\overline{A}}\right) \tag{9.4}$$

$$\frac{dX}{dt} = \mu_{max}X\left(\frac{S}{K_s+S}\right)\left(\frac{A}{K_a+A}\right) - bX \tag{9.5}$$

$$\frac{d\overline{X}}{dt} = \mu_{max}\overline{X}\left(\frac{\overline{S}}{K_s+\overline{S}}\right)\left(\frac{\overline{A}}{K_a+\overline{A}}\right) - b\overline{X} \tag{9.6}$$

where:

S = aqueous phase substrate concentration (ML^{-3})
$\overline{S}$ = substrate concentration in attached biomass (ML^{-3})
A = aqueous phase electron acceptor concentration (ML^{-3})
$\overline{A}$ = electron acceptor concentration in attached biomass (ML^{-3})
X = aqueous phase concentration of unattached biomass (ML^{-3})
$\overline{X}$ = attached biomass concentration; mass of attached cells per volume of aqueous phase (ML^{-3})
E = mass of electron acceptor consumed per mass of substrate biodegraded
β = surface area of a single microcolony (L^2)
k = mass transfer coefficient (LT^{-1})
μ_{max} = maximum specific growth rate (T^{-1})
ρ_x = biomass density; mass of cells per volume of biomass (ML^{-3})
V_c = volume of a single microcolony (L^3)
m_c = mass of cells in a single microcolony; $m_c = r_x V_c$ (M)
Y = yield coefficient; mass of cells produced per mass of substrate biodegraded

K_s = substrate half-saturation coefficient (ML^{-3})

K_a = electron acceptor half-saturation coefficient (ML^{-3})

b = endogenous decay coefficient (T^{-1})

k_{abio} = first-order abiotic rate constant (T^{-1})

t = time (T)

These equations are similar to the system of equations solved by Molz *et al.* [1986] and Chen *et al.* [1992]. Equation 9.1 includes three mechanisms for loss of substrate from the aqueous phase: diffusion of substrate across a stagnant liquid layer into attached biomass; biodegradation of substrate by unattached microorganisms in the aqueous phase; and abiotic loss of the substrate through first-order reactions. The biodegradation reactions are limited by both the substrate and electron acceptor concentrations through the Monod terms.

Equation 9.2 describes the loss of substrate within attached biomass and is written for a single microcolony (Molz *et al.*, 1986). This equation describes the diffusion of substrate into attached biomass, biodegradation of the substrate within the biomass, and abiotic decay of the substrate.

Equations 9.3 and 9.4 describe the loss of the electron acceptor. These equations are of the same form as Eqs. 9.1 and 9.2 in that they describe diffusion across a liquid film and loss in biodegradation reactions. The biodegradation rate expressions are multiplied by the factor E, the mass of electron acceptor consumed per mass of substrate biodegraded. Equations 9.5 and 9.6 describe the growth and decay of unattached and attached biomass, respectively. The relationship between the attached biomass concentration $\overline{X}$ appearing in Eqs. 9.1, 9.3 and 9.6 to the biomass density, microcolony volume and microcolony mass is

$$\overline{X} = \frac{C_c \rho_b m_c}{n\phi} \tag{9.7}$$

where C_c is the number of cells per mass of solid, ρ_b is the bulk density, n is the number of cells per microcolony (a constant), and ϕ is the porosity. Since the biomass density, number of cells per microcolony, porosity, and mass per microcolony are assumed to be constant, changes in $\overline{X}$ actually correspond to changes in C_c, or alternately, to C_c/n, the number of microcolonies (Molz *et al.*, 1986). The area available for transport of species from the aqueous phase to the biomass is directly proportional to $\overline{X}$ because the surface area per microcolony is constant.

If external mass transport is ignored, then the system of six equations is reduced to three equations consisting of Eq. 9.6 and a single equation each for loss of the substrate and electron acceptor:

$$\frac{dS}{dt} = -\frac{\mu_{max}\overline{X}}{Y}\left(\frac{S}{K_s + S}\right)\left(\frac{A}{K_a + A}\right) - k_{abio}S \tag{9.8}$$

$$\frac{dA}{dt} = -\frac{\mu_{max}\overline{X}E}{Y}\left(\frac{S}{K_s + S}\right)\left(\frac{A}{K_a + A}\right) \tag{9.9}$$

where $\overline{X}$ is the concentration of attached biomass and all other concentrations are aqueous phase concentrations.

When biodegradation reactions that involve more than one substrate are being modeled, equations of the same form as Eqs. 9.1 and 9.2 (or 9.8) are solved for each additional substrate. Similarly, equations of the form of Eqs. 9.3 and 9.4 (or 9.9) are solved for each additional electron acceptor. Substrates can be biodegraded by microorganisms using more than one electron acceptor, and each electron acceptor can be used for biodegradation of multiple substrates.

When substrate competition is considered, the half-saturation coefficient of each Monod term is modified in the following manner (Bailey and Ollis, 1986):

$$\frac{S_1}{K_{s,1}\left(1+\frac{S_2}{K_{s,2}}\right)+S_1}$$

where:

S_1, S_2 = concentration of substrates 1 and 2, respectively (ML^{-3})

$K_{s,1}$, $K_{s,2}$ = half-saturation coefficients of substrates 1 and 2, respectively (ML^{-3})

If sequential electron acceptor utilization occurs (e.g., oxygen consumption followed by consumption of nitrate), then the biodegradation rate expressions in the equations for substrate loss, electron acceptor consumption and biomass growth are multiplied by an inhibition factor of the form (Widdowson *et al.*, 1988):

$$\left(\frac{I}{I+C_{ihb}}\right)$$

where I is an experimentally determined inhibition constant. The inhibition factor approaches 0 as the concentration of the inhibiting substance C_{ihb} increases. For nitrate respiration, for example, this term keeps denitrification rates very small until oxygen is nearly exhausted.

When cometabolic reactions are considered, the equations describing the loss of cometabolite and attached biomass growth are, in the case of no mass transfer resistances (Chang and Alvarez-Cohen, 1995):

$$\frac{dC}{dt}=-k_c\overline{X}\left(\frac{C}{K_c+C}\right)\left(\frac{A}{K_a+A}\right)\left(\frac{R}{K_r+R}\right) \tag{9.10}$$

$$\frac{d\overline{X}}{dt}=-\frac{\mu_{max,s}\overline{X}}{Y}\left(\frac{S}{K_s+S}\right)\left(\frac{A}{K_a+A}\right)\left(\frac{R}{K_r+R}\right)-\frac{k_c\overline{X}}{T_c}\left(\frac{C}{K_c+C}\right)\left(\frac{A}{K_a+A}\right)\left(\frac{R}{K_r+R}\right)-b\overline{X} \tag{9.11}$$

where k_c is the maximum specific cometabolite biodegradation rate ($ML^{-3}T^{-1}$), C is the aqueous phase cometabolite concentration, R is the reducing power (NAD(P)H) concentration within the cells, K_r is the NAD(P)H half-saturation constant, K_c is the cometabolite half-saturation coefficient, $\mu_{max,s}$ is the maximum specific growth rate on growth substrate, and T_c is the transformation capacity, defined as the maximum possible mass of substrate biodegraded per mass of biomass. The second expression in Eq. 9.11 describes the deactivation of biomass through cometabolism reactions, which can produce toxic by-products that damage cells (Chang and Alvarez-Cohen, 1995). When reducing power limitations are considered, an equation is also needed to describe the production of NAD(P)H by the growth substrate and the consumption of NAD(P)H by the cometabolite:

$$\frac{dR}{dt} = -k_c E_{rc} \overline{X} \left(\frac{C}{K_c + C} \right) \left(\frac{A}{K_a + A} \right) \left(\frac{R}{K_r + R} \right) + \frac{\mu_{max} E_{rp} \overline{X}}{Y} \left(\frac{S}{K_s + S} \right) \left(\frac{A}{K_a + A} \right) \left(\frac{R}{K_r + R} \right) \tag{9.12}$$

where E_{rc} is the mass of NAD(P)H consumed per mass of cometabolite biodegraded, and E_{rp} is the mass of NAD(P)H produced per mass of growth substrate biodegraded.

9.4 Example Simulations

The multi-phase flow and biodegradation capabilities of the model are demonstrated through the simulation of hypothetical LNAPL and DNAPL spills. In these simulations, the modeling domain consists of a homogeneous, initially uncontaminated, confined aquifer that is 125 m long by 54 m wide by 6 m thick (see Fig. 9.1). The domain is simulated with 25 gridblocks in the x direction, 11 gridblocks in the y direction, and 5 gridblocks in the z direction. Groundwater is flowing in the positive x direction (left to right in all figures) with an average velocity of 0.1 m/day. Other flow and physiochemical parameters are listed in Table 9.1. The spills are modeled by injecting NAPL into the center of gridblock (x = 5, y = 6, z = 1), which is approximately 22 meters from the left boundary. All chemical species are assumed to be non-adsorbing. There is no air phase in these simulations; the top boundary is a no-flow boundary.

For both of these examples, local equilibrium is assumed between the NAPL and the aqueous phase, so that the concentration of organic constituents in the aqueous phase is calculated by the partitioning relationship:

$$C_{i,aq} = C_{i,sol} x_{i,NAPL} \tag{9.13}$$

where $C_{i,aq}$ is the aqueous phase concentration of component i, $C_{i,sol}$ is the aqueous phase solubility of component i, and $x_{i,NAPL}$ is the volume fraction of component i in the NAPL.

9.4.1 LNAPL Simulation Example

Sequential use of electron acceptors and equilibrium partitioning of multiple components into the aqueous phase are illustrated with an example LNAPL simulation. The LNAPL example simulates a leak of 3.8 m^3 of gasoline containing approximately 1% by volume of benzene and 6% by volume of toluene into a shallow, confined aquifer. The leak is assumed to occur over a four-day period. The groundwater initially contains 8 mg/L oxygen and 10 mg/L nitrate. Parameters used for this simulation are listed in Table 9.2.

Figure 9.2 shows the NAPL saturation history in a vertical slice down the center of the aquifer in the x-z plane. As seen in Fig. 9.2, the NAPL moves little once the NAPL lens is established. The NAPL lens gradually decreases in size as the organic constituents dissolve into the flowing groundwater.

As the benzene and toluene partition out of the gasoline into the aqueous phase, they become available to microorganisms as substrates. For simplicity, a single population of microorganisms capable of biodegrading the benzene and toluene is assumed to exist in the aquifer. This biological species biodegrades both benzene and toluene aerobically and biodegrades toluene anaerobically with nitrate as the electron acceptor. Abiotic decay and biodegradation by free-floating microorganisms are assumed to be negligible (k_{abio} and X are 0). Biodegradation kinetic parameters used for the simulation were obtained from Chen *et al.* [1992].

Figure 9.3 compares the concentration of benzene in the aqueous phase at 500 days to the concentration of benzene that would exist if no biodegradation reactions were occurring. This figure shows that significant biodegradation of dissolved benzene has occurred. The toluene plume is also shown in Fig. 9.3. Although the toluene solubility is three times less than the benzene solubility, the maximum toluene concentration in the aqueous phase is higher than the maximum benzene concentration because its concentration in the gasoline is six times the benzene concentration of the gasoline. Toluene concentrations are nearly as low as benzene concentrations at the fringes of the plume because toluene is biodegraded both aerobically and anaerobically, where oxygen is exhausted, but the benzene is not.

The concentrations of benzene, toluene, oxygen and nitrate at 500 days are compared in Fig. 9.4. Oxygen immediately downgradient of the spill is practically exhausted. Nitrate is also nearly exhausted from the area immediately downgradient of the spill because sufficient time has elapsed since oxygen depletion to allow denitrification to occur. However, at the forward edge of the plume, relatively high nitrate concentrations still exist in areas where oxygen has been depleted, but not exhausted.

9.4.2 DNAPL Simulation Example

Different model capabilities are illustrated with a DNAPL simulation in which trichloroethylene (TCE) is biodegraded through cometabolism. In this simulation, 0.028 m^3 of TCE are spilled in a single day. The cometabolic process is illustrated by injecting water containing methane through five injection wells located approximately 24 meters downgradient of the spill. The injected water contains 20 mg/L methane and 8 mg/L oxygen. The water injection rate is 1.4 m^3 per day per well. The groundwater is assumed to contain 8 mg/L oxygen. Parameters used for the DNAPL simulation example are listed in Table 9.3.

A population of methanotrophic microorganisms, capable of biodegrading TCE aerobically through cometabolism, is assumed to exist in the aquifer. The methanotrophs use methane as the primary substrate and oxygen as the electron acceptor. TCE biodegradation is assumed to reduce the active biomass and consume reducing power of the methanotrophs, so that TCE biodegradation both reduces the active biomass concentration and reduces the active biomass's biodegradation effectiveness. Once biomass has become deactivated, it does not become active again. Biodegradation rate parameters were obtained from Chang and Alvarez-Cohen [1995]. External mass transport of chemical species from the aqueous phase to the biomass was ignored for this example.

The effect of the methane injection wells is illustrated in Fig. 9.5, where concentrations of TCE, a hypothetical TCE tracer, oxygen and methane are shown at 170 days. The TCE tracer is simply TCE that is not allowed to biodegrade in the model so that the effects of biodegradation can be seen. Concentration contours of the different constituents are shown in the top 1.2-m layer of the aquifer. Oxygen is depleted downgradient of the plume, but only a small fraction of the oxygen is consumed upgradient of the methane injection wells. Most of the oxygen upgradient of the wells remains because the high TCE concentrations deactivate the biomass and consume reducing power, preventing the TCE from biodegrading. Even with a small TCE spill, TCE concentrations in the aquifer are so high that most biomass immediately downgradient of the spill is rapidly deactivated. Significant TCE biodegradation occurs only where appreciable methane is present to regenerate the microorganism's reducing power and where TCE concentrations are low. These effects can be seen in Fig. 9.5. The high concentration contours of the TCE and TCE tracer are nearly the same, but biodegradation of the TCE causes a slight retardation in the progress of the TCE plume at low concentrations.

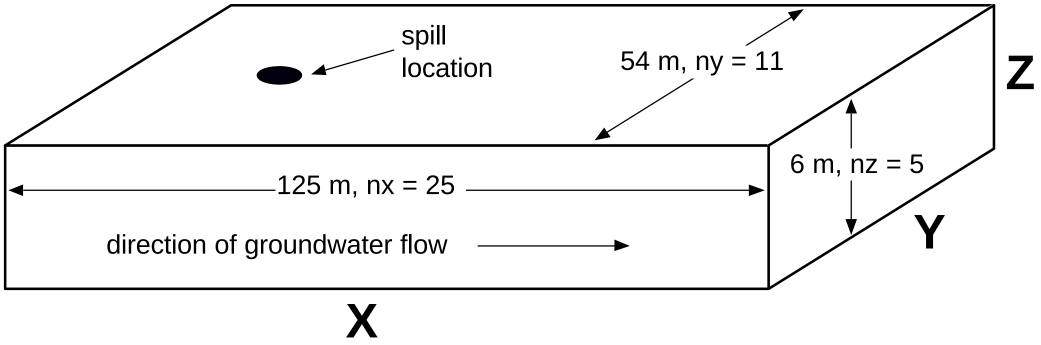


Figure 9.1. Modeling domain size and discretization.

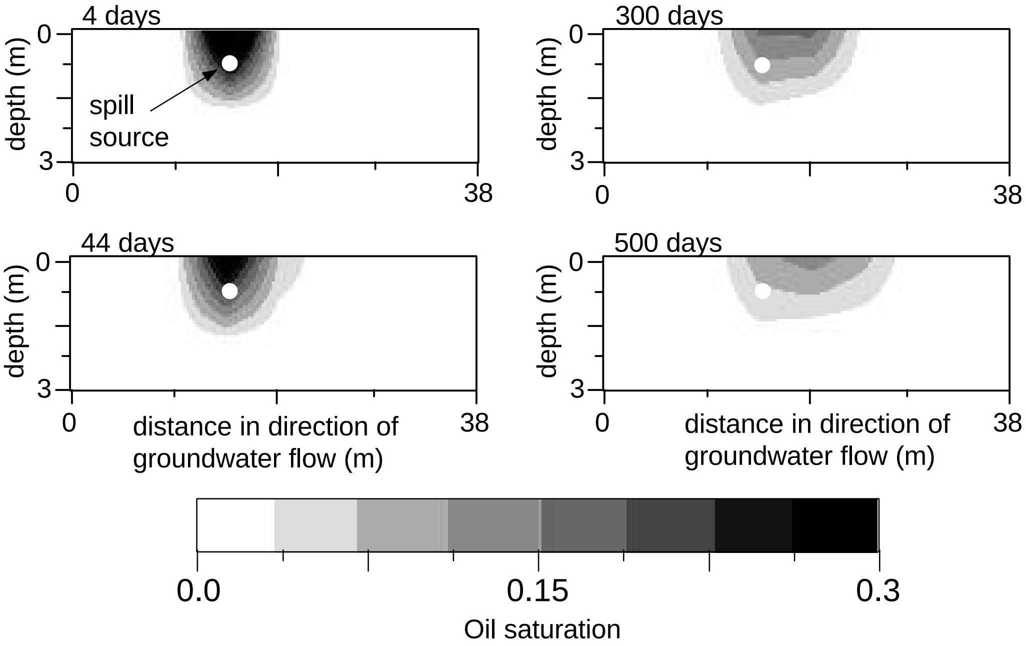


Figure 9.2. NAPL saturation history in the vicinity of a hypothetical gasoline spill. The figure shows a vertical section along the x axis in the center of the aquifer. This gasoline spill is simulated by injecting 3.8 m^3 of gasoline at a depth 0.6 m below the top of the confined aquifer.

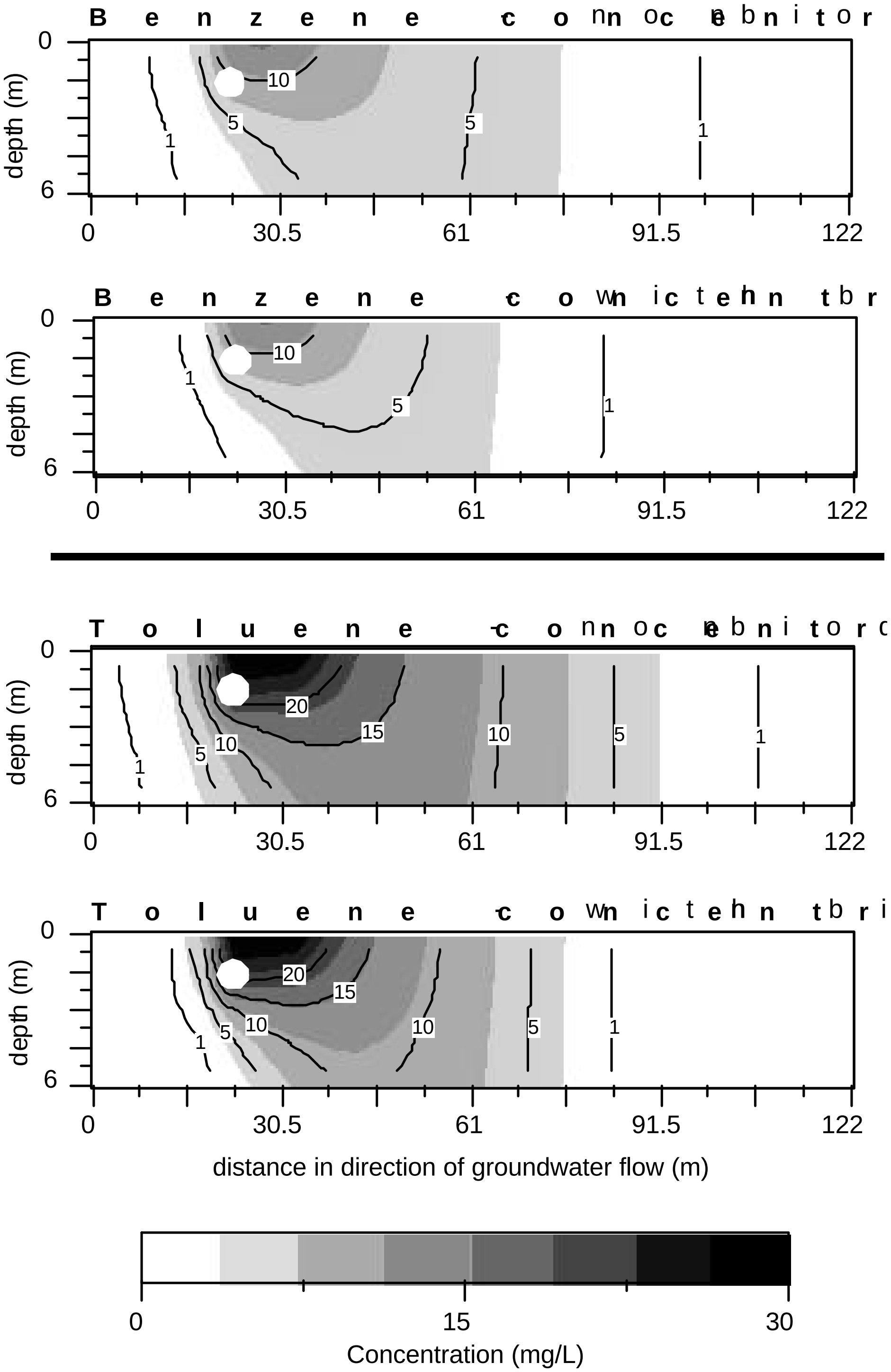


Figure 9.3. Comparison of benzene and toluene concentrations in the aqueous phase 500 days after a gasoline spill. The figure shows a vertical section along the x axis in the center of the aquifer. Gasoline was injected at the location of the white circle. Concentrations of benzene and toluene are compared for the assumptions of no biodegradation and biodegradation of the two compounds.

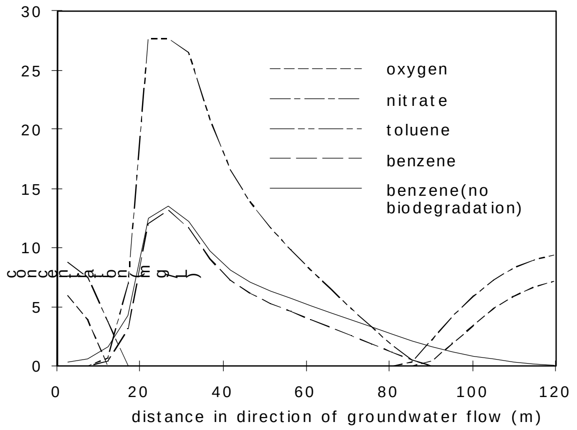


Figure 9.4. Concentrations of benzene without biodegradation, benzene with biodegradation, toluene, oxygen, and nitrate in upper 1.2 m of aquifer along aquifer center line at 500 days.

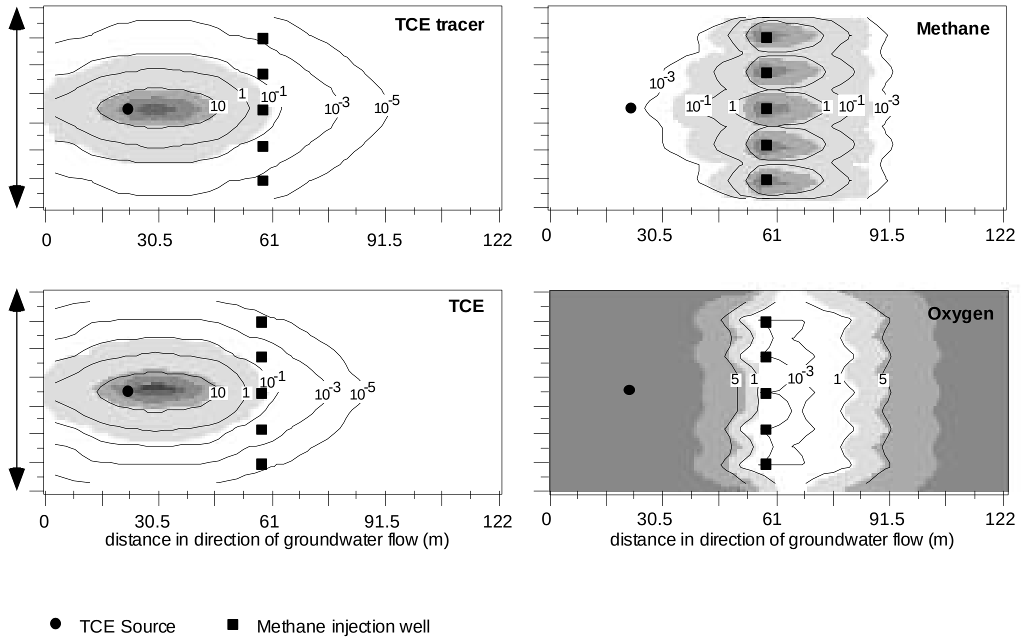


Figure 9.5. Plan view of TCE, a hypothetical TCE tracer, methane and oxygen concentrations in the upper 1.2 m of a confined aquifer 170 days after a TCE spill. All concentrations are mg/L. Groundwater is flowing from left to right at 0.1 m/d. Shading is present for visualization purposes only and does not correspond to specific chemical concentrations. Assumptions are: TCE solubility = 1,100 mg/L; initial oxygen concentration = 8 mg/L; methane concentration in injected water = 20 mg/L. Biodegradation rate parameters are from Chang and Alvarez-Cohen [1995].

Table 9.1. Flow Parameters for All Simulations

average velocity, v (m/d)	0.1
porosity, ϕ	0.38
bulk soil density, ρ_b (g/cm^3)	1.64
longitudinal dispersivity, α_L (m)	5
transverse dispersivity, α_T (m)	0.625
initial oxygen concentration, A_o (mg/L)	8.0
initial nitrate concentration, A_n (mg/L)	10.0

Table 9.2. Parameters for LNAPL Simulation Example

Simulation parameters	
Spill volume (m^3)	3.8
Spill duration (d)	4
Physiochemical parameters	
Density of gasoline (g/cm^3)	0.87
Density of benzene (g/cm^3)	0.87
Density of toluene (g/cm^3)	0.86
Solubility of benzene (mg/L)	1,778
Solubility of toluene (mg/L)	500
Initial benzene concentration in NAPL (volume %)	1.1
Initial toluene concentration in NAPL (volume %)	6.1
Mass transfer coefficient for benzene, κ_b (m^2/d)	4.60×10^{-1}
Mass transfer coefficient for toluene, κ_t (m^2/d)	4.26×10^{-1}
Mass transfer coefficient for oxygen, κ_o (m^2/d)	7.92×10^{-1}
Mass transfer coefficient for nitrate, κ_n (m^2/d)	6.52×10^{-1}
Microbial parameters (from Chen et al., 1992)	
Initial cell concentration, C_c (cells/g soil)	3.8×10^5
Colony population density, n (cells/microcolony)	100
Biomass density, ρ_x (g/cm^3)	1.0
Microcolony surface area, β (m^2/microcolony)	1.19×10^{-10}
Microcolony volume, V_c (m^3/microcolony)	1.0×10^{-16}
Initial attached biomass concentration, $\overline{X}$ (mg/L)	1.64
Maximum specific growth rate on benzene, $\mu_{max,b}$ (d^{-1})	4.15
Maximum specific growth rate on toluene, $\mu_{max,t}$ (d^{-1})	4.95
Yield coefficient for benzene, Y_b (g cells/g benzene)	0.5
Yield coefficient for toluene, Y_t (g cells/g toluene)	0.5
Half-saturation coef. of benzene for oxygen respiration, K_s^{bo} (mg/L)	12.2

Half-saturation coef. of toluene for oxygen respiration, K_s^{to} (mg/L)	17.4

Table 9.2. Parameters for LNAPL Simulation Example

Half-saturation coef. of toluene for nitrate respiration, K_s^{tn} (mg/L)	17.4
Half-saturation coef. of oxygen for benzene biodeg., K_a^{bo} (mg/L)	0.1
Half-saturation coef. of oxygen for toluene biodeg., K_a^{to} (mg/L)	0.01
Half-saturation coef.of nitrate for toluene biodeg., K_a^{tn} (mg/L)	2.6
Endogenous decay coefficient, b (d^{-1})	0.1

Table 9.3. Parameters for DNAPL Simulation Example

Simulation parameters	
Spill volume (m^3)	0.028
Spill duration (d)	1
Physiochemical parameters	
Density of NAPL (g/cm^3)	1.46
Density of TCE (g/cm^3)	1.46
Solubility of TCE (mg/L)	1,100
Initial TCE concentration in NAPL (volume %)	50
Microbial parameters	
Initial biomass concentration, X (mg/L)	4.31
Maximum biodegradation rate of TCE, k_c (mg TCE/mg cells-d)	4.2
Maximum specific growth rate for methane, $\mu_{max,m}$ (d^{-1})	0.31
Yield coefficient for methane, Y (mg cells/mg methane)	0.33
TCE transformation capacity, T_c (mg TCE/mg cells)	0.1
Half-saturation coefficient for TCE, K_c (mg/L)	7.0
Half-saturation coefficient for methane, K_s (mg/L)	1.1
Half-saturation coefficient for reducing power, K_r (mmol of e^-/L)	0.54
Reducing power production coefficient, E_{rp} (mmol e^- produced/mg methane biodegraded)	0.5
Reducing power consumption coefficient, E_{rc} (mmol e^- consumed/ mg TCE biodegraded)	0.15
Initial reducing power concentration in cells, (mmol e^-/mg cells)	0.0005

Section 10
Well Models

10.1 Introduction

In this section, the well models in the UTCHEM simulator are described. The options available are:

- An arbitrary number of producers in any gridblock can be specified (Cartesian grid option only).
- Skin factor (S) and completion interval can be specified.
- Both the injection wells and the producers can be shut in or opened at anytime during the simulation. The well type can also be changed during the simulation (e.g., an injector changed to a producer).
- Each injection well can inject multiple slugs with different component concentrations.
- Wells can be completed in any direction parallel to the axes (Cartesian and Curvilinear grid options only).

10.2 Vertical Wells with Cartesian or Curvilinear Grid Options

Two basic well conditions of constant flow rate or constant flowing bottomhole pressure are implemented. Application of Darcy's law to a wellblock (i,j,k) results in:

$$Q = \sum_{\ell=1}^{n_p} Q_\ell = \sum_{\ell=1}^{n_p} PI_\ell \left(P_{wf} - P_\ell\right) \tag{10.1}$$

where $P_\ell = P_1 + P_{c1\ell}$ and PI is the productivity index. For two-dimensional areal (x-y) and three-dimensional simulation, the PI is given by:

$$PI_\ell = \frac{2\pi\sqrt{k_x k_y}\,\Delta z}{(0.15802)\left(\ln\dfrac{r_o}{r_w} + S\right)} \lambda_{r\ell} \tag{10.2}$$

and for one-dimensional and cross-sectional (x-z) simulation by:

$$PI_\ell = \frac{k_x \Delta y \Delta z}{0.15802 \dfrac{\Delta x}{2}} \lambda_{r\ell} \tag{10.3}$$

where the constant in the above equations is the unit conversion factors where the permeability is in Darcy and gridblock size in ft and $\lambda_{r\ell} = \frac{k_{r\ell}}{\mu_\ell}$ in cp^{-1} to result PI in $(psi)^{-1}$.

The equivalent radius, r_o, is calculated using Peaceman's model (Peaceman, 1983):

$$r_o = 0.28 \frac{\left(\left(\frac{k_x}{k_y} \right)^{1/2} \Delta y^2 + \left(\frac{k_y}{k_x} \right)^{1/2} \Delta x^2 \right)^{1/2}}{\left(\frac{k_x}{k_y} \right)^{1/4} + \left(\frac{k_y}{k_x} \right)^{1/4}} \tag{10.4}$$

The well bottomhole following pressure in any layer k, $P_{wf,k}$ is given by:

$$(P_{wf})_k = (P_{wf})_{k-1} + \bar{\gamma}_k \quad k = 2,..., nbz \tag{10.5}$$

where n_{bz} is the number of layers perforated and

$$\bar{\gamma}_k = \gamma_k \frac{\Delta z_k}{2} + \gamma_{k-1} \frac{\Delta z_{k-1}}{2} \tag{10.6}$$

γ_k are calculated from:

$$\gamma_k = \frac{\sum_{\ell=1}^{n_p} \gamma_\ell PI_\ell}{\sum_{\ell=1}^{n_p} PI_\ell} \tag{10.7}$$

For the producer wellblock, specific weights of the produced fluids, γ_ℓ, are used in the above calculations while for the injection wells, the specific weights of the injected phases are calculated using:

$$\gamma_\ell = \sum_{k=1}^{n_c} \left((C_{inj})_{k,\ell} \right) \gamma_k \tag{10.8}$$

10.2.1 Well Constraints for Injection Wells

10.2.1.1 Rate Constraint

When the phase injection rates, $Q_{inj,\ell}$, are specified, the positive injection rates are allocated to the individual layer k that is perforated according to:

$$Q_\ell = Q_{inj,\ell} \frac{\sum_{\ell=1}^{n_p} PI_\ell}{\sum_{k=1}^{n_{bz}} \sum_{\ell=1}^{n_p} PI_\ell} \tag{10.9}$$

The total injection rate for the ijk block is given by:

$$Q = \sum_{\ell=1}^{n_p} Q_\ell \tag{10.10}$$

The above term is then added to the constant vector of the pressure equation at the ijk block. In Eq. 10.9, it is assumed that the potential gradient between the wellbore and the gridblock pressure is the same for all the layers in the reservoir model. Nolen and Berry [1972] have shown that including the potential differences in Eq. 10.9 may result in stability problems. Equation 10.9 may give erroneous results in the case of large vertical heterogeneity and especially when noncommunicating layers exist. However, in the absence of a very low permeability zone or small crossflow, the above formulation does not produce a significant error.

10.2.1.2 Pressure Constraint

When bottomhole injection pressure for the first perforated layer, $(P_{wf})_{ij,k=1}$, is specified, Eq. 10.1 is used. The term $\sum_{\ell=1}^{n_p} PI_\ell \left(P_{wf} - P_{c1\ell}\right)$ in Eq. 10.1 is added to the constant vector of the pressure equation for block ijk and term $\sum_{\ell=1}^{n_p} PI_\ell$ to the $(P_1)^{n+1}$ term (diagonal element in the pressure matrix).

After the pressure equation is solved, Eq. 10.1 is used to obtain the total injection rate at the end of the time step, Q. The injected phase cuts for each layer are the same as the total injected cuts:

$$Q_\ell \quad Q \frac{Q_{inj,}}{\sum_{\ell=1}^{n_p} Q_{inj,\ell}} \tag{10.11}$$

the phase injection rates, $Q_{inj,\ell}$, specified as input values, are treated as phase cuts.

10.2.2 Well Constraints for Production Wells

10.2.2.1 Rate Constraint

When the total production rate, input as a negative value (Q_{prod}) is specified, the withdrawal rate for each layer k is calculated using:

$$Q = Q_{prod} \frac{\sum_{\ell=1}^{n_p} PI_\ell}{\sum_{k=1}^{n_{bz}} \sum_{\ell=1}^{n_p} PI_\ell} \tag{10.12}$$

and the produced phase cuts are then calculated using:

$$Q_\ell = Q \frac{\lambda_{r\ell}}{\sum_{\ell=1}^{n_p} \lambda_{r\ell}} \tag{10.13}$$

10.2.2.2 Pressure Constraint

When bottomhole pressure for a producer is specified, Eq. 10.1 is used to calculate the total production rate (Q) in the same manner as was described above for the injection well on pressure constraint. The produced phase cuts are then obtained from:

$$Q_\ell = Q \frac{PI_\ell}{\sum_{\ell=1}^{n_p} PI_\ell} \tag{10.14}$$

10.3 Vertical Wells with Radial Grid Option

The boundary conditions for the radial option are

- no vertical flow at the upper and lower boundaries
- a rate constraint well at the center of the reservoir,
- a constant pressure outer boundary that is treated the same as a pressure constraint injector/producer well.

The phase productivity index in the gridblock ijk for the injection or production well is calculated as

$$PI_\ell = \frac{k_x \Delta z}{\frac{\Delta x}{2}} \lambda_{r\ell} \tag{10.15}$$

10.3.1 Rate Constraint Injector

Equations 10.9 and 10.10 are used to calculate the rate allocation to each layer.

10.3.2 Rate Constraint Producer

Equations 10.12 and 10.13 are used to calculate the rate withdrawal from each layer.

10.3.3 External Boundary

The amount of fluid that crosses each layer k from the last gridblock at the open boundary is calculated by

$$Q = \sum_{\ell=1}^{n_p} PI_{\ell} \left((P_1)_e - (P_1)_{i=n_r} \right) \tag{10.16}$$

where the outer boundary aqueous phase pressure $(P_1)_e$ is maintained at the initial pressure for the duration of the simulation as:

$$(P_1)_{e,k} = (P_1)_{e,k-1} + \bar{\gamma}_k \qquad \text{for k = 2,..., nbz} \tag{10.17a}$$

where $\bar{\gamma}_k$ is calculated from Eqs. 10.6 and 10.7. The phase productivity index is calculated as:

$$PI_{\ell} = 6.3266 \frac{2\pi k_x \Delta z}{\ln \frac{r_e}{r_i}} \lambda_{r\ell} \tag{10.17b}$$

where the permeability and radius of the outermost gridblock ($i = n_r$) are used. The calculation is implicit similar to that for the pressure constrained wells discussed above. Once the pressure is known, total rate for each layer is calculated from Eq. 10.16. The phase cuts for the fluids crossing the boundary are calculated from Eq. 10.14.

10.4 Horizontal Well with Cartesian or Curvilinear Grid Options

Horizontal wells use the same well model equations as vertical wells. Only parameters related to the direction of the wellbore were modified. When the wellbore is parallel to the z direction, the calculation of the productivity index uses the gridblock height, •z, the permeability in the x direction, k_x, and the permeability in the y direction, k_y:

$$PI_{\ell} = \frac{2\pi\sqrt{k_x k_y}\,\Delta z}{0.15802\left[\ln\left(\frac{r_o}{r_w}\right) + S\right]} \lambda_{r\ell} \tag{10.18}$$

where the constant 0.15802 is a unit conversion factor. k_x and k_y are in Darcy, •z, r_o, and r_w are in ft, and $\lambda_{r\ell} = k_{r\ell} / \mu_{\ell}$ is in cp^{-1}. The equivalent wellblock radius, r_o, is based on Peaceman [1983] and uses wellblock properties in the x and y directions such as the dimensions •x and •y and the permeability values k_x and k_y:

$$r_o = 0.28 \frac{\left[\left(\frac{k_x}{k_y} \right)^{1/2} \Delta y^2 + \left(\frac{k_y}{k_x} \right)^{1/2} \Delta x^2 \right]^{1/2}}{\left(\frac{k_x}{k_y} \right)^{1/4} + \left(\frac{k_y}{k_x} \right)^{1/4}} \tag{10.19}$$

10.4.1 Productivity Index for Horizontal Wells

The productivity index calculations were generalized for horizontal wells parallel to either the x direction or the y direction by taking into account the pertinent directional properties. When the wellbore is parallel to the x direction, the productivity index calculation uses •x as the wellblock dimension parallel to the wellbore. Since the wellbore is perpendicular to the y and z directions, the productivity index calculation uses the permeability in the y direction and the permeability in the z direction:

$$PI_{\ell} = \frac{2\pi\sqrt{k_y k_z}\,\Delta x}{0.15802\left[\ln\left(\frac{r_o}{r_w}\right)+S\right]}\lambda_{r\ell} \qquad (10.20)$$

When the wellbore is parallel to the y direction, the productivity index calculation uses •y as the wellblock dimension parallel to the wellbore. Since the wellbore is perpendicular to the x and z directions, the productivity index calculation uses the permeability in the x direction and the permeability in the z direction:

$$PI_{\ell} = \frac{2\pi\sqrt{k_x k_z}\,\Delta y}{0.15802\left[\ln\left(\frac{r_o}{r_w}\right)+S\right]}\lambda_{r\ell} \qquad (10.21)$$

10.4.1.1 Equivalent Wellblock Radius for Horizontal Wells (Peaceman, 1983)

The calculations of the equivalent wellblock radius were also generalized for horizontal wells by taking into account reservoir properties perpendicular to the direction of the wellbore. In case the wellbore is parallel to the x direction, the equivalent wellblock radius, based on Peaceman [1983], uses wellblock properties in the y and z directions such as the dimensions •y and •z and the permeability values k_y and k_z:

$$r_o = 0.28\,\frac{\left[\left(\frac{k_y}{k_z}\right)^{0.5}\Delta z^2 + \left(\frac{k_z}{k_y}\right)^{0.5}\Delta y^2\right]^{0.5}}{\left(\frac{k_y}{k_z}\right)^{0.25} + \left(\frac{k_z}{k_y}\right)^{0.25}} \qquad (10.22)$$

In case the wellbore is parallel to the y direction, the equivalent wellblock radius uses wellblock properties in the x and z directions such as the dimensions •x and •z and the permeability values k_x and k_z:

$$r_o = 0.28\,\frac{\left[\left(\frac{k_x}{k_z}\right)^{0.5}\Delta z^2 + \left(\frac{k_z}{k_x}\right)^{0.5}\Delta x^2\right]^{0.5}}{\left(\frac{k_x}{k_z}\right)^{0.25} + \left(\frac{k_z}{k_x}\right)^{0.25}} \qquad (10.23)$$

10.4.1.2 Equivalent Wellblock Radius (Babu *et al.*, 1991)

In addition to Peaceman's formulation [1983], a formulation of the equivalent wellblock radius based on the paper by Babu *et al.* [1991] was implemented in the simulator (Dakhlia *et al*, 1995). As published, the gridblock sizes were assumed uniform and the equations depended on gridblock numbering. However, numerical reservoir simulation is often carried out with non-uniform gridblock sizes. The equations were therefore rearranged so that gridblock sizes were no longer required to be uniform and the equations no longer depended on the gridblock numbering. $\frac{h}{\Delta z}$ was substituted for n_z and $\frac{a}{\Delta x}$ was substituted for n_x. In case an integer was needed, such as in the summation limits, the FORTRAN function NINT was used to calculate the nearest integer to the argument. Therefore, NINT($\frac{h}{\Delta z}$) was substituted for n_z in the summation limit used in S_{xz}. In addition, $\frac{2x_w}{\Delta x}$ was substituted for ν and $\frac{2z_w}{\Delta z}$ was substituted for λ. As a result, the applicability of the formulation was extended to non-uniform grids. The assumption for these substitutions was that away from the wellbore, the effect of a coarse and non-uniform grid was equivalent to the effect of a fine and uniform grid on the pressure behavior near the wellbore.

The resulting formulation is given below for a wellbore parallel to the y direction. In case the wellbore was parallel to either the x or z direction, the pertinent directional variables were modified accordingly.

$$\ln\left(\frac{r_o}{h}\right)=\left[\frac{\pi a}{6h\left(\frac{a}{\Delta x}\right)^2}\sqrt{\frac{k_z}{k_x}}\right]+0.25\ln\left[\frac{k_x}{k_z}\right]-\ln\left[\sin\left(\frac{\pi z_w}{h}\right)\right]-1.84-B_E-S_{xz} \tag{10.24}$$

where the boundary term, B_E, is computed by

$$B_E=\ln(1-E_1)+0.5\ln\left[1-2\cos\left(\frac{2\pi z_w}{h}\right)E_1+E_1^2\right] \tag{10.25}$$

and

$$E_1=\exp\left[-\frac{2\pi\min(x_w,a-x_w)}{h}\sqrt{\frac{k_z}{k_x}}\right] \tag{10.26}$$

and the summation term, S_{xz}, is

$$S_{xz}=\frac{\pi}{\left(\frac{h}{\Delta z}\right)}\sum_{n=1}^{\mathrm{NINT}\left(\frac{h}{\Delta z}\right)-1}\frac{\cos^2\left[\frac{\pi n z_w}{h}\right]\left[1+x_n^{-\left(\frac{2x_w}{\Delta x}\right)}\right]\left[1+x_n^{-2\left(\frac{a-x_w}{\Delta x}\right)}\right]}{\sin\left[\frac{\pi n}{2\left(\frac{h}{\Delta z}\right)}\right]\sqrt{1+\alpha_n^2}\left[1-x_n^{-\left(\frac{2a}{\Delta x}\right)}\right]} \tag{27}$$

with α, α_n, and x_n defined as

$$\alpha=\frac{\Delta x}{\Delta z}\sqrt{\frac{k_z}{k_x}} \tag{10.28}$$

$$\alpha_n = \alpha \sin\left[\frac{\pi n}{2\left(\frac{h}{\Delta z}\right)}\right] \tag{10.29}$$

$$x_n = \left(\alpha_n + \sqrt{1+\alpha_n^2}\right)^2 \tag{10.30}$$

For symmetry purposes, the wellbore location (x_w, z_w) was temporarily adjusted so that

$$x_w = \min(x_w, a - x_w) \tag{10.31}$$

and

$$z_w = \min(z_w, a - z_w) \tag{10.32}$$

Section 11
Effect of Alcohol on Phase Behavior

11.1 Introduction

This section is based on the Ph.D. dissertation by Saad [1989]. The phase behavior calculation for a mixture of water, oil, and surfactant is discussed in Section 2. The effect of alcohol on the phase behavior is discussed here. The presence of alcohol affects the effective salinities and causes a shift in the phase boundaries. The effect of alcohol on the solubility is accounted for by shifting the maximum height of binodal curve. The amount of alcohol that partitions in the excess phase(s) is modeled either by constant partitioning coefficients as in Hirasaki's model (Hirasaki, 1982) or as a function of total composition with the concept of pseudocomponent and pseudophase as in Provoust's model (Prouvost *et al.*, 1984a,b, 1985). Following is a discussion of the UTCHEM phase behavior model in the presence of alcohol (Pope and Nelson, 1978; Prouvost *et al.*, 1984a,b, 1985; Camilleri *et al.*, 1987c; Saad, 1989).

The phase behavior is modeled as a tetrahedric diagram at a fixed salinity. Four pseudocomponents are surfactant, alcohol, oil, and water represented in a tetrahedric diagram. Tielines and binodal curves are located on the ternaries sliced through tetrahedrons. The pseudophases are (1) the aqueous consists of water and alcohol(s), (2) oleic consists of oil and alcohol(s), and (3) microemulsion consists of surfactant and alcohol(s). Similar to the no alcohol mixture, the phase behavior parameters such as binodal curve, plait point and invariant point are calculated as a function of effective salinity using Hand's rule (Hand, 1939).

11.2 Alcohol Partitioning

The two options available in UTCHEM to calculate the alcohol partitioning are based on the models of Hirasaki and Prouvost. Hirasaki's model assumes a constant partition coefficient whereas experimental results show that alcohol partition coefficients vary with total composition. Prouvost extended the pseudophase model to calculate variable alcohol partition coefficients and to be applicable to two alcohols. The following intensive composition parameters are defined in the model:

$$\lambda_j = \frac{C_\kappa^1}{C_1} \tag{11.1}$$

$$\gamma_j = \frac{C_\kappa^2}{C_2} \tag{11.2}$$

$$\sigma_j = \frac{C_\kappa^3}{C_3} \tag{11.3}$$

where for $\kappa = 7$, the value of subscript j = 1 and for $\kappa = 8$, j = 2. C_1, C_2, and C_3 are the overall water, oil, and surfactant volume fractions, respectively. Superscripts 1, 2, and 3 represent the association of alcohol with aqueous, oleic, and microemulsion pseudophases. Therefore, C_7^1 is the volume of alcohol 7 (component 7 in UTCHEM) in the aqueous phase, and C_8^1 is the volume of alcohol 8 (component 8) in the aqueous phase. The partition coefficients used in Hirasaki's model can be defined using the above parameters:

$$K_\kappa^2 = \frac{\gamma_j}{\lambda_j} \tag{11.4}$$

$$K_\kappa^3 = \frac{\sigma_j}{\lambda_j} \tag{11.5}$$

where for $\kappa = 7$, the value of subscript j = 1 and for $\kappa = 8$, j = 2. In Prouvost's model, monomeric alcohol reactions are considered. The following thermodynamic constants are used in the model:

k_{w1} = partition coefficient of monomeric alcohol 7 between aqueous and oleic pseudophases
k_{m1} = partition coefficient of monomeric alcohol 7 between interfacial and oleic pseudophases
k_1 = self-association constant of monomeric alcohol 7 in oleic pseudophase
a = ratio of molar volume of monomeric alcohol 7 to equivalent molar volume of surfactant

k_{w2}, k_{m2}, k_2, and b are similar constants for alcohol 8.

The above parameters are input to the simulator. A material balance gives the following relationships:

$$C_\kappa = \frac{A_j C_1}{D_j + \gamma_j C_2} + \frac{B_j C_3}{E_j} \qquad \text{for } \kappa = 7, j = 1 \text{ ; } \kappa = 8, j = 2 \tag{11.6}$$

where

$$\begin{aligned}
A_1 &= \gamma_1 k_{w1}\left[1 + \gamma_1 + \gamma_2\left(1 + k_2\right)\right] \\
B_1 &= a\gamma_1 k_{m1}\left[1 + \gamma_1 + \gamma_2\left(1 + k_2\right)\right] \\
D_1 &= \left\{\left[1 + \gamma_2 + \gamma_1\left(1 + k_1\right)\right]\left[1 + \gamma_1 + \gamma_2\left(1 + k_2 - k_{w2}\right)\right] - \gamma_1 k_{w1}\left[1 + \gamma_1 + \gamma_2\left(1 + k_2\right)\right]\right\} \\
E_1 &= \left\{\left[1 + \gamma_2 + \gamma_1\left(1 + k_1\right)\right]\left[1 + \gamma_1 + \gamma_2\left(1 + k_2 - k_{m2}\right)\right] - \gamma_1 k_{m1}\left[1 + \gamma_1 + \gamma_2\left(1 + k_2\right)\right]\right\}
\end{aligned} \tag{11.7}$$

$$\begin{aligned}
A_2 &= \gamma_2 k_{w2}\left[1 + \gamma_2 + \gamma_1\left(1 + k_1\right)\right] \\
B_2 &= b\gamma_2 k_{m2}\left[1 + \gamma_2 + \gamma_1\left(1 + k_1\right)\right] \\
D_2 &= \left\{\left[1 + \gamma_1 + \gamma_2\left(1 + k_2\right)\right]\left[1 + \gamma_2 + \gamma_1\left(1 + k_1 - k_{w1}\right)\right] - \gamma_2 k_{w2}\left[1 + \gamma_2 + \gamma_1\left(1 + k_1\right)\right]\right\} \\
E_2 &= \left\{\left[1 + \gamma_1 + \gamma_2\left(1 + k_2\right)\right]\left[1 + \gamma_2 + \gamma_1\left(1 + k_1 - k_{m1}\right)\right] - \gamma_2 k_{m2}\left[1 + \gamma_2 + \gamma_1\left(1 + k_1\right)\right]\right\}
\end{aligned} \tag{11.8}$$

C_7 and C_8 are the overall volume fractions of alcohol 7 and alcohol 8 in the gridblock and are known values from the solution of species conservation equations. Knowing C_7 and C_8, Eqs. 11.7 and 11.8 are solved for γ_1 and γ_2 using the Newton Raphson iteration method, and then the other four intensive parameters are calculated:

$$\lambda_j = \frac{A_j}{D_j} \quad \text{for } j = 1, 2 \tag{11.9}$$

$$\sigma_j = \frac{B_j}{E_j} \quad \text{for } j = 1 , 2 \tag{11.10}$$

Once λ_j, γ_j, and σ_j are determined, alcohol partition coefficients K_κ^2, and K_κ^3 are calculated using Eqs. 11.4 and 11.5. When only a single alcohol is used, Eq. 11.6 reduces to the following cubic equation:

$$A'\,\gamma^3 + B'\,\gamma^2 + C'\,\gamma + D' = 0 \tag{11.11}$$

where

$$A' = (1 + k - k_m)\,(1 + k - k_w) \tag{11.12}$$

$$B' = k_w(1 + k - k_m)\frac{C_1}{C_2} + ak_m(1 + k - k_m)\frac{C_3}{C_2} - (1 + k - k_m)(1 + k - k_w)\frac{C_1}{C_2} + 2 + 2k - k_m - k_w \tag{11.13}$$

$$C' = k_w\frac{C_1}{C_2} + ak_m\frac{C_3}{C_2} - (2 + 2k - k_m - k_w)\frac{C_1}{C_2} + 1 \tag{11.14}$$

$$D' = \frac{C_7}{C_2} \tag{11.15}$$

Then the partition coefficients are calculated using:

$$K_7^2 = \frac{1 + \gamma(1 + k - k_w)}{k_w} \tag{11.16}$$

$$K_7^3 = \frac{a\,k_m[1 + g(1 + k - k_w)]}{k_w[1 + g(1 + k - k_m)]} \tag{11.17}$$

For two alcohols, the overall alcohol volumes are related to the overall volumes of water (C_1), oil (C_2), and surfactant (C_3) pseudocomponents by:

$$C_\kappa = \lambda_j\,C_1 + \gamma_j\,C_2 + \sigma_j\,C_3 \quad \text{for } \kappa = 7, j = 1 \;;\; \kappa = 8, j = 2 \tag{11.18}$$

The above equations, can be written in terms of the alcohol partition coefficients as:

$$C_\kappa = \lambda_j\,C_1 + \lambda_j\,K_\kappa^2\,C_2 + \lambda_j\,K_\kappa^3\,C_3 \quad \text{for } \kappa = 7, j = 1 \;;\; \kappa = 8, j = 2 \tag{11.19}$$

From above equations the parameters λ_j are defined as:

$$\lambda_j = \frac{C_\kappa}{C_1 + K_\kappa^2 C_2 + K_\kappa^3 C_3} \qquad \text{for } j = 1, 2 \tag{11.20}$$

λ_j is then used in calculating the pseudocomponents that are the apexes of the pseudoternary diagram.

C_{P1}= (water volume) + (alcohol volumes associated with water) = C_1 (1 + λ_1 + λ_2) (11.21)

C_{P2} = (oil volume) + (alcohol volumes associated with oil)

$$= C_2(1+\gamma_1+\gamma_2) = C_2(1+\gamma_1 K_7^2 + \lambda_2 K_8^2) \tag{11.22}$$

C_{P3} = (water volume) + (alcohol volumes associated with water)

$$= C_3(1+\sigma_1+\sigma_2) = C_3(1+\gamma_1 K_7^3 + \lambda_2 K_8^3) \tag{11.23}$$

The calculation of the pseudocomponent volumes is summarized below:

1. Using Newton Raphson iteration, calculate γ_1 and γ_2 from Eqs. 11.3 and 11.4.
2. Calculate λ_j and σ_j using Eqs. 11.9 and 11.10.
3. a) Calculate K_κ^2 and K_κ^3 using Eqs. 11.4 and 11.5. If there is only one alcohol, use Eq. 11.11 to calculate γ. Then calculate the partition coefficients using Eqs. 11.16 and 11.17.
   b) If constant partition coefficient option is used, K_κ^2 and K_κ^3 are input parameters.
   c) Calculate λ_j using Eq. 11.20.
4. Calculate the volume of the pseudocomponents, C_{P1}, C_{P2}, and C_{P3}, using Eqs. 11.21-11.23.

Above calculations are made in Subroutines ALCPTN and TWOALC.

11.3 Effective Salinity

Hirasaki [1982] introduced a model to account for the change in optimal salinity with respect to changes in the concentration of alcohol and calcium. Camilleri *et al.* [1987c] extended Hirasaki's model to entire salinity space to define an effective salinity for the case with one alcohol:

$$C_{SE} = \frac{C_{51}}{(1-\beta_6 f_6^S)(1-\beta_\kappa f_\kappa^S)} \tag{11.24}$$

C_{SE} is the effective salinity, and β_6 and β_κ are the slope parameters for calcium and alcohol dilution effects. f_6^S is the fraction of calcium cations associated with surfactant micelles and is given in Section 2. f_κ^S is defined as:

$$f_\kappa^S = \frac{\text{total volume of alcohol associated with surfactant}}{\text{total volume of surfactant pseudocomponent}} = \frac{\sigma}{1+\sigma} \tag{11.25}$$

β_6 and β_κ are determined by matching an experimental salinity requirement diagram such as those reported by Nelson [1982] or equivalent diagrams (Satoh, 1984). For formulations containing only one alcohol,

C_{SEL} and C_{SEU} are constant for a fixed chemical formulation and are determined using Eq. 11.24. If there is no calcium present, Eq. 11.24 represents a group of straight lines which pass through the fixed point (0, $-1/\beta_\kappa$). If calcium is present, then it represents a group of planes which pass through the three fixed points (0, $-1/\beta_\kappa$, 0), (0, 0, $1/\beta_\kappa$), and (0, $-1/\beta_\kappa$, $1/\beta_6$). Due to the fact that Eq. 11.24 is nonlinear, these planes are not flat . The calculated effective salinity becomes negative when $f_6^S > 1/\beta_6$ or β_κ is negative and $f_\kappa^S > 1/|\beta_\kappa|$.

Since different alcohols give different salinity limits, the following effective salinity is defined for the case when there are two alcohols present:

$$C_{SE} = \frac{C_{51}}{(1-\beta_6 f_6^S)(1+\beta_7 f_7^S + \beta_8 f_8^S)} \tag{11.26}$$

where the effective salinity limits are not constant in this case and are calculated by:

$$C_{SEL} \frac{C_{SEL7}\left|\beta_7 f_7^S\right| + C_{SEL8}\left|\beta_8 f_8^S\right|}{\left|\beta_7 f_7^S\right| + \left|\beta_8 f_8^S\right|} \tag{11.27}$$

$$C_{SEU} \frac{C_{SEU7}\left|\beta_7 f_7^S\right| + C_{SEU8}\left|\beta_8 f_8^S\right|}{\left|\beta_7 f_7^S\right| + \left|\beta_8 f_8^S\right|} \tag{11.28}$$

C_{SEL7}, C_{SEL8}, C_{SEU7}, and C_{SEU8} are effective salinity limits for alcohol 7 and 8. C_{SEL7} and C_{SEU7} are determined when alcohol 7 is the only alcohol present and are calculated using Eq. 11.24. Similar independent calculations are made for alcohol 8. For the two alcohol case, f_7^S and f_8^S are defined as:

$$f_\kappa^S = \frac{\text{total volume of alcohol k associated with surfactant}}{\text{total volume of surfactant pseudocomponent}}$$

$$= \frac{\sigma_1}{1+\sigma_1+\sigma_2} = \frac{\lambda_j K_\kappa^3}{1+\lambda_1 K_7^3 + \lambda_2 K_8^3} \quad \text{for } \kappa = 7,\ j = 1\ ;\ \kappa = 8,\ j = 2 \tag{11.29}$$

K_κ^3 and λ_j are calculated as outlined in the previous section.

Once effective salinity is calculated, the phase environment (Fig. 11.1) for each gridblock is determined according to:

$C_{SE} < C_{SEL}$	Type II(-)
$C_{SEL} \bullet C_{SE} \bullet C_{SEU}$	Type III
$C_{SE} > C_{SEU}$	Type II(+)

Effective salinity is calculated in Subroutine CSECAL.

11.4 Flash Calculations

A binodal curve is an intercept of a binodal surface and a pseudoternary plane. The original simulator introduced by Pope and Nelson [1978] could treat nonsymmetric binodal curves; however, the present simulator can treat only a symmetric binodal curve. The effects of alcohol on the height of the binodal curve was included which can increase as the total chemical increases. The following linear relationship between the height of the binodal curve (C_{3max}) and f_{κ}^{S} is used for the case with one alcohol (Fig. 11.2):

$$C_{3max,\kappa m} = m_{\kappa m}\, f_{\kappa}^{S} + C_{\kappa m} \qquad \text{for } m = 0, 1, 2;\ \kappa = 7 \tag{11.30}$$

where m = 0 means at zero salinity, 1 means at optimal salinity, and 2 means at two times the optimal salinity. $m_{\kappa m}$ is the slope for maximum height of binodal curve vs. fraction of alcohol (alcohol 7 or alcohol 8 for the two alcohol case) associated with the surfactant pseudocomponent at salinity m. $C_{\kappa m}$ is the intercept of maximum height of the binodal curve at zero fraction of alcohol (alcohol 7 or alcohol 8 for the two alcohol case) associated with the surfactant pseudocomponent at salinity m. Parameters $m_{\kappa m}$ and $C_{\kappa m}$ are obtained by matching the volume fraction diagrams corresponding to at least three different total chemical (alcohol + surfactant) compositions. For the first iteration, the slope parameters are set to zero and the intercept parameters are adjusted in order to obtain a reasonable match of the volume fraction diagrams; then the slope parameters are obtained. Having obtained the slope parameters, the matching procedure is repeated for further improvements. This matching is done using single alcohol experiments independently for alcohol 7 and alcohol 8 using Eq. 11.30. The variables HBNC70, HBNC71, HBNC72 in Fig. 11.2 are the UTCHEM input parameters for $C_{\kappa m}$ at three values of m. The variables HBNS70, HBNS71, HBNS72 in Fig. 11.2 are the UTCHEM input parameters for $m_{\kappa m}$ at three values of m.

The following equations are used for calculating the height of the binodal curve for the two alcohol case:

$$C_{3max,\kappa m} = m_{\kappa m}\left(f_{7}^{S} + f_{8}^{S}\right) + C_{\kappa m} \qquad \text{for } \kappa = 7 \text{ and } 8 \tag{11.31}$$

$$C_{3maxm} = C_{3max,8m} + \left(C_{3max,7m} - C_{3max,8m}\right)\frac{f_{7}^{S}}{f_{7}^{S} + f_{8}^{S}} = \left(m_{7m} + \frac{C_{7m}}{f_{7}^{S} + f_{8}^{S}}\right) f_{7}^{S} + \left(m_{8m} + \frac{C_{8m}}{f_{7}^{S} + f_{8}^{S}}\right) f_{8}^{S} \tag{11.32}$$

The following Hand equations are used for phase behavior calculations:

$$\frac{C_{P3}}{C_{P2}} = A\left(\frac{C_{P3}}{C_{P1}}\right)^{B} \tag{11.33}$$

$$\frac{C_{P3\ell}}{C_{P2\ell}} = E\left(\frac{C_{P3\ell'}}{C_{P1\ell}}\right)^{F} \tag{11.34}$$

Equation 11.33 defines the binodal curve for all types of phase behavior, and Eq. 11.34 defines the distribution curve (tielines) when two phases exist (Type II(-) or Type II(+)). C_{P1}, C_{P2}, and C_{P3} represent pseudocomponents defined by Eqs. 11.21-11.23. $C_{P2\ell}$, $C_{P3\ell}$, $C_{P1\ell'}$, and $C_{P3\ell'}$ represent phase concentrations of the pseudocomponents in the two pseudophases ℓ and ℓ'. Because pseudocomponent concentrations are in volume fractions, they must add up to one; therefore the following constraints are used:

$$C_{P1}+ C_{P2} + C_{P3} = 1 \tag{11.35}$$

$$C_{P1\ell}+ C_{P2\ell} + C_{P3\ell} = 1 \tag{11.36}$$

$$C_{P1\ell'}+ C_{P2\ell'} + C_{P3\ell'} = 1 \tag{11.37}$$

The total composition, C_{P1}, C_{P2}, and C_{P3}, is known. Therefore there are five equations and six unknowns ($C_{P\kappa\ell}$, $\kappa = 1, 2, 3$, $\ell = 1, 2$). Any phase concentration can be chosen and varied between 0 and 1 to sweep the phase diagram. Since only symmetric binodal curves are modeled in the simulator, parameter B is equal to -1 and parameter F is equal to 1. Parameter A in Eq. 11.33 is related to the height of the binodal curve by:

$$A = \left(\frac{2C_{3\max}}{1 - C_{3\max}} \right)^2 \tag{11.38}$$

Linear interpolation is then used to determine the A parameter for arbitrary effective salinity values. The reason for interpolating A instead of the maximum height of the binodal curve, $C_{3\max}$, is that, at high salinity, $C_{3\max}$ exceeds unity, which means the binodal curve is outside the ternary diagram. To avoid this problem, the interpolation is done on A. The following linear interpolation equations are used:

$$A = (A_0 - A_1)\left(1 - \frac{C_{SE}}{C_{SEOP}}\right) + A_1 \quad \text{for } C_{SE} \bullet C_{SEOP} \tag{11.39}$$

$$A = (A_2 - A_1)\left(1 - \frac{C_{SE}}{C_{SEOP}}\right) + A_1 \quad \text{for } C_{SE} > C_{SEOP} \tag{11.40}$$

where C_{SEOP} is the optimum effective salinity (CSEOP = 1/2 (CSEL+CSEU)).

Parameter E is calculated from the location of the plait point. From the phase distribution equation (Eq. 11.34) and the plait point P:

$$\frac{C_{P3P}}{C_{P2P}} = E\left(\frac{C_{P3P}}{C_{P1P}}\right)^F \tag{11.41}$$

and since the plait point is also on the binodal curve:

$$\frac{C_{P3P}}{C_{P2P}} = A\left(\frac{C_{P3P}}{C_{P1P}}\right)^B \tag{11.42}$$

Also:

$$C_{P1P} + C_{P2P} + C_{P3P} = 1 \tag{11.43}$$

For the case when B = -1 and F = 1 (symmetric binodal curve), all phase concentrations can be calculated explicitly. From Eq. 11.36:

$$C_{P11} = 1 - C_{P21} - C_{P31} \tag{11.44}$$

Now substituting Eq. 11.44 in Eq. 11.33, C_{P31} can be calculated as a function of C_{P21}:

$$C_{P31} = \frac{1}{2}\left(-AC_{P21} + \sqrt{(AC_{P21})^2 + 4AC_{P21}(1 - C_{P21})}\right) \tag{11.45}$$

and from Eq. 11.42:

$$E = \frac{C_{P1P}}{C_{P2P}} \tag{11.46}$$

where C_{P2P}, the oil pseudocomponent concentration at the plait point, is an input parameter in the simulator, and

$$C_{P3P} = \frac{1}{2}\left(-AC_{P2P} + \sqrt{(AC_{P2P})^2 + 4AC_{P2P}(1 - C_{P2P})}\right) \tag{11.47}$$

Then from Eq. 11.36:

$$C_{P1P} = 1 - C_{P2P} - C_{P3P} \tag{11.48}$$

knowing C_{P1P}, parameter E can be calculated from Eq. 11.46. Having calculated C_{P31} and C_{P11} from Eqs. 11.44 and 11.45, C_{P22} is calculated from the following:

$$C_{P22} = \frac{A}{h^2 + Ah + A} \tag{11.49}$$

where

$$h = E\frac{C_{P31}}{C_{P11}} \tag{11.50}$$

Then C_{P32} is calculated from

$$C_{P32} = h\, C_{P22} \tag{11.51}$$

and

$$C_{P12} = 1 - C_{P22} - C_{P32} \tag{11.52}$$

The above calculations are performed when there are only two phases present, for Type II(-) or Type II(+) phase behavior. The only difference between the two cases is that for Type II(-) phase behavior C^*_{P2PR} and for Type II(+) phase behavior C^*_{P2PL}, are used for C_{P2P} in the above equations. The distribution of the three pseudocomponents in the two phases for Type II(-) and Type II(+) phase behavior are summarized below:

11.4.1 For Type II(-) Phase Behavior, $C_{SE} < C_{SEL}$

Known values for this case are C_{3max0}, C_{3max1}, C_{3max2}, C_{SE}, C_{SEL}, C_{SEU}, C^*_{P2PR} and overall concentration of the pseudocomponents, C_{P1}, C_{P2}, and, C_{P3}.

1. Calculate parameter A from Eq. 11.39.
2. Using C^*_{P2PR} calculate C^*_{P3PR} and C^*_{P1PR} using Eqs. 11.47-11.48.
3. Calculate parameter E using Eq. 11.46 and C^*_{P1PR} and C^*_{P2PR}.
4. Vary the value of C_{P21} from 0 to C^*_{P2PR}, calculate C_{P11} and C_{P31} using Eqs. 11.44-11.45.
5. Calculate h from Eq. 11.50.
6. Calculate C_{P22}, C_{P32}, and C_{P12} using Eqs. 11.49-11.52.
7. If $(C_{P32} - C_{P3})(C_{P21} - C_{P2}) - (C_{P31} - C_{P3})(C_{P22} - C_{P2}) \bullet \varepsilon$, where ε is a sufficiently small number (10^{-4}), then stop; otherwise increment C_{P21} using the half interval method and go to step 4.

11.4.2 For Type II(+) Phase Behavior, $C_{SE} > C_{SEU}$

Known values for this case are C_{3max0}, C_{3max1}, C_{3max2}, C_{SEL}, C_{SE}, C_{SEU}, C^*_{P2PL} and overall concentration of the pseudocomponents, C_{P1}, C_{P2}, and .C_{P3}.

1. Calculate parameter A from Eq. 11.40.
2. Using C^*_{P2PL} calculate C^*_{P3PL} and C^*_{P1PL} from Eqs. 11.47-11.48.
3. Calculate parameter E using Eq. 11.46 and C^*_{P1PL} and C^*_{P2PL}.

4-7. Steps 4-7 as in the Type II(-) described above.

For Type III phase behavior, the tie lines for the left (Type II(+)) and the right (Type (-)) lobes are calculated separately. Because of the symmetric binodal curve assumption, the binodal curve is calculated in the same manner as in the Type II(-) and Type II(+) cases. The invariant point M is calculated as follows:

$$a = \frac{C_{SE} - C_{SEL}}{C_{SEU} - C_{SEL}} \tag{11.53}$$

where

$$\frac{a - C_{P2M}}{C_{P3M}} = \text{Cos } 60^\circ \tag{11.54}$$

Therefore, $C_{P3M} = 2(a - C_{P2M})$.

Since the invariant point M is on the binodal curve, Eq. 11.33 can be used to calculate C_{P3M} as a function of C_{P2M} using Eq. 11.45:

$$C_{P3M} = \frac{1}{2}\left(-AC_{P2M} + \sqrt{(AC_{P2M})^2 + 4AC_{P2M}(1 - C_{P2M})}\right) \tag{11.55}$$

Solving Eqs. 11.54-11.55 for C_{P2M}, the following is obtained:

$$C_{P2M} = \frac{2a(4-A) + A \pm \sqrt{(2a(4-A)+A)^2 - 16a^2(4-A)}}{2(4-A)} \tag{11.56}$$

The invariant point should disappear when C_{SE} approaches C_{SEL} (C_{P2M} = 0, a = 0) and when C_{SE} approaches C_{SEU} (C_{P2M} = 1, a = 1). These conditions hold only for the negative sign in Eq. 11.56. Therefore, the composition at the invariant point is determined by Eq. 11.55, Eq. 11.56 with the negative sign, and by

$$C_{P1M} = 1 - C_{P3M} - C_{P2M} \tag{11.57}$$

The plait point for the left lobe of the Type III phase environment must vary between zero and the plait point for the Type II(+) value, C^{*}_{P2PL}. The plait point is calculated by salinity interpolation:

$$C_{P2PL} = C^{*}_{P2PL} + \frac{C_{P2PL}}{C_{SEU} - C_{SEL}}(C_{SE} - C_{SEU}) \tag{11.58}$$

In order to apply the Hand equations to the left lobe, a coordinate transformation is made (Fig. 11.3). The Hand distribution equation in the new coordinate system is :

$$\frac{C'_{P32}}{C'_{P22}} = E\left(\frac{C'_{P31}}{C'_{P11}}\right) \tag{11.59}$$

where

$$C'_{P\,2\ell} = C_{P2\ell} \operatorname{Sec}\theta \tag{11.60}$$

$$C'_{P\,3\ell} = C_{P3\ell} - C_{P2\ell} \tan\theta \tag{11.61}$$

$$C'_{P\,1\ell} = 1 - C'_{P\,2\ell} - C'_{P\,3\ell} \tag{11.62}$$

Now let

$$\beta = \operatorname{Sec}\theta = \frac{\sqrt{(C_{P2M})^2 + (C_{P3M})^2}}{C_{P2M}} \tag{11.63}$$

$$\alpha = \tan\theta = \frac{C_{P3M}}{C_{P2M}} \tag{11.64}$$

Because of the symmetric binodal curve assumption (F=1), E can be calculated explicitly from:

$$E = \frac{C'_{P1P}}{C'_{P2P}} \frac{1-(\beta-\alpha)C_{P2P} - C_{P3P}}{\beta C_{P2P}} \tag{11.65}$$

where C_{P2P} is equal to C_{P2PL} calculated using Eq. 11.58, and C_{P3P} and C_{P1P} are calculated from Eqs. 11.47 and 11.48.

C_{P11} and C_{P31} are calculated by Eqs. 11.44-11.45. Now Eq. 11.59 can be solved as before:

$$C_{P22} = \frac{A}{h'^2 + A\,h' + A} \tag{11.66}$$

where

$$h' = \frac{b\,E\,C'_{P31}}{C'_{P11}} \tag{11.67}$$

and

$$C_{P32} = h'\,C_{P22} \tag{11.68}$$

$$C_{P12} = 1 - C_{P22} - C_{P32} \tag{11.69}$$

Therefore all phase concentrations for the two phases in the left lobe have been determined.

The calculations for the right lobe are very similar to the above calculations for the left lobe. The C_{P2P} value for the plait point in this case varies between 1 and the input value for the Type II(-) case, C^*_{P2PR}, and is calculated by:

$$C_{P2PR} = C^*_{P2PR} + \left(\frac{1-C^*_{P2PR}}{C_{SEU} - C_{SEL}}\right)(C_{SE} - C_{SEL}) \tag{11.70}$$

Then C_{P32} is calculated using Eq. 11.45 but as a function of C_{P12} instead of C_{P21}:

$$C_{P32} = \frac{1}{2}\left(-AC_{P12} + \sqrt{(AC_{P12})^2 + 4AC_{P12}(1-C_{P12})}\right) \tag{11.71}$$

and

$$C_{P22} = 1 - C_{P12} - C_{P32} \tag{11.72}$$

Now let

$$h' = \frac{b\,C'_{P32}}{E\,C'_{P11}} + a \tag{11.73}$$

Then

$$C_{P11} = \frac{A}{h'^2 + A h' + A} \tag{11.74}$$

$$C_{P31} = h' C_{P11} \tag{11.75}$$

$$C_{P21} = 1 - C_{P11} - C_{P31} \tag{11.76}$$

where

$$\alpha = \frac{C_{P3M}}{C_{P1M}} \tag{11.77}$$

$$\beta = \frac{\sqrt{C_{P3M}^2 + C_{P1M}^2}}{C_{P1M}} \tag{11.78}$$

$$C'_{P1\ell} = \beta\, C_{P1\ell} \tag{11.79}$$

$$C'_{P3\ell} = C_{P3\ell} - \alpha\, C_{P1\ell} \tag{11.80}$$

$$C'_{P2\ell} = 1 - C'_{P3\ell} - C'_{P1\ell} \tag{11.81}$$

$$E = \frac{C'_{P1P}}{C'_{P2P}} = \frac{\beta C_{P1P}}{1 - (\beta - \alpha) C_{P1P} - C_{P3P}} \tag{11.82}$$

C'_{P1P} and C'_{P2P} are calculated using Eqs. 11.79-11.81 and Eqs. 11.47-11.48.

When three phases exist, the water and oil pseudocomponents are assumed to contain no surfactant pseudocomponent. This assumption is a consequence of the choice of phase behavior in the three phase region which assumes that the two phase region below the three phase tie triangle is very small; therefore, any composition in the three phase region will have three phases comprising of the surfactant-rich pseudophase with the composition of the invariant point, water-rich pseudophase with the composition of the water pseudocomponent apex, and oil-rich pseudophase with the composition of the oil pseudocomponent apex. Therefore:

$$C_{P11} = C_{P22} = 1 \tag{11.83}$$

$$C_{P21} = C_{P31} = C_{P12} = C_{P32} = 0 \tag{11.84}$$

The composition of the third phase, C_{P13}, C_{P23}, and C_{P33}, is calculated using Eqs. 11.55-11.57. Phase concentrations in the single phase region are the same as the overall composition, $C_{P13} = C_{P1}$, $C_{P23} = C_{P2}$, $C_{P33} = C_{P3}$. The other phase concentrations are zero.

The distribution of the three pseudocomponents in the two or three pseudophases for Type III phase behavior are summarized below:

11.4.3 For Type III Phase Behavior, C_{SEL} •C_{SE} • C_{SEU}

Known values for this case are: C_{3max0}, C_{3max1}, C_{3max2}, C_{SE}, C_{SEL}, C_{SEU}, C^{*}_{P2PR}, C^{*}_{P2PL} and overall concentration of the pseudocomponents, C_{P1}, C_{P2}, and .C_{P3}.

1. Calculate parameter A from Eq. 11.39-11.40.
2. Calculate C_{P2M} from Eqs. 11.56.
3. Calculate C_{P3M} and C_{P1M} from Eqs. 11.55-11.57.
4. <u>If the total composition is in the three phase region:</u>
   - Calculate water and oil pseudophase concentrations from Eqs. 11.83-11.84.
   - $C_{P23} = C_{P2M}$ calculated in step 2. $C_{P33} = C_{P3M}$ and $C_{P13} = C_{P1M}$ calculated in step 3.
5. <u>If the total composition is in Type II(+) lobe of Type III:</u>
   - Calculate C_{P2PL} from Eq. 11.58.
   - Calculate a and b from Eqs. 11.63-11.64.
   - Calculate C_{P3PL} and C_{P1PL} from Eqs. 11.47-11.48 using C_{P2PL}.
   - Calculate parameter E from Eq. 11.65.

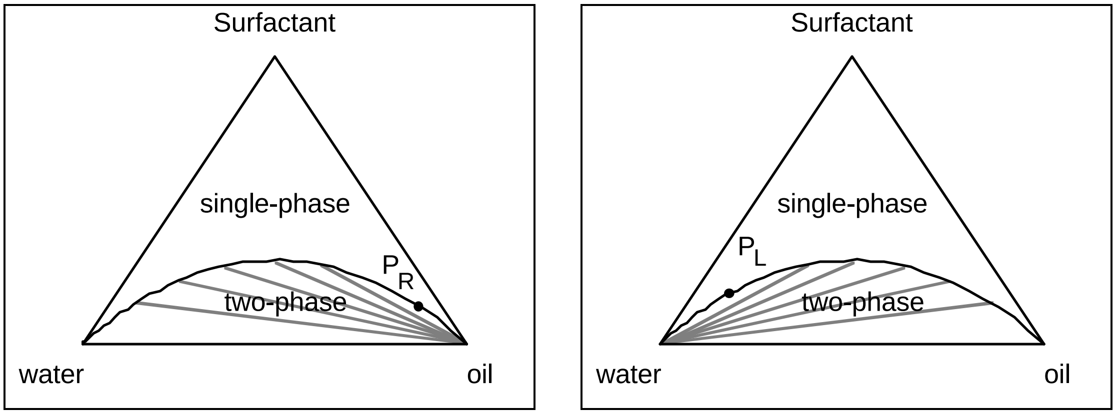
   * Using a value of C_{P21} from 0 to C_{P2PL}, calculate C_{P11} and C_{P31} using Eqs. 11.44-11.45.

   - Calculate C'_{P31} and C'_{P11} from Eqs. 11.61-11.62.
   - Calculate h' from Eq. 11.67.
   - Calculate C_{P22}, C_{P32}, and C_{P12} using Eqs. 11.66, 11.68, and 11.69.
   - If $(C_{P33} - C_{P3}) (C_{P21} - C_{P2}) - (C_{P31} - C_{P3}) (C_{P23} - C_{P2})$ • ε , where ε is a sufficiently small number (10^{-4}), then stop; otherwise increment C_{P21} using the half interval method and go back to step *****.
6. <u>If the total composition is in Type II(-) lobe of Type III:</u>
   - Calculate C_{P2PR} from Eq. 11.70.
   - Calculate α and β from Eqs. 11.77-11.78.
   - Calculate C_{P3PR} and C_{P1PR} from Eqs. 11.47-11.48 using C_{P2PR}.
   - Calculate parameter E from Eq. 11.82.

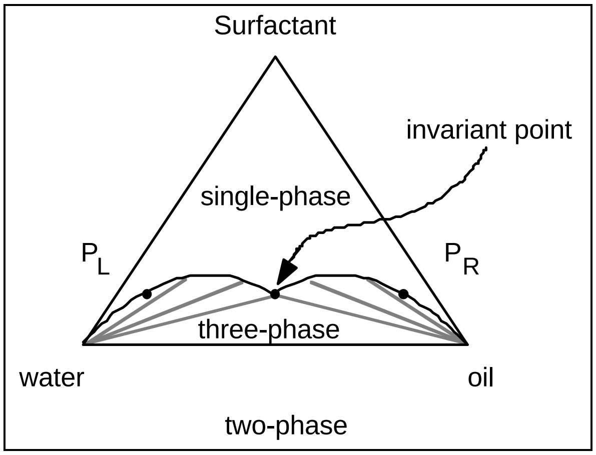
   ** Using a value of C_{P12} from 0 to C_{P1PR}, calculate C_{P32} and C_{P22} using Eqs. 11.71-11.72.

- Calculate C'_{P31} and C'_{P11} from Eqs. 11.79-11.80.
- Calculate h' from Eq. 11.73.
- Calculate C_{P11}, C_{P31}, and C_{P21} using Eqs. 11.74-11.76.
- If $(C_{P32} - C_{P3}) (C_{P23} - C_{P2}) - (C_{P33} - C_{P3}) (C_{P22} - C_{P2}) \bullet \varepsilon$, where ε is a sufficiently small number (10^{-4}), then stop; otherwise increment C_{P12} using the half interval method and go back to step ******.

After the phase composition in the pseudoternary diagram and saturations are determined, the phase concentrations are converted back to the pseudoquaternary diagram using Eqs. 11.21-11.23. Phase compositions are calculated in Subroutine PHCOMP.



a) Type II(-) b) Type II (+)



c) Type III

Figure 11.1. Schematic representations of a) Type II(-), b) Type II(+), and c) Type III.

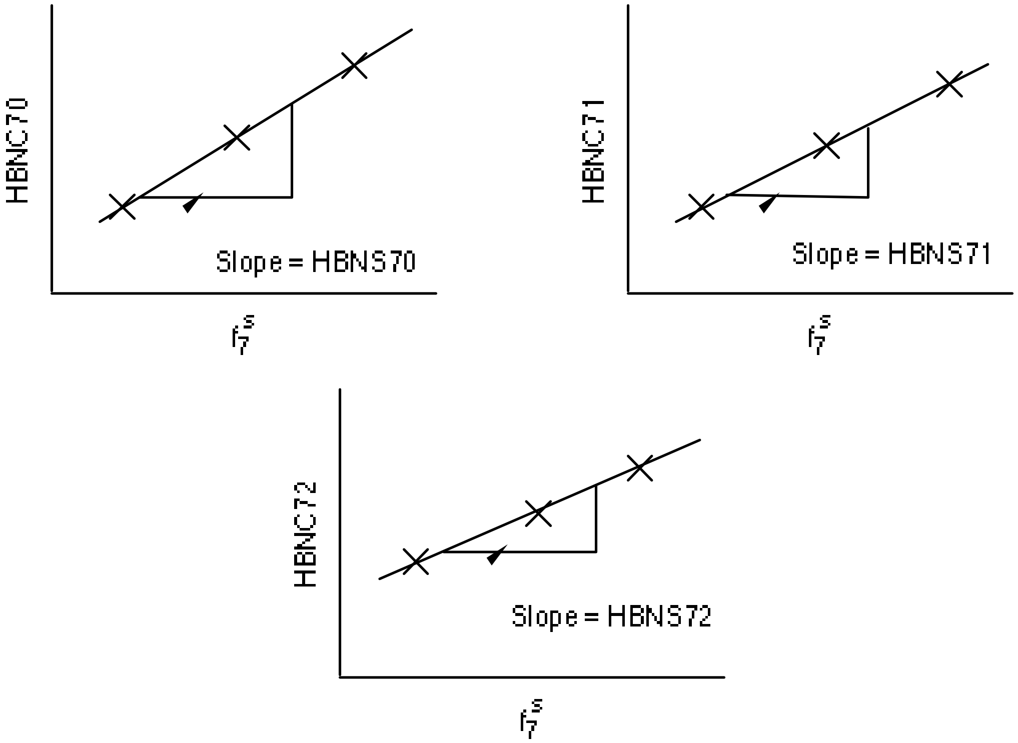


Figure 11.2. Effect of alcohol on the maximum height of binodal curve.

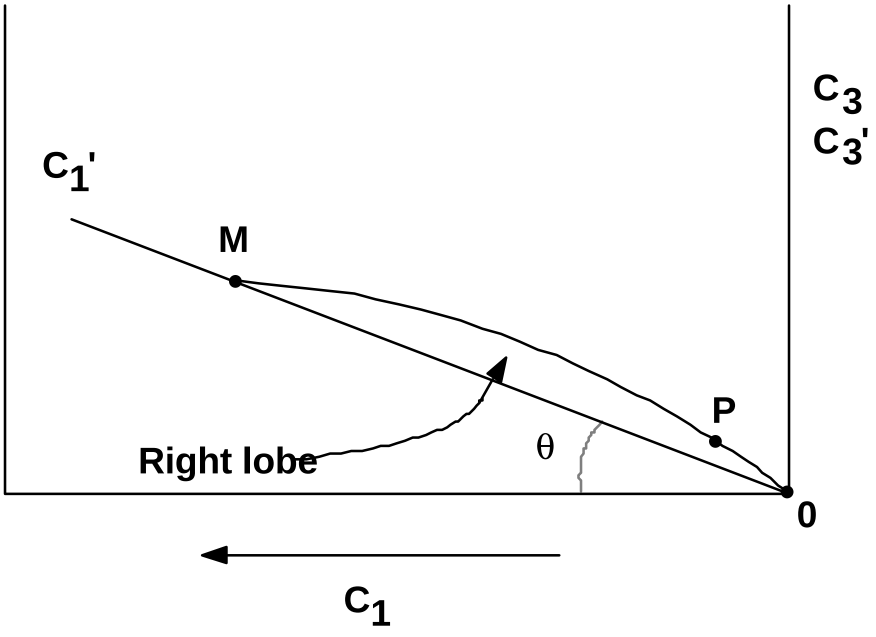


Figure 11.3. Coordinate transformation for Type III.

Section 12
Organic Dissolution Model in UTCHEM

12.1 Introduction

Both equilibrium and rate limited nonequilibrium solubility of organic component in the aqueous phase are modeled in UTCHEM. The rate limited mass transfer equations are used for the enhance solubility of oil in the presence of surfactant. The current implementation in UTCHEM is for under optimum Type II(-) surfactant formulation. However, it can be applied to the Type III phase environment. This section discusses the formulation and the method of solution for the case of single component oil phase. The formulation of the multiple organic oleic phase is given in Section 7.

12.2 Saturated Zone (Gas Phase Is Not Present)

The overall component concentrations for water ($\kappa = 1$), oil ($\kappa = 2$), and surfactant ($\kappa = 3$) in two-phase flow of water/oil or microemulsion/oil from the conservation equations are

$$C_1 = C_{11}S_1 + C_{12}S_2 \qquad (12.1a)$$

$$C_2 = C_{21}S_1 + C_{22}S_2 \qquad (12.1b)$$

$$C_3 = C_{31}S_1 + C_{32}S_2 \qquad (12.1c)$$

where phase 2 refers to the oil phase and phase 1 in this section refers to either water or surfactant rich microemulsion phase.

The overall concentrations for oil, water, and surfactant are obtained solving the conservation equations as below

$$\frac{\partial(\phi C_\kappa)}{\partial t} + \vec{\nabla} \cdot \left(\tilde{F}_{\kappa 1} + \tilde{F}_{\kappa 2}\right) = Q_{\kappa 1} + Q_{\kappa 2} \quad \text{for } \kappa = 1, 2, 3 \qquad (12.2)$$

where the flux term is the sum of the convective and dispersive fluxes as

$$\begin{aligned} \tilde{F}_{\kappa 1} &= C_{\kappa 1}\vec{u}_1 - \phi S_1 \vec{\vec{K}}_{\kappa 1} \cdot \vec{\nabla} C_{\kappa 1} \\ \tilde{F}_{\kappa 2} &= C_{\kappa 2}\vec{u}_2 - \phi S_2 \vec{\vec{K}}_{\kappa 2} \cdot \vec{\nabla} C_{\kappa 2} \end{aligned} \quad \text{for } \kappa = 1 \text{ or } 2 \qquad (12.3)$$

The definitions of the dispersion tensor and the flux are given in Section 2. The nonequilibrium concentration of oil in the aqueous phase is computed from the mass balance on oil species in the aqueous phase and using the first order mass transfer rate equation for oil dissolution as

$$\frac{\partial(\phi S_1 C_{21})}{\partial t} + \vec{\nabla} \cdot \tilde{F}_{21} = Q_{21} + M\left(C_{21}^{eq} - C_{21}\right) \tag{12.4}$$

where C_{21}^{eq} is the known limit of solubility for oil in the aqueous phase. In the absence of the surfactant, the C_{21}^{eq} is the limit of solubility for the specific organic contaminant and when surfactant is present the equilibrium solubility is calculated from the Hand's equations (Section 2). M is the mass transfer coefficient for the dissolution of organic species in the water phase and is assumed to be a constant. Equation 12.4 is solved either explicitly or implicitly as described below.

12.2.1 Organic Solubility

12.2.1.1 Explicit Solution

The new time level, (n+1), concentration of oil solubilized in water is

$$(\phi S_1 C_{21})^{n+1} = (\phi S_1 C_{21})^{n} + (Q_{21} - \vec{\nabla} \cdot \tilde{F}_{21})\Delta t + M\Delta t\left(C_{21}^{eq} - C_{21}^{n}\right) \quad \text{for } C_{21}^{n} < C_{21}^{eq} \tag{12.5}$$

where the right-hand side of the equation is a known quantity. Therefore,

$$(S_1 C_{21})^{n+1} = \frac{(\phi S_1 C_{21})^{n+1}}{\phi^{n+1}} \tag{12.6}$$

since the porosity is known either as a constant or is calculated based on the new time step pressure if rock compressibility is not negligible.

12.2.1.2 Implicit Solution

$$(\phi S_1 C_{21})^{n+1} = (\phi S_1 C_{21})^{n} + (Q_{21} - \vec{\nabla} \cdot \tilde{F}_{21})\Delta t + M\Delta t\left(C_{21}^{eq} - C_{21}^{n+1}\right) \tag{12.7}$$

where we define $\text{RHS} = (\phi S_1 C_{21})^{n} + (Q_{21} - \vec{\nabla} \cdot \tilde{F}_{21})\Delta t + M\Delta t\left(C_{21}^{eq} - C_{21}^{n+1}\right)$.

Substituting for S_1^{n+1} from overall concentration for oil component (Eq. 12.1b) and noting that ***C_{22} = 1 for the flow conditions of oil/water and the Type II(-) with corner plait point*** and the sum of the saturations is equal to one ($S_1 + S_2 = 1$), we have

$$\left(\phi C_{21} \frac{C_2 - 1}{C_{21} - 1}\right)^{n+1} = \text{RHS} \tag{12.8}$$

The above equation can then be rearranged in terms of oil concentration in the aqueous phase (C_{21}) as

$$M\,\Delta t\, C_{21}^2 + \text{bterm}\, C_{21} + \text{cterm} = 0 \tag{12.9}$$

where

$$\text{bterm} = \phi C_2 - \phi - M\Delta t - \text{cterm} \tag{12.10}$$

$$\text{cterm} = (\phi S_1 C_{21})^{n} + \Delta t\left(Q_{21} - \vec{\nabla} \cdot \tilde{F}_{21}\right) + M\,\Delta t\, C_{21}^{eq} \tag{12.11}$$

The solution to the quadratic equation (Eq. 12.9) is

$$\begin{cases} C_{21} = \dfrac{2\text{cterm}}{-\text{bterm} + \sqrt{(\text{bterm})^2 - 4M\,\Delta t(\text{cterm})}} & \text{for bterm} < 0 \\ C_{21} = \dfrac{2\text{cterm}}{-\text{bterm} - \sqrt{(\text{bterm})^2 - 4M\,\Delta t(\text{cterm})}} & \text{for bterm} > 0 \end{cases} \tag{12.12}$$

12.2.2 Phase Saturations

12.2.2.1 Oil/Water Phases (No Surfactant)

Substituting $C_{12} = 0.0$ and $C_{22} = 1.0$, Eqs. 12.1a and 12.1b become

$$\begin{aligned} C_1 &= C_{11} S_1 \\ C_2 &= C_{21} S_1 + S_2 \end{aligned} \tag{12.13}$$

The equilibrium saturations and concentrations are computed first as

$$S_2^{eq} = \frac{C_2 - \min(C_2, K_{ow})}{1 - \min(C_2, K_{ow})} \tag{12.14}$$

$$S_1^{eq} = 1. - S_2^{eq} \tag{12.15}$$

where K_{ow} is the limit of solubility of oil in water at equilibrium in the absence of surfactant or cosolvent and is an input parameter. The minimum in Eq. 12.14 is taken to ensure that the input solubility is not greater than the total oil available in a gridblock.

The nonequilibrium phase saturations and concentrations are computed as described below once the equilibrium organic concentration is solved for from Eq. 12.4.

12.2.2.1.1 Explicit Method

Since the product of water saturation times the oil concentration is known using the explicit solution (Eq. 12.6), the new time step oil saturation from Eq. 12.1b is

$$S_2 = C_2 - (C_{21} S_1)^{n+1} \quad \text{and} \quad S_1 = 1 - S_2 \tag{12.16}$$

The overall oil concentration (C_2) is computed from the oil material balance equation. The phase compositions are then as follows

$$\begin{aligned} C_{11} &= \frac{C_1}{S_1} \\ C_{21} &= \min\left(C_{21}^{eq}\, , \frac{(C_{21} S_1)^{n+1}}{S_1} \right) \\ C_{22} &= 1.0 \end{aligned} \tag{12.17}$$

If the calculated nonequilibrium concentration is greater than the equilibrium value ($C_{21} > C_{21}^{eq}$), the saturations are then set to the equilibrium values calculated from Eqs. 12.14 and 12.15.

12.2.2.1.2 Implicit Method

From the implicit solution of the mass balance equation for oil component in the aqueous phase, we could obtain the nonequilibrium organic dissolution in the aqueous phase (Eq. 12.12). The phase saturations and phase compositions are then calculated as

$$\begin{cases} C_{21}^{\text{noneq}} = \min(C_{21}^{\text{eq}}, C_{21}) \\ S_1 = \dfrac{C_1}{1 - C_{21}^{\text{noneq}}} \\ S_2 = 1 - S_1 \end{cases} \tag{12.18}$$

and

$$\begin{aligned} C_{11} &= \frac{C_1}{S_1} \\ C_{12} &= 0.0 \\ C_{22} &= 1.0 \end{aligned} \tag{12.19}$$

12.2.2.2 Oil/Aqueous Phases (Surfactant Below CMC)

The phase concentrations and saturations are calculated as above and surfactant concentration is

$$C_{31} = \frac{C_3}{S_1} \tag{12.20}$$

12.2.2.3 Oil /Microemulsion Phases (Type II (-) With Corner Plait Point)

For the case of corner plait point we have

$C_{22} = 1.0$, $C_{12} = 0.0$,   and $C_{32} = 0.0$

and the equilibrium concentrations of surfactant, oil, and water in microemulsion phase $\left(C_{11}^{\text{eq}}, C_{21}^{\text{eq}}, C_{31}^{\text{eq}}\right)$ are calculated from Hand's equations described in Section 2. Substituting these in the overall component concentrations, we have

$$\begin{aligned} C_1 &= C_{11} S_1 \\ C_2 &= S_2 + C_{21} S_1 \\ C_3 &= C_{31} S_1 \end{aligned} \tag{12.21}$$

The equilibrium saturations are then computed as

$$\begin{aligned} S_2^{\text{eq}} &= \frac{C_2 - C_{21}^{\text{eq}}}{1 - C_{21}^{\text{eq}}} \\ S_1^{\text{eq}} &= 1 - S_2^{\text{eq}} \end{aligned} \tag{12.22}$$

The nonequilibrium concentration of oil (C_{21} for the implicit solution or $S_1 C_{21}$ for the explicit solution) is computed from Eq. 12.4 using an explicit or implicit method. The following section gives the phase saturations and phase compositions for both the implicit and explicit solutions of the organic mass balance equation.

12.2.2.3.1 Explicit Solution

The phase saturations are computed using the overall oil concentration and the product of microemulsion saturation times organic concentration in the microemulsion phase from Eq. 12.12.

$$\begin{aligned} S_2 &= C_2 - \left(C_{21}S_1\right)^{n+1} \\ S_1 &= 1. - S_2 \end{aligned} \tag{12.23}$$

The phase compositions are then computed as

$$\begin{aligned} C_{11} &= \frac{C_1}{S_1} \\ C_{21} &= \min\left(C_{21}^{eq}, \frac{\left(C_{21}S_1\right)^{n+1}}{S_1} \right) \\ C_{31} &= 1. - C_{11} - C_{21} \\ C_{22} &= 1.0 \\ C_{12} &= 0.0 \\ C_{32} &= 0.0 \end{aligned} \tag{12.24}$$

If the calculated nonequilibrium concentration is greater than the equilibrium value ($C_{21} > C_{21}^{eq}$), the saturations are then set to the equilibrium values.

12.2.2.3.2 Implicit Method

From the implicit solution of mass balance equation for oil component in the microemulsion phase, we could obtain the nonequilibrium organic dissolution (Eq. 12.12). The phase saturations and phase compositions are calculated as

$$\begin{cases} C_{21} = \min(C_{21}^{eq}, C_{21}^{n+1}) \\ S_2 = \dfrac{C_2 - C_{21}}{1 - C_{21}} \\ S_1 = 1 - S_2 \end{cases} \tag{12.25}$$

and

$$\begin{aligned} C_{11} &= \frac{C_1}{S_1} \\ C_{31} &= 1 - C_{11} - C_{21} \\ C_{12} &= 0.0,\ C_{22} = 1.0,\ C_{32} = 0.0 \end{aligned} \tag{12.26}$$

12.3 Vadose Zone

The solubility of organic species in three-phase flow of water/oil/gas in the vadose zone in the absence of surfactant is modeled in UTCHEM. Similar to the previous section, the overall concentrations for oil, water, and gas are obtained solving the conservation equations.

$$\frac{\partial(\phi C_\kappa)}{\partial t} + \vec{\nabla} \cdot \left(\tilde{F}_{\kappa 1} + \tilde{F}_{\kappa 2}\right) = Q_{\kappa 1} + Q_{\kappa 2} \qquad \text{for } \kappa = 1, 2, 8 \tag{12.27}$$

The nonequilibrium concentration of oil in the aqueous phase is calculated from the mass balance on oil species in the aqueous phase and using the first order mass transfer equation for oil solubility as

$$\frac{\partial(\phi S_1 C_{21})}{\partial t} + \vec{\nabla} \cdot \tilde{F}_{21} = Q_{21} + M\left(C_{21}^{eq} - C_{21}\right) \tag{12.28}$$

where the flux term is defined as

$$\tilde{F}_{21} = C_{21}\vec{u}_1 - \phi S_1 \vec{\vec{K}}_{21} \cdot \vec{\nabla} C_{21} \tag{12.29}$$

Equation 12.29 is solved explicitly to obtain the rate-limited solubility of contaminant in the aqueous phase in the vadose zone. The new time level, (n+1), concentration of oil solubilized in water is

$$\left(\phi S_1 C_{21}\right)^{n+1} = \left(\phi S_1 C_{21}\right)^{n} + (Q_{21} - \vec{\nabla} \cdot \tilde{F}_{21})\Delta t + M\Delta t\left(C_{21}^{eq} - C_{21}^{n}\right) \qquad \text{for } C_{21}^{n} < C_{21}^{eq} \tag{12.30}$$

where the right-hand side of the equation is a known quantity. Therefore,

$$\left(S_1 C_{21}\right)^{n+1} = \frac{\left(\phi S_1 C_{21}\right)^{n+1}}{\phi^{n+1}} \tag{12.31}$$

since the porosity is known and the new time step oil saturation from Eq. 12.1b is

$$S_2 = C_2 - \left(C_{21} S_1\right)^{n+1} \tag{12.32}$$

$$S_1 = C_1 - \left(S_1 C_{21}\right)^{n+1} \tag{12.33}$$

and

$$S_4 = 1 - S_1 - S_2 \tag{12.34}$$

where the overall concentrations (C_1 and C_2) are computed from the species conservation equations. The phase compositions are then as follows

$$C_{11} = \frac{C_1}{S_1}$$

$$C_{21} = \min\left(C_{21}^{eq}, \frac{\left(C_{21} S_1\right)^{n+1}}{S_1}\right) \tag{12.34}$$

$$C_{22} = 1.0$$

If the calculated nonequilibrium concentration is greater than the equilibrium value ($C_{21} > C_{21}^{eq}$), the saturations and phase concentrations are set back to those at the equilibrium.

12.4 Nomenclature

$C_{i,\kappa}$ = Total concentration of species κ in gridblock i, L^3/L^3 PV

C_κ = Overall concentration of species κ in the mobile phases, L^3/L^3

C_κ^{eq} = Equilibrium concentration of species κ, L^3/L^3

$C_{\kappa\ell}$ = Concentration of species κ in phase ℓ, L^3/L^3

K = Dispersion coefficient, L^2t^{-1}

$\vec{\vec{K}}_{\kappa\ell}$ = Dispersion tensor for species in phase , L^2

M = Mass transfer coefficient, t^{-1}

Q = Source/sink for species , L^3/T

S = Saturation of phase , L^3/L^3 PV

t = Time, t

t^n, t^{n+1} = Time-step size at n^{th} and $n+1^{th}$ time level, t

$\vec{u}_\ell$ = Darcy flux, Lt^{-1}

Greek Symbols

ϕ = Porosity, fraction

Subscripts

κ = species number

- 1 = Water
- 2 = Oil
- 3 = Surfactant
- 8 = air

ℓ = Phase number

- 1 = Aqueous
- 2 = Oleic
- 3 = Microemulsion
- 4 = Air

Appendix A
UTCHEM 6.1 User's Guide

A.1 INTRODUCTION

UTCHEM is a three-dimensional chemical flooding simulator. The solution scheme is analogous to IMPES, where pressure is solved for implicitly, but concentrations rather than saturations are then solved for explicitly. Phase saturations and concentrations are then solved in a flash routine. An energy balance equation is solved explicitly for reservoir temperature. The energy balance equation includes heat flow between the reservoir and the over- and underburden rocks. The major physical phenomena modeled in the simulator are:

dispersion
diffusion
dilution effects
adsorption for oil, surfactant and polymer
interfacial tension
relative permeability
capillary pressure
hysteresis in relative permeability and capillary pressure
capillary trapping
cation exchange
phase density
compositional phase viscosity
phase behavior (pseudoquaternary)
aqueous reactions
partitioning of chemical species between oil and water
dissolution/precipitation
cation exchange reactions involving more than two cations
in-situ generation of surfactant from acidic crude oil
pH dependent surfactant adsorption
organic biodegradation capability
multiple organic species
equilibrium and nonequilibrium organic dissolution in aqueous phase
dual porosity option for simple phase tracer flow
polymer properties: shear thinning viscosity, inaccessible pore volume, permeability reduction, adsorption
gel properties: viscosity, permeability reduction, adsorption
tracer properties: partitioning, adsorption, radioactive decay, reaction (ester hydrolization), dead-end pore (capacitance)
temperature dependent properties: viscosity, tracer reaction, gel reactions, Surfactant phase behavior
gas mobility reduction due to foam

See Section 2 of this report for the general formulation of the simulator.

A.2 OPERATION OF THE SIMULATOR

The UTCHEM simulator is run on a CRAY J90 at the Texas Advanced Computing Center affiliated with The University of Texas at Austin (UNICOS operating system), a number of DEC Alpha systems (DEC 4000/610, 3000/500 & 3000/300X) at the Department of Petroleum and Geosystems Engineering (OSF/1 operating system), and a DEC Alpha system (DEC 3000/500) at the Department of Petroleum and Geosystems Engineering (OpenVMS operating system), a number of IBM RS6000 workstations, and a WINDOWS-based PC workstation. The same code is executed on all systems, except for the use of double precision (64-bit words) on the DEC, RS6000 and PC machines—we differentiate between "Cray" and "double precision" versions of the code by adding a "V" prior to the version number for the "Cray" version and a "D" prior to the version number for the "double-precision". Several intrinsic Cray functions need to be implemented when not running on the Cray; these routines are "commented" out in the "Cray" version. Please check the source code for additional information about necessary changes when running on different computers.

2.1 Input and Output Files

UTCHEM requires one input file for non-restart runs. The program expects this file to be named INPUT. For restart runs, a restart file (named INPUT2) is required in addition to the original input data file used for the previous run. A detailed input data description is given in Section A.3 of this appendix and the data in the restart data file is documented in Section 4.3 of this appendix. A number of UTCHEM input example files demonstrating a variety of petroleum oil-field and groundwater applications are available to UTCHEM users. The oil-field applications include water, single-well tracer, interwell tracer, polymer, profile control using gel, surfactant/polymer, and high pH alkaline/surfactant/polymer flooding. The groundwater applications include contaminant infiltration, water flushing, partitioning interwell tracer, surfactant enhanced aquifer remediation, and bioremediation.

We provide all users with two sample input files for testing purposes (see distribution disks for copies of the files). The first sample input file (ex01) is for a 3D surfactant/polymer flood. In that file, the surfactant properties are for petroleum sulfonate and the polymer properties are based on the typical data for xanthan gum. CPU usage for the EX01 example run is about 10 minutes on a DEC Alpha 4000/610 and about 153 seconds on a CRAY J90. The second sample input file (EX21) is for a 2-D contamination event in the saturated zone of an aquifer. CPU usage for the EX21 example run is about 264 seconds on a DEC Alpha 4000/610 and about 52 seconds on a CRAY J90. If you would like to receive additional sample input files, please contact Joanna L. Castillo (joanna@mail.utexas.edu or 512-471-3229) for details.

The number of output files generated by UTCHEM varies depending upon several control flags set by the user in the input file. The number of history plot files depends on the value of the MXW parameter in the `PARAM.INC` source file. The FORTRAN unit number for the history plot file is incremented by one for each well. For example, if MXW is equal to three, then three history plot files would be generated corresponding to FORTRAN unit numbers 19, 20, and 21 even if the run only has two wells. The input and output files are summarized in the following table.

Unit Number	File Name	Contents
1	TEMPL	Analytical temp. profile, created if IENG=1 and IANAL=1
2	ECHO	Echo print of the input file information
3	MESH	Number of gridblocks and distances to center of gridblocks in each direction.
4	PROFIL	Formatted profile data; described in Section A.4 of this appendix

5	INPUT	Input data; described in detail in Section A.3 of this appendix
6	TTABLE	Table of time steps and Courant numbers
7	RESTAR	Stored restart run data; described in Section A.4 of this appendix
8	CONCP	Component concentration profile plotting data, created if IPCTOT>0
9	OVERAL	History of overall properties; described in Section A.4 of this appendix
10	GFILEP	Gel property profile plotting data, created if IREACT=1
11	PRESP	Phase pressure profile plotting data, created if IPPRES>0
12	SATP	Phase saturation profile plotting data, created if IPSAT>0
13	TRACP	Phase tracer concentration profile plotting data, created if IPTRAC>0
14	CAPP	Capacitance property profile or dual porosity plotting data, created if IPCAP>1
15	ALKP	Alkaline option related profile plotting data, created if IREACT>1
16	INPUT2	Restart run data (input file created by an earlier run)
17	WARN	Warning messages
18	TEMPP	Temperature profile, created if IENG=1 and IPTEMP=1
19	HIST01	Well history plotting data for well #1; described in Section A.4 of this appendix
20	HIST02	Well history plotting data for well #2
…		
ℓ	HISTℓ	Well history plotting data for last well
ℓ+1	TRAC01	Aqueous (or gas) phase tracer concentration for the 1st tracer at observation points, created if IPOBS>0; described in Section A.4 of this appendix
ℓ+2	TRAC02	Aqueous (or gas) phase tracer concentration for 2nd tracer at observation points
…		
n	TRAC*n*	Aqueous (or gas) phase tracer concentration for the last tracer at observation points

2.2 Source Code Array Dimensions

The parameters in the table below are used by the simulator to define array sizes. All parameter values must be equal to or greater than the size of the grid dimensions specified in the input file, unless otherwise noted. All parameters used in UTCHEM are defined in the `PARAM.INC` source file. This file should be edited **before** compilation and linking of the source code to define the maximum global discretization size. Example `PARAM.INC` source file:

```
PARAMETER (NNX=96,NNY=96,NNZ=2,MXC=11,MXP=3)
PARAMETER (MXW=2,MXWB=2,MXNT=3,MXMO=1)
PARAMETER (MXELE=1,MXFLD=1,MXSLD=1,MXSORB=1,MXACAT=1,MXEX=1)
PARAMETER (MHM=1,MVM=1)
PARAMETER (MAXBIO=9,MAXBS=9,MAXMET=4)
```

The following table contains definitions of the parameter variables used in the `PARAM.INC` file.

Parameter	Definition
NNX	Number of gridblocks in X-direction (must be set equal or larger to NX in the input file)
NNY	Number of gridblocks in Y-direction (must be set equal or larger to NY in the input file)
NNZ	Number of gridblocks in Z-direction (must be set equal or larger to NZ in the input file)
MXC	Maximum number of components (cannot be less than 8)
MXP	Number of phases (must be set equal to 3 when there is no gas phase and must be set equal to 4 if gas is present)
MXW	Maximum number of wells
MXWB	Maximum number of well blocks
MXNT	Maximum number of tracers (check if NT>0)
MXELE	Maximum number of elements (check for IREACT>1)
MXFLD	Maximum number of reactive fluid species (check for IREACT>1)
MXSLD	Maximum number of solids (check for IREACT>1)
MXSORB	Maximum number of adsorbed species (check for IREACT>1)
MXACAT	Maximum number of cations associated with surfactant (check for IREACT>1)
MXEX	Maximum number of insoluble exchangers (check for IREACT>1)
MVH	Maximum number of subgrids in vertical direction (check for ICAP=2)
MHM	Maximum number of subgrids in lateral direction (check for ICAP=2)
MAXBIO	Maximum number of chemical and biological species participating in biodegradation reactions
MAXMET	Maximum number of metabolic combinations of substrate, electron acceptor, and biological species
MAXBS	Maximum number of biological species (check for IBIO=1)
MXMO	Maximum number of organic components (check for NO>1)

2.3 Compilation and Execution on Workstations

The UTCHEM distribution package for workstations contains the following files: `Makefile-alpha`, `PARAM.INC`, `UTCHEMD6P1.for`, `ddriv2.f`, `DPUTIL.for`, `ex01.data`, and `ex21.data`. Make sure you place all seven files in the same directory on your workstation. Then, follow these steps:

1. Split the `UTCHEMD6P1.for` and `DPUTIL.for` files using the UNIX "`fsplit`" command.

2. To build an executable file called `utchem.exe`, issue the command:

```
make -f Makefile-alpha
```

   Note that the example makefile included on the distribution disks assumes the use of the `f77` FORTRAN compiler. You will need to modify the `Makefile-alpha` file if you wish to use another compiler (`xlf` on IBM RS6000 workstations, for example).

3. Run UTCHEM in the background using a command file (in the example below, the file is called `work.job`). Note that the `work.job` file needs to be executable. Use any text editor to create your job file and then issue the command:

```
chmod +x work.job
```

at the UNIX prompt to make sure the `work.job` file is executable. Then, submit the job file by issuing the following command:

```
work.job &
```

at the UNIX prompt. Example `work.job` file:

```
rm -r ex01.dir
mkdir ex01.dir
cd EX01.dir
ln -s ../ex01.data INPUT
time ../utchem.exe
mv TTABLE ex01.ttable
mv ECHO   ex01.echo
mv MESH   ex01.mesh
mv PROFIL ex01.prof
mv CONCP  ex01.con
mv PRESP  ex01.presp
#mv  ALKP ex01.alkp
mv SATP   ex01.satp
mv GFILEP ex01.gel
mv TEMPP  ex01.temp
mv HIST01 ex01.hist01
mv HIST02 ex01.hist02
mv HIST03 ex01.hist03
mv HIST04 ex01.hist04
#mv HIST05 ex01.hist05
#mv HIST06 ex01.hist06
#mv HIST07 ex01.hist07
mv OVERAL ex01.overal
mv RESTAR ex01.rest
mv WARN   ex01.warn
```

The `work.job` file needs to be modified to reflect the directory structure you create for running UTCHEM jobs as well as the names you wish to use for input and output files. See Section A.9 of this appendix for a description of the contents of the `work.job` file.

2.4 Compilation and Execution on the CRAY J90

The UTCHEM distribution package for the Cray contains the following files: `Makefile-cray`, `PARAM.INC`, `UTCHEMV6P1.for`, `SDRIV2.f`, `ex01.data`, and `ex21.data`. Make sure you place all six files in the same directory on your Cray account. Then, follow these steps:

1. Split the `UTCHEMV6P1.for` file using the UNIX "`fsplit`" command.

2. To build an executable file called `utchem.exe`, issue the command:

```
make -f Makefile-cray
```

3. Submit your job request to the Cray. A sample job file follows:

```
workdir="/insert_path/utchem/"
workdir1="/insert_path/utchem/ex01"
set -xS
cd $TMPDIR
ja jacct$$
rcp $workdir/ex01.data INPUT
#rcp $workdir1/ex01.rest INPUT2
rcp $workdir/utchem.exe a.out
a.out
rcp TTABLE  $workdir1/ex01.ttable
rcp ECHO    $workdir1/ex01.echo
rcp MESH    $workdir1/ex01.mesh
rcp PROFIL  $workdir1/ex01.prof
rcp SATP    $workdir1/ex01.satp
rcp TEMPP  $workdir1/ex01.temp
rcp PRESP  $workdir1/ex01.presp
rcp CONCP  $workdir1/ex01.concp
#rcp ALKP   $workdir1/ex01.alkp
rcp GFILEP  $workdir1/ex01.gel
rcp HIST01  $workdir1/ex01.his1
rcp HIST02  $workdir1/ex01.his2
rcp HIST03 $workdir1/ex01.his3
rcp HIST04 $workdir1/ex01.his4
rcp OVERAL  $workdir1/ex01.overal
rcp RESTAR  $workdir1/ex01.rest
rcp WARN    $workdir1/ex01.warn
```

This job file assumes the code and input file reside in a directory called "`utchem`" and that the output files will be placed in the "`ex01`" directory which is one level below the "`utchem`" directory. Replace *`insert_path`* with the actual path to the "`utchem`" directory.

A.3 INPUT DATA DESCRIPTION

The UTCHEM input file consists of comment lines and data lines. All comment lines are ignored by the UTCHEM simulator. It is important to note, however, that the number of comment lines between data lines is fixed. The first twenty-two lines of the input file are reserved for comment lines used to briefly describe the input file. Each data line is preceded by three comment lines (except for the input described in Section 3.5 of this appendix). The input file is basically divided into seven sections and each of those input sections (except Section 3.5) is preceded by an additional seven comment lines. The user should update the comment lines as the input file is modified in order to make using the simulator easier.

All data is free-formatted. This means that for each read statement, it is only necessary to leave a blank space between data elements. Note that the first data element for a given read statement must be on a new line in the input file. Subsequent data elements for that read statement can span as many lines as necessary. Implicit type matching is used; that is, all REAL variables begin with the letters A-H or O-Z and all integer variables begin with the letters I-N.

The following is a list of variables as they are read by UTCHEM. The variable names appear in all-caps on a single line in the order they are read by the program (variables that are new to the latest version of UTCHEM are printed in ***italicized boldface*** as well). Every list of variables is followed by a description of each variable and corresponding units or possible values if applicable. All of the variables listed in the input description will be read by the program unless otherwise noted; therefore, a dummy value will be read by the program for variables not pertinent to the problem being run.

3.1. Title and Reservoir Description Data

The first input section consists of the title and reservoir description data. Please remember that there are 22 comment lines at the beginning of this section and that each data line is preceded by three comment lines.

3.1.1 RUNNO

RUNNO - Run number.

Note: The run number can consist of any combination of alphanumeric characters on a single line (not to exceed 80 characters). This information will be printed as the first line of every output file.

3.1.2 TITLE

TITLE - Title and run description.

Note: The title can consist of any combination of alphanumeric characters spanning three lines in the input file (not to exceed 80 characters per line). The title must span three lines and any of those lines can be blank.

3.1.3 IMODE, IMES, IDISPC, ICWM, ICAP, IREACT, IBIO, ICOORD, ITREAC, ITC, IGAS, IENG

IMODE - Flag indicating if the problem to be run is a first run or a restart simulation.

Possible Values:

1 - First simulation run
2 - Restart simulation

Note: See Section A.4 of this appendix for more details on how to run restart simulations.

IMES - Flag indicating if a constant or automatic time-step is to be used.

Possible Values:

1 - Constant time-step size is used

2 - Automatic time-step size selector based on method of relative changes for the first three components is used

3 - Automatic time-step size selector based on method of relative changes for all the components is used

4 - Automatic time-step size selector based on changes in dimensionless concentration for all the components is used

Note: The automatic time-step selector is recommended. See input lines 3.7.9 through 3.7.13 and Section A.8 of this appendix for more details on the above options.

IDISPC - Flag indicating which type of numerical dispersion control is used.

Possible Values:

0 - Single point upstream method is used

2 - Two point upstream method is used

3 - Improved total variation diminishing third order method is used

Note: These methods are applied to both concentration and relative permeability.

ICWM - Flag indicating if the concentration well model is used or not.

Possible Values:

0 - Concentration well model is not used

1 - Concentration well model is used

Note: The concentration well model (ICWM=1) can only be used with vertical wells (IDIR(M)=3).

ICAP - Flag indicating if the capacitance model is used or not.

Possible Values:

0 - Capacitance model or dual porosity option is not used

1 - Capacitance model is used

2 - Dual porosity option is used for single phase tracer flow

Note: The dual porosity option (ICAP=2) is available only if IMODE=1, IUNIT=0, and ICOORD=1.

IREACT - Flag indicating if gel reactions or alkaline options are used or not.

Possible Values:

0 - Gel reactions are not used

1 - Gel reactions are used

2 - Geochemistry option with no acidic crude is used

3 - Geochemistry option with acidic crude is used

4 - IREACT=2 and gel reactions are used

IBIO - Flag indicating whether or not biodegradation reactions occur

Possible Values:

0 - No biodegradation reactions

1 - Biodegradation reactions occur

ICOORD - Flag indicating which coordinate system is used.

Possible Values:

1 - Cartesian coordinate system is used

2 - Radial coordinate system is used

3 - Cartesian coordinate system with variable-width gridblock is used (2-D cross section only)

4 - Curvilinear grid definition of the X-Z cross section is used (2-D or 3-D)

Note: For ICOORD=4, the 3-D grid consists of the 2-D cross sectional grid repeated at specified intervals (uniform or non-uniform) in the Y direction, according to the definition of DY1. The curvilinear grid option is not available with the temperature equation option.

ITREAC - Flag indicating if a tracer reaction is used or not.

Possible Values:

0 - Tracer reactions are not used
1 - Tracer reactions are used

ITC - Flag indicating if second-order time approximation is used or not.

Possible Values:

0 - Second-order time approximation is not used
1 - Second-order time approximation is used

Note: We recommend that second-order time approximation (ITC=1) only be used with higher-order dispersion methods (IDISPC>1).

IGAS - Flag indicating if gas phase is considered or not.

Possible Values:

0 - Gas is not present
1 - Gas is present
2 - Gas is present and foam option is used

IENG - Flag indicating if temperature variation is considered or not.

Possible Values:

0 - Isothermal simulation
1 - Temperature equation is solved

3.1.4 NX, NY, NZ, IDXYZ, IUNIT

NX - Number of gridblocks along X-axis (ICOORD=1, 3, or 4) or number of gridblocks in radial direction (ICOORD=2).

Note: This value should be equal to or smaller than the NNX parameter in UTCHEM.

NY - Number of gridblocks along Y-axis.

Note: This value should be equal to or smaller than the NNY parameter in UTCHEM. It should be set equal to 1 if the user is running a 1-D problem or a 2-D cross sectional problem. If ICOORD=2, this value is automatically set equal to 1.

NZ - Number of gridblocks along Z-axis.

Note: This value should be equal to or smaller than the NNZ parameter in UTCHEM. It should be set equal to 1 if the user is running a 1-D problem or a 2-D areal problem.

IDXYZ - Flag indicating constant or variable grid size.

Possible Values:

0 - Constant grid size
1 - Variable grid size on a regional basis
2 - Variable grid size

Note: IDXYZ must be set equal to 2 if ICOORD=3.

IUNIT - Flag indicating English or Metric units.

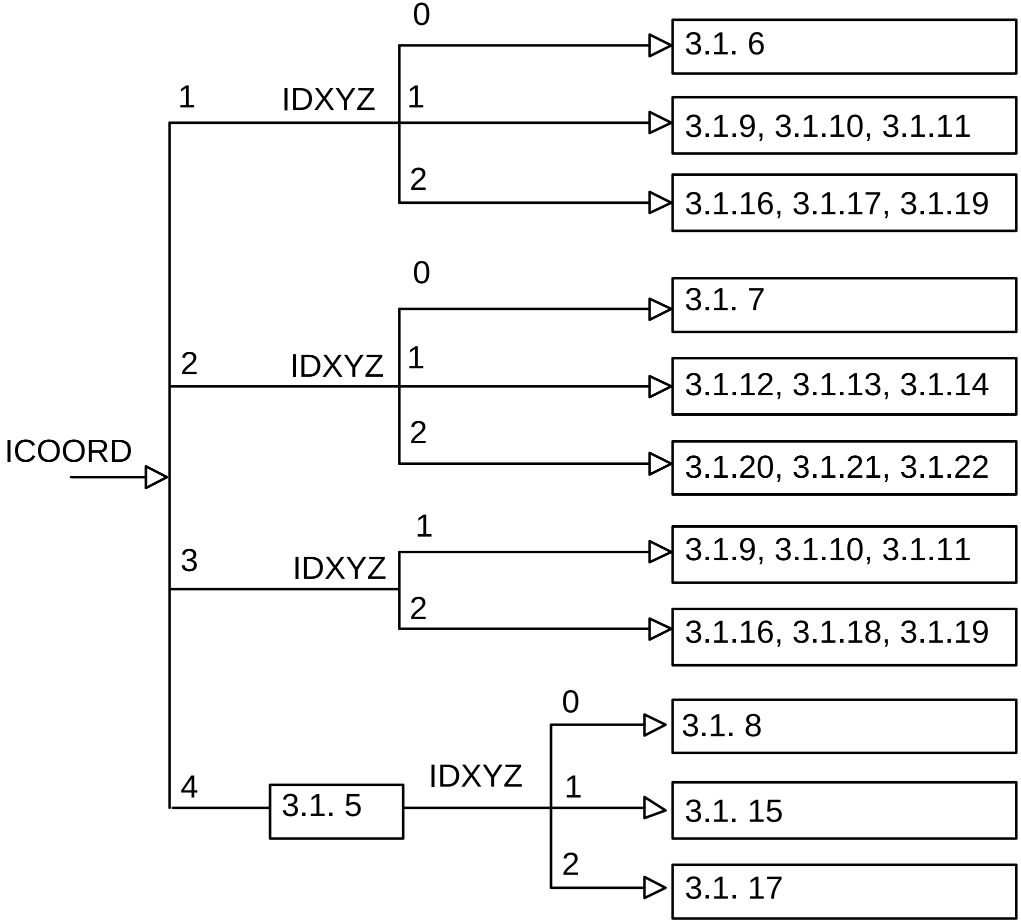
Possible Values:

0 - English unit
1 - Metric unit

Note: UTCHEM must be compiled and run with the NX, NY, and NZ input values being equal to or smaller than the NNX, NNY, and NNZ parameters in the code. All parameters used in UTCHEM are defined in the `PARAM.INC` source file.

Simulation Gridblock Sizes (Lines 3.1.5-3.1.23)

Refer to the following flowchart to help determine which input lines should be used to specify the gridblock size input values for different options:



3.1.5 XCORD(I), ZCORD(I), for I=1, (NX+1)×(NZ+1) (This line is read only if ICOORD=4)

XCORD - Gridblock coordinate of I^{th} corner point in X-direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

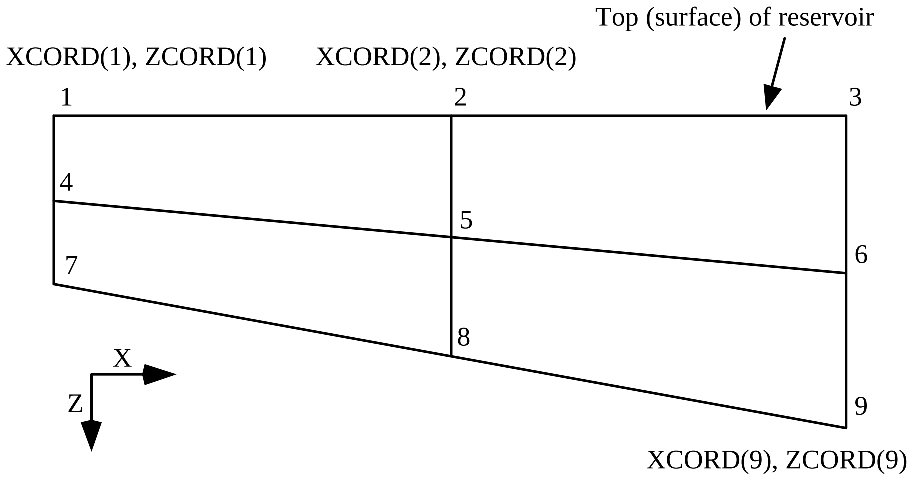
ZCOORD - Gridblock coordinate of I^{th} corner point in Z-direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: The coordinates of the corners (or vertices) of the 2-D X-Z cross section gridblocks are input in pairs as follows:

XCORD(1),	ZCORD(1)
.	.
.	.
.	.
XCORD(nodes),	ZCORD(nodes)

where nodes = (NX+1) × (NZ+1) and is the total number of corner points defining the X-Z cross section and Z is positive downward. The following figure illustrates the input order for an example X-Z cross section grid:



The number of gridblocks is equal to NX × NZ and the number of coordinate pairs (or nodes) is equal to (NX+1) × (NZ+1).

Cautionary warning: The X-Z cross section grid should be constructed by the user such that the curvilinear coordinate system is at least quasi-orthogonal. Departure from orthogonality will lead to numerical errors in the solution.

3.1.6 DX1, DY1, DZ1 (This line is read only if IDXYZ=0 and ICOORD=1 or 3)

DX1 - Gridblock size in X direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

DY1 - Gridblock size in Y direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

DZ1 - Gridblock size in Z direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.7 R(1), DX1, DZ1 (This line is read only if IDXYZ=0 and ICOORD=2)

R(1) - Wellbore radius.
Units: feet (IUNIT=0) or m (IUNIT=1)

DX1 - Distance between nodes in radial direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

DZ1 - Gridblock size in Z direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.8 DY1 (This line is read only if IDXYZ=0 and ICOORD=4)

DY1 - Gridblock size in Y direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.9 II1, II2, DX1 (This line is read only if IDXYZ=1 and ICOORD=1 or 3)

II1 - First index for gridblocks with same size in X direction.

II2 - Last index for gridblocks with same size in X direction.

DX1 - Gridblock size in X direction
Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NX gridblocks in the X direction have been specified. The first line in the set must have II1=1 and the last line must have II2=NX.

Example: If NX=11 and the first three gridblocks in the X direction are 3 feet in size, the fourth through ninth gridblocks in the X direction are 2 feet in size, and the last two gridblocks in the X direction are 2.5 feet in size, this line would need to be repeated three times to fully describe the X direction gridblocks as follows:

1	3	3.0
4	9	2.0
10	11	2.5

3.1.10 JJ1, JJ2, DY1 (This line is read only if IDXYZ=1 and ICOORD=1 or 3)

JJ1 - First index for gridblocks with same size in Y direction.

JJ2 - Last index for gridblocks with same size in Y direction.

DY1 - Gridblock size in Y direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NY gridblocks in the Y direction have been specified. The first line in the set must have JJ1=1 and the last line must have JJ2=NY. See the example for input line 3.1.9.

3.1.11 KK1, KK2, DZ1 (This line is read only if IDXYZ=1 and ICOORD=1 or 3)

KK1 - First index for gridblocks with same size in Z direction.

KK2 - Last index for gridblocks with same size in Z direction.

DZ1 - Gridblock size in Z direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NZ gridblocks in the Z direction have been specified. The first line in the set must have KK1=1 and the last line must have KK2=NZ. See the example for input line 3.1.9.

3.1.12 R(1) (This line is read only if IDXYZ=1 and ICOORD=2)

R(1) - Wellbore radius.

Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.13 II1, II2, DX1 (This line is read only if IDXYZ=1 and ICOORD=2)

II1 - First index for radial node distances of the same size.

II2 - Last index for radial node distances of the same size.

DX1 - Distance between nodes in radial direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until the NX-1 distances between the NX nodes in the radial direction have been specified. The first line in the set must have II1=1 and the last line must have II2=NX-1.

Example: If NX=35 and the first ten gridblocks in the X direction are 1 foot in size and the rest are 2 feet in size, this line would need to be repeated twice to fully describe the radial direction nodes as follows:

1	10	1.0
11	34	2.0

3.1.14 KK1, KK2, DZ1 (This line is read only if IDXYZ=1 and ICOORD=2)

KK1 - First index for gridblocks with same size in Z direction.

KK2 - Last index for gridblocks with same size in Z direction.

DZ1 - Gridblock size in Z direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NZ gridblocks in the Z direction have been specified. The first line in the set must have KK1=1 and the last line must have KK2=NZ. See the example for input line 3.1.9.

3.1.15 JJ1, JJ2, DY1 (This line is read only if IDXYZ=1 and ICOORD=4)
JJ1 - First index for gridblocks with same size in Y direction.
JJ2 - Last index for gridblocks with same size in Y direction.
DY1 - Gridblock size in Y direction.
Units: feet (IUNIT=0) or m (IUNIT=1)
Note: This line is repeated until sizes for each of the NY gridblocks in the Y direction have been specified. The first line in the set must have JJ1=1 and the last line must have JJ2=NY. See the example for input line 3.1.9.

3.1.16 DX(I), for I=1, NX (This line is read only if IDXYZ=2 and ICOORD=1 or 3)
DX(I) - Grid size of Ith block in X direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.17 DY(J), for J=1, NY (This line is read only if IDXYZ=2 and ICOORD=1 or 4)
DY(J) - Grid size of Jth block in Y direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.18 DY(I), for I=1, NX (This line is read only if IDXYZ=2 and ICOORD=3)
DY(I) - Thickness of Ith block.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.19 DZ(K), for K=1, NZ (This line is read only if IDXYZ=2 and ICOORD=1 or 3)
DZ(K) - Grid size of Kth block in Z direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.20 R(1) (This line is read only if IDXYZ=2 and ICOORD=2)
R(1) - Wellbore radius.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.21 DX(I), for I=1, NX-1 (This line is read only if IDXYZ=2 and ICOORD=2)
DX(I) - Distance between the Ith node and the I+1th node in the radial direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.22 DZ(K), for K=1, NZ (This line is read only if IDXYZ=2 and ICOORD=2)
DZ(K) - Grid size of Kth block in Z direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.23 N, NO, NTW, NTA, NGC, NG, ***NOTH***
N - Total number of components in the run (including tracers and reactive components).
Value must be set equal to: N=8+NO+NTW+NTA+NGC+NG+NOTH
NO - Total number of NAPL phase organic components in the run.

Note: If IBIO=1, set NO=0 if no NAPL phase is present and all biodegrading species are present only in the aqueous phase; otherwise, set NO to the number of organic species.

NTW - Number of water/oil tracers.

NTA - Number of oil/gas tracers.

NGC - Number of components for geochemistry option.

NG - Number of gel components.

NOTH - Total number of other chemical and biological species that are considered in biodegradation reactions, including products generated by biodegradation reactions, nutrients required for biological growth, electron acceptors, and biological species.

Note: See Section A.7 of this appendix for the component numbering scheme used in UTCHEM and Section 9 of this report for more details on the microbiological population model options.

3.1.24 ***SPNAME***(I), for I=1, N

SPNAME(I) - Name of Ith species.

Note: The name of each component may not exceed 8 characters and each name must be on a separate line of the input file.

3.1.25 ITRU(I), for I=1, NTW (This line is read only if NTW>0 and ITREAC=1)

ITRU(I) - Flag indicating the units of the Ith water tracer.

Possible Values:

1 - Ith tracer units are in volume %

2 - Ith tracer units are in weight %

3.1.26 ICF(KC), for KC=1, N

ICF(KC) - Flag indicating if KCth component is included in the calculations or not.

Possible Values:

0 - The KCth component is not included in the calculations

1 - The KCth component is included in the calculations

Example: If 11 components are considered but Alcohol 2 is not present, this line would appear as follows:

1 1 1 1 1 1 1 0 1 1 1

3.2 Output Option Data

The second input section consists of output options. Please remember that there are seven comment lines at the beginning of this section and that each data line is preceded by three comment lines.

3.2.1 ICUMTM, ISTOP

ICUMTM - Flag indicating if the output intervals indicated by the CUMPR1, CUMHI1, WRHPV, WRPRF and RSTC variables on input line 3.7.8 are specified in pore volumes or days.

Possible Values:

0 - Data will be written in day intervals

1 - Data will be written in pore volume intervals

Note: The day interval output option (ICUMTM=0) is particularly useful if there is a shut in period.

ISTOP - Flag indicating if the maximum and injection times (variables TMAX on input line 3.3.1 and TINJ on input line 3.7.8) are specified in pore volumes or days.

Possible Values:

0 - TMAX and TINJ are specified in days
1 - TMAX and TINJ are specified in pore volumes

Note: A 3rd variable (ICOPSM) which used to control printing to UNIT 3 is no longer available with the latest version of UTCHEM.

3.2.2 IPRFLG(KC), for KC=1, N

IPRFLG(KC) - Flag indicating if profile of KCth component should be written to UNIT 8.

Possible Values:

0 - Profile of KCth component will not be written
1 - Profile of KCth component will be written

Note: If IPCTOT=0, none of the component profiles will be written.

Example: If 11 components are present and only profiles for the oil, surfactant, and polymer components are desired, this line would appear as follows:

0 1 1 1 0 0 0 0 0 0 0

3.2.3 IPPRES, IPSAT, IPCTOT, IPTRAC, IPCAP, IPGEL, IPALK, IPTEMP, IPOBS, IBPR

IPPRES - Flag indicating if profile of phase pressures should be written to UNIT 11.

Possible Values:

0 - Profile of phase pressures will not be written
1 - Profile of phase pressures will be written

IPSAT - Flag indicating if profile of phase saturations should be written to UNIT 12.

Possible Values:

0 - Profile of phase saturations will not be written
1 - Profile of phase saturations will be written

IPCTOT - Flag indicating if profile of component concentrations should be written to UNIT 8.

Possible Values:

0 - Profile of component concentrations will not be written
1 - Profile of component concentrations will be written

IPTRAC - Flag indicating if profile of tracer phase concentrations should be written to UNIT 13.

Possible Values:

0 - Profile of tracer phase concentrations will not be written
1 - Profile of tracer phase concentrations will be written

IPCAP - Flag indicating if profile of capacitance properties should be written to UNIT 14.

Possible Values:

0 - Profile of capacitance properties will not be written
1 - Profile of capacitance properties will be written

IPGEL - Flag indicating if profile of gel properties should be written to UNIT 10.

Possible Values:

0 - Profile of gel properties will not be written
1 - Profile of gel properties will be written

IPALK - Flag indicating if profile of properties related to the alkaline option should be written to UNIT 15.

Possible Values:

0 - Profile of properties related to the alkaline option will not be written

1 - Profile of properties related to the alkaline option will be written

IPTEMP - Flag indicating if profile of reservoir temperature should be written to UNIT 18.

Possible Values:

0 - Profile of temperature will not be written

1 - Profile of temperature will be written

IPOBS - Flag indicating if aqueous phase tracer concentration at observation points should be written to the TRACxx output files.

Possible Values:

0 - Aqueous phase tracer concentrations at observation points will not be written

1 - Aqueous phase tracer concentrations at observation points will be written

IBPR - Flag indicating if chemical and biological species concentrations in the aqueous phase and within attached biomass should be written to UNITS 4, 8, and HISTℓ.

Possible Values:

0 - Aqueous and intra-biomass concentrations will not be written

1 - Aqueous and intra-biomass concentrations will be written

3.2.4 IPHP, IADS, ICKL, IVEL, IVIS, IPER, ICNM, IRKF, IPHSE, ICSE

IPHP - Flag indicating if oleic and microemulsion phase pressure data should be printed.

Possible Values:

0 - Oleic and microemulsion phase pressure data will not be printed

1 - Oleic and microemulsion phase pressure data will be printed

IADS - Flag indicating if surfactant, polymer, calcium, gel, chromium, hydrogen, and sodium adsorption data should be printed.

Possible Values:

0 - Adsorption data will not be printed

1 - Adsorption data will be printed

ICKL - Flag indicating if component concentration data in each phase should be printed.

Possible Values:

0 - Component concentration data in each phase will not be printed

1 - Component concentration data in each phase will be printed

IVEL - Flag indicating if X, Y, and Z direction phase fluxes should be printed.

Possible Values:

0 - X, Y, and Z direction phase fluxes will not be printed

1 - X, Y, and Z direction phase fluxes will be printed

IVIS - Flag indicating if phase viscosities should be printed.

Possible Values:

0 - Phase viscosities will not be printed

1 - Phase viscosities will be printed

IPER - Flag indicating if relative permeabilities should be printed.

Possible Values:

0 - Relative permeabilities will not be printed

1 - Relative permeabilities will be printed

ICNM - Flag indicating if phase capillary numbers and interfacial tensions should be printed.

Possible Values:

0 - Capillary numbers, residual saturations, and interfacial tensions will not be printed

1 - Capillary numbers, residual saturation, and interfacial tensions will be printed

IRKF - Flag indicating if permeability reduction factors should be printed.

Possible Values:

0 - Permeability reduction factors, polymer viscosities, and equivalent shear rate will not be printed

1 - Permeability reduction factors, polymer viscosities, and equivalent shear rate will be printed

IPHSE - Flag indicating if phase environment indexing should be printed.

Possible Values:

0 - Phase environment indexing will not be printed

1 - Phase environment indexing will be printed

Note: The indices for the phase environment are as follows:

1 - single phase

2 - two phase oil/water or oil/microemulsion or water/microemulsion

3 - three phase oil/microemulsion/water

4 - lobe II(+) of type III

5 - lobe II(-) of type III

ICSE - Flag indicating if effective salinity should be printed.

Possible Values:

0 - Effective salinity information will not be printed

1 - Effective salinity will be printed to PROFIL and history data files

Note: These flags give the option of printing a very detailed description (all flags = 1) every CUMPR1 pore volume interval or a very limited description (all flags = 0) to UNIT 4. See Section A.4 of this appendix for a list of the values that are written to UNIT 4 automatically.

3.2.5 NOBS (This line is read only if IPOBS=1)

NOBS - Number of tracer concentration observation points.

3.2.6 IOBS(I), JOBS(I), KOBS(I), for I=1, NOBS (This line is read only if IPOBS=1 and NOBS>0)

IOBS(I) - Index of Ith observation point in X direction.

JOBS(I) - Index of Ith observation point in Y direction.

KOBS(I) - Index of Ith observation point in Z direction.

Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM.

3.3. Reservoir Properties

The third input section consists of the reservoir properties. Please remember that there are seven comment lines at the beginning of this section and that each data line is preceded by three comment lines.

3.3.1 TMAX

TMAX - Total injection period (maximum simulation time).

Units: days or pore volumes (dependent on value of ISTOP flag in line 3.2.1)

3.3.2 COMPR, PSTAND

COMPR - Rock compressibility.

Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

PSTAND - Reference pressure at which pore volume and fluid compressibilities are specified.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

Reservoir/Aquifer Properties (Lines 3.1.3-3.1.17)

3.3.3 IPOR1, IPERMX, IPERMY, IPERMZ, IMOD

IPOR1 - Flag indicating constant or variable porosity for reservoir.

Possible Values:

- 0 - Constant porosity for whole reservoir
- 1 - Constant porosity for each layer
- 2 - Variable porosity over reservoir

IPERMX - Flag indicating constant or variable X direction permeability (ICOORD=1 or 3) or radial direction permeability (ICOORD=2) for reservoir.

Possible Values:

- 0 - Constant permeability for whole reservoir
- 1 - Constant permeability for each layer in the X direction (ICOORD=1 or 3) or radial direction (ICOORD=2)
- 2 - Variable permeability over reservoir

IPERMY - Flag indicating constant or variable Y direction permeability for reservoir.

Possible Values:

- 0 - Constant permeability for whole reservoir
- 1 - Constant permeability for each layer in the Y direction
- 2 - Variable permeability over reservoir
- 3 - Y direction permeability is dependent on X direction permeability

IPERMZ - Flag indicating constant or variable Z direction permeability for reservoir.

Possible Values:

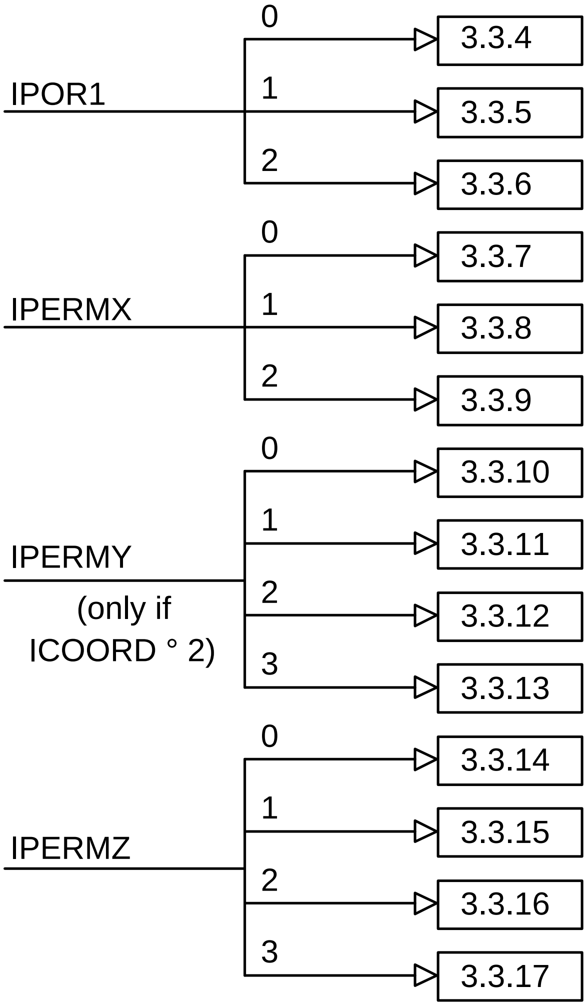
- 0 - Constant permeability for whole reservoir
- 1 - Constant permeability for each layer in the Z direction
- 2 - Variable permeability over reservoir
- 3 - Z direction permeability is dependent on X direction permeability

IMOD - Flag indicating whether the reservoir properties are modified or not.

Possible Values:

- 0 - No property is modified
- 1 - Allow for property modification

Refer to the following flowchart to help determine which input lines should be used to specify the porosity and permeability values for different options:



3.3.4 PORC1 (This line is read only if IPOR1=0)

PORC1 - Reservoir porosity.

Units: fraction

Note: All elements of the POR array will be set equal to PORC1.

3.3.5 POR(K), for K=1, NZ (This line is read only if IPOR1=1)

POR(K) - Porosity of Kth layer.

Units: fraction

Note: NZ values are actually read into a workspace array (WKSP1) and then the first set of NX × NY elements (corresponding to layer 1) of the POR array are set equal to WKSP1(1), the second set of NX × NY elements (corresponding to layer 2) of the POR array are set equal to WKSP1(2), etc.

3.3.6 POR(I), for I=1, NBL (This line is read only if IPOR1=2)

POR(I) - Porosity of Ith gridblock

Units: fraction

Notes:

1) The three-dimensional grid system is being read into a one-dimensional array. The first index (column) of the three-dimensional system varies fastest, the second index (row) varies next fastest, and the third index (layer) varies slowest. The total number of gridblocks, NBL, is NX × NY × NZ.

   Example: If you had a 4 × 3 × 2 system (4 columns—NX=4, 3 rows—NY=3, and 2 layers—NZ=2), the values would be read in the following order:

1,1,1	2,1,1	3,1,1	4,1,1
1,2,1	2,2,1	3,2,1	4,2,1
1,3,1	2,3,1	3,3,1	4,3,1
1,1,2	2,1,2	3,1,2	4,1,2
1,2,2	2,2,2	3,2,2	4,2,2
1,3,2	2,3,2	3,3,2	4,3,2

2) The transmissibilities are set to zero for gridblocks with porosity values less than or equal to 0.01 (ICOORD=1).

3) To specify certain gridblocks as inactive, the user needs to set the porosity for the inactive cells to a very small number (e.g. 10^{-6}).

3.3.7 PERMXC (This line is read only if IPERMX=0)

PERMXC - Permeability of the reservoir in the X direction or in the radial direction (ICOORD=2).

Units: millidarcies = 10^{-3} μm^2

Note: All elements of the PERMX array will be set equal to PERMXC.

3.3.8 PERMX(K), for K=1, NZ (This line is read only if IPERMX=1)

PERMX(K) - Permeability of the Kth layer in the X direction or in the radial direction (ICOORD=2).

Units: millidarcies = 10^{-3} μm^2

Note: See the note for input line 3.3.5.

3.3.9 PERMX(I), for I=1, NBL (This line is read only if IPERMX=2)

PERMX(I) - Permeability of the Ith gridblock in the X direction or in the radial direction (ICOORD=2).

Units: millidarcies = 10^{-3} μm^2

Note: See the note and example for input line 3.3.6 for the order of the permeability values.

3.3.10 PERMYC (This line is read only if IPERMY=0 and ICOORD•2)

PERMYC - Permeability of the reservoir in the Y direction.

Units: millidarcies = 10^{-3} μm^2

Note: All elements of the PERMY array will be set equal to PERMYC.

3.3.11 PERMY(K), for K=1, NZ (This line is read only if IPERMY=1 and ICOORD•2)

PERMY(K) - Permeability of the Kth layer in the Y direction.

Units: millidarcies = 10^{-3} μm^2

Note: See note for input line 3.3.5.

3.3.12 PERMY(I), for I=1, NBL (This line is read only if IPERMY=2 and ICOORD•2)

PERMY(I) - Permeability of the Ith gridblock.

Units: millidarcies = 10^{-3} μm^2

Note: See the note and example for input line 3.3.6 for the order of the permeability values.

3.3.13 FACTY (This line is read only if IPERMY=3 and ICOORD•2)

FACTY - Constant permeability multiplier for Y direction permeability.

Units: dimensionless

Note: The X direction permeabilities are multiplied by FACTY to obtain the Y direction permeabilities.

3.3.14 PERMZC (This line is read only if IPERMZ=0)

PERMZC - Permeability of the reservoir in the Z direction.

Units: millidarcies = 10^{-3} μm^2

Note: All elements of the PERMZ array will be set equal to PERMZC.

3.3.15 PERMZ(K), for K=1, NZ (This line is read only if IPERMZ=1)

PERMZ(K) - Permeability of the Kth layer in the Z direction.

Units: millidarcies = 10^{-3} μm^2

Note: See note for input line 3.3.5.

3.3.16 PERMZ(I), for I=1, NBL (This line is read only if IPERMZ=2)

PERMZ(I) - Permeability of the Ith gridblock.

Units: millidarcies (10^{-3} μm^2)

Note: See the note and example for input line 3.3.6 for the order of the permeability values.

3.3.17 FACTZ (This line is read only if IPERMZ=3)

FACTZ - Constant permeability multiplier for Z direction permeability.

Units: dimensionless

Note: The X direction permeabilities are multiplied by FACTZ to obtain the Z direction permeabilities.

Initial Reservoir/Aquifer Data (Lines 3.3.18-3.3.36)

3.3.18 IDEPTH, IPRESS, ISWI

IDEPTH - Flag indicating type of depth measurement of the top layer.

Possible Values:

0 - Single value for depth of the top layer is specified
1 - Depth of top gridblock (1,1,1) and the reservoir dip angles are specified
2 - Depth of each gridblock in the top layer is specified

Note: If ICOORD=2, this value is automatically set equal to 0. The depth is specified at the middle of a gridblock.

IPRESS - Flag indicating type of reservoir initial pressure measurement.

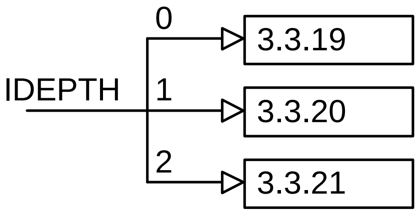
Possible Values:

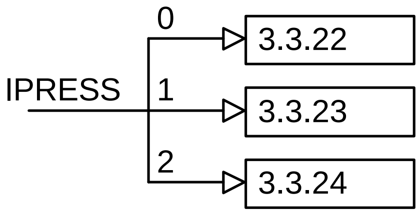
0 - Single value for reservoir initial pressure is used for all gridblocks

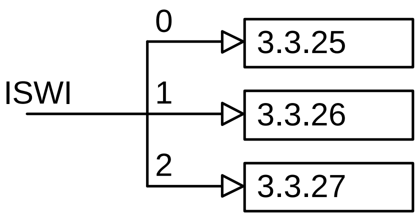
1 - Initial pressure for a point at a specified depth is specified by user
2 - Initial pressure for each gridblock is specified by user

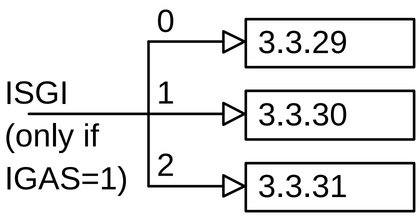
ISWI - Flag indicating type of initial water saturation measurement.
Possible Values:
0 - Single value for initial water saturation is used for all gridblocks
1 - Constant value for water saturation for each layer is specified by user
2 - Initial water saturation for each gridblock is specified by user

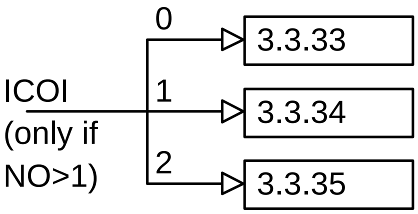
Refer to the following flowchart to help determine which input lines should be used to specify the initial properties such as depth, pressure, initial water saturations, initial gas saturations when IGAS•1, and initial organic concentrations when NO>1:











3.3.19 D111 (This line is read only if IDEPTH=0)

D111 - Depth of the top layer of the reservoir measured from the surface (reference plane), positive downward.
Units: feet (IUNIT=0) or m (IUNIT=1)

Note: If IDEPTH=0 and ICOORD=4, D111 is the reference depth of the first gridblock.

3.3.20 D111, THETAX, THETAY (This line is read only if IDEPTH=1)

D111 - Depth of the first gridblock (1,1,1).
Units: feet (IUNIT=0) or m (IUNIT=1)

THETAX - Reservoir dip angle in X direction, positive downward.
Units: radians

THETAY - Reservoir dip angle in Y direction, positive downward.
Units: radians

Note: If ICOORD=4, set THETAY equal to 0 (dip angle in X-Z plane).

3.3.21 EL(I), for I=1, NX × NY (This line is read only if IDEPTH=2)
EL(I) - Depth of I^{th} gridblock in the top layer (K=1).
Units: feet (IUNIT=0) or m (IUNIT=1)
Note: See the note and example for input line 3.3.6 for the order of the gridblock depths.

3.3.22 PRESS1 (This line is read only if IPRESS=0)
PRESS1 - Initial reservoir pressure.
Units: psi (IUNIT=0) or kPa (IUNIT=1)

3.3.23 PINIT, HINIT (This line is read only if IPRESS=1)
PINIT - Initial reservoir pressure at HINIT depth.
Units: psia (IUNIT=0) or kPa (IUNIT=1)
HINIT - Depth of the point where PINIT initial pressure is specified.
Units: feet (IUNIT=0) or m (IUNIT=1)
Note: Initial pressure is assumed to be the aqueous phase pressure.

3.3.24 P(I), for I=1, NBL (This line is read only if IPRESS=2)
P(I) - Initial pressure of each gridblock in the reservoir.
Units: psia (IUNIT=0) or kPa (IUNIT=1)
Note: See the note and example for input line 3.3.6 for the order of the initial pressure values. This is assumed to be the aqueous phase pressure.

3.3.25 SWI (This line is read only if ISWI=0)
SWI - Initial water saturation for all gridblocks of the reservoir.
Units: fraction of pore volume

3.3.26 S(K,1), for K=1, NZ (This line is read only if ISWI=1)
S(K,1) - Initial water saturation for K^{th} layer.
Units: fraction of pore volume
Note: See the note for input line 3.3.5.

3.3.27 S(I,1), for I=1, NBL (This line is read only if ISWI=2)
S(I,1) - Initial water saturation for I^{th} block.
Units: fraction of pore volume
Note: See the note and example for input line 3.3.6 for the order of the initial water saturation values.

3.3.28 ISGI (This line is read only if IGAS•1)
ISGI - Flag indicating type of initial gas saturation.
Possible Values:
0 - Constant initial gas saturation for whole reservoir
1 - Constant initial gas saturation for each layer
2 - Initial gas saturation for each gridblock is specified by user

3.3.29 SGI (This line is read only if IGAS•1 and ISGI=0)

SGI - Initial gas saturation for all gridblocks of the reservoir.

Units: fraction of pore volume

3.3.30 S(K,4), for K=1, NZ (This line is read only if IGAS•1 and ISGI=1)

S(K,4) - Initial gas saturation for K^{th} layer.

Units: fraction of pore volume

Note: See the note for input line 3.3.5.

3.3.31 S(I,4), for I=1, NBL (This line is read only if IGAS•1 and ISGI=2)

S(I,4) - Initial gas saturation for I^{th} gridblock.

Units: fraction of pore volume

Note: See the note and example for input line 3.3.6 for the order of the initial gas saturation values.

Initial Organic Concentrations (Lines 3.3.32-3.3.35) — This section is **required only if** the multiple organic option is used **(NO>1)**.

3.3.32 ICOI (This line is read only if NO>1)

ICOI - Flag indicating type of initial oil phase compositions.

Possible Values:

- 0 - Constant initial oil phase concentration for whole reservoir
- 1 - Constant initial oil phase concentration for each layer
- 2 - Initial oil phase concentration for each gridblock

3.3.33 COI(KO), for KO=1, NO (This line is read only if NO>1 and ICOI=0)

COI(KO) - Initial oil phase concentration for oil component KO for the reservoir.

Units: volume fraction

3.3.34 COI(K,KO), for K=1, NZ, for KO=1, NO (This line is read only if NO>1 and ICOI=1)

COI(K, KO) - Initial oil phase concentration for oil component KO at K^{th} layer.

Units: volume fraction

3.3.35 COI(I,KO), for I=1, NBL, for KO=1,NO (This line is read only if NO>1 and ICOI=2)

COI(I,KO) - Initial oil phase concentration for oil component KO at I^{th} gridblock.

Units: volume fraction

Reservoir Property Modification Data (Lines 3.3.36-3.3.46) — This section is **required only if IMOD=1**.

3.3.36 IMPOR, IMKX, IMKY, IMKZ, IMSW (This line is read only if IMOD=1)

IMPOR - Flag indicating whether the porosity is modified or not.

Possible Values:

- 0 - No modification is considered in porosity values
- 1 - Allow modification in porosity

IMKX- Flag indicating whether the permeability in the X direction is modified or not.

Possible Values:

0 - No modification is considered in X permeability
1 - Allow modification in X permeability

IMKY- Flag indicating whether the permeability in the Y direction is modified or not.
Possible Values:
0 - No modification is considered in Y permeability
1 - Allow modification in Y permeability

IMKZ- Flag indicating whether the permeability in the Z direction is modified or not.
Possible Values:
0 - No modification is considered in Z permeability
1 - Allow modification in Z permeability

IMSW- Flag indicating whether the initial water saturation is modified or not.
Possible Values:
0 - No modification is considered in initial water saturation values
1 - Allow modification in initial water saturation

3.3.37 NMOD0 (This line is read only if IMOD=1 and IMPOR=1)
NMOD0 - Number of regions with modified porosity.

3.3.38 IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX (This line is read only if IMOD=1 and NMOD>0)
IMIN - The first index in X direction.
IMAX - The last index in X direction.
JMIN - The first index in Y direction.
JMAX - The last index in Y direction.
KMIN - The first index in Z direction.
KMAX - The last index in Z direction.
IFACT - Flag indicating how porosity is modified.
Possible Values:
1 - Replace porosity with FACTX
2 - Multiply porosity by FACTX
3 - Add FACTX to porosity
FACTX - The constant used to modify the porosity value.
Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD0 times.

3.3.39 NMOD1 (This line is read only if IMOD=1 and IMKX=1)
NMOD1 - Number of regions with modified X permeability.

3.3.40 IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX (This line is read only if IMOD=1 and NMOD1>0)
IMIN - The first index in X direction.
IMAX - The last index in X direction.
JMIN - The first index in Y direction.
JMAX - The last index in Y direction.
KMIN - The first index in Z direction.
KMAX - The last index in Z direction.
IFACT - Flag indicating how X permeability is modified.

Possible Values:

1 - Replace X permeability with FACTX
2 - Multiply X permeability by FACTX
3 - Add FACTX to X permeability

FACTX - The constant used to modify the X permeability value.

Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD1 times.

3.3.41 NMOD2 (This line is read only if IMOD=1 and IMKY=1)

NMOD2 - Number of regions with modified Y permeability.

3.3.42 IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX (This line is read only if IMOD=1 and NMOD2>0)

IMIN - The first index in direction.
IMAX - The last index in X direction.
JMIN - The first index in Y direction.
JMAX - The last index in Y direction.
KMIN - The first index in Z direction.
KMAX - The last index in Z direction.
IFACT - Flag indicating how Y permeability is modified.

Possible Values:

1 - Replace Y permeability with FACTX
2 - Multiply Y permeability by FACTX
3 - Add FACTX to Y permeability

FACTX - The constant used to modify the Y permeability value.

Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD2 times.

3.3.43 NMOD3 (This line is read only if IMOD=1 and IMKZ=1)

NMOD3 - Number of regions with modified Z permeability.

3.3.44 IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX **(This** line is read only if IMOD=1 and NMOD3>0)

IMIN - The first index in X direction.
IMAX - The last index in X direction.
JMIN - The first index in Y direction.
JMAX - The last index in Y direction.
KMIN - The first index in Z direction.
KMAX - The last index in Z direction.
IFACT - Flag indicating how Z permeability is modified.

Possible Values:

1 - Replace Z permeability with FACTX
2 - Multiply Z permeability by FACTX
3 - Add FACTX to Z permeability

FACTX - The constant used to modify the Z permeability value.

Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD3 times.

3.3.45 NMOD4 (This line is read only if IMOD=1 and IMSW=1)
NMOD4 - number of regions with modified initial water saturation.

3.3.46 IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX (This line is read only if IMOD=1 and NMOD4>0)
IMIN - The first index in X direction.
IMAX - The last index in X direction.
JMIN - The first index in Y direction.
JMAX - The last index in Y direction.
KMIN - The first index in Z direction.
KMAX - The last index in Z direction.
IFACT - Flag indicating how initial water saturation is modified.
Possible Values:
1 - Replace initial water saturation with FACTX
2 - Multiply initial water saturation by FACTX
3 - Add FACTX to initial water saturation
FACTX - The constant used to modify the initial water saturation value.
Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD4 times.

3.3.47 ***NMOD5*** (This line is read only if IMOD=1, IMSW=1, and IGAS•1)
NMOD5 - number of regions with modified initial gas saturation.

3.3.48 ***IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX*** (This line is read only if IMOD=1 and NMOD5>0)
IMIN - The first index in X direction.
IMAX - The last index in X direction.
JMIN - The first index in Y direction.
JMAX - The last index in Y direction.
KMIN - The first index in Z direction.
KMAX - The last index in Z direction.
IFACT - Flag indicating how initial gas saturation is modified.
Possible Values:
1 - Replace initial gas saturation with FACTX
2 - Multiply initial gas saturation by FACTX
3 - Add FACTX to initial gas saturation
FACTX - The constant used to modify the initial gas saturation value.
Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD5 times.

3.3.49 C50, C60
C50 - Initial brine salinity.
Units: meq/ml of brine
Note: This is assumed to be all the anions (in equivalents).
C60 - Initial divalent cation concentration of brine.
Units: meq/ml of brine

Note: C50 and C60 are replaced by the input values of C5I and C6I on input line 3.5.34 when IREACT>1.

3.4 General Physical Property Data

The fourth input section consists of the general physical property data. Please remember that there are seven comment lines at the beginning of this section and that each data line is preceded by three comment lines.

Surfactant/Cosolvent Phase Behavior Data (Lines 3.4.1-3.4.21)

3.4.1 C2PLC, C2PRC, EPSME, IHAND

C2PLC - Oil concentration at plait point in type II(+) region.
Units: volume fraction

C2PRC - Oil concentration at plait point in type II(-) region.
Units: volume fraction

EPSME - Critical micelle concentration (CMC)—minimum surfactant concentration for the formation of micelles.
Units: volume fraction

IHAND - Flag to specify whether modified Hand's rule is considered or not.
Possible Values:
0 - Original Hand's rule is considered for phase behavior (default)
1 - Modified Hand's rule is considered for Phase behavior

Note: The option of IHAND=1 is available only for oil/microemulsion, Type II(-) phase behavior, and IMASS=1.

3.4.2 IFGHBN

IFGHBN - Flag indicating type of phase behavior parameters.
Possible
0 - Input height of binodal curve (default)
1 - Input solubilization ratio (new option)

Note: The input height of binodal curve option (IFGHBN=1) is currently only available for the multiple organic option (NO>1). The effect of temperature or alcohol on phase behavior is not currently modeled for IFGHBN=1. See Sections 2 & 11 of this report for more details on the input height of binodal curve option and Section 7 for more details on the input solubilization ratio option.

Binodal Curve Input Option (Lines 3.4.3-3.4.11) — This section is **required only if IFGHBN=0**.

3.4.3 HBNS70, HBNC70, HBNS71, HBNC71, HBNS72, HBNC72 (This line is read only if IFGHBN=0)

HBNS70 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1 associated with surfactant at zero salinity.
Units: volume fraction

HBNC70 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 1 (associated with surfactant at zero salinity.
Units: volume fraction

HBNS71 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1 associated with surfactant at optimal salinity.
Units: volume fraction

HBNC71 - Intercept of maximum height of binodal curve at zero fraction of Alcohol associated with surfactant at optimal salinity.
Units: volume fraction

HBNS72 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1 associated with surfactant at twice optimal salinity.
Units: volume fraction

HBNC72 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 1 associated with surfactant at twice optimal salinity.
Units: volume fraction
Note: If alcohol is not present, the maximum height of binodal curves at three different salinities are the only parameters used in the phase behavior calculations.

3.4.4 HBNT70, HBNT71, HBNT72, CSET (This line is read if IFGHBN=0 and IENG=1)

HBNT70 - Slope of height of binodal curve versus temperature at zero salinity
Units: volume fraction/(•F) (IUNIT=0) or volume fraction/•C (IUNIT=1)

HBNT71 - Slope of height of binodal curve versus temperature at optimal salinity
Units: volume fraction /(•F) (IUNIT=0) or volume fraction/•C (IUNIT=1)

HBNT72 - Slope of height of binodal curve versus temperature at twice optimal salinity
Units: volume fraction /(•F) (IUNIT=0) or volume fraction/•C (IUNIT=1)

CSET - The Slope parameter, $\beta_{T,}$ for temperature dependency of the three-phase window
Units: (•F)$^{-1}$ (IUNIT=0) or (•C)$^{-1}$ (IUNIT=1)

3.4.5 HBNS80, HBNC80, HBNS81, HBNC81, HBNS82, HBNC82 (This line is read if IFGHBN=0)

HBNS80 - Slope for maximum height of binodal curve vs. fraction of Alcohol 2 associated with surfactant at zero salinity.
Units: volume fraction

HBNC80 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2 associated with surfactant at zero salinity.
Units: volume fraction

HBNS81 - Slope of maximum height of binodal curve vs. fraction of Alcohol 2 associated with surfactant at optimal salinity.
Units: volume fraction

HBNC81 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2 associated with surfactant at optimal salinity.
Units: volume fraction

HBNS82 - Slope for maximum height of binodal curve vs. fraction of Alcohol 2 associated with surfactant at twice optimal salinity.
Units: volume fraction

HBNC82 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2 associated with surfactant at twice optimal salinity.
Units: volume fraction

3.4.6 CSEL7, CSEU7, CSEL8, CSEU8 (This line is read if IFGHBN=0)

CSEL7 - Lower effective salinity limit for type III phase region determined when Alcohol 1 and calcium approach zero.
Units: meq/ml

CSEU7 - Upper effective salinity limit for type III phase region determined when Alcohol 1 and calcium approach zero.
Units: meq/ml

CSEL8 - Lower effective salinity limit for type III phase region determined when Alcohol 2 and calcium approach zero.
Units: meq/ml

CSEU8 - Upper effective salinity limit for type III phase region determined when Alcohol 2 and calcium approach zero.
Units: meq/ml

3.4.7 BETA6, BETA7, BETA8 (This line is read if IFGHBN=0)

BETA6 - The effective salinity slope parameter for calcium.
Units: dimensionless

BETA7 - The effective salinity slope parameter for Alcohol 1.
Units: dimensionless

BETA8 - The effective salinity slope parameter for Alcohol 2.
Units: dimensionless

3.4.8 IALC, OPSK7O, OPSK7S, OPSK8O, OPSK8S (This line is read if IFGHBN=0)

IALC - Flag indicating choice of alcohol partition model to use.
Possible Values:
0 - Hirasaki's model will be used
1 - Prouvost's model will be used

OPSK7O - Alcohol partition coefficient (oil/water) for Alcohol 1.
Units: dimensionless

OPSK7S - Alcohol partition coefficient (surfactant/water) for Alcohol 1.
Units: dimensionless

OPSK8O - Alcohol partition coefficient (oil/water) for Alcohol 2.
Units: dimensionless

OPSK8S - Alcohol partition coefficient (surfactant/water) for Alcohol 2.
Units: dimensionless

Note: If IALC=0 then OPSK7O, OPSK7S, OPSK8O, and OPSK8S remain fixed. If OPSK7O, OPSK7S, OPSK8O, and OPSK8S are equal to zero and IALC=0, then alcohol is lumped with surfactant as a single component (total chemical). OPSK7O, OPSK7S, OPSK8O, and OPSK8S are only used when Hirasaki's model is chosen. See Section 11 of this report for more details on the alcohol partition models.

3.4.9 NALMAX, EPSALC (This line is read if IFGHBN=0)

NALMAX - Maximum number of iterations for alcohol partitioning for two alcohol system.
Note: The suggested value is 20 and a value of zero would result in no iterations.

EPSALC - Tolerance for convergence of iterations for two alcohol system.
Note: Suggested values are 10^{-3} and 10^{-4}.

3.4.10 AKWC7, AKWS7, AKM7, AK7, PT7 (This line is read if IFGHBN=0)

AKWC7, AKWS7 - Parameters used to determine partition coefficient of monomeric Alcohol 1 between aqueous and oleic pseudophases.
Units: dimensionless

AKM7 - Partition coefficient of monomeric Alcohol 1 between surfactant and oleic pseudophases.
Units: dimensionless

AK7 - Self-association constant of Alcohol 1 in oleic pseudophase.
Units: dimensionless

PT7 - Ratio of molar volume of Alcohol 1 to equivalent molar volume of surfactant.
Units: dimensionless

3.4.11 AKWC8, AKWS8, AKM8, AK8, PT8 (This line is read if IFGHBN=0)

AKWC8, AKWS8 - Parameters used to determine partition coefficient of monomeric Alcohol 2 between aqueous and oleic pseudophases.
Units: dimensionless

AKM8 - Partition coefficient of monomeric Alcohol 2 between surfactant and oleic pseudophases.
Units: dimensionless

AK8 - Self-association constant of Alcohol 2 in oleic pseudophase.
Units: dimensionless

PT8 - Ratio of molar volume of Alcohol 2 to equivalent molar volume of surfactant.
Units: dimensionless

Solubilization Ratio Input Option (Lines 3.4.12-3.4.21) — These lines are **required only if** the phase behavior calculation is based on the solubilization ratio **(IFGHBN=1)**.

3.4.12 IOD (This line is read if IFGHBN=1 and NO>1)

IOD - Flag indicating whether phase behavior depends on organic composition
Possible Values:
- 0 - Phase behavior and properties depend on organic composition
- 1 - Phase behavior and properties are independent of organic composition (default)

3.4.13 NCOMP (This line is read only if IFGHBN=1 and IOD=0)

NCOMP - Number of organic components in the first solubility measurement.

3.4.14 ONAME(I) for I=1, NCOMP (This line is read only if IFGHBN=1 and IOD=0)

ONAME(I) - Name of organic species in the first solubility measurement. Currently the values in the following table can be specified.

ONAME Value	Formula	Name	Molecular Weight	Equivalent Alkane Carbon No. (EACN)
DECANE	$C_{10}H_{22}$	Decane	142	10
OCTANE	C_8H_{18}	Octane	114	8
HEXANE	C_6H_{14}	Hexane	86	6

PCE	C_2Cl_4	Tetrachloro-ethylene	165.8	2.9
PXYLEN		P-xylene	106	2
TOLUEN		Toluene	92	1
CCL4	CCl_4	Carbon tetrachloride	153.8	-0.06
TCE	C_2HCl_3	Trichloro-ethylene	131.4	-3.81
DCB	1,2-$C_6H_4Cl_2$	1,2-dichloro-benzene	146.9	-4.89
TCA	CH_3CCl_3	1,1,1-trichloro-ethene	133.35	-2.5
DCE	1,2-$C_2H_4Cl_2$		98.9	-12.1
CHCL3	$CHCl_3$		119.4	-13.67
CH2CL2	CH_2Cl_2		84.9	-13.79
C2CL4	1,1,2,2-$C_2H_2Cl_4$		167.8	-22.15

3.4.15 OCOMP(I), for I=1, NCOMP (This line is read only if IFGHBN=1 and IOD=0)

OCOMP(I) - concentration of Ith organic component in the first solubility measurement.
Units: mole fraction

3.4.16 CS0, SCS0, CS1, SCS1, CS2, SCS2, DCS20 (This line is read only if IFGHBN=1)

CS0 - Effective salinity which is between the lower and optimal effective salinity limits for type III phase region; CSEL<CS0<CSEOP.
Units: meq/ml

SCS0 - Solubility at CS0.
Units: volume fraction

CS1 - Optimal effective salinity (CSEOP).
Units: meq/ml•

SCS1 - Solubility at CS1.
Units: volume fraction

CS2 -Effective salinity which is between the optimal and the upper effective salinity limits for type III phase region ; CSEOP<CS2<CSEU.
Units: meq/ml•

SCS2 - Solubility at CS2.
Units: volume fraction

DCS20 - The difference of the upper and the lower effective salinity limits for type III phase region; C_{SEU} - C_{SEL}.

3.4.17 NCOMP (This line is read only if IFGHBN=1 and IOD=0)

NCOMP - Number of organic components in the second solubility measurement.

3.4.18 ONAME(I), for I=1, NCOMP (This line is read only if IFGHBN=1 and IOD=0)

ONAME(I) - Name of organic species in the second solubility measurement.
Note: See input line 3.4.14 for a list of available species names.

3.4.19 OCOMP(I), for I=1, NCOMP (This line is read only if IFGHBN=1 and IOD=0)

OCOMP(I) - concentration of Ith organic component in the second solubility measurement.
Units: mole fraction

3.4.20 CS0, SCS0, CS1, SCS1, CS2, SCS2, DCS20 (This line is read only if IFGHBN=1 and IOD=0)

CS0 - Effective salinity which is between the lower and optimal effective salinity limits for type III phase region; CSEL<CS0<CSEOP.
Units: meq/ml

SCS0 - Solubility at CS0.
Units: volume fraction

CS1 - Optimal effective salinity.
Units: meq/ml

SCS1 - Solubility at CS1.
Units: volume fraction

CS2 -Effective salinity which is between the optimal and the upper effective salinity limits for type III phase region ; CSEOP<CS2<CSEU.
Units: meq/ml

SCS2 - Solubility at CS2.
Units: volume fraction

DCS20 - The difference of the upper and the lower effective salinity limits for type III phase region; C_{SEU} - C_{SEL}.

Note: These values are the phase behavior information for the second organic mixture.

3.4.21 BETA6 (This line is read only if IFGHBN=1)

BETA6 - The effective salinity slope parameter for calcium.
Units: dimensionless

Interfacial Tension Data (Lines 3.4.22-3.4.25)

3.4.22 IFT

IFT - This flag indicates which interfacial tension correlation is used.
Possible Values:
- 0 - Healy and Reed's correlation will be used
- 1 - Huh's correlation will be used

Note: See Section 2 of this report for more details on the interfacial tension model options.

3.4.23 G11, G12, G13, G21, G22, G23 (This line is read only if IFT=0)

G11, G12, G13 - Interfacial tension parameters for water-microemulsion interface.
G21, G22, G23 - Interfacial tension parameters for oil-microemulsion interface.
Units: Dimensionless

3.4.24 CHUH, AHUH (This line is read only if IFT=1)

CHUH - Constant in modified Huh's interfacial tension correlation.
Typical Values: 0.1 - 0.35

AHUH - Constant in modified Huh's interfacial tension correlation
Typical values: 5 - 20

3.4.25 XIFTW

XIFTW - $\log_{10} \sigma_{wo}$ where σ_{wo} is the interfacial tension of the water-oil interface.

Units: dynes/cm = mN/m

Organic Mass Transfer Data (Lines 3.4.26-3.4.29)

3.4.26 IMASS

IMASS - Flag indicating the choice of oil solubility in water.

Possible Values

0 - No solubility of oil in water in the absence of surfactant

1 - Allow for solubility of oil in water in the absence of surfactant or allow for nonequilibrium transfer of oil in water

3.4.27 WSOL, CNEM2, ISOL (This line is read only if NO•1 and IMASS=1 and IGAS=0 with surfactant being present)

WSOL - Equilibrium concentration of oil in water in the absence of surfactant.

Units: volume fraction

CNEM2 - Coefficient of nonequilibrium mass transfer of oil in aqueous phase with or without surfactant.

Units: vol. of water/(bulk vol.-day)

Note: The input value of zero for CNEM2 represents an equilibrium mass transfer. The nonequilibrium mass transfer (CNEM2>0) calculation is valid for type II(-) with the plait point in the corner (C2PLC=0) and in the absence of gas phase (IGAS=0).

ISOL - Flag indicating the solution scheme for the nonequilibrium mass transfer calculations

Possible Values

0 - Implicit method is used

1 - Explicit method is used

Note: The explicit method (ISOL=1) is the only option available when gas is present (IGAS•1).

Note: See Section 12 of this report for more details on the rate limited organic dissolution model.

3.4.28 (WSOL(KO), for KO=1, NO), CNEM2, ISOL (This line read only if NO>1, IMASS=1, and IGAS=0 with surfactant being present)

WSOL(KO) - Water/oil equilibrium partition coefficient for oil component KO in the absence of surfactant

Units: volume fraction

CNEM2 - Coefficient of nonequilibrium mass transfer of oil components in aqueous phase when surfactant is present.

Units: vol. of water / (bulk vol.-day)

ISOL - Flag indicating whether the mass transfer calculation is implicit or explicit when surfactant is present.

Possible Values:

0 - Implicit method is used

1 - Explicit method is used

3.4.29 CNEMK(KO), for KO=1, NO (This line read only if NO>1, IMASS=1, and WSOL(KO)>0)

CNEMK(KO) - Coefficient of nonequilibrium mass transfer of oil component KO in aqueous phase when surfactant is not present.

Units: vol. of water / (bulk vol.-day)

Note: See Section 7 of this report for more details on the rate limited multiple organic dissolution model.

3.4.30 ITRAP, T11, T22, T33

ITRAP - Flag indicating whether residual saturations and relative permeabilities are dependent on capillary number or not.

Possible Values:

- 0 - Residual saturations are not dependent on capillary number; endpoint and exponent of relative permeability curves are constant
- 1 - Residual saturations and relative permeabilities are dependent on capillary number
- 2 - Residual saturations and relative permeabilities are dependent on trapping number

Note: ITRAP=2 is currently not available with the curvilinear grid option (ICOORD=4) or when gas is present (IGAS•1)

T11 - Capillary desaturation curve parameter for aqueous phase.

T22 - Capillary desaturation curve parameter for oleic phase.

T33 - Capillary desaturation curve parameter for microemulsion phase.

Note: Options ITRAP=1 and ITRAP=2 are identical for 1-d displacement in the vertical direction with zero capillary pressure. See Section 2 of this report for more information on the capillary and trapping number options.

Relative Permeability Data (Lines 3.4.31-3.4.57)

3.4.31 IPERM, IHYST, IPARK

IPERM - Flag indicating which relative permeability and capillary pressure model is used.

Possible Values:

- 0 - Imbibition Corey
- 1 - First drainage Corey (only for two phase water/oil flow)
- 2- Parker and Lenhard's model

Note: See Section 2 of this report for more details on this option.

IHYST - Flag indicating whether the hysteresis is used with Parker and Lenhard's model (IPERM=2)

Possible Values:

- 0 - Hysteretic model is not used
- 1 - Hysteretic model is used

Note: See Section 3 of this report for more details on this option.

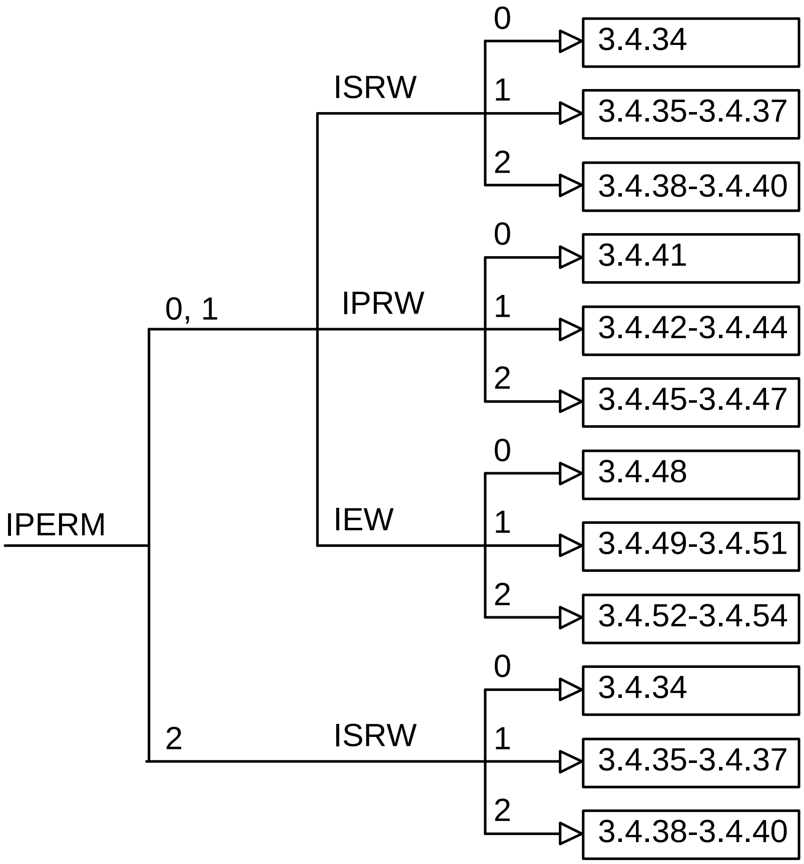
IPARK - Flag indicating the model used to calculate the oil trapping for hysteretic model

Possible Values:

- 0 - Kalurachchi and Parker's model is used
- 1 - Parker and Lenhard's model is used

Low Capillary Number Data (Lines 3.4.32-3.4.54)

Refer to the following flowchart to help determine which input lines should be used to specify the relative permeability parameters for different options:



3.4.32 ISRW, IPRW, IEW (This line is read only for IPERM< 2)

ISRW - Flag indicating type of residual saturation.

Possible Values:

0 - Constant residual saturation for entire reservoir
1 - Constant residual saturation for each layer
2 - Residual saturation for each gridblock

IPRW - Flag indicating type of endpoint relative permeability.

Possible Values:

0 - Constant endpoint relative permeability for entire reservoir
1 - Constant endpoint relative permeability for each layer
2 - Constant endpoint relative permeability for each gridblock

IEW - Flag indicating type of relative permeability exponent.

Possible Values:

0 - Constant relative permeability exponent for entire reservoir
1 - Constant relative permeability exponent for each layer
2 - Constant relative permeability exponent for each gridblock

3.4.33 ISRW (This line is read only if IPERM=2)

ISRW - Flag indicating type of residual saturation.

Possible Values:

0 - Constant residual saturation for entire reservoir
1 - Constant residual saturation for each layer
2 - Residual saturation for each gridblock

3.4.34 S1RWC, S2RWC, S3RWC (This line is read only if ISRW=0)

S1RWC - Residual saturation of aqueous phase displaced by oil at low capillary number for entire reservoir.

Units: fraction

S2RWC - Residual saturation of oleic phase displaced by water at low capillary number for entire reservoir.

Units: fraction

S3RWC - Residual saturation of microemulsion phase displaced by water at low capillary number for entire reservoir.

Units: fraction

3.4.35 S1RWC(K), for K=1, NZ (This line is read only if ISRW=1)

S1RWC(K) - Residual saturation of aqueous phase displaced by oil or gas at low capillary number for Kth layer.

Units: fraction

Note: S1RWC(K) must begin a separate line in the input file for each layer.

3.4.36 S2RWC(K), for K=1, NZ (This line is read only if ISRW=1)

S2RWC(K) - Residual saturation of oleic phase displaced by water at low capillary number for Kth layer.

Units: fraction

Note: S2RWC(K) must begin a separate line in the input file for each layer.

3.4.37 S3RWC(K), for K=1, NZ (This line is read only if ISRW=1)

S3RWC(K) - Residual saturation of microemulsion phase displaced by water or oil at low capillary number for Kth layer.

Units: fraction

Note: S3RWC(K) must begin a separate line in the input file for each layer.

3.4.38 S1RW(I), for I=1, NBL (This line is read only if ISRW=2)

S1RW(I) - Residual saturation of aqueous phase displaced by oil or gas at low capillary number for Ith gridblock.

Units: fraction

3.4.39 S2RW(I), for I=1, NBL (This line is read only if ISRW=2)

S2RWC(K) - Residual saturation of oleic phase displaced by water at low capillary number for Ith gridblock.

Units: fraction

3.4.40 S3RW(I), for I=1, NBL (This line is read only if ISRW=2)

S3RW(I) - Residual saturation of microemulsion phase displaced by water or oil at low capillary number for I^th gridblock.
Units: fraction

Relative Permeability Endpoint and Exponent Data (Lines 3.4.41-3.4.54) — These lines are **required only if** Corey function (**IPERM<2**) is used.

3.4.41 P1RWC, P2RWC, P3RWC (This line is read only if IPERM<2 and IPRW=0)

P1RWC - End point relative permeability of water at low capillary number for entire reservoir.
Units: dimensionless

P2RWC - End point relative permeability of oil at low capillary number for entire reservoir.
Units: dimensionless

P3RWC - End point relative permeability of microemulsion at low capillary number for entire reservoir.
Units: dimensionless

3.4.42 P1RWC(K), for K=1, NZ (This line is read only if IPERM<2 and IPRW=1)

P1RWC(K) - Constant endpoint relative permeability of water at low capillary number for K^th layer.
Units: dimensionless

3.4.43 P2RWC(K), for K=1, NZ (This line is read only if IPERM<2 and IPRW=1)

P2RWC(K) - Constant endpoint relative permeability of oil at low capillary number for K^th layer.
Units: dimensionless

3.4.44 P3RWC(K), for K=1, NZ (This line is read only if IPERM<2 and IPRW=1)

P3RWC(K) - Constant endpoint relative permeability of microemulsion at low capillary number for K^th layer.
Units: dimensionless

3.4.45 P1RW(I), for I=1, NBL (This line is read only if IPERM<2 and IPRW=2)

P1RW(I) - Endpoint relative permeability of water at low capillary number for I^th gridblock.
Units: dimensionless

3.4.46 P2RW(I), for I=1, NBL (This line is read only if IPERM<2 and IPRW=2)

P2RW(I) - Endpoint relative permeability of oil at low capillary number for I^th gridblock.
Units: dimensionless

3.4.47 P3RW(I), for I=1, NBL (This line is read only if IPERM<2 and IPRW=2)

P3RW(I) - Endpoint relative permeability of microemulsion at low capillary number for I^th gridblock.
Units: dimensionless

3.4.48 E1WC, E2WC, E3WC (This line is read only if IPERM<2 and IEW=0)

E1WC - Phase relative permeability exponent for aqueous phase at low capillary number for entire reservoir.
Units: dimensionless

E2WC - Phase relative permeability exponent for oleic phase at low capillary number for entire reservoir.
Units: dimensionless

E3WC - Phase relative permeability exponent for microemulsion phase at low capillary number system for entire reservoir.
Units: dimensionless

3.4.49 E1WC(K), for K=1, NZ (This line is read only if IPERM<2 and IEW=1)

E1WC(K) - Relative permeability exponent of aqueous phase at low capillary number for Kth layer.
Units: dimensionless

3.4.50 E2WC(K), for K=1, NZ (This line is read only if IPERM<2 and IEW=1)

E2WC(K) - Relative permeability exponent of oleic phase at low capillary number for Kth layer.
Units: dimensionless

3.4.51 E3WC(K), for K=1, NZ (This line is read only if IPERM<2 and IEW=1)

E3WC(K) - Relative permeability exponent of microemulsion phase at low capillary number for Kth layer.
Units: dimensionless

3.4.52 E1W(I), for I=1, NBL (This line is read only if IPERM<2 and IEW=2)

E1W(I) - Relative permeability exponent of aqueous phase at low capillary number for Ith gridblock.
Units: dimensionless

3.4.53 E2W(I), for I=1, NBL (This line is read only if IPERM<2 and IEW=2)

E2W(I) - Relative permeability exponent of oleic phase at low capillary number for Ith gridblock.
Units: dimensionless

3.4.54 E3W(I), for I=1, NBL (This line is read only if IPERM<2 and IEW=2)

E3W(I) - Relative permeability exponent of microemulsion phase at low capillary number for Ith gridblock.
Units: dimensionless

<u>High Capillary Number Data (Lines 3.4.55-3.4.57)</u> — These lines are **required only if <u>ITRAP=1</u>** or **<u>ITRAP=2</u>**.

3.4.55 S1RC, S2RC, S3RC (This line is read only if ITRAP=1 or 2)

S1RC - Residual saturation of aqueous phase at high capillary number.
Units: fraction

S2RC - Residual saturation of oleic phase at high capillary number.
Units: fraction

S3RC - Residual saturation of microemulsion phase at high capillary number.

Units: fraction

Note: The residual saturations at high capillary number can not be set equal to those at low capillary number.

3.4.56 P1RC, P2RC, P3RC (This line is read only for ITRAP=1 or 2 and IPERM< 2)

P1RC - End point relative permeability of aqueous phase at high capillary number condition.

Units: dimensionless

P2RC - End point relative permeability of oleic phase at high capillary number condition.

Units: dimensionless

P3RC - End point relative permeability of microemulsion phase at high capillary number condition.

Units: dimensionless

3.4.57 E13C, E23C, E31C (This line is read only for ITRAP=1 or 2 and IPERM< 2)

E13C, E23C, E31C - Parameters used for calculating exponents for relative permeability calculations at high capillary number.

Units: dimensionless

Viscosity Data (Lines 3.4.58-3.4.63)

3.4.58 VIS1, VIS2, TSTAND

VIS1 - Water viscosity at reference temperature.

Units: cp = mPa.s

VIS2 - Oil viscosity at reference temperature.

Units: cp = mPa.s

TSTAND - Reference temperature

Units: •F (IUNIT=0) or •C (IUNIT=1)

Note: For IENG=0, if TSTAND=0.0, the water component viscosity will be constant and equal to the input value VIS1. If TSTAND>0.0, water component viscosity will be calculated as a function of reservoir temperature, pressure, and local salinity for each gridblock.

3.4.59 IOVIS (This line read only if NO>1)

IOVIS - Flag indicating whether the viscosity is a function of organic composition.

Possible Values:

0 - Viscosity does not depend on the organic species concentration.
1 - Viscosity depends on the organic species concentration.

Note: See Section 2 of this report for more information on the IOVIS=0 option and Section 7 for more information on the IOVIS=1 option.

3.4.60 OVIS(K), for K=1, NO (This line is read only if NO>1 and IOVIS=1)

OVIS(K) - Viscosity for organic component K at reference temperature.

Units: cp = mPa.s

3.4.61 VIS4, VSLOPG (This line is read only if IGAS•1)

VIS4 - Gas viscosity at reference temperature and reference pressure.

Units: cp = mPa.s

VSLOPG - Slope of gas viscosity.

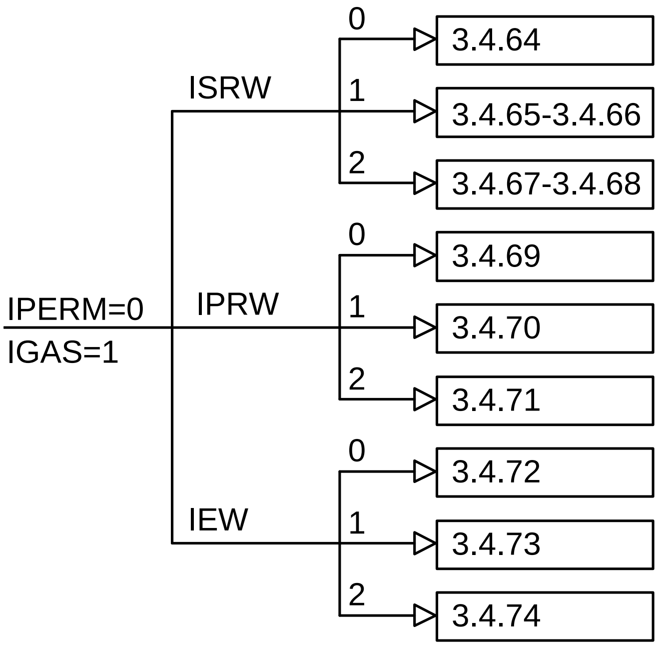
Units: (psi)$^{-1}$ (IUNIT=0) or (kPa)$^{-1}$ (IUNIT=1)

3.4.62 BVI(1), BVI(2) (This line is read only if IENG=1)
BVI(1) - Parameter for calculating water viscosity as a function of reservoir temperature.
Units: (•K)$^{-1}$
BVI(2) - Parameter for calculating oil viscosity as a function of reservoir temperature.
Units: (•K)$^{-1}$

3.4.63 BVI(4) (This line is read only if IGAS•1 and IENG=1)
BVI(4) - Parameter for calculating gas viscosity as a function of reservoir temperature.
Units: (•K)$^{-1}$

Corey Option Gas Relative Permeability Data (Lines 3.4.64-3.4.75) — These lines are **required only if IGAS•1** and **IPERM=0**.

Refer to the following flowchart to help determine which input lines should be used to specify the gas relative permeability parameters for different options:



3.4.64 S2RWC4, S4RWC (This line is read only if ISRW=0)
S2RWC4 - Constant residual oil saturation to displacing gas phase for entire reservoir.
Units: fraction
S4RWC - Constant residual gas saturation for entire reservoir.
Units: fraction

3.4.65 S2RWC4(K), for K=1, NZ (This line is read only if ISRW=1)
S2RWC4(K) - Constant residual oil saturation to displacing gas phase for Kth layer.
Units: fraction

3.4.66 S4RWC(K), for K=1, NZ (This line is read only if ISRW=1)
S4RWC(K) - Constant residual gas saturation for Kth layer.
Units: fraction

3.4.67 S2RW4(I), for I=1, NBL (This line is read only if ISRW=2)
S2RW4(I) - Constant residual oil saturation to displacing gas phase for Ith gridblock.
Units: fraction

3.4.68 S4RW(I), for I=1, NBL (This line is read only if ISRW=2)
S4RW(I) - Residual gas saturation for Ith gridblock.
Units: fraction

3.4.69 P4RWC (This line is read only if IPRW=0)
P4RWC - Constant gas endpoint relative permeability for entire reservoir.
Units: dimensionless

3.4.70 P4RWC(K), for K=1, NZ (This line is read only if IPRW=1)
P4RWC(K) - Constant gas endpoint relative permeability for Kth layer.
Units: dimensionless

3.4.71 P4RW(I), for I=1, NBL (This line is read only if IPRW=2)
P4RW(I) - Constant gas endpoint relative permeability for Ith gridblock.
Units: dimensionless

3.4.72 E4WC (This line is read only if IEW=0)
E4WC - Constant gas relative permeability exponent for entire reservoir.
Units: dimensionless

3.4.73 E4WC(K), for K=1, NZ (This line is read only if IEW=1)
E4WC(K) - Constant gas relative permeability exponent for Kth layer.
Units: dimensionless

3.4.74 E4WC(I), for I=1, NBL (This line is read only if IEW=2)
E4WC(I) - Constant gas relative permeability exponent for Ith gridblock.
Units: dimensionless

3.4.75 S4RC, P4RC, E4C, T44 (This line is read only if ITRAP=1)
S4RC - Residual gas saturations at high capillary number.
Units: fraction
P4RC - Gas endpoint relative permeability at high capillary number.
Units: dimensionless
E4C - Gas relative permeability exponent at high capillary number.
Units: dimensionless
T44 - Gas phase trapping parameter.
Units: dimensionless

3.4.76 XIFTG, ***XIFTGW*** (This line is read only if IGAS•1)
XIFTG - Log of interfacial tension between gas and oil.
Units: dyne/cm = mN/m
XIFTGW - Log of interfacial tension between gas and water.
Units: dyne/cm = mN/m

Microemulsion Viscosity Data (Line 3.4.77)

3.4.77 ALPHAV(I), for I=1, 5
ALPHAV(I) - Compositional phase viscosity parameters.
Units: dimensionless
Note: All five viscosity parameters must be positive values.
Note: See Section 2 of this report for more information on the compositional viscosity model.

Polymer Property Data (Lines 3.4.78-3.4.81) — See Section 2 of this report for information on the polymer property models.

3.4.78 AP1, AP2, AP3
AP1, AP2, AP3 - Parameters used for calculating polymer viscosity at zero shear rate as a function of polymer and electrolyte concentrations.
Units: $(\text{wt. \%})^{-1}$, $(\text{wt. \%})^{-2}$, $(\text{wt. \%})^{-3}$

3.4.79 BETAP, CSE1, SSLOPE
BETAP - Parameter for calculating the effective divalent salinity used to calculate polymer viscosity.
Units: dimensionless
CSE1 - Value below which the polymer viscosity is considered to be independent of salinity.
Units: meq/ml
SSLOPE - Slope of viscosity vs. effective salinity on a log-log plot—assumed to be constant.
Units: dimensionless
Note: This value is usually large and negative for hydrolyzed polyacrylamides and small and positive for polysaccharides.

3.4.80 GAMMAC, GAMHF, POWN
GAMMAC - Coefficient in shear rate equation below.
Units: $\frac{\text{day}\left(\text{darcy}\right)^{1/2}}{\text{ft}-\text{sec}}$ (IUNIT=0) or $\frac{\text{day}\left(\mu\text{m}^2\right)^{1/2}}{\text{m}-\text{sec}}$ (IUNIT=1)
GAMHF - Shear rate at which polymer viscosity is one half polymer viscosity at zero shear rate.
Units: sec^{-1}
POWN - Exponent for calculating shear rate dependence of polymer viscosity.
Units: dimensionless

3.4.81 IPOLYM, EPHI3, EPHI4, BRK, CRK
IPOLYM - Flag indicating type of polymer partitioning.
Possible Values:

0 - All polymer exists in aqueous phase if aqueous phase exists; otherwise, it exists completely in microemulsion phase

1 - Partitioning of polymer to water component is constant

EPHI3 - Effective porosity for surfactant—ratio of apparent porosity for surfactant to actual porosity.

Units: dimensionless

EPHI4 - Effective porosity for polymer—ratio of apparent porosity for polymer to actual porosity.

Units: dimensionless

BRK - Parameter for calculating permeability reduction factor.

Units: $\dfrac{\text{volume of polymer} - \text{rich phase}}{\text{weight\% polymer}}$

CRK - Parameter for calculating permeability reduction factor.

Units: $(\text{darcy})^{1/2}$ $(100\ \text{g/g})^{-1/3}$ = $(\mu\text{m}^2)^{1/2}$ $(100\ \text{g/g})^{-1/3}$)

Note: EPHI3 and EPHI4 are used to account for inaccessible pore volume in the case of surfactant and polymer.

$$\phi_{\text{surfactant}} = \phi \times \text{EPHI3}$$

$$\phi_{\text{polymer}} = \phi \times \text{EHPI4}$$

The effect of permeability reduction or residual resistance is to reduce the mobility of the polymer rich phase. This is accounted for by multiplying the viscosity of the phase by BRK.

Component Density Data (Lines 3.4.82-3.4.88)

3.4.82 DEN1, DEN2, ***DEN23***, DEN3, DEN7, DEN8, IDEN, IODEN

DEN1 - Specific weight or density of water (Component 1).

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN2 - Specific weight or density of oil (Component 2).

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN23 - Coefficient of oil in microemulsion phase density calculations.

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN3 - Specific weight or density of surfactant (Component 3).

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN7 - Specific weight or density of Alcohol 1 (Component 7).

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN8 - Specific weight or density of Alcohol 2 (when IGAS=0) or gas (when IGAS•1) (Component 7).

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

IDEN - Flag indicating if gravity effect should be considered.

Possible Values:

1 - Do not consider gravity effect

2 - Consider gravity effect

IODEN - Flag indicating if specific weight/density is a function of organic species concentration for NO>1.

Possible Values:

0 - Does not depend on organic species concentration

1 - Depends on organic species concentration

Note: See Section 2 of this report for information on the IODEN=0 option or Section 7 for information on the IODEN=1 option.

Note: Specific weight for pure water is 0.433 psi/ft (density of 1 g/cm^3). IODEN must be set to 1 if any non-aqueous phase species (those with indices < (8+NO)) participate in biodegradation equations.

Multiple Organic Density Data (Lines 3.4.83-3.4.84) — These lines are **required only if IODEN=1 and NO>1**.

3.4.83 DNOILC(K), for K=1, NO (This line is read only if IODEN=1 and NO>1)

DNOILC(K) - Specific weight or density of organic component K for oleic phase.

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

3.4.84 DNOME(K), for K=1, NO (This line is read only if IODEN=1 and NO>1)

DNOME(K) - Specific weight or density of organic component K for microemulsion phase.

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

Multiple Organic Data (Lines 3.4.85-3.4.88) — These lines are **required only if NO>1.** Furthermore, if (**IFGHBN=1** and **IOD=0**) or **IOVIS=1**.

3.4.85 INAME (This line is read only if NO>1 and ((IFGHBN=1 and IOD=0) or IOVIS=1)))

INAME - Flag indicating whether name of the organic components will be provided by user.

Possible Values:

0 - Name of the organic components will be provided; the molecular weight and equivalent alkane carbon number will be obtained from the built-in database

1 - Molecular weight and equivalent alkane carbon number for each organic components will be provided.

3.4.86 ONAME(K), for K=1, NO (This line is read only if NO>1 and ((IFGHBN=1 and IOD=0) or IOVIS=1)) and INAME=0)

ONAME(K) - Name of organic component K. See input line 3.4.14 for a list of valid component names.

3.4.87 OMWT(K), for K=1, NO (This line is read only if NO>1 and ((IFGHBN=1 and IOD=0) or IOVIS=1)) and INAME=1)

OMWT(K) - Molecular weight for organic component K.

3.4.88 OEACN(K), for K=1, NO (This line is read only if NO>1 and ((IFGHBN=1 and IOD=0) or IOVIS=1)) and INAME=1)

OEACN(K) - equivalent alkane carbon number for organic component K.

Note: See Section 7 of this report for information on the equivalent alkane carbon number.

3.4.89 ISTB

ISTB - Flag indicating the units to be used when printing injection and production rates.

Possible Values:

0 - Rates printed at bottomhole condition in ft^3 or m^3

1 - Rates printed at surface condition in bbls

3.4.90 FVF(L), for L=1, MXP (This line is read only if ISTB=1 and IUNIT=0)
FVF(L) - Formation volume factor for L^{th} phase.
Units: SCF/ft^3
Note: MXP=3 when IGAS=0 and MXP=4 when IGAS•1.

Fluid Compressibility Data (Lines 3.4.91-3.4.93)

3.4.91 COMPC(1), COMPC(2), COMPC(3), COMPC(7), COMPC(8)
COMPC(1) - Compressibility of brine (Component 1).
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)
COMPC(2) - Compressibility of oil (Component 2).
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)
COMPC(3) - Compressibility of surfactant (Component 3).
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)
COMPC(7) - Compressibility of Alcohol 1 (Component 7).
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)
COMPC(8) - Compressibility of Alcohol 2 (when IGAS=0) or gas (when IGAS•1) (Component 8).
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)
Note: For incompressible fluids, values of zero should be used for the COMPC values listed above.

3.4.92 ICOMPO (This line is read only if NO>1)
ICOMPO - Flag indicating whether each organic component has different compressibility.
Possible Values:
0 - All organic components have the same compressibility as COMPC(2)
1 - Each organic component has different compressibility

3.4.93 COMPO(K), for K=1, NO (This line is read only if NO>1 and ICOMPO=1)
COMPO(K) - Compressibility of organic component K.
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

Capillary Pressure Data (Lines 3.4.94-3.4.117) — See Section 2 of this report for capillary pressure information.

3.4.94 ICPC, IEPC, IOW
ICPC - Flag indicating type of capillary pressure endpoint.
Possible Values:
0 - Constant capillary pressure endpoint for entire reservoir
1 - Constant capillary pressure endpoint for each layer
2 - Capillary pressure endpoint for each gridblock
IEPC - Flag indicating type of capillary pressure exponent.
Possible Values:
0 - Constant capillary pressure exponent for entire reservoir
1 - Constant capillary pressure exponent for each layer
2 - Capillary pressure exponent for each gridblock

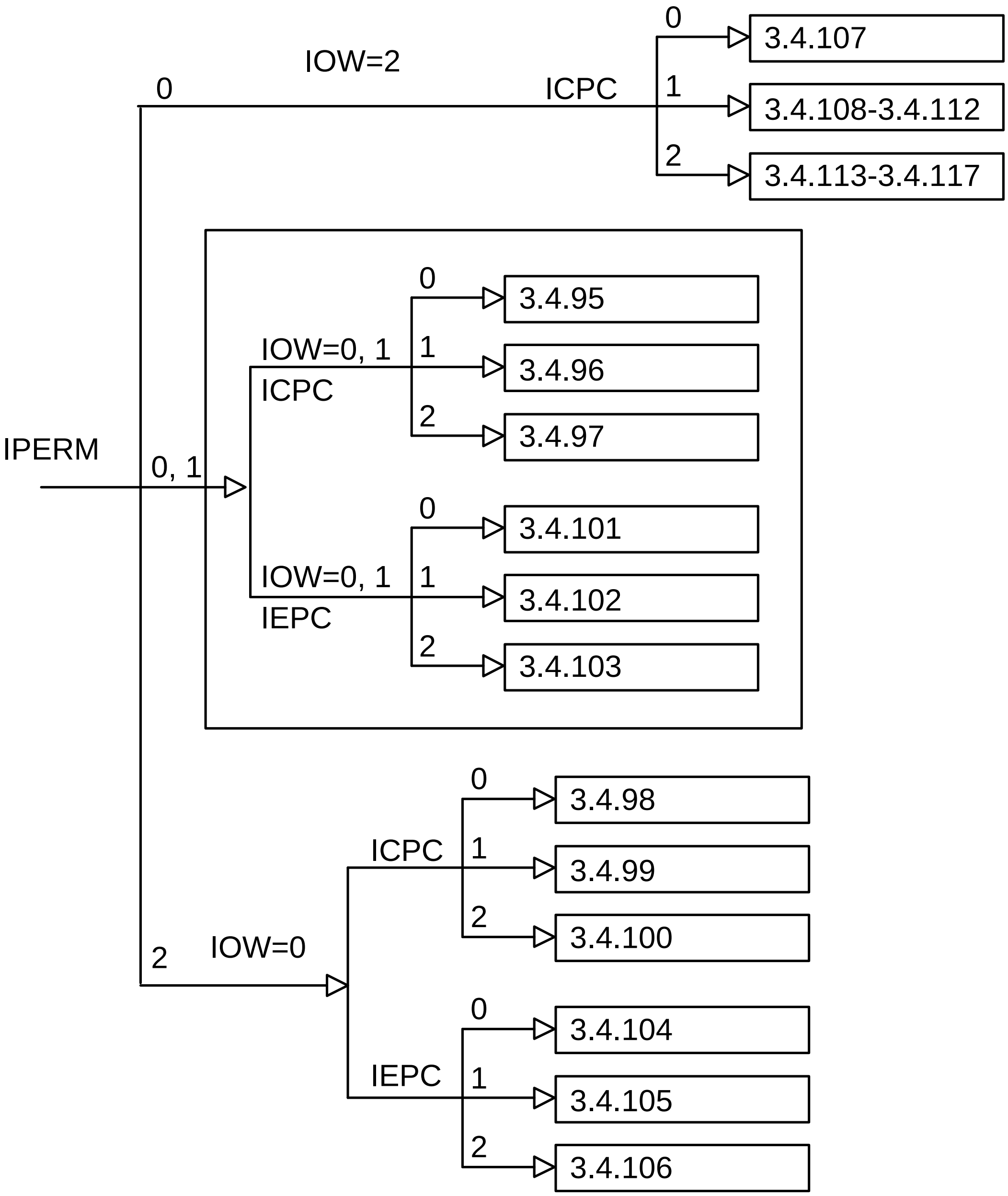
IOW - Flag indicating the wettability for two-phase oil/water capillary pressure calculations using imbibition Corey function (IPERM=0).

Possible Values:

0 - The capillary pressure curve is for strongly water-wet rock (default)
1 - The capillary pressure curve is for strongly oil-wet rock
2 - The capillary pressure curve is for mixed-wet rocks

Note: IOW=1 and 2 are available only for IPERM=0.

Refer to the following flowchart to help determine which input lines should be used to specify the capillary pressure data for different options:



<u>Capillary Pressure Data for Strongly Water- or Oil-Wet Rocks (Lines 3.4.95-3.4.106)</u> — These lines are **required only if <u>IOW<2</u>**.

3.4.95 CPC0 (This line is read only if IOW<2 and ICPC=0 and IPERM<2)
CPC0 - Capillary pressure endpoint for entire reservoir.
Units: $\mathrm{psi}\cdot\sqrt{\mathrm{darcies}}$ (IUNIT=0) or $\mathrm{kPa}\cdot\sqrt{\mu\mathrm{m}^2}$ (IUNIT=1)

3.4.96 CPC(K), for K=1, NZ (This line is read only if IOW<2 and ICPC=1 and IPERM<2)
CPC(K) - Capillary pressure endpoint for Kth layer.
Units: $\mathrm{psi}\cdot\sqrt{\mathrm{darcies}}$ (IUNIT=0) or $\mathrm{kPa}\cdot\sqrt{\mu\mathrm{m}^2}$ (IUNIT=1)

3.4.97 CPC(I), for I=1, NBL (This line is read only if IOW<2 and ICPC=2 and IPERM<2)
CPC(I) - Capillary pressure endpoint for Ith gridblock.
Units: $\mathrm{psi}\cdot\sqrt{\mathrm{darcies}}$ (IUNIT=0) or $\mathrm{kPa}\cdot\sqrt{\mu\mathrm{m}^2}$ (IUNIT=1)

3.4.98 CPC0 (This line is read only if IOW=0 and ICPC=0 and IPERM=2)
CPC0 - van Genuchten capillary pressure parameter, α, for entire reservoir.
Units: $\left(\mathrm{psi}\cdot\sqrt{\mathrm{darcies}}\right)^{-1}$ (IUNIT=0) or $\sqrt{\mu\mathrm{m}^2}$ / kPa (IUNIT=1)

3.4.99 CPC(K), for K=1, NZ (This line is read only if IOW=0 and ICPC=1 and IPERM=2)
CPC(K) - van Genuchten capillary pressure parameter, α, for Kth layer.
Units: $\left(\mathrm{psi}\cdot\sqrt{\mathrm{darcies}}\right)^{-1}$ (IUNIT=0) or $\sqrt{\mu\mathrm{m}^2}$ / kPa (IUNIT=1)

3.4.100 CPC(I), for I=1, NBL (This line is read only if IOW=0 and ICPC=2 and IPERM=2)
CPC(I) - van Genuchten capillary pressure parameter, α, for Ith gridblock.
Units: $\left(\mathrm{psi}\cdot\sqrt{\mathrm{darcies}}\right)^{-1}$ (IUNIT=0) or $\sqrt{\mu\mathrm{m}^2}$ / kPa (IUNIT=1)

3.4.101 EPC0 (This line is read only if IOW<2 and IEPC=0 and IPERM<2)
EPC0 - Capillary pressure exponent for entire reservoir.
Units: dimensionless

3.4.102 EPC(K), for K=1, NZ (This line is read only if IOW<2 and IEPC=1 and IPERM<2)
EPC(K) - Capillary pressure exponent for Kth layer.
Units: dimensionless

3.4.103 EPC(I), for I=1, NBL (This line is read only if IOW<2 and IEPC=2 and IPERM<2)
EPC(I) - Capillary pressure exponent for Ith gridblock.
Units: dimensionless

3.4.104 EPC0 (This line is read only if IOW=0 and IEPC=0 and IPERM=2)
EPC0 - van Genuchten capillary pressure parameter, n, for entire reservoir.
Units: dimensionless

3.4.105 EPC(K), for K=1, NZ (This line is read only if IOW=0 and IEPC=1 and IPERM=2)

EPC(K) - van Genuchten capillary pressure parameter, n, for Kth layer.
Units: dimensionless

3.4.106 EPC(I), for I=1, NBL (This line is read only if IOW=0 and IEPC=2 and IPERM=2)

EPC(I) - van Genuchten capillary pressure parameter, n, for Ith gridblock.
Units: dimensionless

<u>Capillary Pressure Data for Mixed-Wet Rocks (Lines 3.4.107-3.4.117)</u> — These lines are **required only if <u>IPERM=0</u>** and **<u>IOW=2</u>**.

3.4.107 CPCW, EPCW, CPCO, EPCO, SSTAR (This line is read only if IPERM=0 and IOW=2 and ICPC=0)

CPCW - Capillary pressure endpoint for entire reservoir for positive branch.
Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

EPCW - Capillary pressure exponent for entire reservoir for positive branch.
Units: dimensionless

CPCO - Capillary pressure endpoint for entire reservoir for negative branch.
Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

EPCO - Capillary pressure exponent for entire reservoir for negative branch.
Units: dimensionless

SSTAR - Water saturation where the capillary pressure is zero.
Units: dimensionless

3.4.108 CPCW(K), for K=1, NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=1)

CPCW - Capillary pressure endpoint for kth layer for positive branch.
Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

3.4.109 EPCW(K), for K=1, NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=1)

EPCW (K) - Capillary pressure exponent for entire reservoir.
Units: dimensionless

3.4.110 CPCO(K), for K=1, NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=1)

CPCO (K) - Capillary pressure endpoint for Kth layer for negative branch.
Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

3.4.111 EPCO(K), for K=1, NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=1)

EPCO (K) - Capillary pressure exponent for Kth layer for negative branch.
Units: dimensionless

3.4.112 SSTAR(K), for K=1, NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=1)

SSTAR (K) - Water saturation for Kth layer where the capillary pressure is zero.
Units: dimensionless

3.4.113 CPCW(I), for I=1, NBL (This line is read only if IPERM=0 and IOW=2 and ICPC=2)

CPCW (I) - Capillary pressure endpoint for Ith gridblock for positive branch.

Units: psi$\sqrt{\text{darcies}}$ (IUNIT=0) or kPa$\sqrt{\mu\text{m}^2}$ (IUNIT=1)

3.4.114 EPCW(I), for I=1, NBL (This line is read only if IPERM=0 and IOW=2 and ICPC=2)

EPCW (I) - Capillary pressure exponent for Ith gridblock for positive branch.

Units: dimensionless

3.4.115 CPCO(I), for I=1, NBL (This line is read only if IPERM=0 and IOW=2 and ICPC=2)

CPCO - Capillary pressure endpoint for Ith gridblock for negative branch.

Units: psi$\sqrt{\text{darcies}}$ (IUNIT=0) or kPa$\sqrt{\mu\text{m}^2}$ (IUNIT=1)

3.4.116 EPCO(I), for I=1, NBL (This line is read only if IPERM=0 and IOW=2 and ICPC=2)

EPCO - Capillary pressure exponent for Ith gridblock for negative branch.

Units: dimensionless

3.4.117 SSTAR(I), for I= 1, NBL (This line is read only if IPERM=0 and IOW=2 and ICPC=2)

SSTAR (I) - Water saturation in Ith gridblock where the capillary pressure is zero.

Units: dimensionless

<u>Diffusion and Dispersion Data (Lines 3.4.118-3.4.125)</u>

3.4.118 D(KC,1), for KC=1, N

D(KC,1) - Molecular diffusion coefficient of KCth component in aqueous phase.

Units: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

3.4.119 D(KC,2), for KC=1, N

D(KC,2) - Molecular diffusion coefficient of KCth component in oleic phase.

Units: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

3.4.120 D(KC,3), for KC=1, N

D(KC,3) - Molecular diffusion coefficient of KCth component in microemulsion phase.

Units: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

3.4.121 D(KC,4), for KC=1, N (This line is read only if IGAS•1)

D(KC,4) - Molecular diffusion coefficient of KCth component in gas phase.

Units: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

Note: The input diffusion coefficient should be divided by tortuosity (D/τ) where the value of tortuosity is greater than one.

3.4.122 ALPHAL(1), ALPHAT(1)

ALPHAL(1) - Longitudinal dispersivity of aqueous phase.

Units: feet (IUNIT=0) or m (IUNIT=1)

ALPHAT(1) - Transverse dispersivity of aqueous phase.

Units: feet (IUNIT=0) or m (IUNIT=1)

3.4.123 ALPHAL(2), ALPHAT(2)
ALPHAL(2) - Longitudinal dispersivity of oleic phase.
Units: feet (IUNIT=0) or m (IUNIT=1)
ALPHAT(2) - Transverse dispersivity of oleic phase.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.4.124 ALPHAL(3), ALPHAT(3)
ALPHAL(3) - Longitudinal dispersivity of microemulsion phase.
Units: feet (IUNIT=0) or m (IUNIT=1)
ALPHAT(3) - Transverse dispersivity of microemulsion phase.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.4.125 ALPHAL(4), ALPHAT(4) (This line is read only if IGAS•1)
ALPHAL(4) - Longitudinal dispersivity of gas phase.
Units: feet (IUNIT=0) or m (IUNIT=1)
ALPHAT(4) - Transverse dispersivity of gas phase.
Units: feet (IUNIT=0) or m (IUNIT=1)

Adsorption Data (Lines 3.4.126-3.4.129)

3.4.126 IADSO
IADSO - Flag to specify organic adsorption calculation.
Possible Values
0 - Organic adsorption calculation is not considered
1 - Organic adsorption calculation is considered

3.4.127 FOC, AKOC, DENS (This line is read only if IADSO=1 and NO•1)
FOC - fraction of organic carbon in soil.
Units: dimensionless
AKOC - Organic adsorption coefficient.
Units: $\frac{\mu\text{g adsorbed}/\text{g organic carbon}}{\mu\text{g}/\text{ml solution}}$
DENS - grain density
Units: lb/ft^3 (IUNIT=0), g/cc (IUNIT=1)
Note: See Section 2 of this report for information on the organic adsorption model.

3.4.128 FOC, (AKOCK(K), for K=1, NO), DENS (This line is read only if IADSO=1 and NO>1)
FOC - Fraction of organic carbon in soil.
Units: dimensionless
AKOCK(K) - Organic adsorption coefficient for oil component K.
Units: $\frac{\mu\text{g adsorbed}/\text{g organic carbon}}{\mu\text{g}/\text{ml solution}}$
DENS - grain density.
Units: lb/ft^3 (IUNIT=0), g/cc (IUNIT=1)
Note: See Section 7 of this report for information on the multiple organic adsorption model.

3.4.129 AD31, AD32, B3D, AD41, AD42, B4D, IADK, IADS1, FADS

AD31 - Surfactant adsorption parameter.
Units: dimensionless

AD32 - Surfactant adsorption parameter.
Units: ml/meq

B3D - Surfactant adsorption parameter.
Units: $\frac{\text{volume of water}}{\text{volume of surfactant}}$

AD41 - Polymer adsorption parameter.
Units: dimensionless

AD42 - Polymer adsorption parameter.
Units: ml/meq

B4D - Polymer adsorption parameter.
Units: $\frac{\text{volume of water}}{\text{weight\% polymer}}$

IADK - Permeability dependent adsorption flag
Possible Values:
- 0 - Surfactant and polymer adsorption is independent of permeability
- 1 - Surfactant and polymer adsorption is dependent on permeability

IADS1 - Flag to specify the competitive surfactant adsorption in the presence of polymer
Possible Values:
- 0 - Surfactant and polymer adsorption are independent
- 1 - Competitive surfactant and polymer adsorption is considered

FADS - Parameter to adjust the competitive adsorption calculation

Note: See Section 2 of this report for information on the surfactant and polymer adsorption model.

3.4.130 QV, XKC, XKS, EQW

QV - Cation exchange capacity of clays.
Units: meq/ml of pore volume

XKC - Cation exchange constant for clays.
Units: $(\text{meq/ml})^{-1}$

XKS - Cation exchange constant for surfactant.
Units: $(\text{meq/ml})^{-1}$

EQW - Equivalent weight of surfactant.

Note: See Section 2 of this report for information on the cation exchange model.

Tracer Data (Lines 3.4.131-3.4.143) — These lines are **required only if NTW+NTA>0**. See Section 4 of this report for more details on tracer modeling in UTCHEM.

3.4.131 TK(I), for I=1, NTW+NTA (This line is read only if NTW+NTA>0)

TK(I) - Tracer partitioning coefficient for I^{th} water/oil tracer at initial chloride concentration and reference temperature. A value of 0.0 indicates a water or gas tracer and a value of -1.0 indicates an oil tracer.
Units: fraction

3.4.132 TKS(I), for I=1, NTW (This line is read only if NTW>0)

TKS(I) - Parameter for calculating water/oil tracer partitioning coefficient for I^{th} tracer as a function of salinity.
Units: $(meq/ml)^{-1}$

3.4.133 TKT(I), for I=1, NTW+NTA (This line is read only if NTW+NTA>0 and IENG=1)

TKT(I) - Parameter for calculating tracer partitioning coefficient for I^{th} tracer as a function of reservoir temperature.
Units: $(•F)^{-1}$ (IUNIT=0) or $(•C)^{-1}$ (IUNIT=1)

3.4.134 RDC(I), for I=1, NTW+NTA (This line is read only if NTW+NTA>0)

RDC(I) - Radioactive decay coefficient for I^{th} tracer. A value of 0.0 indicates a non–radioactive tracer.
Units: 1/days

3.4.135 RET(I), for I=1, NTW+NTA (This line is read only if NTW+NTA>0)

RET(I) - Tracer adsorption parameter (adsorbed concentration/flowing concentration). A value of 0.0 indicates no retardation.
Units: dimensionless

Dead-end Pore Model Data (Lines 3.4.136-3.4.139) — These lines are **required only if NTW+NTA>0 and ICAP=1**.

3.4.136 FFL(1), FFH(1), CM(I,1), for I=1, NTW+NTA (This line is read only if NTW+NTA>0 and ICAP=1)

FFL(1) - Water phase flowing fraction at fractional flow = 0.0.
Units: dimensionless

FFH(1) - Water phase flowing fraction at fractional flow = 1.0.
Units: dimensionless

CM(I,1) - Mass transfer coefficients for I^{th} tracer in water phase.
Units: 1/sec

3.4.137 FFL(2), FFH(2), CM(I,2), for I=1, NTW+NTA (This line is read only if NTW+NTA>0 and ICAP=1)

FFL(2) - Oil phase flowing fraction at fractional flow = 0.0.
Units: dimensionless

FFH(2) - Oil phase flowing fraction at fractional flow = 1.0.
Units: dimensionless

CM(I,2) - Mass transfer coefficients for I^{th} tracer in oil phase.
Units: 1/sec

3.4.138 FFL(3), FFH(3), CM(I,3), for I=1, NTW+NTA (This line is read only if NTW+NTA>0 and ICAP=1)

FFL(3) - Microemulsion phase flowing fraction at fractional flow = 0.0.
Units: dimensionless

FFH(3) - Microemulsion phase flowing fraction for at fractional flow = 1.0.
Units: dimensionless

CM(I,3) - Mass transfer coefficients for I^{th} tracer in microemulsion phase.
Units: 1/sec

3.4.139 FFL(4), FFH(4), CM(I,4), for I=1, NTW+NTA (This line is read only if NTW+NTA>0 and ICAP=1 and IGAS•1)

FFL(4) - Value of flowing fraction for gas phase when fractional flow = 0.0.
Units: dimensionless

FFH(4) - Value of flowing fraction for gas phase when fractional flow = 1.0.
Units: dimensionless

CM(I,4) - Mass transfer coefficients for I^{th} tracer in gas phase.
Units: 1/sec

<u>Reacting Tracer Data (Lines 3.4.140-3.4.143)</u> — The following lines are **required only if <u>NTW>0</u> and <u>ITREAC=1</u>**.

3.4.140 NRT, TAK(I), for I=1, NRT (This line is read only if NTW>0 and ITREAC=1)

NRT - Number of reacting tracers.
Possible Values: 1 or 2

TAK(I) - Rate constant for a first-order aqueous phase reaction at reference temperature for reacting tracer I
Units: days^{-1}

Note: First reacting tracer is tracer 2 hydrolyzes to form tracer 3. The second reacting tracer if present is tracer 4 hydrolyzes to form tracer 5.

3.4.141 TMW(I), for I=1, NTW (This line is read only if NTW>0 and ITREAC=1)

TMW(I) - Molecular weight of the I^{th} tracer.
Units: The user can specify the molecular weight in any unit as long as the units are the same for all the tracers. It is assumed that the reaction of 1 mole of primary tracer produces 1 mole of secondary tracer. If not, use "equivalent" molecular weights.

3.4.142 TDEN(I), for I=1, NTW (This line is read only if NTW>0 and ITREAC=1)

TDEN(I) - Density of the I^{th} tracer.
Units: g/cm^3

3.4.143 TAKT(I), for I=1, NRT (This line is read only if NTW>0 and ITREAC=1 and IENG=1)

TAKT(I) - Parameter for calculating rate constant for a first-order aqueous phase reaction as a function of reservoir temperature for reacting tracer I.
Units: (•K)$^{-1}$

Dual Porosity Data (Lines 3.4.144-3.4.162) — This section is **required for dual porosity option (ICAP=2) only**. This option works only with English unit (IUNIT=0) and the Cartesian coordinate (ICOORD=1). See Section 5 of this report for more details on this option. The capability of dual porosity option at this time is limited to single phase water and one tracer component. Restart capability (IMODE=2) is not currently available for the dual porosity option.

3.4.144 NSUB, MSUB, ISUB (This line is read only if ICAP=2)
NSUB – Number of subgrids in lateral direction.
MSUB – Number of subgrids in vertical direction.
ISUB – Mode of subgridding
Possible Values:
0 - Uniform matrix block dimension
1 - Variable matrix block size dimension in each direction
2 - Variable matrix block dimension in whole reservoir

3.4.145 XL1, YL1, ZL1 (This line is read only if ICAP=2 and ISUB=0)
XL1, YL1 and ZL1 – Uniform matrix block sizes in x y, and z directions.
Units: feet

3.4.146 II1, II2, XL1 (This line is read only if ICAP=2 and ISUB=1)
II1, II2 - First and last index for gridblocks with same size in X direction.
XL1– Matrix block size in X direction.
Units: feet

3.4.147 JJ1, JJ2, YL1 (This line is read only if ICAP=2 and ISUB=1)
JJ1, JJ2 - First and last index for gridblocks with same size in Y direction.
YL1 – Matrix block size in Y direction.
Units: feet

3.4.148 KK1, KK2, ZL1 (This line is read only if ICAP=2 and ISUB=1)
KK1, KK2 - First and last index for gridblocks with same size in Z direction
ZL1 – Matrix block size in Z direction.
Units: feet

3.4.149 XL(I), for I=1, NBL (This line is read only if ICAP=2 and ISUB=2)
XL(I) - Matrix block size in X direction for Ith reservoir gridblock.
Units: feet

3.4.150 YL(I), for I=1, NBL (This line is read only if ICAP=2 and ISUB=2)
YL(I) - Matrix block size in Y direction for Ith reservoir gridblock.
Units: feet

3.4.151 ZL(I), for I=1, NBL (This line is read only if ICAP=2 and ISUB=2)
ZL(I), - Matrix block size in Z direction for Ith reservoir gridblock.
Units: feet

3.4.152 VFRACM(J), for J=1, NSUB (This line is read only if ICAP=2)

VFRACM(J) – Volume fraction of Jth subgrid. These values are used to generate subgrids in the lateral direction.

3.4.153 ZFRACM(J), for J=1, MSUB (This line is read only if ICAP=2)

ZFRACM – Thickness fraction of Jth vertical subgrid. These values are used to generate subgrids in the vertical direction.

3.4.154 KPH, KKX, KKZ (This line is read only if ICAP=2)

KPH – Flag for matrix porosity distribution.

Possible Values:

- 0 - Uniform matrix porosity
- 1 - Variable matrix porosity

KKX – Flag for diffusion coefficient distribution in lateral direction in matrix.

Possible Values:

- 0 - Uniform matrix diffusion coefficient
- 1 - Uniform matrix diffusion coefficient in each reservoir layer
- 2 - Variable matrix diffusion coefficient at each reservoir node

KKZ – Flag for diffusion coefficient distribution in vertical direction in matrix.

Possible Values:

- 0 - Uniform matrix diffusion coefficient
- 1 - Uniform matrix diffusion coefficient in each reservoir layer
- 2 - Variable matrix diffusion coefficient at each reservoir node

3.4.155 PHIC (This line is read only if ICAP=2 and KPH=0)

PHIC – Matrix porosity.

3.4.156 PORCM(I,1,1), for I=1, NBL (This line is read only if ICAP=2 and KPH=1)

PORCM(I,1,1) – Matrix porosity of the Ith reservoir node.

3.4.157 DMC (This line is read only if ICAP=2 and KKX=0)

DMC – Matrix diffusion coefficient in lateral direction.

Units: ft^2/day

3.4.158 DMX(K), for K=1, NZ (This line is read only if ICAP=2 and KKX=1)

DMX(K) – Matrix diffusion coefficient in Kth reservoir layer in lateral direction.

Units: ft^2/day

3.4.159 DMX(I), for I=1, NBL (This line is read only if ICAP=2 and KKX=2)

DMX(I) – Matrix diffusion coefficient at Ith reservoir node in lateral direction.

Units: ft^2/day

3.4.160 DMC (This line is read only if ICAP=2 and KKZ=0)

DMC – Matrix diffusion coefficient in vertical direction.

Units: ft^2/day

3.4.161 DMZ(K), for K=1, NZ (This line is read only if ICAP=2 and KKZ=1)

DMZ(K) – Matrix diffusion coefficient in Kth reservoir layer in vertical direction.

Units: ft^2/day

3.4.162 DMZ(I), for I=1, NBL (This line is read only if ICAP=2 and KKZ=2)

DMZ(I) – Matrix diffusion coefficient at Ith reservoir node in vertical direction.

Units: ft^2/day

Gel Reaction Data (Lines 3.4.163-3.4.167) — These lines are **required only if IREACT=1 or IREACT=4 and NG>0**. Refer to Section 6 of this report for more details on this option.

3.4.163 KGOPT, AK1, AK2, SCR, X4, X13, X14, X16, WM4 (This line is read only if IREACT=1 or 4 and NG>0)

KGOPT - Flag to specify the gelation type used.

Possible Values:

1 - Polymer/chromium chloride gel
2 - Polymer/chromium malonate gel
3 - Silicate gel

AK1 - Kinetic rate coefficient for NG1 and NG2 at reference temperature (KGOPT=1).

Units: ppm^{-1} days^{-1}

AK2 - Kinetic rate coefficient for gel at reference temperature .

Units: (mole/liter)$^{1-X4-X14+X16}$ days^{-1} for KGOPT=1
(mole/liter)$^{1-X4-X13+X16}$ days^{-1} for KGOPT=2
(mole/liter)$^{1-X4+X14}$ days^{-1} for KGOPT=3

SCR - Stoichiometric ratio in mass between Cr^{3+} and polymer.

Units: dimensionless

X4 - Exponent to be used for polymer or silicate in gelation reaction.

Units: dimensionless

X13 - Exponent to be used for component (NG2) in gelation reaction for KGOPT=2.

Units: dimensionless

X14 - Exponent to be used for the third gel option component (NG3) in gelation reaction.

Units: dimensionless

X16 - Exponent to be used for hydrogen ion component (NG5) of gelation reaction.

Units: dimensionless

WM4 - Molecular weight of polymer (KGOPT=1 or 2) or silicate (KGOPT=3).

Units: g/mole

Note: The following tables define different gelation options and corresponding gel components.

For IREACT=1:

Component No.	**KGOPT=1**	**KGOPT=2**	**KGOPT=3**
4	Polymer	Polymer	Silicate
NG1	$Na_2Cr_2O_7$	-	-
NG2	CSN_2H_4	Malonate ion	-
NG3	Cr(III)	Cr(III)	OH^-
NG4	Gel	Gel	Gel
NG5	Hydrogen	Hydrogen	-

For IREACT=4:

Component NO.	KGOPT=1	KGOPT=2
4	Polymer	Polymer
NGC1	Sodium	Sodium
NGC2	Hydrogen	Hydrogen
NGC3	Magnesium	Magnesium
NGC4	Carbonate	Carbonate
NGC5	Chromium*	Chromium*
NGC6	Silica	Silica
NG1	$Na_2Cr_2O_7$	-
NG2	CSN_2H_4	Malonate ion
NG3	Cr(III)**	Cr(III)**
NG4	Gel	Gel

Where NG and NGC are the gel option and geochemistry option species.

3.4.164 AK1T, AK2T (This line is read only if IREACT=1 or 4 and NG>0 and IENG=1)

AK1T - Parameter for calculating Kinetic rate coefficient for Cr^{3+} as a function of reservoir temperature.

Units: $(\bullet K)^{-1}$

AK2T - Parameter for calculating Kinetic rate coefficient for gel as a function of reservoir temperature.

Units: $(\bullet K)^{-1}$

3.4.165 AG1, AG2, CRG, AGK, BGK (This line is read only if IREACT=1 or 4 and NG>0)

AG1 - Flory-Huggins parameter for gel viscosity.

Units: cp ppm^{-1} = m = Pa.s ppm^{-1}

AG2 - Flory-Huggins parameter for gel viscosity.

Units: cp ppm^{-2} = mPa.s ppm^{-2}

CRG - Constant in the dimensionless pore radius reduction group. This constant depends on the gel type.

Units: $\sqrt{\text{darcy}}(\text{wt}\%)^{1/3} = \sqrt{\mu m^2}(\text{wt}\%)^{1/3}$

AGK, BGK - Permeability reduction parameters for Langmuir correlation with gel concentration.

Units: dimensionless

3.4.166 A15D, B15D, ICREX, A14D, B14D, CRNAK, HNAK, C160 (This line is read only if IREACT=1 or 4 and NG>0)

A15D, B15D - Gel adsorption parameters.

Units: vol. of water / ppm gel

ICREX - Flag indicating if Cr^{3+} will be allowed to exchange with clays.

Possible Values:

0 - Cr^{3+} exchange with clays is not allowed

1 - Cr^{3+} exchange with clays is allowed

A14D, B14D - Chromium adsorption parameters.

Units: vol. of water / ppm chromium
CRNAK - Chromium-sodium exchange reaction equilibrium constant.
HNAK - Hydrogen-sodium exchange reaction equilibrium constant.
C160 - Initial hydrogen ion concentration.
Units: meq/ml
Note: The input values of CRNAK, HNAK, and C160 are ignored for IREACT=4

3.4.167 IP1, IP2 (This line is read only if IREACT=1 or 4 and NG>0 and NY=1 and NZ=1)
IP1, IP2 - Gridblock locations where calculated pressure values should be printed to UNIT 19.
Note: These values are intended to be used for comparison with pressure tab data of 1-D experiments.

Temperature Data (Lines 3.4.168-3.4.171) — These lines are **required only if** temperature variation is considered in the simulation for **IENG=1**.

3.4.168 TEMPI (This line is read only if IENG=1)
TEMPI- Constant initial reservoir temperature.
Units: •F (IUNIT=0) or •C (IUNIT=1)

3.4.169 DENS, CRTC, CVSPR, (CVSPL(L), for L=1, MXP) (This line is read only if IENG=1)
DENS - Reservoir rock density.
Units: lb/ft^3 (IUNIT=0) or g/cm^3 (IUNIT=1)
CRTC - Reservoir thermal conductivity.
Units: Btu (day-ft-•F)$^{-1}$ (IUNIT=0) or kJ (day-m-•K)$^{-1}$ (IUNIT=1)
CVSPR - Reservoir rock heat capacity.
Units: Btu (lb-•F)$^{-1}$ (IUNIT=0) or kJ (kg-•K)$^{-1}$ (IUNIT=1)
CVSPL(L) - Phase L heat capacity (MXP is equal to 3 (IGAS=0) or 4 (IGAS•1)).
Units: Btu (lb-•F)$^{-1}$ (IUNIT=0) or kJ (kg-•K)$^{-1}$ (IUNIT=1)

3.4.170 IHLOS, IANAL (This line is read only if IENG=1)
IHLOS - Flag indicating if the heatloss calculation to overburden and underburden rock is considered or not.
Possible Values:
0 - Heatloss is not considered
1 - Heatloss is considered
IANAL - Flag indicating if the temperature profile is calculated from analytical solution (only 1-D).
Possible Values:
0 - Analytical solution is not considered
1 - Analytical solution is considered

3.4.171 TCONO, DENO, CVSPO, TCONU, DENU, CVSPU (This line is read only if IHLOS=1 and if IENG=1)
TCONO - Thermal conductivity of overburden rock.
Units: Btu (day-ft-•F)$^{-1}$ (IUNIT=0) or kJ (day-m-•K)$^{-1}$ (IUNIT=1)
DENO - Density of overburden rock.
Units: lb/ft^3 (IUNIT=0) or g/cm^3 (IUNIT=1)

CVSPO - Heat capacity of overburden rock.
Units: Btu (lb-•F)$^{-1}$ (IUNIT=0) or kJ (kg-•K)$^{-1}$ (IUNIT=1)
TCONU - Thermal conductivity of underburden rock.
Units: Btu (day-ft-•F)$^{-1}$ (IUNIT=0) or kJ (day-m-•K)$^{-1}$ (IUNIT=1)
DENU - Density of underburden rock.
Units: lb/ft^3 (IUNIT=0) or g/cm^3 (IUNIT=1)
CVSPU - Heat capacity of underburden rock.
Units: Btu (lb-•F)$^{-1}$ (IUNIT=0) or kJ (kg-•K)$^{-1}$ (IUNIT=1)

Foam Model Data (Lines 3.4.172 and 3.4.173) — These lines are **required only if** the foam option is considered (**IGAS=2**).

3.4.172 RFMAX, SOSTAR, CSTAR, EPXLO, SHRTN, VELGR (This line is read only if IGAS=2)
RFMAX- Maximum foam "R" parameter.
Units: dimensionless
SOSTAR - Critical oil saturation above which foam is not generated.
Units: dimensionless
CSTAR - Critical surfactant concentration below which foam is not generated.
Units: volume fraction
EPXLO - Water saturation tolerance parameter in foam model.
Units: dimensionless
SHRTN - Gas shear thinning exponent.
Units: dimensionless
VELGR - Reference gas velocity.
Units: ft/day (IUNIT=0) or m/day (IUNIT=1)

3.4.173 SWSTAR(I), for I=1, NBL (This line is read only if IGAS=2)
SWSTAR(I)- Water saturation at critical capillary pressure for Ith gridblock.
Units: dimensionless
Note: SWSTAR(I) is assumed to be corrected for the permeability used in the simulation.

3.5 Physical Property Data for Geochemical Options

The fifth input section consists of physical property data for geochemistry option and it is **required only** if **IREACT>1**. The data for this section is generated by a preprocessor program (EQBATCH) and does not have the same format as the rest of the input data for UTCHEM. This input section is read by a separate routine called GEOREAD not preceded by the usual seven comment lines and individual data lines are not preceded by three comment lines. Section A.5 of this appendix gives an example for the list of elements, fluid species, solid species, and adsorbed species for geochemical options. See Section 8 of this report for information on the EQBATCH program.

3.5.1 IRSPS, IPHAD
IRSPS - Flag indicating if the reactive species concentrations should be printed.
Possible Values:
0 - Reactive species concentrations will not be printed
1 - Independent aqueous reactive species, solid species, and sorbed species concentrations will be printed

2 - All aqueous species, solid species, and sorbed species concentrations will be printed

IPHAD - Flag indicating whether surfactant adsorption is pH dependent or not.

Possible Values:

0 - Surfactant adsorption is not pH dependent

1 - Surfactant adsorption is pH dependent

3.5.2 PHC, PHT, PHT1, HPHAD (This line is read only if IPHAD>0)

PHC - Critical pH above which surfactant adsorption is pH dependent.

PHT - Extrapolated pH value at zero surfactant adsorption.

PHT1 - pH value above which surfactant adsorption is constant.

HPHAD - Fraction of the low-pH adsorption plateau retained at a pH above PHT1.

3.5.3 CSELP, CSEUP (This line is read only if IREACT=3)

CSELP - Lower optimum salinity limit for generated surfactant.

Units: meq/ml

CSEUP - Upper optimum salinity limit for generated surfactant.

Units: meq/ml

3.5.4 NELET, NFLD, NSLD, NSORB, NACAT, ICHRGE

NELET - Total number of elements less non reacting element.

NFLD - Total number of fluid species.

NSLD - Total number of solid species.

NSORB - Total number of sorbed species.

NACAT - Total number of surfactant associated cations.

ICHRGE - Flag indicating whether an oxygen balance or a charge balance will be used.

Possible Values:

0 - Oxygen balance used

1 - Charge balance in solution used

Note: If solid SiO_2 is considered, the oxygen balance must be used.

3.5.5 NIAQ, NEX, NSLEL, NSURF1

NIAQ - Total number of independent fluid species.

NEX - Total number of insoluble exchangers.

NSLEL - Total number of elements comprising the solid species.

NSURF1 - Position number corresponding to the insitu generated surfactant anion in the fluid species array FLDSPS.

Note: NSURF1 is automatically set to 0 by the program if IREACT=2.

3.5.6 NH, NNA, NCA, NMG, NCARB

NH - Position number corresponding to the hydrogen element in the element array ELEMNT.

NNA - Position number corresponding to the sodium element in the element array ELEMNT.

NCA - Position number corresponding to the calcium element in the element array ELEMNT.

NMG - Position number corresponding to the magnesium element in the element array ELEMNT.

NCARB - Position number corresponding to the carbonate pseudo-element in the element array ELEMNT.

Note: A value of zero is required if the element is not considered.

3.5.7 NALU, NSILI, NOXY

NALU - Position number corresponding to the aluminum element in the element array ELEMNT.

NSILI - Position number corresponding to the silicon element in the element array ELEMNT.

NOXY - Position number corresponding to the oxygen element in the element array ELEMNT.

Note: A value of zero is required if the element is not considered.

3.5.8 NACD (This line is read only if IREACT=3)

NACD - Position number corresponding to the petroleum acid pseudo-element in the element array ELEMNT.

3.5.9 NCR, NHFD, NCRFD (This line is read only if IREACT=4)

NCR - Position number corresponding to the chromium element in the element array ELEMNT.

NHFD - Position number corresponding to the hydrogen ion element in the fluid species array FLDSPS.

NCRFD - Position number corresponding to the CR(III) ion in the fluid species array FLDSPS.

3.5.10 ELEMNT(I), ELCRG(I) for I=1, NELET

ELEMNT(I) - Name of the Ith element.

ELCRG(I) - Charge for Ith element

Note: The name of each element may not exceed 32 characters and each name and charge must be on a separate line of the input file. The order in which these elements must be listed corresponds to the order in which the injection concentrations need to be specified on input line 3.7.7.a with the exceptions of calcium and chloride (if they exist) since Components 5 and 6 are reserved for these elements.

3.5.11 FLDSPS(I), for I=1, NFLD

FLDSPS(I) - Name of the Ith fluid species.

Note: The name of each fluid species may not exceed 32 characters and each name must be on a separate line of the input file. If IREACT=3, the last fluid species must be HA_w (petroleum acid in water).

3.5.12 SLDSPS(I), for I=1, NSLD (This line is read only if NSLD>0)

SLDSPS(I) - Name of the Ith solid species.

Note: The name of each solid may not exceed 32 characters and each name must be on a separate line of the input file.

3.5.13 SORBSP(I), for I=1, NSORB (This line is read only if NSORB>0)

SORBSP(I) - Name of the Ith adsorbed cation.

Note: The name of each adsorbed cation may not exceed 32 characters and each name must be on a separate line of the input file.

3.5.14 ACATSP(I), for I=1, NACAT (This line is read only if NACAT>0)

ACATSP(I) - Name of the Ith surfactant adsorbed cation.

Note: The name of each surfactant adsorbed cation may not exceed 32 characters and each name must be on a separate line of the input file.

3.5.15 NSORBX(I), for I=1, NEX (This line is read only if NSORB>0)

NSORBX(I) - Number of cations for I^th^ exchanger.

3.5.16 AR(I,J), for J=1, NFLD, for I=1, NELET << or >>

AR(I,J), for J=1, NFLD, for I=1, NELET-1

AR(I,J) - Stoichiometric coefficient of I^{th} element in J^{th} fluid species.

Note: If ICHRGE=0, then NFLD × NELET values are required by the program. If ICHRGE=1, then NFLD × (NELET-1) values are required by the program.

3.5.17 BR(I,J), for J=1, NSLD, for I=1, NELET << or >>

BR(I,J), for J=1, NSLD, for I=1, NELET-1 (This line is read only if NSLD>0)

BR(I,J) - Stoichiometric coefficient of I^{th} element in J^{th} solid species.

Note: If ICHRGE=0, then NSLD × NELET values are required by the program. If ICHRGE=1, then NSLD × (NELET-1) values are required by the program.

3.5.18 DR(I,J), for J=1, NSORB, for I=1, NELET << or >>

DR(I,J), for J=1, NSORB, for I=1, NELET-1 (This line is read only if NSORB>0)

DR(I,J) - Stoichiometric coefficient of I^{th} element in J^{th} sorbed species.

Note: If ICHRGE=0, then NSORB × NELET values are required by the program. If ICHRGE=1, then NSORB × (NELET-1) values are required by the program.

3.5.19 ER(I,J), for J=1, NACAT, for I=1, NELET << or >>

ER(I,J), for J=1, NACAT, for I=1, NELET-1 (This line is read only if NACAT>0)

ER(I,J) - Stoichiometric coefficient of I^{th} element in J^{th} surfactant associated cation.

Note: If ICHRGE=0, then NACAT × NELET values are required by the program. If ICHRGE=1, then NACAT × (NELET-1) values are required by the program.

3.5.20 BB(I,J), for J=1, NIAQ+NSORB+NACAT, for I=1, NFLD+NSORB+NACAT

BB(I,J) - Exponent of the J^{th} independent fluid species concentration when the I^{th} fluid species is expressed in terms of independent species concentrations.

3.5.21 EXSLD(I,J), for J=1, NIAQ, for I=1, NSLD (This line is read only if NSLD>0)

EXSLD(I,J) - Exponent of the J^{th} independent fluid species concentration in the solubility product definition of the I^{th} solid.

3.5.22 CHARGE(I), for I=1, NFLD

CHARGE(I) - Charge of the I^{th} fluid species.

3.5.23 SCHARG(I,J), for J=1, NSORBX(I), for I=1, NEX (This line is read only if NSORB>0)

SCHARG(I,J) - Charge of the J^{th} sorbed species on the I^{th} exchanger.

3.5.24 EQK(I), for I=1, NFLD

EQK(I) - Equilibrium constant for I^{th} fluid species when expressed in independent species concentrations only.

3.5.25 EXK(I,J), for J=1, NSORBX(I)-1, for I=1, NEX (This line is read only if NEX>0)

EXK(I,J) - Exchange equilibrium constant for J^{th} exchange equilibrium of the I^{th} insoluble exchanger.

3.5.26 EXEX(I,J,K), for K=1, NIAQ+NSORB+NACAT, for J=1, NSORBX(I)-1, for I=1, NEX (This line is read only if NEX>0)

EXEX(I,J,K) - Exponent of K^{th} independent species in J^{th} equilibrium relation of the I^{th} exchanger

3.5.27 REDUC(I,J), for J=1, NSORBX(I)-1, for I=1, NEX (This line is read only if NEX>0)

REDUC(I,J) - Valence difference of the two cations involved in the exchange reaction J on exchanger I.

Note: This value is positive if the higher valence cation bulk concentration has a positive exponent in EXEX(I,J) definition and is negative otherwise.

3.5.28 EXCAI(I), for I=1, NEX (This line is read only if NEX>0)

EXCAI(I) - Exchange capacity of I^{th} insoluble exchanger.

Units: meq/ml pore volume

3.5.29 SPK(I), for I=1, NSLD (This line is read only if NSLD•1)

SPK(I) - Solubility product of I^{th} solid defined in terms of independent fluid species concentrations only.

3.5.30 CHACAT(I), for I=1, NACAT (This line is read only if NACAT•1)

CHACAT(I) - Charge of I^{th} surfactant associated cation.

3.5.31 ACATK(I), for I=1, NACAT-1 (This line is read only if NACAT•1)

ACATK(I) - Equilibrium constant for I^{th} exchange equilibrium for cation exchanges on surfactant.

3.5.32 EXACAT(I,J) for J=1, NIAQ+NSORB+NACAT, for I=1, NACAT-1 (This line is read only if NACAT•1)

EXACAT(I,J) - Exponent of J^{th} independent species in I^{th} equilibrium for cation exchange on surfactant.

3.5.33 CI(J), for J=1, NACAT (This line is read only if NACAT•1)

CI(J) - Initial concentration of J^{th} surfactant associated cation.

Units: moles/liter pore volume

3.5.34 C5I, C6I

C5I - Initial concentration of non-reacting anions.

Units: equivalents/liter

C6I - Initial concentration of calcium in aqueous phase.

Units: equivalents/liter

3.5.35 CELAQI(J), for J=1, NGC

CELAQI(J) - Initial concentrations of J^{th} geochemistry component.

Units: equivalents/liter

3.5.36 CAC2I (This line is read only if IREACT=3)

CAC2I - Initial concentration of acid in oil.

Units: moles/liter oil

3.5.37 CAQI(J), for J=1, NIAQ

CAQI(J) - Initial guesses for J^{th} independent species concentration.

Units: moles/liter water

3.5.38 CSLDI(I), for I=1, NSLD (This line is read only NSLD>0)

CSLDI(I) - Initial concentration of I^{th} solid.

Units: moles/liter pore volume

3.5.39 CSORBI(I), for I=1, NSORB (This line is read only if NSORB>0)

CSORBI(I) - Initial concentration of I^{th} adsorbed cation.

Units: moles/liter pore volume

3.5.40 C1I, C2I (This line is read only if IREACT=3)

C1I - Initial concentration of water in aqueous phase.

Units: volume fraction

C2I - Initial concentration of oil in oleic phase.

Units: volume fraction

3.5.41 ACIDIS, EQWPS (This line is read only if IREACT=3)

ACIDIS - Dissociation constant of the petroleum acid.

EQWPS - Equivalent weight of petroleum acid.

3.6 Data for Biodegradation Option

The sixth input section consists of physical property data that is **required only if IBIO=1**. This section includes the biodegradation and mass transfer parameters required to model the biodegradation of chemical species. This section is read only if IBIO=1. The data is read by a separate subroutine called BIOREAD, and is input in the standard UTCHEM format. Section 9 of this report gives more details on this option.

3.6.1 DIAMP, DENBLK, CMIN, ***EPSBIO***

DIAMP - Average particle size diameter (used to calculate mass transfer coefficient). A value of DIAMP must be input whether or not mass transfer is considered. The value is ignored if mass transfer is not considered.

Units: cm

DENBLK - Bulk density of the porous medium (mass of porous medium per unit total volume).

Units: g/cm^3

CMIN - Minimum concentration of substrate and electron acceptor that is of interest. This parameter is used for two purposes. First, if concentrations of all substrates and electron acceptors in a gridblock are below CMIN, then biodegradation reactions are assumed negligible at the gridblock and are not modeled. Second, when the concentration of all substrates and electron acceptors fall below CMIN during solution of the biodegradation reaction expressions, further biodegradation reactions are assumed to be negligible and program execution returns to the main program.

Units: mg/L

EPSBIO - Convergence tolerance for solution of the biodegradation equations.

Note: Values of 10^{-4} to 10^{-6} are recommended, although larger values can also result in accurate simulations. Small values ensure accurate solutions of the biodegradation equations but increase run times, while larger values decrease run times at the expense of some accuracy.

3.6.2 NBC, NMET, IBKIN

NBC - Total number of chemical and biological species that are considered in biodegradation reactions, including oil components, surfactants, products generated by abiotic and biodegradation reactions, nutrients required for biological growth, electron acceptors, and biological species.

NMET - Number of substrate-electron acceptor-biological species metabolic combinations. Include combinations of biodegrading products-electron acceptor-biological species for each product that also biodegrades.

IBKIN - Flag specifying the type of biodegradation kinetics.

Possible Values:

0 - No reaction (useful for restart runs)
1 - Monod kinetics and external mass transfer resistances
2 - Monod kinetics with no mass transfer
3 - Instantaneous kinetics (stoichiometric reactions)

Note: First order kinetics can be also be modeled by adjusting the values of the Monod parameters. See input line 3.6.6 below.

3.6.3 ***KC(I)***, ***ITYPE(I)***, CINIT(I), ***RABIO(I)***, ***NPABIO(I)***, for I=1, NBC

Note: One line is required for each chemical and biological species that participates in biodegradation reactions.

KC(I) - Index of the Ith chemical or biological species.

ITYPE(I) - Flag indicating whether the I'th component is a chemical or biological species.

Possible values:

1 - The Ith component is a chemical species
2 - The Ith component is a biological species

CINIT(I) - Initial concentration of chemical or free-floating (unattached) biological species I in the aqueous phase.

Units: mg/ℓ

Note: Although a value of CINIT must be entered for organic species that participate in biodegradation reactions, these values are ignored by the program. Initial concentrations of these components are input on input lines 3.3.32 through 3.3.35.

RABIO(I) - First-order abiotic reaction rate constant.

Units: 1/days

Note: Although a value of RABIO can be specified for biological as well as chemical species, biomass decay should not be controlled with RABIO. Instead, use the parameters ENDOG and ENDOGB to control endogenous decay of unattached and attached biomass, respectively. RABIO should normally be set to 0.0 for biological species.

NPABIO(I) - Number of products generated by a first-order abiotic reaction of chemical species I.

Note: A value must be entered for biological species as well, although the value is ignored by the program because generation of products from decay of biomass is not allowed.

3.6.4 ***KC(I)***, DENBIO(I), RCOL(I), TCOL(I), COLNUM(I), ENDOG(I), ENDOGB(I), CBI(I), CBIOMN(I) for I=1, NBS

Note: One line is required for each biological species.

KC(I) - Index of the biological species.

DENBIO(I) - density of attached biological species I (biofilm density).

Units: g cells / cm^3 biomass

RCOL(I) - radius of an attached microcolony of biological species I.

Units: cm

Note: The parameter RCOL is used to calculate the surface area of a single attached microcolony. Although microcolonies are assumed to be disk-shaped by the model, the user may specify any desired surface area per microcolony using RCOL. TCOL can then be adjusted to obtain the desired volume of the microcolony since the thickness of the microcolony does not affect external mass transfer into the attached biomass.

TCOL(I) - Thickness of a single attached microcolony of biological species I.

Units: cm

COLNUM(I) - Number of bacterial cells per microcolony of biological species I.

Units: cells/colony

ENDOG(I) - endogenous decay coefficient of *unattached* cells of biological species I.

Units: 1/days

ENDOGB(I) - endogenous decay coefficient of *attached* cells of biological species I.

Units: 1/days

CBI(I) - Number of attached bacterial cells of biological species I per gram of dry soil.

Units: cells/gram of solid.

CBIOMN(I) - Lower limit of number of attached bacterial cells of biological species I.

Units: cells/gram of solid.

Note: A population of attached microorganisms, sustained by naturally occurring organic matter, is assumed to exist in the porous media regardless of the concentration of other chemical species. This concentration is CBIOMN, and the concentration of biomass is not allowed to fall below this value.

3.6.5 ISUB(I), IEA(I), IBS(I), BRMAX(I), BRMAXB(I), YXS(I), AKS(I), AKA(I), FEA(I), for I=1, NMET

Note: One line is read for each metabolic combination.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

BRMAX(I) - maximum specific growth rate of *unattached* microorganisms for metabolic combination I.

Units: 1/days

BRMAXB(I) - Maximum specific growth rate of *attached* microorganisms for metabolic combination I.

Units: 1/days

YXS(I) - Yield coefficient for metabolic combination I.

Units: mg/ℓ

AKS(I) - Substrate half-saturation coefficient for metabolic combination I.

Units: mg/ℓ

AKA(I) - Electron acceptor half-saturation coefficient for metabolic combination I.

Units: mg/ℓ

FEA(I) - Electron acceptor utilization coefficient (mass of electron acceptor consumed per mass of substrate biodegraded).

3.6.6 ISUB(I), IEA(I), IBS(I), NCOMPS(I), NIHB(I), NPROD(I), NNUT(I), ICOMET(I), for I=1, NMET

Note: One line is read for each metabolic combination.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

NCOMPS(I) - Number of other substrates competing with substrate ISUB in metabolic combination I.

NIHB(I) - Number of other chemical species that inhibit metabolic combination I.

NPROD(I) - Number of products generated from metabolic combination I.

NNUT(I) - Number of nutrients that limit the biodegradation rate through Monod terms for metabolic combination I.

ICOMET(I) - Flag indicating whether or not the substrate in metabolic combination I is biodegraded through aerobic cometabolism.

Possible Values:

0 - Substrate ISUB(I) serves as a primary substrate

1 - Substrate ISUB(I) is biodegraded through aerobic cometabolism

Note: Users may specify multiple competing substrates, nutrients, and inhibiting constituents for each metabolic combination. Substrate competition, inhibition and cometabolism cannot be modeled if instantaneous kinetics are selected. However, values for the biodegradation rate parameters must be specified even if instantaneous kinetics are specified.

First-order biodegradation kinetics can be modeled by using a very large value of K_S, and adjusting the ratio of $m_{\max}/K_S$ to be equal to the desired first-order biodegradation rate coefficient.

3.6.7 ISUB(I), IEA(I), IBS(I), (ICSUB(I,J), for J=1, Number of competing substrates), for I=1, NMET (This line is read only if there are competing substrates)

Note: One line is read for each metabolic combination for which there is substrate competition between two or more substrates.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

ICSUB(J) - Indices of other substrates that compete with substrate ISUB(I) in metabolic combination I.

Note: The number of input lines required must equal the number of species that are competing, since complementary lines are required to fully describe the competition. For example, if substrate 12 in metabolic combination 12-15-16 must compete with substrates 13 and 14 that are also biodegraded by biological species 16 using electron acceptor 15, then the required input lines are:

12	15	16	13	14
13	15	16	12	14
14	15	16	12	13

3.6.8 ISUB(I), IEA(I), IBS(I), IHB(I), BSIHB(I), for I=1, Number of metabolic combination and inhibiting compound associations (This line is only read if there are metabolic combination and inhibiting compound associations)

Note: One input line is read for each association of metabolic combination and inhibiting compound.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

IHB(I) - Index of chemical species that inhibits metabolic combination I.

BSIHB(I) - Inhibition constant for metabolic combination I.

Units: mg/ℓ

Note: The total number of lines are

$$I = \sum_{J=1}^{NMET} NIHB(J).$$

For example, suppose there are two substrate-electron acceptor-biological species metabolic combinations: 9-10-12 and 9-11-12. Metabolic combination 9-10-12 is inhibited by the substrate itself (9) and electron acceptor 11, while metabolic combination 9-11-12 is inhibited by only the substrate. Then the input lines for this scenario would be:

9	10	12	9	0.001
9	10	12	11	0.001
9	11	12	9	0.001

3.6.9 ISUB(I), IEA(I), IBS(I), IPR(I), FPR(I), for I=1, Number of biodegradation product formation and metabolic combination associations (This line is read only if there are biodegradation product formation described with Monod kinetics and metabolic combination associations)

Note: One line is read for each association of product formation and metabolic combination.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

IPR(I) - Index of product generated by metabolic combination I.

FPR(I) - Product generation coefficient (stoichiometric ratio - mass of product generated per mass of substrate biodegraded).

Note: Number of lines are

$$I = \sum_{J=1}^{NMET} NPRODT(J).$$

For example, if metabolic combination 9-14-15 generates products 10 and 11, and metabolic combination 12-14-15 generates product 13, then the input lines would be:

9	14	15	10	2.0
9	14	15	11	1.0
12	14	15	13	1.5

Parameters for generation of products through first-order reactions are described on input line 3.6.10.

3.6.10 ***ISUB(I), IPR(I), FPR(I)***, for I=1, Number of products generated by first-order reactions of the biodegradation species. (This line is read only if there are products of first-order reactions of biological species)

ISUB(I) - Index of chemical species that reacts abiotically to generate a product.

IPR(I) - Index of product generated by abiotic reaction of ISUB(I).

FPR(I) - Product generation coefficient (stoichiometric ratio - mass of product generated per mass of reactant reacted).

Note: Number of lines are

$$I = \sum_{J=1}^{NBC} NPABIO(J).$$

For example, if the abiotic products 11, 12 and 13 were generated from the first-order reaction of biodegradation species 9 and 10, then the input lines would be:

```
9     11    1.0
9     12    1.0
10    13    2.0
```

3.6.11 ISUB(I), IEA(I), IBS(I), INUT(I), AKN(I), FN(I), for I=1, Number of metabolic combination and limiting nutrient associations (This line is read only if there are metabolic combination and limiting nutrient associations)

Note: One line is read for each association of metabolic combination and limiting nutrient.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

INUT(I) - Index of nutrient limiting the rate of biodegradation through a Monod term in metabolic combination I.

AKN(I) - Nutrient half-saturation coefficient for metabolic combination I.

Units: mg/ℓ

FN(I) - Nutrient utilization coefficient (mass of nutrient consumed per mass of substrates biodegraded) for metabolic combination I.

Note: Number of lines are $I = \sum_{J=1}^{NMET} NNUTT(J).$

3.6.12 ISUB(I), IEA(I), IBS(I), TC(I), IRLIM(I), for I=1, Number of cometabolic combinations for which aerobic cometabolism exists (This line is read only if there are cometabolic combinations for which aerobic cometabolism exists for at least one metabolic combination specified in line 3.6.6)

Note: One input line is required for each cometabolic combination for which aerobic cometabolism exists.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

TC(I) - Transformation capacity for cometabolism of substrate ISUB(I) (mass of substrate utilized per mass of biomass destroyed).

IRLIM(I) - Flag indicating whether reducing power limitations are considered for cometabolic combination I.

Possible Values:

0 - No reducing power limitations are considered

1 - Cometabolic reaction consumes reducing power

Note: Reducing power limits the biodegradation rate through Monod terms in the manner of Chang and Alvarez-Cohen [1995]. The loss of a biological species' reducing power reduces its activity toward all substrates, not just the cometabolite.

Note: The total number of lines are $I = \sum_{J=1}^{NMET} COMET(J)$.

3.6.13 ISUB(I), IEA(I), IBS(I), IGROW(I), REDI(I), AKR(I), FRP(I), FRC(I), for I=1, Number of cometabolic biodegradation reactions in which reducing power limitations are considered (This line is read only if there are cometabolic biodegradation reactions in which reducing power limitations are considered and IRLIM(I)>0 for at least one metabolic combination specified in line 3.6.11)

Note: One line is required for each cometabolic biodegradation reaction in which reducing power limitations are considered.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

IGROW(I) - Index of growth substrate for cometabolism of substrate ISUB(I).

REDI(I) - Initial intracellular reducing power (NADH) concentration.

Units: mmol/mg of biomass

AKR(I) - Reducing power half-saturation coefficient.

Units: mmol/mg of biomass

FRP(I) - Reducing power generation coefficient for metabolic combination (IGROW(I), IEA(I), IBS(I) (mmol reducing power generated per mg of growth substrate consumed).

FRC(I) - Reducing power consumption coefficient for cometabolic combination (ISUB(I), IEA(I), IBS(I)) (mmol reducing power consumed per mg of substrate consumed by cometabolism).

Note: The total number of lines are

$$I = \sum_{J=1}^{K} IRLIM(J)$$

where

$$K = \sum_{J=1}^{NMET} COMET(J).$$

3.7 Recurrent Injection/Production Data Set

The sixth input section consists of the recurrent injection/production well data. Please remember that there are seven comment lines at the beginning of this section and that each line is preceded by three comment lines.

3.7.1 IBOUND

IBOUND - The flag to specify if constant potential boundaries at the left and right sides of the simulation model are specified.

Possible Values:

0 - No boundary is specified
1 - Boundary is specified

Note: This option of IBOUND=1 is not currently available for the vadose zone or when gas is present (IGAS•1)

3.7.2 IBL, IBR (This line is read only if IBOUND=1)

IBL - The flag to specify if the left hand side constant potential boundary is specified.

Possible Values:

0 - No boundary is specified
1 - Boundary is specified

IBR - The flag to specify if the right hand side constant potential boundary is specified.

Possible Values:

0 - No boundary is specified
1 - Boundary is specified

3.7.3 PBL, C1BL, C5BL, C6BL (This line is read only if IBOUND=1 and IBL=1)

PBL- Pressure at the center of the top layer at the left boundary.

Units: psia (IUNIT=0) or kPa (IUNIT=1)

C1BL- Concentration of water in aqueous phase at the left boundary.

Units: volume fraction

C5BL - Concentration of chloride in aqueous phase at the left boundary.

Units: meq/ml

C6BL - Concentration of calcium in aqueous phase at the left boundary.

Units: meq/ml

3.7.4 PBR, C1BR, C5BR, C6BR (This line is read only if IBOUND=1 and IBR=1)

PBR - Pressure at the center of the top layer at the right boundary.

Units: psia (IUNIT=0) or kPa (IUNIT=1)

C1BR - Concentration of water in aqueous phase at the right boundary.

Units: volume fraction

C5BR - Concentration of chloride in aqueous phase at the right boundary.

Units: meq/ml

C6BR - Concentration of calcium in aqueous phase at the right boundary.

Units: meq/ml

Note: For the biodegradation option (IBIO=1), the concentrations of all species considered at the boundary are set to the initial concentrations.

3.7.5 NWELL, IRO, ITIME, NWREL

NWELL - Number of wells used for the simulation including the pseudowells to mimic an open boundary.

Note: If ICOORD=2, NWELL must be equal to 1 and the MXW parameter in the source code must be set equal to 2.

IRO - Flag indicating the equivalent well radius model to be used.

Possible Values:

1 - Babu and Odeh model is used

2 - Peaceman model is used

Note: The Babu and Odeh model (IRO=1) does not work for ICOORD=4.

ITIME - Flag indicating the units to be used when specifying the minimum and maximum time step.

Possible Values:

0 - Minimum and maximum time steps are input in days

1 - Minimum and maximum time steps are input as Courant numbers

Note: This option is only used if IMES>1 and is not a shut-in period. If IMES=1, this flag is ignored. For a shut-in period you need to use ITIME=0

NWREL - Number of actual wells used for the simulation excluding the pseudowells.

Note: The history data are written only for NWREL wells.

Note: See Section A.8 of this appendix for more details on the Courant number and time step selection options.

The following values for minimum and maximum Courant numbers are recommended for different simulations as follows:

Process	Min. Courant #	Max. Courant #
Waterflood/tracer	0.04	0.4
Polymerflood	0.02	0.2
Surfactant/polymerflood	0.01	0.1
Geochemical process	0.01	0.1

See Section 10 of this report for well model information.

3.7.6 The data on input lines 3.7.6.a through 3.7.6.d are repeated for M=1 to NWELL times.

Important note: Input the actual wells first (NWREL) and then the pseudowells.

3.7.6.a IDW(M), IW(M), JW(M), IFLAG(M), RW(M), SWELL(M), IDIR(M), IFIRST(M), ILAST(M), IPRF(M)

IDW(M) - Well I.D. number for the Mth well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: This number is used by UTCHEM to keep track of which well is being described in the recurrent injection/production well section. The history profile data for the well indicated by IDW(M) will be written to FORTRAN UNIT number 18 + IDW(M).

IW(M) - First index of the reservoir gridblock containing the Mth well.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

Note: If the Mth well is completed parallel to the X-axis, IW(M) is the Y direction index—if the well is completed parallel to the Y- or Z-axis, IW(M) is the X direction index. See example below.

If ICOORD=2, IW(1)=JW(1)=1.

JW(M) - Second index of the reservoir gridblock containing the Mth well.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

Note: If the Mth well is completed parallel to the X- or Y-axis, JW(M) is the Z direction index—if the well is completed parallel to the Z-axis, JW(M) is the Y direction index. See example below.

If ICOORD=2, IW(1)=JW(1)=1.

IFLAG(M) - Flag indicating type of well constraint specification for Mth well.

Possible Values:

1 - Rate constrained injection well

2 - Pressure constrained production well (This option is available only if ICOORD=1 or 3)

3 - Pressure constrained injection well (This option is available only if ICOORD=1 or 3)

4 - Rate constrained production well

RW(M) - Radius of Mth well.

Units: feet (IUNIT=0) or m (IUNIT=1)

SWELL(M) - Skin factor for Mth well.

Units: dimensionless

IDIR(M) - Flag indicating the direction in which the Mth well is completed.

Possible Values:

1 - Well completed parallel to the X-axis

2 - Well completed parallel to the Y-axis

3 - Well completed parallel to the Z-axis

Note: If ICOORD=2, IDIR(1) must be equal to 3.

IFIRST(M) - Index of the first block in which the Mth well is completed.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

ILAST(M) - Index of the last block in which the Mth well is completed.

Possible Values: Between IFIRST(M) and the number of gridblocks in the pertinent direction, inclusive

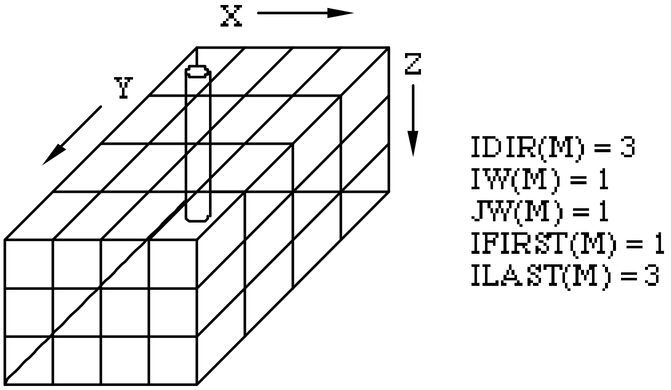
IPRF(M) - Flag indicating if partial completion of the well is considered.

Possible Values:

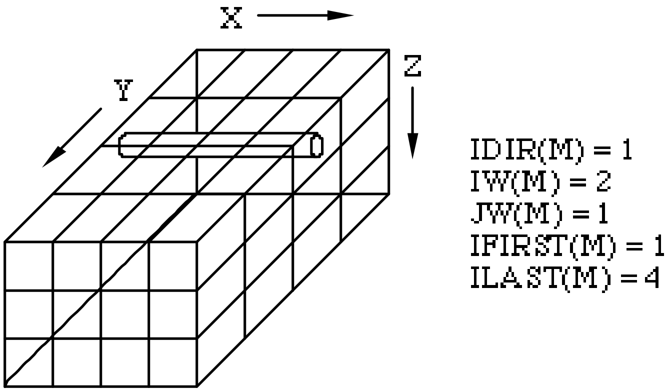
0 - The well is fully completed

1 - The well is partially completed

Example: For a vertical well (completed through all the layers) as illustrated in the 4 × 4 × 3 example below, note the values of IDIR(M), IW(M), JW(M), IFIRST(M), and ILAST(M):



For a horizontal well (completed from the first to last gridblock in the X direction and parallel to the X-axis) as illustrated in the 4 × 4 × 3 example below, note the values of IDIR(M), IW(M), JW(M), IFIRST(M), and ILAST(M):



Note: Horizontal wells can be used for 2-D X-Y or 3-D simulations.

3.7.6.b KPRF(M,IWB), for IWB=1, NWBC (This line is read only if IPRF=1)

KPRF(M,IWB) - Flag indicating if the IWB^th well block of the M^th well is perforated or not.

Possible Values:

0 - The well block is not perforated

1 - The well block is perforated

3.7.6.c WELNAM(M)

WELNAM(M) - Name of the M^th well.

Note: The name can consist of any combination of up to 18 alphanumeric characters. This information will be printed—along with the well I.D. number, IDW(M)—at the beginning of the history output files.

3.7.6.d ICHEK(M), PWFMIN(M), PWFMAX(M), QTMIN(M), QTMAX(M)

ICHEK(M) - The flag to specify whether to check the rate or pressure caps for the M^th well.

Possible Values:

0 - There will be no check on the rate or pressure limits and no automatic shut in for the pressure constraint injector

1 - There will be no automatic shut in for the pressure constraint injector but the pressure or rate limits are checked

2 - There will be both the automatic shut in and the check on the pressure or rate limits

PWFMIN(M) - Minimum flowing bottom hole pressure (specified at the top layer) for the M^th well.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

PWFMAX(M) - Maximum flowing bottom hole pressure (specified at the top layer) for the M^th well.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

QTMIN(M) - Minimum total flow rate (specified at the top layer) for the M^th well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

QTMAX(M) - Maximum total flow rate (specified at the top layer) for the Mth well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

Note: – PWFMIN(M) and PWFMAX(M) are the pressure caps for a rate constraint injector or producer well. QTMIN(M) and QTMAX(M) are the total rate caps for a pressure constraint injector or producer well. If the Mth pressure constraint injector or producer produces at total rate less than QTMIN(M), the Mth well will be switched to a rate constraint well with total rate of QTMIN(M) for the rest of the injector or production period. On the other hand, if the total rate is greater than the QTMAX(M), the Mth well then will be switched to a rate constraint well with the total rate of QTMAX(M). The similar concept is applied to a rate constraint injector or producer.

– The user can skip the well control calculation by specifying very small values for QTMIN(M) and PWFMIN(M) and very large values for QTMAX(M) and PWFMAX(M).

– The code still has the automatic option for shut in of a pressure constraint injector injecting at a rate of less than QTMIN(M).

3.7.7 The data on input lines 3.7.7.a, 3.7.7.b, 3.7.7.c, and 3.7.7.d are repeated for M=1 to NWELL times.

Notes: – For injection wells that are on rate constraint only injection rates and concentrations for each phase are listed. For injection wells that are on pressure constraint the injection pressure is also specified. In this case the injection rates are treated as phase cuts in the injected fluid. For producer pressure constraint only the bottom hole pressure is specified. For producer rate constraint only the total production rate is specified.

– The user can shut in a pressure constraint well by specifying a negative bottom hole pressure or a rate constraint well by specifying a value of zero for rate (QI).

3.7.7.a ID(M), (QI(M,L), (C(M,KC,L), for KC=1, N), for L=1, MXP) (This set of data is read only if IFLAG(M)=1 or 3)

ID(M) - Well I.D. number for the Mth well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: See note for IDW(M) on input line 3.7.6.a.

QI(M,L) - Injection rate of Lth phase in Mth well (see note below).

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

C(M,KC,L) - Concentration of KCth component in Lth phase in Mth well.

Units: vary according to component (see note below)

Notes: – See Section A.7 of this appendix for component and phase numbering scheme and the concentration units for each species.

– The KC index changes the fastest, the L index changes the next fastest, and the M index changes the slowest. A separate data line should be in the input file for each phase—that is, M × L lines will be read by the program. MXP is equal to 3 (IGAS=0) or 4 (IGAS•1).

3.7.7.b ID(M), PWF(M) (This line is read only if IFLAG(M)=2 or 3)

ID(M) - Well I.D. number for the Mth well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: See note for IDW(M) on input line 3.7.6.a. For IFLAG(M)=3, the rates (QI(M,L)) are used an injected volume fraction for each phase.

PWF(M) - Flowing bottom hole pressure for the Mth well.

Units: psia (IUNIT=0) or kPa (IUNIT=1)

3.7.7.c ID(M), TEMINJ(M) (This line is read only if IENG=1 and IFLAG(M)=1 or 3)

ID(M) - Well I.D. number for the Mth well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: See note for IDW(M) on input line 3.7.6.a.

TEMINJ(M) - Injection temperature for Mth well.

Units: •F (IUNIT=0) or •C (IUNIT=1)

3.7.7.d ID(M), QI(M,1) (This line is read only if IFLAG(M)=4)

ID(M) - Well I.D. number for the Mth well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: See note for IDW(M) on input line 3.7.6.a.

QI(L) - Total production rate for Mth well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

Note: This value needs to be input as a negative number.

3.7.8 TINJ, CUMPR1, CUMHI1, WRHPV, WRPRF, RSTC

TINJ - Cumulative injection time.

Units: days or pore volumes (dependent on value of ISTOP flag on input line 3.2.1)

CUMPR1 - Indicates interval at which profiles should be written to UNIT 4.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

CUMHI1 - Indicates interval at which production data should be written to UNIT 4.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

WRHPV - Indicates interval at which production histories should be written to output file(s) for history plotting.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

Note: If WRHPV > total pore volume injected or maximum simulation time, the data will not be printed. The unit number of the file to be written to starts at 19 and continues upward. For example, for a run with three producers, UNITS 19, 20 and 21 would be used. The history of reservoir properties and overall rates from all the producing wells is written to UNIT 9.

WRPRF - Indicates interval at which concentration, pressure, saturation, tracer phase concentration, capacitance property, gel property, alkaline property, and temperature profiles should be written to UNITS 8, 11, 12, 13, 14, 10, 15, and 18 respectively.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

Note: If WRPRF > total pore volume injected or maximum simulation time, the data will not be written.

RSTC - Indicates the interval at which restart data should be written to UNIT 7.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

Note: A 7th variable (CUMH12) which used to control production data printing to UNIT 3 is no longer available with the latest version of UTCHEM.

Time Step Selection Data (Lines 3.7.9-3.7.13)

See Section A.8 of this appendix for more details on the time step selection options.

3.7.9 DT (This line is read only if IMES=1 and ITIME=0)
DT - Time step size for constant time step option.
Units: days

3.7.10 DT, DCLIM, DTMAX, DTMIN (This line is read only if IMES=2 and ITIME=0)
DT - Initial time step size.
Units: days
DCLIM - Tolerance for concentration change for the first three components.
Units: volume fraction
DTMAX - Maximum time step size.
Units: days
DTMIN - Minimum time step size.
Units: days

3.7.11 DT, DCLIM, CNMAX, CNMIN (This line is read only if IMES=2, ITIME=1, and at least one well is not shut-in.)
DT - Initial time step size.
Units: days
DCLIM - Tolerance for concentration changes for the first three components.
Units: volume fraction
CNMAX - Maximum Courant number.
Units: dimensionless
CNMIN - Minimum Courant number.
Units: dimensionless

3.7.12 DT, (DELC(KC), for KC=1, N), DTMAX, DTMIN (This line is read only if IMES=3 or 4 and ITIME=0)
DT - Initial time-step size.
Units: days
DELC(KC) - Tolerance for concentration change of KCth component (IMES=3) or relative tolerance for concentration change of KCth component (IMES=4).
Units: IMES=3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 3.7.7.a)
IMES=4: dimensionless
Note: DELC(KC) is the dimensionless relative change in concentration. For example: DELC(3)=0.1 indicates a 10% change in concentration of component 3.
DTMAX - Maximum time step size.
Units: days
DTMIN - Minimum time step size.
Units: days

3.7.13 DT, (DELC(KC), for KC=1, N), CNMAX, CNMIN (This line is read only if IMES=3 or 4, ITIME=1, and all the wells are not shut-in)

DT - Initial time step size.

Units: days

DELC(KC) - Tolerance for concentration change of KCth component (IMES=3) or relative tolerance for concentration change of KCth component (IMES=4).

Units: IMES=3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 3.7.7.a)

IMES=4: dimensionless

CNMAX - Maximum Courant number.

Units: dimensionless

CNMIN - Minimum Courant number.

Units: dimensionless

IMPORTANT NOTE: The data on lines 3.7.14 through 3.7.23 describe the changes in boundary conditions and are repeated until the injected time (TINJ on input line 3.7.8) is greater than or equal to the maximum simulation time (TMAX on input line 3.3.1).

3.7.14 IRO, ITIME, (IFLAG(M), for M=1, NWELL)

IRO - Flag indicating the equivalent well radius model to be used.

Possible Values:

1 - Babu and Odeh model is used

2 - Peaceman model is used

ITIME - Flag indicating the units to be used when specifying the minimum and maximum time step.

Possible Values:

0 - Minimum and maximum time steps are input in days

1 - Minimum and maximum time steps are input as Courant numbers

Note: This option is only used if IMES>1 and it is not a shut-in period. If IMES=1, this flag is ignored.

IFLAG(M) - Flag indicating type of well constraint specification for Mth well.

Possible Values:

1 - Rate constrained injection well

2 - Pressure constrained production well (This option is available only if ICOORD=1 or 3)

3 - Pressure constrained injection well (This option is available only if ICOORD=1 or 3)

4 - Rate constrained production well

3.7.15 NWEL1

NWEL1 - Number of wells with changes in location (IW(M), JW(M)), skin, direction, perforation, name, or minimum and maximum bottomhole pressure or minimum or maximum rate.

3.7.16 The data on input lines 3.7.16.a through 3.7.16.d are repeated for M=1 to NWEL1 times.

3.7.16.a ID, IW(ID), JW(ID), RW(ID), SWELL(ID), IDIR(ID), IFIRST(ID), ILAST(ID), IPRF(ID)

ID - Well ID number with changes from the previous slug injection period.

IW(ID) - First index of the reservoir gridblock containing the IDth well.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

Note: See note for input line 3.7.6.a.

JW(ID) - Second index of the reservoir gridblock containing the IDth well.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

Note: See note for input line 3.7.6.a.

RW(ID) - Radius of IDth well.

Units: feet (IUNIT=0) or m (IUNIT=1)

SWELL(ID) - Skin factor for IDth well.

Units: dimensionless

IDIR(ID) - Flag indicating the direction in which the IDth well is completed.

Possible Values:

1 - Well completed parallel to the X-axis
2 - Well completed parallel to the Y-axis
3 - Well completed parallel to the Z-axis

Note: If ICOORD=2, IDIR(1) must be equal to 3.

IFIRST(ID) - Index of the first block in which the IDth well is completed.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

ILAST(ID) - Index of the last block in which the IDth well is completed.

Possible Values: Between IFIRST(ID) and the number of gridblocks in the pertinent direction, inclusive

Note: At this time, UTCHEM assumes the well is completed continuously between IFIRST(ID) and ILAST(ID).

IPRF(ID) - Flag indicating if partial completion of the well is considered.

Possible Values:

0 - The well is fully completed
1 - The well is partially completed

3.7.16.b KPRF(ID,IWB), for IWB=1, NWBC (This line is read only if IPRF=1)

KPRF(ID,IWB) - Flag indicating if the IWBth well block of the IDth well is perforated or not.

Possible Values:

0 - The well block is not perforated
1 - The well block is perforated

3.7.16.c WELNAM(ID)

WELNAM(ID) - Name of the IDth well.

Note: The name can consist of any combination of up to 18 alphanumeric characters. This information will be printed—along with the well I.D. number, IDW(ID)—at the beginning of the history output files.

3.7.16.d ICHEK(ID), PWFMIN(ID), PWFMAX(ID), QTMIN(ID), QTMAX(ID)

ICHEK(ID) - The flag to specify whether to check the rate or pressure caps for the IDth well.

Possible Values:

0 - There will be no check on the rate or pressure limits and no automatic shut in for the pressure constraint injector

1 - There will be no automatic shut in for the pressure constraint injector but the user specified pressure or rate limits are checked

2 - There will be both the automatic shut in and the check on the user specified pressure or rate limits

PWFMIN(ID) - Minimum flowing bottom hole pressure (specified at the top layer) for the IDth well.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

PWFMAX(ID) - Maximum flowing bottom hole pressure (specified at the top layer) for the IDth well.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

QTMIN(ID) - Minimum total flow rate (specified at the top layer) for the IDth well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

QTMAX(ID) - Maximum total flow rate (specified at the top layer) for the IDth well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

Note: See the note for input line 3.7.6.d.

3.7.17 NWEL2, (IDWW(J), for J=1, NWEL2)

NWEL2 - Number of wells with changes in rate, concentration or bottomhole pressure.

IDWW(J) - ID number for Jth well with changes.

3.7.18 The data on input lines 3.7.18.a through 3.7.18.d are repeated for M=1 to NWEL2 times.

3.7.18.a ID, QI(ID,L), (C(ID,KC,L), for KC=1,N), for L=1, MXP (This set of data is read only if IFLAG(ID)=1 or 3)

ID - Well ID number with changes from the previous slug injection period.

QI(ID,L) - Injection rate of Lth phase in IDth well (see note for input line 3.7.7.a).

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

C(ID,KC,L) - Concentration of KCth component in Lth phase for IDth well.

Units: vary according to component (see note for line 3.7.7.a)

Note: If IGAS=0, then MXP=3. If IGAS•1, then MXP=4.

3.7.18.b ID, PWF(ID) (This line is read only if IFLAG(ID)=2 or 3)

ID - Well ID number with changes from the previous slug injection period.

PWF(ID) - Flowing bottom hole pressure for the IDth well.

Units: psia (IUNIT=0) or kPa (IUNIT=1)

3.7.18.c ID, TEMINJ(ID) (This line is read only if IENG=1 and IFLAG(ID)=1 or 3)

ID - Well ID number with changes from the previous slug injection period.

TEMINJ(ID) - Injection temperature for the IDth well.

Units: •F (IUNIT=0) or •C (IUNIT=1)

3.7.18.d ID, QI(ID,1) (This line is read only if IFLAG(ID)=4)

ID - Well ID number with changes from the previous slug injection period.

QI(ID,1) - Total production rate for IDth well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)
Note: This value needs to be input as a negative number.

3.7.19 TINJ, CUMPR1, CUMHI1, WRHPV, WRPRF, RSTC

TINJ - Cumulative injection time.
Units: days or pore volumes (dependent on value of ISTOP flag on input line 3.2.1)

CUMPR1 - Indicates interval at which profiles should be written to UNIT 4.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

CUMHI1 - Indicates interval at which production data should be written to UNIT 4.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

WRHPV - Indicates interval at which production histories should be written to output file(s) for history plotting.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)
Note: If WRHPV > total pore volume injected or maximum simulation time, the data will not be printed. The unit number of the file to be written to starts at 19 and continues upward. For example, for a run with three producers, UNITS 19, 20, and 21 would be used. The history of reservoir properties and the total rate from all the producing wells is written to UNIT 9.

WRPRF - Indicates interval at which concentration, pressure, saturation, tracer phase concentration, capacitance property, pressure difference, gel property, alkaline property, and temperature profiles should be written to UNITS 8, 11, 12, 13, 14, 10, 15 and 18 respectively.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)
Note: If WRPRF > total pore volume injected or maximum simulation time, the data will not be written.

RSTC - Indicates the interval at which restart data should be written to UNIT 7.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

Note: A 7th variable (CUMH12) which used to control production data printing to UNIT 3 is no longer available with the latest version of UTCHEM.

3.7.20 DT (This line is read only if IMES=1 and ITIME=0)

DT - Time step size for constant time step option.
Units: days

3.7.21 DT, DCLIM, DTMAX, DTMIN (This line is read only if IMES=2 and ITIME=0)

DT - Initial time step size.
Units: days

DCLIM - Tolerance for concentration change for the first three components.
Units: volume fraction

DTMAX - Maximum time step size.
Units: days

DTMIN - Minimum time step size.
Units: days

3.7.22 DT, DCLIM, CNMAX, CNMIN (This line is read only if IMES=2, ITIME=1, and at least one well is not shut-in)

DT - Initial time step size.

Units: days

DCLIM - Tolerance for concentration changes for the first three components.

Units: volume fraction

CNMAX - Maximum Courant number.

Units: dimensionless

CNMIN - Minimum Courant number.

Units: dimensionless

3.7.23 DT, (DELC(KC), for KC=1, N), DTMAX, DTMIN (This line is read only if IMES=3 or 4 and ITIME=0)

DT - Initial time-step size.

Units: days

DELC(KC) - Tolerance for concentration change, •$C_{lim,\kappa}$, of KCth component (IMES=3) or relative tolerance for concentration change of KCth component (IMES=4).

Units: IMES=3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 3.7.7.a)

IMES=4: dimensionless

DTMAX - Maximum time step size.

Units: days

DTMIN - Minimum time step size.

Units: days

3.7.24 DT, (DELC(KC), for KC=1, N), CNMAX, CNMIN (This line is read only if IMES=3 or 4, ITIME=1, and reservoir is not shut-in)

DT - Initial time step size.

Units: days

DELC(KC) - Tolerance for concentration change of KCth component (IMES=3) or relative tolerance for concentration change of KCth component (IMES=4).

Units: IMES=3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 3.7.7.a)

IMES=4: dimensionless

CNMAX - Maximum Courant number.

Units: dimensionless

CNMIN - Minimum Courant number.

Units: dimensionless

A.4 OUTPUT FILES

The following sections describe: (4.1) data that is automatically written to the profile data file, (4.2) restart run procedure, (4.3) data written to stored restart data file, (4.4) data written to history files for each well, (4.5) data written to history of reservoir properties and overall injection and production rates from all the wells, and (4.6) data written to aqueous phase tracer concentration data files.

4.1 Default Data Written to Profile Data File

The information in the following lists is always written to the profile data file (PROFIL) and is not controlled by the various print control flags in the input files.

Printed at each CUMHI1 interval:

- Time, number of time steps
- Time step size
- Courant number
- Cumulative pore volume injected
- Original in place for each component
- Cumulative injection for each component
- Cumulative production for each component
- Amount retained for each component
- Relative error for each component
- Fraction of oil recovered
- If IREACT • 2:
    - Average number of iterations, computation time
- For each well:
    - Position of the well, first and last well block completed
    - Cumulative injection/production
    - Bottomhole pressure for each well block
    - All well related information (such as pressure for each phase, phase concentration, phase cut, etc.)
    - Producer wellbore temperature and phase cut and concentration

Printed at each CUMPR1 interval:

- Reservoir temperature if IENG=1
- Phase saturation profile for each phase
- Aqueous phase pressure profile
- Concentration of each component in the fluid
- If IBIO=1 and IBPR=1:
    - Concentration of aqueous phase biodegradation species
    - If IBKIN=1:
        - Concentration of biodegradation species within attached biomass
- If tracers are present and ICAP•0:
    - Flowing concentration
    - Dendiritic concentration
    - Flowing saturation
    - Dendiritic saturation

4.2 Restart Run Procedure

The restart procedure is available with UTCHEM. This enables a user to continue a run past the initial time period or to break a large run up into smaller segments. Each time you run UTCHEM, a file called RESTAR is created. This file (described in Section 6.3) contains all the information necessary to continue the run at a later time. In order to do so, the user needs to:

1.- Rename the output file RESTAR from the previous run to INPUT2

2.- Set the variable IMODE equal to 2 on line 3.1.3 of input file INPUT

3.- Change the value of TMAX on input line 3.3.1 of file INPUT to the new injection period being simulated in the restart run

4.- Change the value of TINJ on input line 3.7.8 of file INPUT if appropriate

5.- Add additional information for input lines 3.7.14 through 3.7.24 of file INPUT if the well conditions are different for the new injection period

Note: Make sure the source code you run the restart problem (IMODE=2) has the same values for the array sizes in the parameter statement as the one used in original run (IMODE=1).

4.3 Data Written to Stored Restart Run Data File

The information in the following list is always written to the stored restart data file (RESTAR). If the user is running a RESTART run, this data file needs to be renamed to correspond to the INPUT2 input file. The values in parentheses are the FORTRAN variable names as they appear in the code.

Printed at the end of each run:
- Time (T), injection time (TINJ), time step size (DT), number of time steps (ICNT)
- New slug injection or restart flag (IINJ), number of time step reduction (INEC), cumulative pore volume injection (CUMPV), number of blocks in X-direction minus 1 (NXM1)
- Cumulative injection (CUMI), cumulative production (CUMP), original in place (OIP) for each component
- Cumulative injection/production (CUMQI and CUMQP) for each well
- Phase concentration (C), phase saturation (S), effective salinity (CSE), overall concentration (CTOT), number of phases (NPHASE)
- If ICOORD=2:
  - Boundary concentration (CE), boundary pressure (PE)
- Viscosity (VIS), relative permeability (RPERM), injection rate (QI), total rate for each well (QT), phase rate (Q), bottomhole pressure (PWF)
- Pressure (P)
- If IADSO=1:
  - Organic adsorption (C2ADSS)
- If LMO=1:
  - Multiple organic adsorption (CS1DSK)
- Surfactant adsorption (C3ADSS), surfactant adsorption parameter (A3DS), polymer adsorption (C4ADSS)

Permeability reduction factor (RKF), calcium concentration (C6JO), calcium adsorbed by clay (C6ADSS), calcium adsorbed by surfactant (C6HATS)
Alcohol 7 partitioning coefficient (X7OLD), alcohol 8 partitioning coefficient (X8OLD)
Oil breakthrough (BTO), tracer breakthrough (TBT), tracer injection concentration (CINJT), tracer retardation factor (TRD)
Lower effective salinity (CSEL), upper effective salinity (CSEU)
Density (DEN), capillary pressure (PRC)
Total surfactant (TSURF)
If IPERM=2 and IHYST=1:
    Minimum water saturation (SWMIN)
If ICAP=1:
    Dendiritic concentration (CD), dendiritic saturation (SD), flowing saturation (SF), total flowing concentration (CTF)
If NG•0:
    Chromium adsorption (C14ADS), gel adsorption (C15ADS), cation exchange capacity of clay (QW)
If IENG=1:
    Cum. heat inj. (CUMHI), cum. heat prod. (CUMHP), temperature (TEM), total volumetric heat capacity (TVHC)
If IENG=1 and IHLOS=1:
    Cum. heat loss (TQLOS), integral for overburden and underburden heatloss calculations (RINO, RINU), time of change of overburden temp. from the reservoir block (TTCHG), overburden temperature (TEMPOB), underburden temperature (TEMPUB)
If IENG =1 and ICOORD =2:
    Boundary enthalpy (ENTHE)
If IREACT >1:
    Solid concentration (CSLDT), adsorbed concentration (CSORBT), species concentration (CAQSP), surf. associated cation concentration (CACATT), cation concentration (CACAT)
    Cumulative no. of iteration for geochem option (ITCUM)
If IBIO =1:
    Concentrations of attached biomass and intra-biomass concentrations of chemical species (CB)
    Concentrations of reducing power in aqueous phase biomass (RED) and attached biomass (REDB)

4.4 Data Written to Well History Plotting Data File(s)

The information in the following list is always written to the well history plotting data files (HIST01-HISTℓ) for each production well.

Printed at each WRHPV interval:

Cumulative pore volume, time [days], cumulative production [ft^3, m^3, or STB], water oil ratio, cumulative oil recovery, total production rate [ft^3/day, m^3/day, or STB/day]
If IGAS =1: Water cut, oil cut, microemulsion cut, gas cut
Wellbore pressure for each well block [psi or kPa]
If IENG =1: Wellbore temperature [•F or •C]

For I=1, N:
- If ICF(I) =1: phase concentration for component N (C(I,L), L=1,MXP), total concentration of component N (CTOT(I))

If IREACT>1 or ICF(3)=1: Lower effective salinity, upper effective salinity, effective salinity

If IBIO =1 and IBPR =1:
- Concentrations of attached biomass and intra-biomass concentrations of chemical species (CMGL) [mg/ℓ]

If IBIO=1, IBPR=1, and there are cometabolic biodegradation reactions in which reducing power limitations are considered:
- Concentrations of reducing power (NADH) in aqueous phase and attached biomass

If IREACT >1:
- Independent species concentration (CAQSP(KK), KK=1, NIAQ) [mole/liter of water]
- If IRSPS >0: Dependent species concentration (CAQSP(KK), KK=NIAQ+1,NFLD) [mole/liter of water]
- If IREACT =3 or 5: Phase concentration of injected + generated surfactant (PSURF(I,L), L=1,3), total concentration of injected + generated surfactant (TSURF)
- If NSLD >0: Concentration of solid components (CSLDT(KK), KK=1, NSLD) [mole/liter of pore volume]
- If ICNM >0: Log_{10} of interfacial tension between water/microemulsion and oil/microemulsion (XIFT1, XIFT2) [dyne/cm]

The information in the following list is always written to the well history plotting data files for each injection well.

Printed at each WRHPV interval:
- Cumulative pore volume, time in days, cumulative injection [ft^3, m^3, or STB], injection rate [ft^3/day, m^3/day, or STB/day]
- Wellbore pressure for each well block [psi or kPa]
- Pressure drop between the wells (for the specific case of one injector and one producer only) or pressure drop between the pressure tabs (when NG>0, NY=1, NZ=1, see line 3.4.167) [psi or kPa]

4.5 Data Written to Overall History Plotting Data File

The information in the following list is always written to the overall history plotting data file (OVERAL).

Printed at each WRHPV interval:
- Cumulative pore volume, time in days, volumetric averaged reservoir pressure (psi or kPa), cumulative oil produced (%OOIP), cumulative oil produced (bbls or m^3), volumetric averaged reservoir temperature (•F or •C) (only if IENG=1)
- Total injection rate (B/D or m^3/day), total production rate (B/D or m^3/day), total fluid injected (1000 bbls or m^3), total fluid produced (1000 bbls or m^3) [Note: The fluid injected and produced values are calculated for the last time step before the print interval.]

Overall production rate for each phase (QBAR(L) for L=1, MXP where MXP=3 if IGAS=0 and MXP=4 if IGAS =1) (B/D or m^3/day)

Average cut for each phase (FBAR(L) for L=1, MXP where MXP=3 if IGAS=0 and MXP=4 if IGAS =1)

Average saturation for each phase (SBAR(L) for L=1, MXP where MXP=3 if IGAS=0 and MXP=4 if IGAS =1)

If ICF(3)=1: Cumulative surfactant injected (bbls or m^3), Cumulative surfactant produced (bbls or m^3), adsorbed surfactant (bbls or m^3), retained surfactant (bbls or m^3), adsorbed surfactant (ml/ml PV)

If ICF(4)=1: Cumulative polymer injected (wt%), Cumulative polymer produced (wt%), adsorbed polymer (wt%), retained polymer (wt%), adsorbed polymer (wt. % / PV)

4.6 Data Written to Tracer Concentration Observation Point Data File(s)

The information in the following list is written to the tracer observation history plotting data files (TRAC01-TRAC*n*) for each tracer (if IPOBS=0).

Printed at each WRHPV interval:

Time in days, cumulative pore volume

If IGAS=0:

Aqueous phase tracer concentration at NOBS observation locations

If IGAS•1:

Gas phase tracer concentration at NOBS observation locations

A.5 GEOCHEMISTRY OPTION (IREACT>1)

This section gives an example list of elements and reactive species for the geochemistry options of IREACT=2 or IREACT=4.

Elements or pseudo-element:	Hydrogen (reactive), Sodium, Calcium, Magnesium, Carbonate, Aluminum, Silicon, Oxygen, Chlorine, S (Injected surfactant)
Independent aqueous or oleic species:	H^+, Na^+,Ca^{2+}, Mg^{2+}, Al^{3+}, CO_3^{2-} , Cl^-, S^-, H_4SiO_4, H_2O
Dependent aqueous or oleic species:	$Ca(OH)^+$, $Mg(OH)^+$, $Al(OH)^{2-}$,$Al(OH)_2^-$, $Ca(HCO_3)^+$, $Mg(HCO_3)^+$, OH^-, HCO_3^- , $H_3SiO_4^-$, $H_2SiO_4^{2-}$, $HSi_2O_6^{3-}$, $Si_2O_5^{2-}$, $Al(OH)_4^-$, H_2CO_3, $CaCO_3^o$, $MgCO_3^o$
Solid species:	$CaCO_3$ (Calcite), $Al_2Si_2O_5(OH)_4$ (Kaolinite), $MgCO_3$ (Magnesite), $NaAlSi_2O_6.H_2O$ (Analcite), SiO_2 (Silica), $Mg(OH)_2$ (Magnesium Hydroxide)
Adsorbed cations on rock surface:	$\overline{H}^+$, $\overline{Na}^+$, $\overline{Ca}^{2+}$, $\overline{Mg}^{2+}$
Adsorbed cations on micelles:	$\overline{\overline{Na}}^+$, $\overline{\overline{Ca}}^{2+}$, $\overline{\overline{Mg}}^{2+}$

Aqueous reactions	**Equilibrium constant**

$H_2O \overset{K_1^{eq}}{\rightleftharpoons} H^+ + OH^-$	$K_1^{eq} = [H^+]\ [OH^-]$
$H^+ + CO_3^{2-} \overset{K_2^{eq}}{\rightleftharpoons} HCO_3^-$	$K_2^{eq} = \dfrac{\left[HCO_3^-\right]}{[H^+]\left[CO_3^{2-}\right]}$
$Ca^{2+} + H_2O \overset{K_3^{eq}}{\rightleftharpoons} Ca(OH)^+ + H^+$	$K_3^{eq} = \dfrac{[Ca(OH)^+]\ [H^+]}{[Ca^{2+}]}$
$Mg^{2+} + H_2O \overset{K_4^{eq}}{\rightleftharpoons} Mg(OH)^+ + H^+$	$K_4^{eq} = \dfrac{[Mg(OH)^+]\ [H^+]}{[Mg^{2+}]}$
$Al^{3+} + H_2O \overset{K_5^{eq}}{\rightleftharpoons} Al(OH)^{2+} + H^+$	$K_5^{eq} = \dfrac{[Al(OH)^{2+}][H^+]}{[Al^{3+}]}$
$Al^{3+} + 2H_2O \overset{K_6^{eq}}{\rightleftharpoons} Al(OH)_2^+ + 2H^+$	$K_6^{eq} = \dfrac{[Al(OH)_2^+][H^+]^2}{[Al^{3+}]}$

Aqueous reactions (cont.)	**Equilibrium constant** (cont.)
$Al^{3+} + 4H_2O \overset{K_7^{eq}}{\rightleftharpoons} Al(OH)_4^- + 4H^+$	$K_7^{eq} = \dfrac{[Al(OH)_4^-][H^+]^4}{[Al^{3+}]}$
$H_4SiO_4 \overset{K_8^{eq}}{\rightleftharpoons} H^+ + H_3SiO_4^-$	$K_8^{eq} = \dfrac{[H^+][H_3SiO_4^-]}{[H_4SiO_4]}$
$H_4SiO_4 \overset{K_9^{eq}}{\rightleftharpoons} 2H^+ + H_2SiO_4^{2-}$	$K_9^{eq} = \dfrac{[H^+]^2[H_2SiO_4^{2-}]}{[H_4SiO_4]}$
$Ca^{2+} + H^+ + CO_3^{2-} \overset{K_{10}^{eq}}{\rightleftharpoons} Ca(HCO_3)^+$	$K_{10}^{eq} = \dfrac{\left[Ca(HCO_3)^+\right]}{[Ca^{2+}]\left[CO_3^{2-}\right][H^+]}$
$Mg^{2+} + H^+ + CO_3^{2-} \overset{K_{11}^{eq}}{\rightleftharpoons} Mg(HCO_3)^+$	$K_{11}^{eq} = \dfrac{\left[Mg(HCO_3)^+\right]}{[Mg^{2+}]\left[CO_3^{2-}\right][H^+]}$
$2H^+ + CO_3^{2-} \overset{K_{12}^{eq}}{\rightleftharpoons} H_2CO_3$	$K_{12}^{eq} = \dfrac{[H_2CO_3]}{\left[CO_3^{2-}\right][H^+]^2}$
$2H_4SiO_4 \overset{K_{13}^{eq}}{\rightleftharpoons} 2H_2O + 3H^+ + HSi_2O_6^{3-}$	$K_{13}^{eq} = \dfrac{[H^+]^3[HSi_2O_6^{3-}]}{[H_4SiO_4]^2}$
$2H_4SiO_4 \overset{K_{14}^{eq}}{\rightleftharpoons} 2H^+ + 3H_2O + Si_2O_5^{2-}$	$K_{14}^{eq} = \dfrac{[H^+]^2[Si_2O_5^{2-}]}{[H_4SiO_4]^2}$

Solid species	**Solubility product**
$CaCO_3$	$K_1^{sp} = [Ca^{2+}]\left[CO_3^{2-}\right]$
$MgCO_3$	$K_2^{sp} = [Mg^{2+}]\left[CO_3^{2-}\right]$
SiO_2	$K_3^{sp} = [H_4SiO_4]$
$Al_2Si_2O_5(OH)_4$	$K_4^{sp} = [H^+]^{-6}[Al^{3+}]^2[H_4SiO_4]^2$
$NaAlSi_2O_6.H_2O$	$K_5^{sp} = [H^+]^{-4}[Na^+][Al^{3+}][H_4SiO_4]^2$
$Mg(OH)_2$	$K_6^{sp} = [Mg^{2+}][H^+]^{-2}$

Exchange reactions (on matrix)	**Exchange equilibrium constant**
$2\overline{Na}^{+} + Ca^{2+} \overset{K_1^{ex}}{\rightleftharpoons} 2Na^{+} + \overline{Ca}^{2+}$	$K_1^{ex} = \frac{[\overline{Ca}^{2+}][Na^{+}]^{2}}{[Ca^{2+}][\overline{Na}^{+}]^{2}}$
$2\overline{Na}^{+} + Mg^{2+} \overset{K_2^{ex}}{\rightleftharpoons} 2Na^{+} + \overline{Mg}^{2+}$	$K_2^{ex} = \frac{[\overline{Mg}^{2+}][Na^{+}]^{2}}{[Mg^{2+}][\overline{Na}^{+}]^{2}}$
$\overline{H}^{+} + Na^{+} + OH^{-} \overset{K_3^{ex}}{\rightleftharpoons} \overline{Na}^{+} + H_2O$	$K_3^{ex} = \frac{[Na^{+}][\overline{H}^{+}]}{[\overline{Na}^{+}][H^{+}]}$

Exchange reactions (on micelle)	**Exchange equilibrium constant**
$2\overline{\overline{Na}}^{+} + Ca^{2+} \overset{K_1^{exm}}{\rightleftharpoons} 2Na^{+} + \overline{\overline{Ca}}^{2+}$	$K_1^{exm} = \frac{[\overline{\overline{Ca}}^{2+}][Na^{+}]^{2}}{[\overline{\overline{Na}}^{+}]^{2}[Ca^{2+}]}$ where $K_1^{exm} = \beta_1^{exm}\,[S^{-}]$
$2\overline{\overline{Na}}^{+} + Mg^{2+} \overset{K_2^{exm}}{\rightleftharpoons} 2Na^{+} + \overline{\overline{Mg}}^{2+}$	$K_2^{exm} = \frac{[\overline{\overline{Mg}}^{2+}][Na^{+}]^{2}}{[\overline{\overline{Na}}^{+}]^{2}[Mg^{2+}]}$ where $K_2^{exm} = \beta_2^{exm}\,[S^{-}]$

A.6 MAIN PROGRAM FLOW OUTLINE

The following outline represents the basic flow through the main program of UTCHEM (that is, the order in which major subroutines are called).

I. INOUT
   A. FILE1
   B. PRINTS
   C. PRINTI
   D. INNAME (called only if NO>1 and IOD is not equal to 1)
   E. MOPPST (called only if NO>1)
      1. SLV2EQ
   F. PRINTO (called only if NO>1)
   G. WMEACN (called only if NO>1 and IOD is not equal to 1)
   H. GEOREAD (called only if IREACT>1)
   I. BIOREAD (called only if IBIO=1)
   J. METRIC (called only if IUNIT=1)
   K. WELLIX
      1. RADIUS
   L. FILE3
   M. FILE2
   N. GRDFAC
II. RSTART (called only if IMODE=2)
   A. NSLUG
   B. WELLIX
      1. RADIUS
III. TIME0
   A. OMOFR (called only if NO>1)
   B. DENSTY
IV. TRAN1
V. ASIGN1
VI. TRANS (Transmissibilities)
VII. SOLMAT (Pressure Eq.)
   A. WELL
   B. BUNDRY (called only if IBOUND=1)
   C. JCG
VIII. QRATE
IX. CONEQ (Conservation Eq.)
   A. GEL
X. ADSORB
XI. REACTR (called only if IREACT>1)
   A. RENAM1
   B. TOTALS
   C. MANIPL
   D. JACUP
      1. GAUSS
      2. SOLVE
   E. RENAM2

- XII. CSECAL
  - A. ALCPTN (called only if IALC=1)
    - 1. TWOALC
    - 2. CUBIC
  - B. CSEOD (called only if NO>1 and IOD is not equal to 1)
  - C. IONCNG
  - D. PHASC (called only if surfactant is not present and IREACT<1)
    - 1. NONEQ
    - 2. ODISWO (called only if NO>1)
      - a. NONEQK
  - E. PHCOMP (called only if surfactant is present or IREACT>1)
    - 1. NONEQ
    - 2. ODISWO
    - 3. TIELIN
      - a. TRY
    - 4. REVISE
    - 5. VGAMMA
    - 6. SINGLE
    - 7. ODISTM (called only if IHAND=0)
    - 8. ODISTM1 (called only if IHAND=1)
- XIII. BIOSOLVE (called only if IBIO=1)
  - A. INST (called only if IBKIN =3)
  - B. SDRIV2 (called only if IBKIN = 1 or 2 and running Cray version of code)
    - 1. F
    - 2. G
  - C. DDRIV2 (called only if IBKIN = 1 or 2 and running double precision version of code)
    - 1. F
    - 2. G
- XIV. OMOFR (called only if NO>1)
- XV. TCAP (called only if ICAP=1)
- XVI. TDIFFU (called only if ICAP=2)
- XVII. DENSTY
- XVIII. ASIGN2
- XIX. ENGBAL (called only if IENG=1)
- XX. LAUWER (called only if IENG=1 and IANAL=1)
- XXI. CAPNUM (called only if ITRAP=1)
- XXII. TRAPNO (called only if ITRAP=2 and IGAS=0)
- XXIII. TRAP (called only if IGAS=0)
- XXIV. TRAPG (called only if IGAS•1)
- XXV. HYST1 (called only if IPERM=2)
- XXVI. UTFOAM (called only if IGAS=2)
- XXVII. VISCOS
- XXVIII. WELLCK
- XXIX. OUTDT1
- XXX. OUTDT2
  - A. PRINTI

- B. PRINTS

XXXI. NSLUG
- A. WELLIX
  - 1. RADIUS

XXXII. RSTART

XXXIII. Go to step V (ASIGN1) if not done

XXXIV. SUMTAB

A.7 PHASES AND SPECIES IN UTCHEM

This section gives the component numbering scheme in UTCHEM and the unit for each component.

The following values for L correspond to the indicated phase:

L	Phase
1	Aqueous phase
2	Oleic phase
3	Microemulsion phase
4	Gas phase

The following indices correspond to the indicated components [corresponding concentration units are listed in square brackets]:

For all values of IREACT:

Index	Component [conc. units]
1	Water [volume fraction]
2	Oil [volume fraction]
3	Surfactant [volume fraction]
4	Polymer or silicate (KGOPT=3) [weight percent]
5	Total nonsorbing anions concentration, assumed to all be chloride anions [meq/ml]
6	Divalent cations, assumed to all be calcium for IREACT<2 [meq/ml]
7	Alcohol 1 [volume fraction]
8	Alcohol 2 or Gas [volume fraction]

Organic species (IBIO=0 and NO>1):

Index	Component [conc. units]
9	First organic species [volume fraction]
8+NO	Last organic species [volume fraction]

Tracers (NT>0):

Index	Component [conc. units]
9+NO	First tracer [*dependent on user input*]
8+NO+NTW+NTA	Last tracer [*dependent on user input*]

Geochemistry option species (IREACT=2 or IRECAT=3):

Index	Component [conc. units]
9+NO+NTW+NTA	First geochemistry component [meq/ml]
8+NO+NTW+NTA+NGC	Last geochemistry component [meq/ml]

Gel model species (IREACT=1 and NG>0):

Index	**KGOPT=1** Component [conc. units]	**KGOPT=2** Component [conc. units]	**KGOPT=3** Component [conc. units]
NG1*	$Na_2Cr_2O_7$ [ppm]	—	—
NG2	CSN_2H_4 [ppm]	Malonate ion [ppm]	—
NG3	Cr^{3+} [ppm]	Cr^{3+} [ppm]	OH^- [ppm]
NG4	Gel [ppm]	Gel [ppm]	Gel [ppm]
NG5	Hydrogen [meq/ml]	Hydrogen [meq/ml]	—

*where NG1 = 9+NO+NTW+NTA

Geochemistry/Gel option species (IREACT=4 and NG>0):

Index	Component [conc. units]
9+NO+NTW+NTA	First geochemistry component [meq/ml]
8+NO+NTW+NTA+NGC	Last geochemistry component [meq/ml]

Index	**KGOPT=1** Component [conc. units]	**KGOPT=2** Component [conc. units]
NG1*	$Na_2Cr_2O_7$ [ppm]	—
NG2	CSN_2H_4 [ppm]	Malonate ion [ppm]
NG3	Cr^{3+} [ppm]	Cr^{3+} [ppm]
NG4	Gel [ppm]	Gel [ppm]

*where NG1 = 9+NO+NTW+NTA+NGC

Biological model species (IBIO=1):

Index	Component [conc. units]
9+NO+NTW+NTA+NGC+NG	First biological species [mg/ℓ]
8+NO+NTW+NTA+NGC+NG+NOTH	Last biological species [mg/ℓ]

A.8 TIME-STEP SELECTION

This section discusses the automatic time-step selection options available in UTCHEM: (E.1) selector based on method of relative changes for the first three components, (E.2) selector based on method of relative changes for all the components, and (E.3) selector based on changes in dimensionless concentration for all the components.

The Courant number, C, is defined as:

$$C = \frac{Q \ \Delta t}{\Delta x \ \Delta y \ \Delta z \ \phi}$$

where Q is maximum injection/production per wellblock.

8.1 Method of Relative Changes for First Three Components (IMES=2)

Minimum and maximum time step in days (option ITIME=0):

The time step selection is based on the method of relative changes for the first three components (water, oil, and surfactant) as:

$$\Delta t^{n+1} = \Delta t^{n} \min\left(\frac{\Delta C_{lim}}{\max\limits_{i=1}^{NBL} \left| \Delta C_{i,\kappa} \right|} \right) \quad \kappa = 1, 2, 3 \qquad \text{(E.1)}$$

where $\bullet t^{n+1}$ is limited to: $\bullet t_{min} \bullet \bullet t^{n+1} \bullet \bullet t_{max.}$ $\bullet t_{min}$ and $\bullet t_{max}$ are the input time step values and ΔC_{lim} is the input value for concentration tolerance (DCLIM) on input line 3.7.10.

Minimum and maximum time step in days (option ITIME=1):

The minimum and maximum time steps in days are computed based on the minimum and maximum Courant number as:

$$\Delta t_{min} = \frac{CNMIN}{\min\limits_{M=1}^{nwell} \left(\max\limits_{i=1}^{nwbc} \frac{Q_i}{\Delta x_i \ \Delta y_i \ \Delta z_i \ \phi_i} \right)}$$

and

$$\Delta t_{max} = \frac{CNMAX}{\min\limits_{M=1}^{nwell} \left(\max\limits_{i=1}^{nwbc} \frac{Q_i}{\Delta x_i \ \Delta y_i \ \Delta z_i \ \phi_i} \right)}$$

where Courant number (C) is limited to: CNMIN•C•CNMAX. CNMIN and CNMAX are the input Courant number values in line 3.7.11. The time step is then calculated from Eq. E.1.

8.2 Method of Relative Changes for All Components (IMES=3)

For IMES=3, the method of relative changes is applied to all the components in the simulation run:

$$\Delta t^{n+1} = \Delta t^{n} \min\left(\frac{\Delta C_{lim,\kappa}}{\max\limits_{i=1}^{NBL} \left| \Delta C_{i,\kappa} \right|} \right) \quad \kappa = 1, ..., n_c$$

where •t^{n+1} is limited to: •t_{min}••t^{n+1}••t_{max}. •$C_{lim,\kappa}$ is a fraction of the initial or injected concentration (whichever is larger) of the KCth component, DELC(KC) in input lines 3.7.12 or 3.7.13. For example: •$C_{lim,3} = 0.1 \times C_3$ where C_3 is the total concentration of component 3. If •$C_{lim,\kappa}$ of the KCth component is entered as zero, that component is not considered in the time-step size selection.

8.3 Method of Relative Changes Using Dimensionless Concentration for All Components (IMES=4)

For IMES=4, the method of relative changes is applied to all the components in the simulation run:

$$\Delta t^{n+1} = \Delta t^{n} \min\left(\frac{R_{lim,\kappa}}{\max\limits_{i=1}^{NBL} \left| \dfrac{\Delta C_{i,\kappa}}{C_{i,\kappa}} \right|} \right) \quad \kappa = 1, ..., n_c$$

where •t^{n+1} is limited to: •t_{min}••t^{n+1}••$t_{max.}$ $R_{lim,\kappa}$ is the input dimensionless relative change in concentration of component κ (DELC(KC)) on input lines 3.7.12 or 3.7.13. For example $R_{lim,3}$=0.1 indicates a 10% change in concentration of Component 3.

A.9 DESCRIPTION OF work.job FILE

This section contains a detailed description of the contents of the example `work.job` file found in Section 2.3 of this appendix.

Command line	**Description**
`rm -r EX01.dir`	Removes the `EX01.dir` directory if it already exists. Make sure you've copied files from previous runs (if you want to save them) to another location before executing the `work.job` file because all files in the `EX01.dir` directory will be deleted when the directory is deleted.
`mkdir EX01.dir`	Create a subdirectory in which to place the new simulation results.
`cd EX01.dir`	Make `EX01.dir` the current working directory.
`ln -s ../ex01.data INPUT`	Create a symbolic link to the `ex01.data` input data file (which is located up one level in the directory structure). When the program looks for the file `INPUT`, it will automatically be pointed to the `ex01.data` file.
`time ../utchem.exe`	Run the program (which is located up one level in the directory structure).

`mv TTABLE ex01.ttable`
`mv ECHO   ex01.echo`
`mv MESH   ex01.mesh`
`mv PROFIL ex01.prof`
`mv CONCP  ex01.con`
`mv PRESP  ex01.presp`
`#mv  ALKP ex01.alkp`
`mv SATP   ex01.satp`
`mv GFILEP ex01.gel`
`mv TEMPP  ex01.temp`
`mv HIST01 ex01.hist01`
`mv HIST02 ex01.hist02`
`mv HIST03 ex01.hist03`
`mv HIST04 ex01.hist04`
`#mv HIST05 ex01.hist05`
`#mv HIST06 ex01.hist06`
`#mv HIST07 ex01.hist07`
`mv OVERAL ex01.overal`
`mv RESTAR ex01.rest`
`mv WARN   ex01.warn`
	Change the default UTCHEM output file names to something more meaningful. The main reason for doing this optional step is to simplify identification of files at a later date. Files that do not appear as part of the current run are commented out using the pound sign (#) in the first column of the `work.job` file.

`gzip *`	Add this line to the `work.job` file to compress all files in order to save space (if necessary).

Appendix B
UTCHEM Local Grid Refinement User's Guide

B.1 INTRODUCTION

UTCHEM is a three-dimensional chemical flooding simulator. The solution scheme is analogous to IMPES, where pressure is solved for implicitly, but concentrations rather than saturations are then solved for explicitly. Phase saturations and concentrations are then solved in a flash routine. An energy balance equation is solved explicitly for reservoir temperature. The energy balance equation includes heat flow between the reservoir and the over- and underburden rocks. The major physical phenomena modeled in the simulator are:

dispersion
dilution effects
adsorption
interfacial tension
relative permeability
capillary trapping
cation exchange
phase density
compositional phase viscosity
phase behavior (pseudoquaternary)
aqueous reactions
partitioning of chemical species between oil and water
dissolution/precipitation
cation exchange reactions involving more than two cations
in-situ generation of surfactant from acidic crude oil
pH dependent adsorption
polymer properties: shear thinning viscosity, inaccessible pore volume, permeability reduction, adsorption
gel properties: viscosity, permeability reduction, adsorption
tracer properties: partitioning, adsorption, radioactive decay, reaction (ester hydrolization)
temperature dependent properties: viscosity, tracer reaction, gel reactions

The following options are available with UTCHEM: isothermal or non-isothermal conditions, a constant or variable time-step, constant pressure or constant rate well conditions, horizontal and vertical wells, and a radial or cartesian geometry. Please refer to the dissertation “Field Scale Simulation of Chemical Flooding” by Naji Saad [1989] for a more detailed discussion of the UTCHEM simulator and its formulation.

B.2 LOCAL GRID REFINEMENT SPECIFICATIONS

This section describes the special requirements unique to the Local Grid Refinement (LGR) version of UTCHEM.

Input Notes:
This code is applicable to water flooding, Surfactant flooding and Tracer flooding.

Can use components: (1, 2, 3, 5, 6, 7, 8, 9, 10, 11)

Methods
Single Point upstream, 2 point upstream, higher order

Models
Water flooding
Salinity
Adsorption
Tracer
Surfactant / alcohol
phase behavior
Capillary number
Interfacial Tension
Full tensor physical diffusion
Capillary pressure
Solubilization (oil in water)
hysteresis
Wells - Peaceman Model
Global flow gradient
Gravity
Variable Permeability

The reservoir is initially defined by a coarse grid (called a base grid) with NXCxNYCxNZC standard cells (gridblocks).

Subject to memory limitations any combination of the base grid cells can be refined by one local level NXFxNYFxNZF which is of fixed resolution for all refined cells.

The locally refined cells are called ZONES.

Memory and ARRAYS.
Arrays must be set in PARAMS.INC and UTCHEMLGR.FOR

Edit PARAMS.INC to see 3 sections:

1) UTwork space, 2) Coarse, 3) Fine

Coarse and Fine correspond to the base grid and Zone requirements respectively. Note NREFI defines maximum number of zones and *total* memory is proportional to

NXXCxNYYCxNZZC + NREFI * NXXFxNYYFxNZZF
+
max(NXXCxNYYCxNZZC , NXXFxNYYFxNZZF)

UTwork space arrays = max(Coarse, Fine)

e.g. NNX = max (NNXC, NNXF)

UTBASE.F only contains work space arrays; e.g., NNX only (not NNXC or NNXF)

LOCAL REFINEMENT = ADD ZONES

New Input Parameters

The input data set consists of the usual UTCHEM data set for the base grid, and a UTCHEM data set for each ZONE (i.e., each refined base cell) again with appropriate minor modifications described below. The input format is identical to the standard UTCHEM manual in each case.

Coordinate Definition

LGR is used with ICOORD = 1

For **BASE** grid data set

```
READ (5,*) NXC,NYC,NZC,IDXYZ,IUNIT
READ (5,*) DXC,DYC,DZC
```

For **ZONE** data set

```
READ (5,*) NXF,NYF,NZF,IDXYZ,IUNIT
READ (5,*) DXF,DYF,DZF
```

(Must have NXF > 1, NYF > 1, NZF > 1 in 3-D)

Note: for uniform grids

DXF = DXC / NXF
DYF = DYC / NYF
DZF = DZC / NZF

otherwise for non-uniform grids

$$\mathrm{DXC} = \sum_j \mathrm{DXF}_j, \quad \mathrm{DYC} = \sum_j \mathrm{DYF}_j, \quad \mathrm{DZC} = \sum_j \mathrm{DZF}_j$$

Note: neighboring non-uniform grids must have the same spacing in the direction tangential to the common interface.

Gravity

D111 is the depth of the center of the first BASE cell in the top layer.

If a coarse cell is refined the corresponding depths of the local ZONE cells are appropriately defined by the code.

Set D111 = 0 in all ZONE domain data sets following the BASE data set.

Permeability

A pre-processing program LGRPERM is supplied which will extract portions of a *fine grid* global permeability map that correspond to zones chosen by the user.

The approach is as follows;

Define a base grid.

Refine the base grid to a specified level.

Create a fine grid permeability map for the entire fine domain then use LGRPERM to define the permeability maps for the local zones. An LGR simulation can then be performed with the specified zones that correspond locally to the fine domain. In effect some base cells are unrefined and appropriate upscaling should be employed for rock properties of these cells. At present LGRPERM assigns an average value to these cells.

Alternatively the user is free to define the local variation over each zone.

Caution: The larger the grid interface ratio (number of fine cells adjacent to a coarse cell) the larger the potential for error in the solution. A large variation in permeability over the interface may give rise to spurious pressure distributions, and in extreme cases may even cause convergence problems for the pressure equation solver.

WELL DATA

Inflow - Outflow

A fine zone can be adjacent to an inflow or out flow boundary. In this case the local zone data set is of identical format to the standard spec and

IBOUND =1.

If the zone is adjacent to an inflow boundary

IBL = 1, IBR = 0.

If the zone is adjacent to an outflow boundary

IBL = 0, IBR = 1.

WELLS

Wells can either be completed through adjoining base cells which are NOT refined, OR through adjoining ZONES. Wells are NOT allowed to be completed across any coarse-fine interface between a ZONE and a non-refined base cell.

Spatial (i,j,k) Indexing

Base grid: as per standard.

Zones: as per standard with respect to the local domain. The well spatial (i,j,k) indexing works with respect to the local domain.

Each well has a globally unique ID number; i.e., upon entering a new domain the "counting" of the wells begins from *current ID number + 1* . If a well is completed through neighboring zones then it has the same ID in both zones, otherwise the same ID cannot be assigned to different wells in separate domains.

Caution: By definition, the method will give relatively poor results if wells are placed in fine cells at coarse/fine interfaces of the grid.

SLUGS

Slug data for the base grid and all zones is tagged on the very end of the entire input file. First input the base grid well data modifications followed by each of the ZONE well data modifications as per standard spec**.** If the base grid or a ZONE is not modified or has no wells then this is flagged by

8 standard lines

CC
CC
then input
IRO,ITIME, (IFLAG(IDW(M)), M= 1 , NWELL)

enter all zeros if no wells,
or
repeat previous data if wells unchanged.
CC
CC
-1

Similarly repeat for each unchanged well in a domain.

NOTE: TINJ should have the same time value for each domain section until the very last specification of TINJ, which should have TINJ > TMAX.

Restart Data

Currently a single line is added to the top of the restart data set to handle well data for the zones.

Enter

1

for each existing zone (of the first simulation) not containing a well and for each new zone that has been added.

Enter

-1

for each existing zone (of the first simulation) containing a well so that the restart well data is read, this data can only be modified via a slug.

The order of entry is strictly according to the occurrence of each zone with respect to the global index IIG(L) = I + (J - 1) * NXC + (K - 1) * NXC*NYC.

e.g., if in the first simulation there are 3 zones with a well in the first zone and 5 restart zones are flagged, then (assuming the new zone global indices are greater than the first zone global index) upon restarting the calculation enter

-1 1 1 1 1

OUTPUT

The output is written per domain in standard UTCHEM format. The base cell and refinement number are printed at the top of each domain data set, "layers" now refers to layers in the local domain.

The velocity field is written for each cell face of each zone. Therefore neighboring interior zones will have the same face velocity field at the common interface locations.

B.3 OPERATION OF THE SIMULATOR

The UTCHEM simulator is run on a CRAY Y/MP at the University of Texas High Performance Computing Facility (UNICOS operating system), a number of DEC Alpha systems (DEC 4000/610, 3000/500 & 3000/300X) at the Department of Petroleum and Geosystems Engineering (OSF/1 operating system), and a DEC Alpha system (DEC 3000/500) at the Department of Petroleum and Geosystems Engineering (OpenVMS operating system). The same code is executed on all three systems, except for the use of double precision (64-bit words) on the DEC machines—we differentiate between "Cray" and "DEC" versions of the code by adding a "V" prior to the version number for the "Cray" version and a "D" prior to the version number for the "DEC" (or double-precision) version. Several intrinsic Cray functions need to be implemented when not running on the Cray; these routines are "commented" out in the "Cray" version. Please check the source code for additional information about necessary changes when running on different computers.

B.3.1 Input and Output Files

UTCHEM requires one input file for non-restart runs. For restart runs, a restart file is required in addition to the original input data file used for the previous run. A detailed input data description is given in section B.3 of this appendix and the data in the restart data file is documented in section B.6. The number of output files generated by UTCHEM varies depending upon several control flags set by the user in the input file. The number of history plot files depends on the value of the MXW parameter in the source code. The FORTRAN unit number for the history plot file is incremented by one for each well. For example, if MXW is equal to three, then three history plot files would be generated corresponding to FORTRAN unit numbers 19, 20, and 21 even if the run only has two wells. The input and output files are summarized in the following table.

Unit Number	File Name	Contents
1	TEMPL	Analytical temp. profile, created if IENG=1 and IANAL=1
2	ECHO	Echo print of the input file information
3	SUMARY	Summary data
4	PROFIL	Formatted profile data; described in section 6.1 of this appendix
5	INPUT	Input data; described in detail in section B.3 of this appendix
6	TTABLE	Table of time steps and Courant numbers
7	RESTAR	Stored restart run data; described in section 6.3 of this appendix
8	CONCP	Component concentration profile plotting data, created if IPCTOT>0
9	OVERAL	History of overall properties; described in section 6.5 of this appendix
10	GFILEP	Gel property profile plotting data, created if IREACT=1
11	PRESP	Phase pressure profile plotting data, created if IPPRES>0
12	SATP	Phase saturation profile plotting data, created if IPSAT>0
13	TRACP	Phase tracer concentration profile plotting data, created if IPTRAC>0
14	CAPP	Capacitance property profile plotting data, created if IPCAP>1
15	ALKP	Alkaline option related profile plotting data, created if IREACT>1
16	INPUT2	Restart run data (input file created by an earlier run)
17	WARN	Warning messages
18	TEMPP	Temperature profile, created if IENG =1 and IPTEMP=1
19	HIST01	Well history plotting data for well #1; described in section 6.4 of this appendix
20	HIST02	Well history plotting data for well #2
…		
ℓ	HISTℓ	Well history plotting data for last well
ℓ+1	TRAC01	Aqueous phase tracer concentration at 1st observation point , created if IPOBS>0; described in section 6.6 of this appendix
ℓ+2	TRAC02	Aqueous phase tracer concentration at 2nd observation point
…		
n	TRAC*n*	Aqueous phase tracer concentration at last observation point

B.3.2 Source Code Array Dimensions

The parameters in the following table are used by the simulator to define array sizes. All the parameter values must be equal to or greater than the size of the grid dimensions specified in the input file, unless otherwise noted. Additionally, all instances of each parameter must be the same throughout the code, so if you want to change the value of one of the parameters, please make sure you make a global substitution. Please see the note in Section 2 on memory and arrays for LGR code.

Parameter	Definition

NNX	Number of gridblocks in X-direction (must be set equal or larger to NX in the input file)
NNY	Number of gridblocks in Y-direction (must be set equal or larger to NY in the input file)
NNZ	Number of gridblocks in Z-direction (must be set equal or larger to NZ in the input file)
MXC	Maximum number of components (cannot be less than 8)
MXP	Number of phases (must be set equal to 3 when there is no gas phase and must be set equal to 4 if gas is present)
MXW	Maximum number of wells
MXWB	Maximum number of well blocks
MXNT	Maximum number of tracers
MXELE	Maximum number of elements
MXFLD	Maximum number of reactive fluid species
MXSLD	Maximum number of solids
MXSORB	Maximum number of adsorbed species
MXACAT	Maximum number of cations associated with surfactant
MXEX	Maximum number of insoluble exchangers

B.4 INPUT DATA DESCRIPTION

The UTCHEM input file consists of comment lines and data lines. All comment lines are ignored by the UTCHEM simulator. It is important to note, however, that the number of comment lines between data lines is fixed. The first twenty-two lines of the input file are reserved for comment lines used to briefly describe the input file. Each data line is preceded by three comment lines (except for the input described in section 4.5 of this appendix). The input file is basically divided into six sections and each of those input sections (except section 4.5 of this appendix) is preceded by an additional seven comment lines. The user should update the comment lines as the input file is modified in order to make using the simulator easier.

All data is free-formatted. This means that for each read statement, it is only necessary to leave a blank space between data elements. Note that the first data element for a given read statement must be on a new line in the input file. Subsequent data elements for that read statement can span as many lines as necessary. Implicit type matching is used; that is, all REAL variables begin with the letters A-H or O-Z and all integer variables begin with the letters I-N.

The following is a list of variables as they are read by UTCHEM. The variable names appear in all-caps on a single line in the order they are read by the program. Every list of variables is followed by a description of each variable and corresponding units or possible values if applicable. All of the variables listed in the input description will be read by the program unless otherwise noted; therefore, a dummy value will be read by the program for variables not pertinent to the problem being run.

B.4.1 Title and Reservoir Description Data

The first input section consists of the title and reservoir description data. Please remember that there are 22 comment lines at the beginning of this section and that each data line is preceded by three comment lines.

4.1.1 RUNNO

RUNNO - Run number.

Note: The run number can consist of any combination of alphanumeric characters on a single line (not to exceed 80 characters). This information will be printed as the first line of every output file.

4.1.2 TITLE

TITLE - Title and run description.

Note: The title can consist of any combination of alphanumeric characters spanning three lines in the input file (not to exceed 80 characters per line). Please note that the title must span three lines and that any of those lines can be blank.

4.1.3 NRINIT, IRESTZONE

NRINIT - Number of refined zones.

IRESTZONE - Number of refined zones for restart run.

4.1.4 IXG(J), IYG(J), IZG(J), for J=1, NRINIT

IXG(J), IYG(J), IZG(J) - Base grid integer coordinates of the refined cells.

4.1.5 IXRG(J), IYRG(J), IZRG(J), for J=1, NRINIT (This line is read only if IRESTZONE > 0)

IXRG(J), IYRG(J), IZRG(J) - Base grid integer coordinates of the cells to be refined at restart. Repeat for IRESTZONE refined base cells.

4.1.6 IMODE, IMES, IDISPC, ICWM, ICAP, IREACT, ICOORD, ITREAC, ITC, IGAS, IENG

IMODE - Flag indicating if the problem to be run is a first run or a restart problem.

Possible Values:

1 - First run problem
2 - Restart problem

IMES - Flag indicating if a constant or automatic time-step is to be used.

Possible Values:

1 - Constant time-step size is used
2 - Automatic time-step size selector based on method of relative changes for the first three components is used
3 - Automatic time-step size selector based on method of relative changes for all the components is used
4 - Automatic time-step size selector based on changes in dimensionless concentration for all the components is used

Note: The automatic time-step selector is recommended. See input lines 4.5.9 through 4.5.12 for more details on the above options. In addition, IMES=1 is the **only option** fully tested with the **LGR code.**

IDISPC - Flag indicating which type of numerical dispersion control is used.

Possible Values:

0 - Single point upstream method is used
1 - Chaudhari's method is used (this method is not available if ICOORD = 2)
2 - Two point upstream method is used
3 - Improved total variation diminishing third order method is used

Note: These methods are applied to both concentration and relative permeability.

ICWM - Flag indicating if the concentration well model is used or not.

Possible Values:

0 - Concentration well model is not used
1 - Concentration well model is used
Note: The concentration well model (ICWM = 1) can only be used with vertical wells (IDIR(M) = 3).

ICAP - Flag indicating if the capacitance model is used or not.
Possible Values:
0 - Capacitance model is not used
1 - Capacitance model is used

IREACT - Flag indicating if gel reactions or alkaline options are used or not.
Possible Values:
0 - Gel reactions are not used
1 - Gel reactions are used
2 - Alkaline option 1 (no silicon, aluminum, or acid)
3 - Alkaline option 2 (no silicon or aluminum; with acidic crude)
4 - Alkaline option 3 (with silicon and aluminum; no acid)
5 - Alkaline option 4 (with silicon, aluminum, and acidic crude)
6 - Alkaline option 3 and gel reactions are used
Note: IREACT=0 is the **only option** available with the **LGR code**.

ICOORD - Flag indicating which coordinate system is used.
Possible Values:
1 - Cartesian coordinate system is used
2 - Radial coordinate system is used
3 - Cartesian coordinate system with variable-width gridblock is used (2-D cross section only)
4 - Curvilinear grid definition of the X-Z cross section is used (2-D or 3-D)
Note: For ICOORD=4, the 3-D grid consists of the 2-D cross sectional grid repeated at specified intervals (uniform or non-uniform) in the Y direction, according to the definition of DY1. The curvilinear grid option is not available for the temperature equation option (IENG must be set to 0 on this input line). In addition, ICOORD=1 is the **only option** available with the **LGR code**.

ITREAC - Flag indicating if a tracer reaction is used or not.
Possible Values:
0 - Tracer reaction is not used
1 - Tracer reaction is used

ITC - Flag indicating if second-order time approximation is used or not.
Possible Values:
0 - Second-order time approximation is not used
1 - Second-order time approximation is used
Note: We recommend that second-order time approximation (ITC = 1) only be used with higher-order dispersion methods (IDISPC > 1).

IGAS - Flag indicating if gas phase is considered or not.
Possible Values:
0 - Gas is not present
1 - Gas is present

IENG - Flag indicating if temperature variation is considered or not.
Possible Values:
0 - Isothermal simulation

1 - Temperature equation is solved

Note: IENG must be set equal to 0 if the curvilinear grid option (ICOORD=4 on this input line) option is used. In addition, IENG=0 is the **only option** available with the **LGR code**.

4.1.7 NX, NY, NZ, IDXYZ, IUNIT

NX - Number of gridblocks along X-axis (ICOORD = 1 or 3) or number of gridblocks in radial direction (ICOORD = 2).

Note: This value should be equal to or smaller than the NNX parameter in UTCHEM.

NY - Number of gridblocks along Y-axis.

Note: This value should be equal to or smaller than the NNY parameter in UTCHEM. It should be set equal to 1 if the user is running a 1-D problem or a 2-D cross sectional problem. If ICOORD = 2, this value is automatically set equal to 1.

NZ - Number of gridblocks along Z-axis.

Note: This value should be equal to or smaller than the NNZ parameter in UTCHEM. It should be set equal to 1 if the user is running a 1-D problem or a 2-D areal problem.

IDXYZ - Flag indicating constant or variable grid size.

Possible Values:

0 - Constant grid size
1 - Variable grid size on a regional basis
2 - Variable grid size

Note: IDXYZ must be set equal to 2 if ICOORD = 3.

IUNIT - Flag indicating English or Metric units.

Possible values:

0 - English unit
1 - Metric unit

Note: UTCHEM must be compiled and run with the NX, NY, and NZ input values being equal to or smaller than the NNX, NNY, and NNZ parameters in the code. All 38 occurrences of the NNX, NNY, and NNZ parameters in the code must be set to the same values which must be equal to or larger than the NX, NY, and NZ input values. Additionally, since parameter statements are used for dimensioning arrays in UTCHEM, any time any parameter statement is changed in the FORTRAN source code, all occurrences of that parameter statement must be changed (and set to the same value throughout the code) or the code will not function properly.

4.1.8 XCORD (I), ZCORD(I), for I = 1, (NX+1) × (NZ+1) (This line is read only if ICOORD = 4)

XCORD - Gridblock coordinate of Ith corner point in X-direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

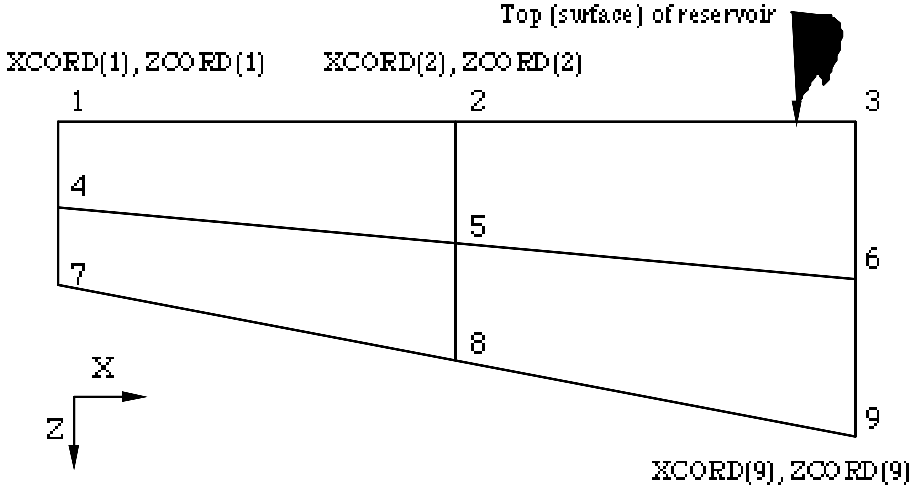
ZCOORD - Gridblock coordinate of Ith corner point in Z-direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: The coordinates of the corners (or vertices) of the 2-D X-Z cross section gridblocks are input in pairs as follows:

```
XCORD(1),          ZCORD(1)
   .                  .
   .                  .
   .                  .
XCORD(nodes),      ZCORD(nodes)
```

where nodes = (NX+1) × (NZ+1) and is the total number of corner points defining the X-Z cross section and Z is positive downward. The following figure illustrates the input order for an example X-Z cross section grid:



The number of gridblocks is equal to NX × NZ and the number of coordinate pairs (or nodes) is equal to (NX+1) × (NZ+1).

Cautionary warning: The X-Z cross section grid should be constructed by the user such that the curvilinear coordinate system is at least quasi-orthogonal. Departure from orthogonality will lead to numerical errors in the solution.

4.1.9 DX1, DY1, DZ1 (This line is read only if IDXYZ = 0 and ICOORD = 1)

DX1 - Gridblock size in X direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

DY1 - Gridblock size in Y direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

DZ1 - Gridblock size in Z direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

4.1.10 R(1), DX1, DZ1 (This line is read only if IDXYZ = 0 and ICOORD = 2)

R(1) - Wellbore radius.
Units: feet (IUNIT=0) or m (IUNIT=1)

DX1 - Distance between nodes in radial direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

DZ1 - Gridblock size in Z direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

4.1.11 DY1 (This line is read only if IDXYZ = 0 and ICOORD = 4)

DY1 - Gridblock size in Y direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

4.1.12 II1, II2, DX1 (This line is read only if IDXYZ = 1 and ICOORD = 1 or 3)

II1 - First index for gridblocks with same size in X direction.

II2 - Last index for gridblocks with same size in X direction.

DX1 - Gridblock size in X direction

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NX gridblocks in the X direction have been specified. The first line in the set must have II1 = 1 and the last line must have II2 = NX.

Example: If NX = 11 and the first three gridblocks in the X direction are 3 feet in size, the fourth through ninth gridblocks in the X direction are 2 feet in size, and the last two gridblocks in the X direction are 2.5 feet in size, this line would need to be repeated three times to fully describe the X direction gridblocks as follows:

1 3 3.0
4 9 2.0
10 11 2.5

4.1.13 JJ1, JJ2, DY1 (This line is read only if IDXYZ = 1 and ICOORD = 1 or 3)

JJ1 - First index for gridblocks with same size in Y direction.

JJ2 - Last index for gridblocks with same size in Y direction.

DY1 - Gridblock size in Y direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NY gridblocks in the Y direction have been specified. The first line in the set must have JJ1 = 1 and the last line must have JJ2 = NY. See the example for input line 4.1.9.

4.1.14 KK1, KK2, DZ1 (This line is read only if IDXYZ = 1 and ICOORD = 1 or 3)

KK1 - First index for gridblocks with same size in Z direction.

KK2 - Last index for gridblocks with same size in Z direction.

DZ1 - Gridblock size in Z direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NZ gridblocks in the Z direction have been specified. The first line in the set must have KK1 = 1 and the last line must have KK2 = NZ. See the example for input line 4.1.9.

4.1.15 R(1) (This line is read only if IDXYZ = 1 and ICOORD = 2)

R(1) - Wellbore radius.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.1.16 II1, II2, DX1 (This line is read only if IDXYZ = 1 and ICOORD = 2)

II1 - First index for radial node distances of the same size.

II2 - Last index for radial node distances of the same size.

DX1 - Distance between nodes in radial direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until the NX-1 distances between the NX nodes in the radial direction have been specified. The first line in the set must have II1 = 1 and the last line must have II2 = NX-1.

4.1.17 KK1, KK2, DZ1 (This line is read only if IDXYZ = 1 and ICOORD = 2)

KK1 - First index for gridblocks with same size in Z direction.

KK2 - Last index for gridblocks with same size in Z direction.

DZ1 - Gridblock size in Z direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NZ gridblocks in the Z direction have been specified. The first line in the set must have KK1 = 1 and the last line must have KK2 = NZ. See the example for input line 4.1.9.

4.1.18 JJ1, JJ2, DY1 (This line is read only if IDXYZ=1 and ICOORD=4)

JJ1 - First index for gridblocks with same size in Y direction.

JJ2 - Last index for gridblocks with same size in Y direction.

DY1 - Gridblock size in Y direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NY gridblocks in the Y direction have been specified. The first line in the set must have JJ1 = 1 and the last line must have JJ2 = NY. See the example for input line 4.1.9.

4.1.19 DX(I), for I = 1, NX (This line is read only if IDXYZ = 2 and ICOORD = 1 or 3)

DX(I) - Grid size of Ith block in X direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.1.20 DY(J), for J = 1, NY (This line is read only if IDXYZ = 2 and ICOORD = 1 or 4)

DY(J) - Grid size of Jth block in Y direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.1.21 DY(I), for I = 1, NX (This line is read only if IDXYZ = 2 and ICOORD = 3)

DY(I) - Thickness of Ith block.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.1.22 DZ(K), for K = 1, NZ (This line is read only if IDXYZ = 2 and ICOORD = 1 or 3)

DZ(K) - Grid size of Kth block in Z direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.1.23 R(1) (This line is read only if IDXYZ = 2 and ICOORD = 2)

R(1) - Wellbore radius.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.1.24 DX(I), for I = 1, NX-1 (This line is read only if IDXYZ = 2 and ICOORD = 2)

DX(I) - Distance between the Ith node and the I+1th node in the radial direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.1.25 DZ(K), for K = 1, NZ (This line is read only if IDXYZ = 2 and ICOORD = 2)

DZ(K) - Grid size of Kth block in Z direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.1.26 N, NTW, NTA, NG

N - Total number of components in the run (including tracers and reactive components).

Possible Values: 1 – 21

NTW - Number of water/oil tracers.

Possible Values: see note

NTA - Number of oil/gas tracers.
Possible Values: see note

NG - Number of gel components.
Possible Values: 4 or 5 when IREACT = 1
4 when IREACT = 6

Note: The combined total number of water/oil and oil/gas tracers (NTW+NTA) must be:

1) less than or equal to MXNT (see section 3.2) and
2) between 0 and 3 (inclusive) if IREACT>1 or between 0 and 13 (inclusive) if IREACT=1.

The components will be listed in the following order for the corresponding values of IREACT:

Index	Component (IREACT = 0)	Component (IREACT = 1)	Component (IREACT = 2)	Component (IREACT = 3)	Component (IREACT = 4)	Component (IREACT = 5)	Component (IREACT = 6)
1	Water	Water	Water	Water	Water	Water	Water
2	Oil	Oil	Oil	Oil	Oil	Oil	Oil
3	Surfactant	Surfactant	Surfactant	Surfactant	Surfactant	Surfactant	Surfactant
4	Polymer	Polymer	Polymer	Polymer	Polymer	Polymer	Polymer
5	Chloride	Chloride	Chloride	Chloride	Chloride	Chloride	Chloride
6	Calcium	Calcium	Calcium	Calcium	Calcium	Calcium	Calcium
7	Alcohol 1	Alcohol 1	Alcohol 1	Alcohol 1	Alcohol 1	Alcohol 1	Alcohol 1
8	Alcohol 2 or Gas	Alcohol 2 or Gas	Alcohol 2 or Gas	Alcohol 2 or Gas	Alcohol 2 or Gas	Alcohol 2 or Gas	Alcohol 2 or Gas
9	Tracer 1	Tracer 1	Tracer 1	Tracer 1	Tracer 1	Tracer 1	Tracer 1
10	Tracer 2	Tracer 2	Tracer 2	Tracer 2	Tracer 2	Tracer 2	Tracer 2
11	Tracer 3	Tracer 3	Tracer 3	Tracer 3	Tracer 3	Tracer 3	Tracer 3
12	Tracer 4	$Na_2Cr_2O_7$	Sodium	Sodium	Sodium	Sodium	Sodium
13	Tracer 5	CSN_2H_4	Hydrogen	Hydrogen	Hydrogen	Hydrogen	Hydrogen
14	Tracer 6	Cr^{3+}	Magnesium	Magnesium	Magnesium	Magnesium	Magnesium
15	Tracer 7	Gel	Carbonate	Carbonate	Carbonate	Carbonate	Carbonate
16	Tracer 8	Hydrogen	—	Acid Comp. of Crude Oil	Aluminum	Aluminum	Aluminum
17	Tracer 9	—	—	—	Silica	Silica	Silica
18	Tracer 10	—	—	—	—	Acid Comp. of Crude Oil	$Na_2Cr_2O_7$
19	Tracer 11	—	—	—	—	—	CSN_2H_4
20	Tracer 12	—	—	—	—	—	Cr^{3+}
21	Tracer 13	—	—	—	—	—	Gel

If IREACT > 0, N must be set to the maximum number of components shown for each case in the above table, whether all the components are present or not. For example, if IREACT = 3, N must be set to 16. The shaded cells indicate options **not available** to the **LGR code**.

4.1.27 TRNAME(IT), for IT = 1, NTW+NTA (This line is read only if NTW+NTA > 0)

TRNAME(IT) - Name of ITth tracer.

Note: The name of each tracer may not exceed 16 characters and each name must be on a separate line of the input file.

4.1.28 ITRU(I), for I = 1, NTW (This line is read only if NTW > 0 and ITREAC = 1)

ITRU(I) - Flag indicating the units of the Ith tracer.

Possible Values:

1 - Ith tracer units are in volume %
2 - Ith tracer units are in weight %

4.1.29 ICF(KC), for KC = 1, N

ICF(KC) - Flag indicating if KCth component is included in the concentration calculations or not.

Possible Values:

0 - The KCth component is not included in the calculations
1 - The KCth component is included in the calculations

Example: If 11 components are considered but Alcohol 2 is not present, this line would appear as follows:

1 1 1 1 1 1 1 0 1 1 1

B.4.2 **Output Option Data**

The second input section consists of output options. Please remember that there are seven comment lines at the beginning of this section and that each data line is preceded by three comment lines.

4.2.1 ICOPSM, ICUMTM, ISTOP

ICOPSM - Flag indicating if data will be written to UNIT 3.

Possible Values:

0 - Data will be written to UNIT 3 as directed by CUMHI2 flag
1 - Data will not be written to UNIT 3

ICUMTM - Flag indicating if the output intervals indicated by the CUMPR1, CUMHI1, CUMHI2, WRHPV, WRPRF and RSTC variables on input line 4.5.8 are specified in pore volumes or days.

Possible Values:

0 - Data will be written in pore volume intervals
1 - Data will be written in day intervals

Note: The day interval output option (ICUMTM = 1) is particularly useful if there is a shut in period.

ISTOP - Flag indicating if the maximum and injection times (variables TMAX on input line 4.3.1 and TINJ on input line 4.6.8) are specified in pore volumes or days.

Possible Values:

0 - TMAX and TINJ are specified in days
1 - TMAX and TINJ are specified in pore volumes

4.2.2 IPRFLG(KC), for KC = 1, N

IPRFLG(KC) - Flag indicating if profile of KCth component should be written to UNIT 8.

Possible Values:

0 - Profile of KCth component will not be written

1 - Profile of KCth component will be written

Note: If IPCTOT=0, none of the component profiles will be written.

Example: If 11 components are present and only profiles for the oil, surfactant, and polymer components are desired, this line would appear as follows:

0 1 1 1 0 0 0 0 0 0 0

4.2.3 IPPRES, IPSAT, IPCTOT, IPTRAC, IPCAP, IPGEL, IPALK, IPTEMP

IPPRES - Flag indicating if profile of phase pressures should be written to UNIT 11.

Possible Values:

0 - Profile of phase pressures will not be written
1 - Profile of phase pressures will be written

IPSAT - Flag indicating if profile of phase saturations should be written to UNIT 12.

Possible Values:

0 - Profile of phase saturations will not be written
1 - Profile of phase saturations will be written

IPCTOT - Flag indicating if profile of component concentrations should be written to UNIT 8.

Possible Values:

0 - Profile of component concentrations will not be written
1 - Profile of component concentrations will be written

IPTRAC - Flag indicating if profile of tracer phase concentrations should be written to UNIT 13.

Possible Values:

0 - Profile of tracer phase concentrations will not be written
1 - Profile of tracer phase concentrations will be written

IPCAP - Flag indicating if profile of capacitance properties should be written to UNIT 14.

Possible Values:

0 - Profile of capacitance properties will not be written
1 - Profile of capacitance properties will be written

IPGEL - Flag indicating if profile of gel properties should be written to UNIT 10.

Possible Values:

0 - Profile of gel properties will not be written
1 - Profile of gel properties will be written

IPALK - Flag indicating if profile of properties related to the alkaline option should be written to UNIT 15.

Possible Values:

0 - Profile of properties related to the alkaline option will not be written
1 - Profile of properties related to the alkaline option will be written

IPTEMP - Flag indicating if profile of reservoir temperature should be written to UNIT 18.

Possible Values:

0 - Profile of temperature will not be written
1 - Profile of temperature will be written

4.2.4 IPHP, IADS, ICKL, IVEL, IVIS, IPER, ICNM, IRKF, IPHSE, ICSE

IPHP - Flag indicating if oleic and microemulsion phase pressure data should be printed.

Possible Values:

0 - Oleic and microemulsion phase pressure data will not be printed
1 - Oleic and microemulsion phase pressure data will be printed

IADS - Flag indicating if surfactant, polymer, calcium, gel, chromium, hydrogen, and sodium adsorption data should be printed.

Possible Values:

0 - Adsorption data will not be printed
1 - Adsorption data will be printed

ICKL - Flag indicating if component concentration data in each phase should be printed.

Possible Values:

0 - Component concentration data in each phase will not be printed
1 - Component concentration data in each phase will be printed

IVEL - Flag indicating if X, Y, and Z direction phase fluxes should be printed.

Possible Values:

0 - X, Y, and Z direction phase fluxes will not be printed
1 - X, Y, and Z direction phase fluxes will be printed

IVIS - Flag indicating if phase viscosities should be printed.

Possible Values:

0 - Phase viscosities will not be printed
1 - Phase viscosities will be printed

IPER - Flag indicating if relative permeabilities should be printed.

Possible Values:

0 - Relative permeabilities will not be printed
1 - Relative permeabilities will be printed

ICNM - Flag indicating if phase capillary numbers and interfacial tensions should be printed.

Possible Values:

0 - Capillary numbers and interfacial tensions will not be printed
1 - Capillary numbers and interfacial tensions will be printed

IRKF - Flag indicating if permeability reduction factors should be printed.

Possible Values:

0 - Permeability reduction factors, polymer viscosities, and equivalent shear rate will not be printed
1 - Permeability reduction factors, polymer viscosities, and equivalent shear rate will be printed

IPHSE - Flag indicating if phase environment indexing should be printed.

Possible Values:

0 - Phase environment indexing will not be printed
1 - Phase environment indexing will be printed

Note: The indices for the phase environment are as follows:

1 - single phase
2 - two phase oil/water or oil/microemulsion or water/microemulsion
3 - three phase oil/microemulsion/water
4 - lobe II(+) of type III
5 - lobe II(-) of type III

ICSE - Flag indicating if effective salinity should be printed.

Possible Values:

0 - Effective salinity information will not be printed
1 - Effective salinity will be printed to PROFIL and history data files

Note: These flags give the option of printing a very detailed description (all flags = 1) every CUMPR1 pore volume interval or a very limited description (all flags = 0) to UNIT 4. See section B.6 for a list of the values that are written to UNIT 4 automatically.

4.3 Reservoir Properties

The third input section consists of the reservoir properties. Please remember that there are seven comment lines at the beginning of this section and that each data line is preceded by three comment lines.

4.3.1 TMAX

TMAX - Total injection period (maximum simulated time).

Units: days or pore volumes (dependent on value of ISTOP flag in line 4.2.1)

4.3.2 COMPR, PSTAND

COMPR - Rock compressibility.

Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

PSTAND - Reference pressure at which pore volume and fluid compressibilities are specified.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

4.3.3 IPOR1, IPERMX, IPERMY, IPERMZ

IPOR1 - Flag indicating constant or variable porosity for reservoir.

Possible Values:

0 - Constant porosity for whole reservoir
1 - Constant porosity for each layer
2 - Variable porosity over reservoir

IPERMX - Flag indicating constant or variable X direction permeability (ICOORD = 1 or 3) or radial direction permeability (ICOORD = 2) for reservoir.

Possible Values:

0 - Constant permeability for whole reservoir
1 - Constant permeability for each layer in the X direction (ICOORD = 1 or 3) or radial direction (ICOORD = 2)
2 - Variable permeability over reservoir

IPERMY - Flag indicating constant or variable Y direction permeability for reservoir.

Possible Values:

0 - Constant permeability for whole reservoir
1 - Constant permeability for each layer in the Y direction
2 - Variable permeability over reservoir
3 - Y direction permeability is dependent on X direction permeability

IPERMZ - Flag indicating constant or variable Z direction permeability for reservoir.

Possible Values:

0 - Constant permeability for whole reservoir
1 - Constant permeability for each layer in the Z direction
2 - Variable permeability over reservoir
3 - Z direction permeability is dependent on X direction permeability

4.3.4 PORC1 (This line is read only if IPOR1 = 0)

PORC1 - Reservoir porosity.

Units: fraction

Note: All elements of the POR array will be set equal to PORC1.

4.3.5 POR(K), for K = 1, NZ (This line is read only if IPOR1 = 1)

POR(K) - Porosity of Kth layer.

Units: fraction

Note: NZ values are actually read into a workspace array (WKSP1) and then the first set of NX × NY elements (corresponding to layer 1) of the POR array are set equal to WKSP1(1), the second set of NX × NY elements (corresponding to layer 2) of the POR array are set equal to WKSP1(2), etc.

4.3.6 POR(I), for I = 1, NX × NY × NZ (This line is read only if IPOR1 = 2)

POR(I) - Porosity of Ith gridblock

Units: fraction

Note: The three-dimensional grid system is being read into a one-dimensional array. The first index (column) of the three-dimensional system fastest, the second index (row) varies next fastest, and the third index (layer) varies slowest.

Example: If you had a 4 × 3 × 2 system (4 columns—NX=4, 3 rows—NY=3, and 2 layers—NZ=2), the values would be read in the following order:

1,1,1	2,1,1	3,1,1	4,1,1
1,2,1	2,2,1	3,2,1	4,2,1
1,3,1	2,3,1	3,3,1	4,3,1
1,1,2	2,1,2	3,1,2	4,1,2
1,2,2	2,2,2	3,2,2	4,2,2
1,3,2	2,3,2	3,3,2	4,3,2

4.3.7 PERMXC (This line is read only if IPERMX = 0)

PERMXC - Permeability of the reservoir in the X direction (ICOORD = 1 or 3) or in the radial direction (ICOORD = 2).

Units: millidarcies = 10^{-3} μm^2

Note: All elements of the PERMX array will be set equal to PERMXC.

4.3.8 PERMX(K), for K = 1, NZ (This line is read only if IPERMX = 1)

PERMX(K) - Permeability of the Kth layer in the X direction (ICOORD = 1 or 3) or in the radial direction (ICOORD = 2).

Units: millidarcies = 10^{-3} μm^2

Note: See the note for input line 4.3.5.

4.3.9 PERMX(I), for I = 1, NX × NY × NZ (This line is read only if IPERMX = 2)

PERMX(I) - Permeability of the Ith gridblock in the X direction (ICOORD = 1 or 3) or in the radial direction (ICOORD = 2).

Units: millidarcies = 10^{-3} μm^2

Note: See the note and example for input line 4.3.6 for the order of the permeability values.

4.3.10 PERMYC (This line is read only if IPERMY = 0 and ICOORD = 1 or 3)

PERMYC - Permeability of the reservoir in the Y direction.

Units: millidarcies = 10^{-3} μm^2
Note: All elements of the PERMY array will be set equal to PERMYC.

4.3.11 PERMY(K), for K = 1, NZ (This line is read only if IPERMY = 1 and ICOORD = 1 or 3)
PERMY(K) - Permeability of the Kth layer in the Y direction.
Units: millidarcies = 10^{-3} μm^2
Note: See note for input line 4.3.5.

4.3.12 PERMY(I), for I = 1, NX × NY × NZ (This line is read only if IPERMY = 2 and ICOORD = 1 or 3)
PERMY(I) - Permeability of the Ith gridblock.
Units: millidarcies = 10^{-3} μm^2
Note: See the note and example for input line 4.3.6 for the order of the permeability values.

4.3.13 FACTY (This line is read only if IPERMY = 3 and ICOORD = 1 or 3)
FACTY - Constant permeability multiplier for Y direction permeability.
Units: dimensionless
Note: The X direction permeabilities are multiplied by FACTY to obtain the Y direction permeabilities.

4.3.14 PERMZC (This line is read only if IPERMZ = 0)
PERMZC - Permeability of the reservoir in the Z direction.
Units: millidarcies = 10^{-3} μm^2
Note: All elements of the PERMZ array will be set equal to PERMZC.

4.3.15 PERMZ(K), for K = 1, NZ (This line is read only if IPERMZ = 1)
PERMZ(K) - Permeability of the Kth layer in the Z direction.
Units: millidarcies = 10^{-3} μm^2
Note: See note for input line 4.3.5.

4.3.16 PERMZ(I), for I = 1, NX × NY × NZ (This line is read only if IPERMZ = 2)
PERMZ(I) - Permeability of the Ith gridblock.
Units: millidarcies (10^{-3} μm^2)
Note: See the note and example for input line 4.3.6 for the order of the permeability values.

4.3.17 FACTZ (This line is read only if IPERMZ = 3 and ICOORD = 1 or 3)
FACTZ - Constant permeability multiplier for Z direction permeability.
Units: dimensionless
Note: The X direction permeabilities are multiplied by FACTZ to obtain the Z direction permeabilities.

4.3.18 IDEPTH, IPRESS, ISWI
IDEPTH - Flag indicating type of depth measurement of the top layer.
Possible Values:

0 - Single value for depth of the top layer is specified
1 - Depth of top gridblock (1,1,1) and the reservoir dip angles are specified
2 - Depth of each gridblock in the top layer is specified
Note: If ICOORD = 2, this value is automatically set equal to 0.
The depth is specified at the middle of a gridblock.

IPRESS - Flag indicating type of reservoir initial pressure measurement.
Possible Values:
0 - Single value for reservoir initial pressure is used for all gridblocks
1 - Initial pressure for a point at a specified depth is specified by user
2 - Initial pressure for each gridblock is specified by user

ISWI - Flag indicating type of initial water saturation measurement.
Possible Values:
0 - Single value for initial water saturation is used for all gridblocks
1 - Constant value for water saturation for each layer is specified by user
2 - Initial water saturation for each gridblock is specified by user

4.3.19 D111 (This line is read only if IDEPTH = 0)
D111 - Depth of the top layer of the reservoir measured from the surface (reference plane), positive downward.
Units: feet (IUNIT=0) or m (IUNIT=1)
Note: If IDEPTH=0 and ICOORD=4, D111 is the reference depth of the first gridblock.

4.3.20 D111, THETAX, THETAY (This line is read only if IDEPTH = 1)
D111 - Depth of the first gridblock (1,1,1).
Units: feet (IUNIT=0) or m (IUNIT=1)
THETAX - Reservoir dip angle in X direction, positive downward.
Units: radians
THETAY - Reservoir dip angle in Y direction, positive downward.
Units: radians
Note: If ICOORD=4, set THETAY equal to 0 (dip angle in X-Z plane).

4.3.21 EL(I), for I = 1, NX × NY (This line is read only if IDEPTH = 2)
EL(I) - Depth of Ith gridblock in the top layer (K=1).
Units: feet (IUNIT=0) or m (IUNIT=1)
Note: See the note and example for input line 4.3.6 for the order of the gridblock depths.

4.3.22 PRESS1 (This line is read only if IPRESS = 0)
PRESS1 - Initial reservoir pressure.
Units: psi (IUNIT=0) or kPa (IUNIT=1)

4.3.23 PINIT, HINIT (This line is read only if IPRESS = 1)
PINIT - Initial reservoir pressure at HINIT depth.
Units: psia (IUNIT=0) or kPa (IUNIT=1)
HINIT - Depth of the point where PINIT initial pressure is specified.
Units: feet (IUNIT=0) or m (IUNIT=1)
Note: Initial pressure is assumed to be the aqueous phase pressure.

4.3.24 P(I), for I = 1, NX × NY × NZ (This line is read only if IPRESS = 2)

P(I) - Initial pressure of each gridblock in the reservoir.

Units: psia (IUNIT=0) or kPa (IUNIT=1)

Note: See the note and example for input line 4.3.6 for the order of the initial pressure values. This is assumed to be the aqueous phase pressure.

4.3.25 SWI (This line is read only if ISWI = 0)

SWI - Initial water saturation for all gridblocks of the reservoir.

Units: fraction of pore volume

4.3.26 S(K,1), for K = 1, NZ (This line is read only if ISWI = 1)

S(K,1) - Initial water saturation for K^{th} layer.

Units: fraction of pore volume

Note: See the note for input line 4.3.5.

4.3.27 S(I,1), I = 1, NX × NY × NZ (This line is read only if ISWI = 2)

S(I,1) - Initial water saturation for I^{th} block.

Units: fraction of pore volume

Note: See the note and example for input line 4.3.6 for the order of the initial water saturation values.

4.3.28 ISGI (This line is read only if IGAS = 1)

ISGI - Flag indicating type of initial gas saturation.

Possible Values:

0 - Constant initial gas saturation for whole reservoir
1 - Constant initial gas saturation for each layer
2 - Initial gas saturation for each gridblock is specified by user

4.3.29 SGI (This line is read only if IGAS = 1 and ISGI = 0)

SGI - Initial gas saturation for all gridblocks of the reservoir.

Units: fraction of pore volume

4.3.30 S(K,4), for K = 1, NZ (This line is read only if IGAS = 1 and ISGI = 1)

S(K,4) - Initial gas saturation for K^{th} layer.

Units: fraction of pore volume

Note: See the note for input line 4.3.5.

4.3.31 S(I,4), I = 1, NX × NY × NZ (This line is read only if IGAS = 1 and ISGI = 2)

S(I,4) - Initial gas saturation for I^{th} block.

Units: fraction of pore volume

Note: See the note and example for input line 4.3.6 for the order of the initial gas saturation values.

4.3.32 C50, C60

C50 - Initial brine salinity.

Units: meq/ml of brine

Note: This is assumed to be all the anions (in equivalents).

C60 - Initial divalent cation concentration of brine.

Units: meq/ml of brine

Note : C50 and C60 are replaced by the input values of C5I and C6I in line 4.5.33 when IREACT>1.

B.4.4 Physical Property Data

The fourth input section consists of the physical property data. Please remember that there are seven comment lines at the beginning of this section and that each data line is preceded by three comment lines.

4.4.1 C2PLC, C2PRC, EPSME

C2PLC - Oil concentration at plait point in type II(+) region.

Units: volume fraction

C2PRC - Oil concentration at plait point in type II(-) region.

Units: volume fraction

EPSME - Critical micelle concentration (CMC)—minimum surfactant concentration for the formation of micelles.

Units: volume fraction

4.4.2 HBNS70, HBNC70, HBNS71, HBNC71, HBNS72, HBNC72

HBNS70 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1—Component 7—associated with surfactant at zero salinity.

Units: volume fraction

HBNC70 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 1—Component 7—associated with surfactant at zero salinity.

Units: volume fraction

HBNS71 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1—Component 7—associated with surfactant at optimal salinity.

Units: volume fraction

HBNC71 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 1—Component 7—associated with surfactant at optimal salinity.

Units: volume fraction

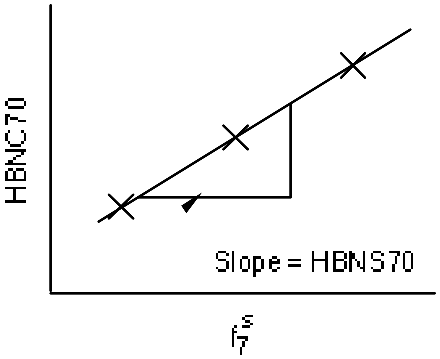
HBNS72 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1—Component 7—associated with surfactant at twice optimal salinity.

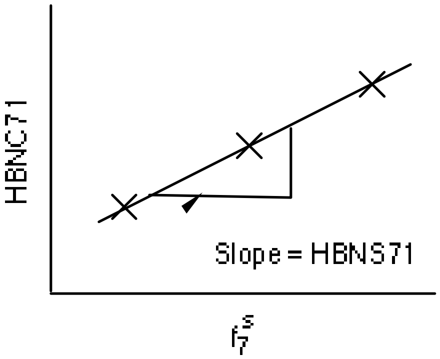
Units: volume fraction

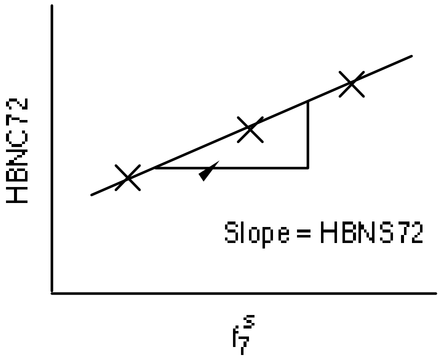
HBNC72 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 1—Component 7—associated with surfactant at twice optimal salinity.

Units: volume fraction

Note: These parameters are obtained by matching the volume fraction diagrams corresponding to at least three different total chemical (alcohol + surfactant) compositions. For the first iteration, the slope parameters are set to zero and the intercept parameters are adjusted in order to obtain a reasonable match of the volume fraction diagrams. Then the slope parameters are obtained as follows:







Having obtained the slope parameters, the matching procedure is repeated for further improvements. See Satoh's thesis for example.

4.4.3 HBNS80, HBNC80, HBNS81, HBNC81, HBNS82, HBNC82

HBNS80 - Slope for maximum height of binodal curve vs. fraction of Alcohol 2—Component 8—associated with surfactant at zero salinity.
Units: volume fraction

HBNC80 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2—Component 8—associated with surfactant at zero salinity.
Units: volume fraction

HBNS81 - Slope of maximum height of binodal curve vs. fraction of Alcohol 2—Component 8—associated with surfactant at optimal salinity.
Units: volume fraction

HBNC81 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2—Component 8—associated with surfactant at optimal salinity.
Units: volume fraction

HBNS82 - Slope for maximum height of binodal curve vs. fraction of Alcohol 2—Component 8—associated with surfactant at twice optimal salinity.
Units: volume fraction

HBNC82 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2—Component 8—associated with surfactant at twice optimal salinity.
Units: volume fraction

Note: See the note for input line 4.4.2 to see how values should be determined.

4.4.4 CSEL7, CSEU7, CSEL8, CSEU8

CSEL7 - Lower effective salinity limit for type III phase region determined when Alcohol 1—Component 7—and calcium approach zero.
Units: meq/ml

CSEU7 - Upper effective salinity limit for type III phase region determined when Alcohol 1—Component 7—and calcium approach zero.
Units: meq/ml

CSEL8 - Lower effective salinity limit for type III phase region determined when Alcohol 2—Component 8—and calcium approach zero.
Units: meq/ml

CSEU8 - Upper effective salinity limit for type III phase region determined when Alcohol 2—Component 8—and calcium approach zero.
Units: meq/ml

Note: The values are calculated as follows:

$$\mathrm{CSEU7} = \lim_{\substack{f_6^s \to 0 \\ f_7^s \to 0}} \left(C_{SEU}\right)$$

$$\mathrm{CSEL7} = \lim_{\substack{f_6^s \to 0 \\ f_7^s \to 0}} \left(C_{SEL}\right)$$

$$\mathrm{CSEU8} = \lim_{\substack{f_6^s \to 0 \\ f_8^s \to 0}} \left(C_{SEU}\right)$$

$$\mathrm{CSEL8} = \lim_{\substack{f_6^s \to 0 \\ f_8^s \to 0}} \left(C_{SEL}\right)$$

and

$$C_{SE} = \frac{C_{51}}{\left(1 - \beta_6 f_6^s\right)\left(1 + \beta_7 f_7^s + \beta_8 f_8^s\right)}$$

4.4.5 BETA6, BETA7, BETA8

BETA6 - The C_{SE} slope parameter, β_6, for calcium.
Units: dimensionless

BETA7 - The C_{SE} slope parameter, β_7, for Alcohol 1—Component 7.
Units: dimensionless

BETA8 - The C_{SE} slope parameter, β_8, for Alcohol 2—Component 8.
Units: dimensionless

Note: See notes for input line 4.4.4.
BETA6 is limited to less than $\frac{1}{f_6^s}$

4.4.6 IALC, OPSK7O, OPSK7S, OPSK8O, OPSK8S

IALC - Flag indicating choice of alcohol partition model to use.
Possible Values:
0 - Hirasaki's model will be used

1 - Prouvost's model will be used

OPSK7O - Alcohol partition coefficient (oil/water) for Alcohol 1—Component 7.
Units: dimensionless

OPSK7S - Alcohol partition coefficient (surfactant/water) for Alcohol 1—Component 7.
Units: dimensionless

OPSK8O - Alcohol partition coefficient (oil/water) for Alcohol 2—Component 8.
Units: dimensionless

OPSK8S - Alcohol partition coefficient (surfactant/water) for Alcohol 2—Component 8.
Units: dimensionless

Note: If IALC = 0 then OPSK7O, OPSK7S, OPSK8O, and OPSK8S remain fixed. If OPSK7O, OPSK7S, OPSK8O, and OPSK8S are equal to zero and IALC = 0, then alcohol is lumped with surfactant as a single component (total chemical). OPSK7O, OPSK7S, OPSK8O, and OPSK8S are only used when Hirasaki's model is chosen.

4.4.7 NALMAX, EPSALC

NALMAX - Maximum number of iterations for alcohol partitioning for two alcohol system.
Note: The suggested value is 20 and a value of zero would result in no iterations.

EPSALC - Tolerance for convergence of iterations for two alcohol system.
Note: Suggested values are 10^{-3} and 10^{-4}.

4.4.8 AKWC7, AKWS7, AKM7, AK7, PT7

AKWC7, AKWS7 - Parameters used to determine partition coefficient of monomeric Alcohol 1—Component 7—between aqueous and oleic pseudophases.
Units: dimensionless

AKM7 - Partition coefficient of monomeric Alcohol 1—Component 7—between surfactant and oleic pseudophases.
Units: dimensionless

AK7 - Self-association constant of Alcohol 1—Component 7—in oleic pseudophase.
Units: dimensionless

PT7 - Ratio of molar volume of Alcohol 1—Component 7—to equivalent molar volume of surfactant.
Units: dimensionless

Note: These values can be calculated using PROPACK and are only required when using Prouvost's model (IALC = 1).

4.4.9 AKWC8, AKWS8, AKM8, AK8, PT8

AKWC8, AKWS8 - Parameters used to determine partition coefficient of monomeric Alcohol 2—Component 8—between aqueous and oleic pseudophases.
Units: dimensionless

AKM8 - Partition coefficient of monomeric Alcohol 2—Component 8—between surfactant and oleic pseudophases.
Units: dimensionless

AK8 - Self-association constant of Alcohol 2—Component 8—in oleic pseudophase.
Units: dimensionless

PT8 - Ratio of molar volume of Alcohol 2—Component 8—to equivalent molar volume of surfactant.
Units: dimensionless

Note: These values can be calculated using PROPACK and are only required when using Prouvost's model (IALC = 1).

4.4.10 G11, G12, G13, G21, G22, G23 (This line is read only if IFT = 0)

G11, G12, G13 - Interfacial tension parameters for water-microemulsion interface.

G21, G22, G23 - Interfacial tension parameters for oil-microemulsion interface.

Units : Dimensionless

Note: The equations used to calculate the interfacial tension parameters are discussed in Camilleri, *et. al.* [1987b].

4.4.11 XIFTW

XIFTW - $\log_{10} \sigma_{wo}$ where σ_{wo} is the interfacial tension of the water-oil interface.

Units: dynes/cm = mN/m

4.4.12 IMASS

IMASS - Flag indicating the choice of oil solubility in water.

Possible Values

- 0 - No solubility of oil in water in the absence of surfactant (component number 3)
- 1 - Allow for solubility of oil in water in the absence of surfactant or allow for nonequilibrium transfer of oil in water

4.4.13 WSOL, CNEM2 (This line is read only if IMASS=1 and IGAS=0 in the presence of surfactant (component no.3))

WSOL - Equilibrium concentration of oil in water in the absence of surfactant.

Units: volume fraction

CNEM2 - Coefficient of nonequilibrium mass transfer of oil in aqueous phase with or without surfactant, M

Units: vol. of water/(bulk vol.-day)

Note: The input value of zero for CNEM2 represents an equilibrium mass transfer. The non-equilibrium mass transfer (CNEM2>0) calculation is valid for type II(-) and lobe II(-) of type III with the plait point in the corner (C2PLC = 0) and in the absence of gas phase (IGAS=0).

$$\frac{\partial\left(S_\ell C_{2\ell}\phi\right)}{\partial t} = M\left(C_{2\ell}^{eq} - C_{2\ell}\right) \text{ , for } \ell = 1 \text{ or } 3$$

$C_{2\ell}^{eq}$ is the computed composition from the hand equations when the surfactant is present and is the input value of WSOL in the absence of surfactant or when the surfactant concentration is below CMC.

4.4.14 ITRAP, T11, T22, T33

ITRAP - Flag indicating whether residual saturations and relative permeabilities are dependent on capillary number or not.

Possible Values:

- 0 - Residual saturations are not dependent on capillary number; endpoint and exponent of relative permeability curves are constant
- 1 - Residual saturations and relative permeabilities are dependent on capillary number

T11 - Capillary desaturation curve parameter, T_1, for aqueous phase.

T22 - Capillary desaturation curve parameter, T_2, for oleic phase.

T33 - Capillary desaturation curve parameter, T_3, for microemulsion phase.

Note: The expressions for capillary desaturation are:

$$S_{\ell r} - S_{\ell rc} = \frac{S_{\ell rw} - S_{\ell rc}}{1 + T_\ell N_{c\ell}}, \quad \ell=1,2,3$$

where

$$N_{c\ell} = (2.23x10^{-5}) \frac{\sqrt{\left(k_x \frac{\partial \Phi}{\partial x}\right)^2 + \left(k_y \frac{\partial \Phi}{\partial y}\right)^2 + \left(k_z \frac{\partial \Phi}{\partial z}\right)^2}}{\sigma_{\ell\ell'}}, \ell=1,2,3$$

For $\ell = 1$, $\sigma_{\ell\ell'} = \sigma_{wm}$. For $\ell = 2$, $\sigma_{\ell\ell'} = \sigma_{mo}$. For $\ell = 3$, $\sigma_{\ell\ell'} = \sigma_{wm}$ if the aqueous phase is mobile, σ_{mo} otherwise.

T11, T22, and T33 are determined by matching experimental capillary desaturation curves.

4.4.15 IPERM

IPERM - Flag indicating the saturation history direction for relative permeability and capillary pressure calculations

Possible Values:

0 - Imbibition Corey
1 - First drainage Corey (only for IOW=0 and two phase water/oil flow)

4.4.16 ISRW, IPRW, IEW

ISRW - Flag indicating type of residual saturation.

Possible Values:

0 - Constant residual saturation for entire reservoir
1 - Constant residual saturation for each layer
2 - Residual saturation for each gridblock

IPRW - Flag indicating type of endpoint relative permeability.

Possible Values:

0 - Constant endpoint relative permeability for entire reservoir
1 - Constant endpoint relative permeability for each layer
2 - Constant endpoint relative permeability for each gridblock

IEW - Flag indicating type of relative permeability exponent.

Possible Values:

0 - Constant relative permeability exponent for entire reservoir
1 - Constant relative permeability exponent for each layer
2 - Constant relative permeability exponent for each gridblock

4.4.17 S1RWC, S2RWC, S3RWC (This line is read only if ISRW = 0)

S1RWC - Residual saturation of aqueous phase displaced by oil at low capillary number for entire reservoir.

Units: fraction

S2RWC - Residual saturation of oleic phase displaced by water at low capillary number for entire reservoir.

Units: fraction

S3RWC - Residual saturation of microemulsion phase displaced by water at low capillary number for entire reservoir.
Units: fraction

4.4.18 S1RWC(K), for K = 1, NZ (This line is read only if ISRW = 1)
S1RWC(K) - Residual saturation of aqueous phase displaced by oil or gas at low capillary number for Kth layer.
Units: fraction

4.4.19 S2RWC(K), for K = 1, NZ (This line is read only if ISRW = 1)
S2RWC(K) - Residual saturation of oleic phase displaced by water at low capillary number for Kth layer.
Units: fraction

4.4.20 S3RWC(K), for K = 1, NZ (This line is read only if ISRW = 1)
S3RWC(K) - Residual saturation of microemulsion phase displaced by water or oil at low capillary number for Kth layer.
Units: fraction
Note: See the note for input line 4.4.42. Additionally, S3RWC(K) must begin a separate line in the input file for each layer.

4.4.21 S1RW(I), for I = 1, NX × NY × NZ (This line is read only if ISRW = 2)
S1RW(I) - Residual saturation of aqueous phase displaced by oil or gas at low capillary number for Ith gridblock.
Units: fraction

4.4.22 S2RW(I), for I = 1, NX × NY × NZ (This line is read only if ISRW = 2)
S2RWC(K) - Residual saturation of oleic phase displaced by water at low capillary number for Ith gridblock.
Units: fraction

4.4.23 S3RW(I), for I = 1, NX × NY × NZ (This line is read only if ISRW = 2)
S3RW(I) - Residual saturation of microemulsion phase displaced by water or oil at low capillary number for Ith gridblock.
Units: fraction

4.4.24 P1RWC, P2RWC, P3RWC (This line is read only if IPRW = 0)
P1RWC - End point relative permeability of water at low capillary number for entire reservoir.
Units: dimensionless
P2RWC - End point relative permeability of oil at low capillary number for entire reservoir.
Units: dimensionless
P3RWC - End point relative permeability of microemulsion at low capillary number for entire reservoir.
Units: dimensionless

4.4.25 P1RWC(K), for K = 1, NZ (This line is read only if IPRW = 1)

P1RWC(K) - Constant endpoint relative permeability of water at low capillary number for Kth layer.
Units: dimensionless

4.4.26 P2RWC(K), for K = 1, NZ (This line is read only if IPRW = 1)

P2RWC(K) - Constant endpoint relative permeability of oil at low capillary number for Kth layer.
Units: dimensionless

4.4.27 P3RWC(K), for K = 1, NZ (This line is read only if IPRW = 1)

P3RWC(K) - Constant endpoint relative permeability of microemulsion at low capillary number for Kth layer.
Units: dimensionless

Note: See the note for input line 4.4.42. Additionally, P1RWC(K) must begin a separate line in the input file for each layer.

4.4.28 P1RW(I), for I = 1, NX × NY × NZ (This line is read only if IPRW = 2)

P1RW(I) - Endpoint relative permeability of water at low capillary number for Ith gridblock.
Units: dimensionless

4.4.29 P2RW(I), for I = 1, NX × NY × NZ (This line is read only if IPRW = 2)

P2RWC(K) - Endpoint relative permeability of oil at low capillary number for Ith gridblock.
Units: dimensionless

4.4.30 P3RW(I), for I = 1, NX × NY × NZ (This line is read only if IPRW = 2)

P3RW(I) - Endpoint relative permeability of microemulsion at low capillary number for Ith gridblock.
Units: dimensionless

4.4.31 E1WC, E2WC, E3WC (This line is read only if IEW = 0)

E1WC - Phase relative permeability exponent for aqueous phase at low capillary number for entire reservoir.
Units: dimensionless

E2WC - Phase relative permeability exponent for oleic phase at low capillary number for entire reservoir.
Units: dimensionless

E3WC - Phase relative permeability exponent for microemulsion phase at low capillary number system for entire reservoir.
Units: dimensionless

4.4.32 E1WC(K), for K = 1, NZ (This line is read only if IEW = 1)

E1WC(K) - Relative permeability exponent of aqueous phase at low capillary number for Kth layer.
Units: dimensionless

4.4.33 E2WC(K), for K = 1, NZ (This line is read only if IEW = 1)

E2WC(K) - Relative permeability exponent of oleic phase at low capillary number for Kth layer.

Units: dimensionless

4.4.34 E3WC(K), for K = 1, NZ (This line is read only if IEW = 1)

E3WC(K) - Relative permeability exponent of microemulsion phase at low capillary number for K^{th} layer.
Units: dimensionless

Note: See the note for input line 4.4.42. Additionally, E1WC(K) must begin a separate line in the input file for each layer.

4.4.35 E1W(I), for I = 1, NX × NY × NZ (This line is read only if IEW = 2)

E1W(I) - Relative permeability exponent of aqueous phase at low capillary number for I^{th} gridblock.
Units: dimensionless

4.4.36 E2W(I), for I = 1, NX × NY × NZ (This line is read only if IEW = 2)

E2WC(K) - Relative permeability exponent of oleic phase at low capillary number for I^{th} gridblock.
Units: dimensionless

4.4.37 E3W(I), for I = 1, NX × NY × NZ (This line is read only if IEW = 2)

E3W(I) - Relative permeability exponent of microemulsion phase at low capillary number for I^{th} gridblock.
Units: dimensionless

4.4.38 S1RC, S2RC, S3RC

S1RC - Residual saturation of aqueous phase at high capillary number.
Units: fraction
S2RC - Residual saturation of oleic phase at high capillary number.
Units: fraction
S3RC - Residual saturation of microemulsion phase at high capillary number.
Units: fraction

4.4.39 P1RC, P2RC, P3RC

P1RC - End point relative permeability of aqueous phase at high capillary number condition.
Units: dimensionless
P2RC - End point relative permeability of oleic phase at high capillary number condition.
Units: dimensionless
P3RC - End point relative permeability of microemulsion phase at high capillary number condition.
Units: dimensionless

4.4.40 E13C, E23C, E31C

E13C, E23C, E31C - Parameters used for calculating exponents for relative permeability calculations at high capillary number.
Units: dimensionless

Note: For IGAS = 0, imbibition Corey relative permeabilities are calculated from:

$$k_{r\ell} = k_{r\ell}^{o} \left(S_{n\ell}\right)^{e_\ell}, \quad \ell = 1, 2, 3$$

where

$$S_{n\ell} = \frac{S_\ell - S_{\ell r}}{1 - S_{1r} - S_{2r} - S_{3r}}$$

$$k^o_{r\ell} = k^o_{r\ell w} \qquad \text{for ITRAP=0}$$

$$k^o_{r\ell} = k^o_{r\ell w} + \frac{S_{\ell' rw} - S_{\ell' r}}{S_{\ell' rw} - S_{\ell' rc}}\left(k^o_{r\ell c} - k^o_{r\ell w}\right) \qquad \text{for ITRAP =1}$$

and

$$e_\ell = e_{\ell w} \qquad \text{for ITRAP=0}$$

$$e_\ell = e_{\ell w} + \frac{S_{\ell' rw} - S_{\ell' r}}{S_{\ell' rw} - S_{\ell' rc}}\left(e_{\ell c} - e_{\ell w}\right) \qquad \text{for ITRAP=1}$$

The phase indices are assigned values according to the type of flow:

for water/oil: $\ell = 1$, $\ell' = 2$, $e_{\ell c}$ = E13C, $e_{\ell W}$ = E1W

for water/microemulsion: $\ell = 1$, $\ell' = 3$, $e_{\ell c}$ = E23C, $e_{\ell W}$ = E2W

for oil/microemulsion: $\ell = 2$, $\ell' = 3$, $e_{\ell c}$ = E31C, $e_{\ell W}$ = E3W

For two phase oil/water drainage (IPERM =1), S_{2r} is set to 0.0.

4.4.41 VIS1, VIS2, TSTAND

VIS1 - Water viscosity at reference temperature, $\mu_{1,ref}$.

Units: cp = mPa.s

VIS2 - Oil viscosity at reference temperature, $\mu_{2,ref}$.

Units: cp = mPa.s

TSTAND - Reference temperature, T_{ref}.

Units: •F (IUNIT=0) or •C (IUNIT=1)

Note: For IENG=0, If TSAND = 0.0, the water component viscosity will be constant and equal to the input value VIS1. If TSATND > 0.0, water component viscosity will be calculated as a function of reservoir temperature, pressure, and local salinity for each gridblock.

4.4.42 VIS4, VSLOPG (This line is read only if IGAS = 1)

VIS4 - Gas viscosity at reference temperature and reference pressure, $\mu_{4,ref}$.

Units: cp = mPa.s

VSLOPG - Slope of gas viscosity, $\mu_{4,s}$.

Units: $(\text{psi})^{-1}$ (IUNIT=0) or $(\text{kPa})^{-1}$ (IUNIT=1)

Note: Gas viscosity is computed from:

$$\mu_4 = \mu_{4,ref}\left(1 + \mu_{4,s}\left(P_1 - \text{PSTAND}\right)\right)$$

4.4.43 BVI(1), BVI(2) (This line is read only if IENG = 1)

BVI(1) - Parameter for calculating water viscosity as a function of reservoir temperature, b_1.

Units: $(\text{•K})^{-1}$

BVI(2) - Parameter for calculating oil viscosity as a function of reservoir temperature, b_2.

Units: $(\text{•K})^{-1}$

Note: The phase viscosities as a function of temperature are calculated from:

$$\mu_\ell = \mu_{\ell,\mathrm{ref}} \exp\left(b_\ell \left(\frac{1}{T} - \frac{1}{T_{\mathrm{ref}}} \right) \right) \qquad \text{for } \ell = 1,2$$

where T and T_{ref} are in absolute •K.

4.4.44 BVI(4) (This line is read only if IGAS =1 and IENG = 1)

BVI(4) - Parameter for calculating gas viscosity as a function of reservoir temperature, b_4.

Units: $(•K)^{-1}$

Note: Gas viscosity as a function of temperature is computed from:

$$\mu_4 = \mu_{4,\mathrm{ref}} \left(1 + \mu_{4,s} (P - \mathrm{PSTAND})\right) \exp\left(1 + b_4 \left(\frac{1}{T} - \frac{1}{T_{\mathrm{ref}}} \right) \right)$$

where T and T_{ref} are in absolute •K.

4.4.45 S2RWC4, S4RWC (This line is read only if IGAS = 1 and ISRW = 0)

S2RWC4 - Constant residual oil saturation to displacing gas phase for entire reservoir.

Units: fraction

S4RWC - Constant residual gas saturation for entire reservoir.

Units: fraction

4.4.46 S2RWC4(K), for K = 1, NZ (This line is read only if IGAS = 1 and ISRW = 1)

S2RWC4(K) - Constant residual oil saturation to displacing gas phase for K^{th} layer.

Units: fraction

4.4.47 S4RWC(K), for K = 1, NZ (This line is read only if IGAS = 1 and ISRW = 1)

S4RWC(K) - Constant residual gas saturation for K^{th} layer.

Units: fraction

4.4.48 S2RW4(I), for I = 1, NX × NY × NZ (This line is read only if IGAS = 1 and ISRW = 2)

S2RW4(I) - Constant residual oil saturation to displacing gas phase for I^{th} gridblock.

Units: fraction

4.4.49 S4RW(I), for I = 1, NX × NY × NZ (This line is read only if IGAS = 1 and ISRW = 2)

S4RW(I) - Residual gas saturation for I^{th} gridblock.

Units: fraction

4.4.50 P4RWC (This line is read only if IGAS = 1 and IPRW = 0)

P4RWC - Constant gas endpoint relative permeability for entire reservoir.

Units: dimensionless

4.4.51 P4RWC(K), for K = 1, NZ (This line is read only if IGAS = 1 and IPRW = 1)

P4RWC(K) - Constant gas endpoint relative permeability for K^{th} layer.

Units: dimensionless

4.4.52 P4RW(I), for I = 1, NX × NY × NZ (This line is read only if IGAS = 1 and IPRW = 2)

P4RW(I) - Constant gas endpoint relative permeability for I^{th} gridblock.

Units: dimensionless

4.4.53 E4WC (This line is read only if IGAS = 1 and IEW = 0)
E4WC - Constant gas relative permeability exponent for entire reservoir.
Units: dimensionless

4.4.54 E4WC(K), for K = 1, NZ (This line is read only if IGAS = 1 and IEW = 1)
E4WC(K) - Constant gas relative permeability exponent for Kth layer.
Units: dimensionless

4.4.55 E4WC(I), for I = 1, NX × NY × NZ (This line is read only if IGAS = 1 and IEW = 2)
E4WC(I) - Constant gas relative permeability exponent for Ith gridblock.
Units: dimensionless

4.4.56 S4RC, P4RC, E4C, T44, XIFTG (This line is read only if IGAS = 1)
S4RC - Residual gas saturations at high capillary number.
Units: fraction
P4RC - Gas endpoint relative permeability at high capillary number.
Units: dimensionless
E4C - Gas relative permeability exponent at high capillary number.
Units: dimensionless
T44 - Gas phase trapping parameter.
Units: dimensionless
XIFTG - Log of interfacial tension between gas and either water or oil.
Units: dyne/cm = mN/m

4.4.57 ALPHA1, ALPHA2, ALPHA3, ALPHA4, ALPHA5
ALPHA1 - Compositional phase viscosity parameter α_1.
ALPHA2 - Compositional phase viscosity parameter α_2.
ALPHA3 - Compositional phase viscosity parameter α_3.
ALPHA4 - Compositional phase viscosity parameter α_4.
ALPHA5 - Compositional phase viscosity parameter α_5.
Note: Compositional phase viscosity is calculated as:

$$\begin{aligned}\mu_\ell = \; & C_{1\ell}\, \mu_p \exp[\alpha_1 (C_{2\ell} + C_{3\ell})] + \\ & C_{2\ell}\, \mu_o \exp[\alpha_2 (C_{1\ell} + C_{3\ell})] + \\ & C_{3\ell}\, \alpha_3 \exp[\alpha_4 C_{1\ell} + \alpha_5 C_{2\ell}]\end{aligned}$$

Polymer viscosity •p is replaced by water viscosity when no polymer is present.

4.4.58 AP1, AP2, AP3
AP1, AP2, AP3 - Parameters used for calculating polymer viscosity at zero shear rate as a function of polymer and electrolyte concentrations.
Units: (wt. %)-1, (wt. %)-2, (wt. %)-3
Note: Polymer viscosity at zero shear rate, •o, is given by:

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Ap1, Ap2, and Ap3 are empirical constants for a given polymer and are measured experimentally.

4.4.59 BETAP, CSE1, SSLOPE

BETAP - Parameter, •P, for calculating the effective divalent salinity, CSEP, used to calculate polymer viscosity (see the note for input line 4.4.60).

Units: dimensionless

Note: C_{SEP} is given by:

$$C_{SEP} = \frac{C_9 + \beta_p C_6}{C_1}$$

CSE1 - Value below which the polymer viscosity is considered to be independent of salinity (minimum value of CSEP—see the note for input line 4.4.60).

Units: meq/ml

SSLOPE - Slope, Sp, of μ_o vs. C_{SEP} on a log-log plot—assumed to be constant (see the note for input line 4.4.60).

Units: dimensionless

Note: This value is usually large and negative for hydrolyzed polyacrylamides and small and positive for polysaccharides.

4.4.60 GAMMAC, GAMHF, POWN

GAMMAC - Coefficient, $\dot{\gamma}_c$, in shear rate equation below.

Units: $\frac{\text{day}(\text{darcy})^{1/2}}{\text{ft} - \text{sec}}$ (IUNIT=0) or $\frac{\text{day}(\mu\text{m}^2)^{1/2}}{\text{m} - \text{sec}}$ (IUNIT=1)

GAMHF - Shear rate, $\dot{\gamma}_{1/2}$, at which polymer viscosity is one half polymer viscosity at zero shear rate.

Units: sec^{-1}

POWN - Exponent, P_α, for calculating shear rate dependence of polymer viscosity.

Units: dimensionless

Note: The shear rate dependence of polymer viscosity is modeled by Meter's equation:

$$\mu_p = \mu_\infty + \frac{\mu_o - \mu_\infty}{1 + \left[\frac{\dot{\gamma}_{eq}}{\dot{\gamma}_{1/2}}\right]^{P_\alpha - 1}}$$

where the equivalent shear rate $\dot{\gamma}_{eq}$ is calculated as:

$$\dot{\gamma}_{eq} = \left(\frac{3n+1}{4n}\right)^{\frac{n}{n-1}} \frac{4uc}{\sqrt{8kk_{rw}\phi s_w}} = \dot{\gamma}_c \frac{u}{\sqrt{kk_{rw}\phi s_w}}$$

where u is in ft/day, k is in Darcies, and $\dot{\gamma}_{eq}$ is in 1/sec. Using n = 0.8 and with the unit conversion we have $\dot{\gamma}_c$ = 3.94 C. The value of shear rate coefficient C can be calculated as:

$$C = \left(4.8\, N_v^{0.167}\right)^{\frac{1}{1-P_\alpha}}$$

where N_v is in cm/sec. N_v is a dimensional group called viscosity number computed as:

$$N_v = \frac{\sqrt{k\,k_{rw}\,\phi s_w}}{\Theta_o u^{n-1}}$$

Please refer to Wreath [1989] and Wreath, et al. [1990] for more detail.

4.4.61 IPOLYM, EPHI3, EPHI4, BRK, CRK

IPOLYM - Flag indicating type of polymer partitioning.

Possible values:

0 - All polymer exists in aqueous phase if aqueous phase exists; otherwise, it exists completely in microemulsion phase

1 - Partitioning of polymer to water component is constant

EPHI3 - Effective porosity for surfactant—ratio of apparent porosity for surfactant to actual porosity.

Units: dimensionless

EPHI4 - Effective porosity for polymer—ratio of apparent porosity for polymer to actual porosity.

Units: dimensionless

BRK - Parameter for calculating permeability reduction factor R_k.

Units: $\frac{\text{volume of polymer} - \text{rich phase}}{\text{weight\% polymer}}$

CRK - Parameter for calculating permeability reduction factor R_k.

Units: $(\text{darcy})^{1/2}\ (100\ \text{g/g})^{-1/3} = (\mu\text{m}^2)^{1/2}\ (100\ \text{g/g})^{-1/3})$

Note: EPHI3 and EPHI4 are used to account for inaccessible pore volume in the case of surfactant and polymer.

$$\phi_{\text{surfactant}} = \phi \times \text{EPHI3}$$

$$\phi_{\text{polymer}} = \phi \times \text{EHPI4}$$

The effect of permeability reduction or residual resistance is to reduce the mobility of the polymer rich phase. This is accounted for by multiplying the viscosity of the phase by R_k.

4.4.62 DEN1, DEN2, DEN3, DEN7, DEN8, IDEN

DEN1 - Specific weight, γ_1, or density of water—Component 1.

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN2 - Specific weight, γ_2, or density of oil—Component 2.

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN3 - Specific weight, γ_3, or density of surfactant—Component 3.

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN7 - Specific weight, γ_7, or density of Alcohol 1—Component 7.

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN8 - Specific weight, γ_8, or density of Alcohol 2 (when IGAS = 0) or gas (when IGAS = 1) — Component 8.

Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

IDEN - Flag indicating if gravity effect should be considered.

Possible values:

1 - Do not consider gravity effect

2 - Consider gravity effect

Note: Specific weight for pure water is 0.433 psi/ft (density of 1 g/cm^3)

4.4.63 ISTB

ISTB - Flag indicating the units to be used when printing injection and production rates.

Possible Values:

0 - Rates printed at bottomhole condition in ft^3 or m^3
1 - Rates printed at surface condition in BBLS

4.4.64 FVF(L), for L = 1, MXP (This line is read only if ISTB = 1 and IUNIT=0)
FVF(L) - Formation volume factor for L^{th} phase.
Units: SCF/ft^3
Note: MXP = 3 when IGAS = 0 and MXP = 4 when IGAS = 1.

4.4.65 COMPC(1), COMPC(2), COMPC(3), COMPC(7), COMPC(8)
COMPC(1) - Compressibility of brine—Component 1.
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)
COMPC(2) - Compressibility of oil—Component 2.
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)
COMPC(3) - Compressibility of surfactant—Component 3.
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)
COMPC(7) - Compressibility of Alcohol 1—Component 7.
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)
COMPC(8) - Compressibility of Alcohol 2 (when IGAS = 0) or gas (when IGAS = 1) — Component 8.
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)
Note: For incompressible fluids, values of zero should be used for the COMPC values listed above.

4.4.66 ICPC, IEPC, IOW
ICPC - Flag indicating type of capillary pressure endpoint, c_{pc}.
Possible Values:
0 - Constant capillary pressure endpoint for entire reservoir
1 - Constant capillary pressure endpoint for each layer
2 - Capillary pressure endpoint for each gridblock
IEPC - Flag indicating type of capillary pressure exponent, n_{pc}.
Possible Values:
0 - Constant capillary pressure exponent for entire reservoir
1 - Constant capillary pressure exponent for each layer
2 - Capillary pressure exponent for each gridblock
IOW - Flag indicating the wettability for capillary pressure calculations.
Possible Values:
0 - The capillary pressure curve is for water-wet rock
1 - The capillary pressure curve is for oil-wet rock (zero at residual water saturations)

4.4.67 CPC0 (This line is read only if ICPC = 0)
CPC0 - Capillary pressure endpoint for entire reservoir, c_{pc}.
Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

4.4.68 CPC(K), for K = 1, NZ (This line is read only if ICPC = 1)
CPC(K) - Capillary pressure endpoint for K^{th} layer, c_{pc}.

Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

4.4.69 CPC(I), for I = 1, NX × NY × NZ (This line is read only if ICPC = 2)

CPC(I) - Capillary pressure endpoint for Ith gridblock, c_{pc}.

Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

4.4.70 EPC0 (This line is read only if IEPC = 0)

EPC0 - Capillary pressure exponent for entire reservoir, n_{pc}.

Units: dimensionless

4.4.71 EPC(K), for K = 1, NZ (This line is read only if IEPC = 1)

EPC(K) - Capillary pressure exponent for Kth layer, n_{pc}.

Units: dimensionless

4.4.72 EPC(I), for I = 1, NX × NY × NZ (This line is read only if IEPC = 2)

EPC(I) - Capillary pressure exponent for Ith gridblock, n_{pc}.

Units: dimensionless

Note: The CPC and EPC values are determined by curve fitting a plot of water-oil capillary pressure vs. normalized water saturation (see the note for input line 4.4.42). For imbibition two phases:

$$P_{C\ell\ell'} = c_{pc}\sqrt{\frac{\phi}{k_a}}\frac{\sigma_{\ell\ell'}}{\sigma_{wo}}\left(1 - S_{n\ell}\right)^{n_{pc}}$$

For three phases:

$$P_{C13} = P_{Cwm} = c_{pc}\sqrt{\frac{\phi}{k_a}}\frac{\sigma_{wm}}{\sigma_{wo}}\left(1 - S_{n1}\right)^{n_{pc}}$$

and

$$P_{C32} = P_{Cmo} = c_{pc}\sqrt{\frac{\phi}{k_a}}\frac{\sigma_{mo}}{\sigma_{wo}}\left(\frac{S_{n2}}{S_{n3} + S_{n2}}\right)^{n_{pc}}$$

For two phase oil/water drainage (IPERM =1):

$$P_{Cow} = c_{pc}\sqrt{\frac{\phi}{k_a}}\left(\frac{S_w - S_{wr}}{1 - S_{wr}}\right)^{n_{pc}}$$

The value for n_{pc} <u>must</u> be non-zero.

4.4.73 D(KC,1), for KC = 1, N

D(KC,1) - Molecular diffusion coefficient of KCth component in aqueous phase.

Units: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

4.4.74 D(KC,2), for KC = 1, N

D(KC,2) - Molecular diffusion coefficient of KCth component in oleic phase.

Units: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

4.4.75 D(KC,3), for KC = 1, N

D(KC,3) - Molecular diffusion coefficient of KCth component in microemulsion phase.

Units: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

4.4.76 D(KC,4), for KC = 1, N (This line is read only if IGAS = 1)

D(KC,4) - Molecular diffusion coefficient of KCth component in gas phase.

Units: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

4.4.77 ALPHAL(1), ALPHAT(1)

ALPHAL(1) - Longitudinal dispersivity of aqueous phase.

Units: feet (IUNIT=0) or m (IUNIT=1)

ALPHAT(1) - Transverse dispersivity of aqueous phase.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.4.78 ALPHAL(2), ALPHAT(2)

ALPHAL(2) - Longitudinal dispersivity of oleic phase.

Units: feet (IUNIT=0) or m (IUNIT=1)

ALPHAT(2) - Transverse dispersivity of oleic phase.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.4.79 ALPHAL(3), ALPHAT(3)

ALPHAL(3) - Longitudinal dispersivity of microemulsion phase.

Units: feet (IUNIT=0) or m (IUNIT=1)

ALPHAT(3) - Transverse dispersivity of microemulsion phase.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.4.80 ALPHAL(4), ALPHAT(4) (This line is read only if IGAS = 1)

ALPHAL(4) - Longitudinal dispersivity of gas phase.

Units: feet (IUNIT=0) or m (IUNIT=1)

ALPHAT(4) - Transverse dispersivity of gas phase.

Units: feet (IUNIT=0) or m (IUNIT=1)

4.4.81 AD31, AD32, B3D, AD41, AD42, B4D

AD31 - Surfactant adsorption parameter, a_{31}.

Units: $\frac{\text{volume of phase } \ell}{\text{pore volume}}$

AD32 - Surfactant adsorption parameter, a_{32}.

Units: ml/meq

B3D - Surfactant adsorption parameter, b_3.

Units: $\frac{1}{\text{volume of surfactant in phase } \ell}$

AD41 - Polymer adsorption parameter, a_{41}.

Units: dimensionless

AD42 - Polymer adsorption parameter, a_{42}.

Units: ml/meq

B4D - Polymer adsorption parameter, b_4.

Units: $\frac{\text{volume of water}}{\text{weight\% polymer}}$

Note: Langmuir-type isotherms are used to model surfactant and polymer adsorption. Surfactant adsorption is irreversible with respect to surfactant concentration:

$$\overline{C}_3 = \frac{a_3 C_{3\ell}}{1 + b_3 C_{3\ell}}$$

Units: $\frac{\text{volume of adsorbed surfactant}}{\text{pore volume}}$

$a_3 = a_{31} + a_{32} C_{SE}$

When $a_{32} = 0$, there will be no salinity dependence.

A Langmuir-type isotherm is used to describe the adsorption level of polymer, component 4, as a function of the concentration of polymer in the water as:

$$\overline{C}_4 = \frac{a_4 C_4^*}{1 + b_4 C_4^*}$$

Units: $\frac{\text{weight\% adsorbed polymer}}{\text{volume of water}}$

where $C_4^* = \frac{\tilde{C}_4 - \overline{C}_4}{C_1}$ and $a_4 = a_{41} + a_{42} C_{SEP}$

4.4.82 QV, XKC, XKS, EQW

QV - Cation exchange capacity of clays.

Units: meq/ml of pore volume

XKC - Cation exchange constant, β^C, for clays.

Units: $(\text{meq/ml})^{-1}$

XKS - Cation exchange constant, β^S, for surfactant.

Units: $(\text{meq/ml})^{-1}$

EQW - Equivalent weight of surfactant.

Note: The cation exchange model is:

$$\frac{\left(\overline{C}_9\right)^2}{\overline{C}_6} = \beta^C Q_v \frac{\left(C_9^o\right)^2}{C_6^o} \quad \text{for clay}$$

$$\frac{\left(C_9^s\right)^2}{C_6^s} = \beta^C C_3 \frac{\left(C_9^o\right)^2}{C_6^o} \quad \text{for micelles}$$

EQW must be non-zero.

4.4.83 TK(I), for I = 1, NTW+NTA (This line is read only if NTW+NTA > 0)

TK(I) - Tracer partitioning coefficient, $K_{\kappa,ref}$, for Ith water/oil tracer at initial chloride (C_{50}) concentration and reference temperature (TSTAND). A value of 0.0 indicates a water or gas tracer and a value of -1.0 indicates an oil tracer.

Units: fraction

Note: $K_{\kappa,ref} = \frac{C_{\kappa o}}{C_{\kappa w}}$ for oil/water tracer

$K_{\kappa,\mathrm{ref}} = \frac{C_{\kappa o}}{C_{\kappa g}}$ for oil/gas tracer

4.4.84 TKS(I), for I = 1, NTW (This line is read only if NTW > 0)

TKS(I) - Parameter for calculating water/oil tracer partitioning coefficient, K_κ, for Ith tracer as a function of salinity, TKS_k.

Units: $(\mathrm{meq/ml})^{-1}$

Note: $K_\kappa = K_{\kappa,\mathrm{ref}}\left(1 + TKS_\kappa(C_{51} - C_{50})\right)$

4.4.85 TKT(I), for I = 1, NTW+NTA (This line is read only if NTW+NTA > 0 and IENG = 1)

TKT(I) - Parameter for calculating tracer partitioning coefficient, K_κ, for Ith tracer as a function of reservoir temperature, TKT_k.

Units: $(\bullet F)^{-1}$ (IUNIT=0) or $(\bullet C)^{-1}$ (IUNIT=1)

Note: $K_\kappa = K_{\kappa,\mathrm{ref}}\left(1 + TKT_\kappa(T - T_{\mathrm{ref}})\right)$

4.4.86 RDC(I), for I = 1, NTW+NTA (This line is read only if NTW+NTA > 0)

RDC(I) - Radioactive decay coefficient, λ_κ, for Ith tracer. A value of 0.0 indicates a non–radioactive tracer.

Units: 1/days

Note: $C = C_0\, e^{-\lambda_\kappa (t - t_0)}$

where

$$\lambda_k = -\frac{\ln(0.5)}{t_{1/2,k}}$$

$t_{1/2,k}$ = half life of radioactive tracer, day

4.4.87 RET(I), for I = 1, NTW+NTA (This line is read only if NTW+NTA > 0)

RET(I) - Tracer retardation factor D_S—adsorbed concentration/flowing concentration. A value of 0.0 indicates no retardation.

Units: dimensionless

Note: The retardation factor is defined as:

$$D_S = \frac{\overline{C}}{C} = \frac{(1-\phi)\rho_r a_T}{\phi \rho_\ell C_{T\ell}}$$

where $\ell = 1$ for oil/water tracer and $\ell = 4$ for gas/water tracer.

This factor causes a reduction in tracer velocity:

$$V_t = \frac{u/\phi}{1 + D_S}$$

4.4.88 FFL(1), FFH(1), CM(I,1), for I = 1, NTW (This line is read only if NTW > 0 and ICAP = 1)

FFL(1) - Value of flowing fraction for phase 1 when fractional flow = 0.0.

Units: dimensionless

FFH(1) - Value of flowing fraction for phase 1 when fractional flow = 1.0.

Units: dimensionless

CM(I,1) - Mass transfer coefficients for Ith tracer in phase 1.

Units: 1/sec

4.4.89 FFL(2), FFH(2), CM(I,2), for I = 1, NTW (This line is read only if NTW > 0 and ICAP = 1)

FFL(2) - Value of flowing fraction for phase 2 when fractional flow = 0.0.

Units: dimensionless

FFH(2) - Value of flowing fraction for phase 2 when fractional flow = 1.0.

Units: dimensionless

CM(I,2) - Mass transfer coefficients for I^{th} tracer in phase 2.

Units: 1/sec

4.4.90 FFL(3), FFH(3), CM(I,3), for I = 1, NTW (This line is read only if NTW > 0 and ICAP = 1)

FFL(3) - Value of flowing fraction for phase 3 when fractional flow = 0.0.

Units: dimensionless

FFH(3) - Value of flowing fraction for phase 3 when fractional flow = 1.0.

Units: dimensionless

CM(I,3) - Mass transfer coefficients for I^{th} tracer in phase 3.

Units: 1/sec

4.4.91 TAK1 (This line is read only if NTW > 0 and ITREAC = 1)

TAK1 - Rate constant for a first-order aqueous phase reaction at reference temperature (T_{ref}) in which Tracer 2 (component 10) hydrolyzes to form Tracer 3 (component 11) according to $C_{11,1}$ = TAK1 $C_{10,1}$.

Units: $days^{-1}$

4.4.92 TMW(I), for I = 1, NTW (This line is read only if NTW > 0 and ITREAC = 1)

TMW(I) - Molecular weight of the I^{th} tracer.

Units: The user can specify the molecular weight in any unit as long as the units are the same for all the tracers. It is assumed that the reaction of 1 mole of primary tracer produces 1 mole of secondary tracer. If not, use "equivalent" molecular weights.

4.4.93 TDEN(I), for I = 1, NTW (This line is read only if NTW > 0 and ITREAC = 1)

TDEN(I) - Density of the I^{th} tracer.

Units: g/cm^3

4.4.94 TAKT (This line is read only if NTW > 0 and ITREAC = 1 and IENG = 1)

TAKT - Parameter for calculating rate constant for a first-order aqueous phase reaction as a function of reservoir temperature.

Units: $(\bullet K)^{-1}$

Note: $\mathrm{TAK} = \mathrm{TAK1}\ \exp\left(\mathrm{TAKT}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right)$

4.4.95 AK1, AK2, SCR, X4, X14, X16, WM4 (This line is read only if NG>0)

AK1 - Kinetic rate coefficient for Cr^{3+} at reference temperature (T_{ref}), $AK1_{ref}$.

Units: ppm^{-1} $days^{-1}$

AK2 - Kinetic rate coefficient for gel at reference temperature (T_{ref}), $AK2_{ref}$.

Units: (mole/liter)$^{1\text{-X4-X14+X16}}$ days^{-1}

Note: In order to achieve the same results achieved in versions previous to UTCHEM-V-5.0, please use the following conversion:

$$\mathrm{AK2}_{\mathrm{new}} = \frac{\mathrm{SCR} \times \mathrm{M}_{\mathrm{Cr}^{3+}} \times \mathrm{M}^{2}_{\mathrm{polymer}} \times 10^{9}}{(1 + \mathrm{SCR})} \mathrm{AK2}_{\mathrm{old}}$$

SCR - Stoichiometric ratio in mass between Cr^{3+} and polymer.

Units: dimensionless

Note: $\mathrm{SCR} = \dfrac{\mathrm{n} \times \mathrm{M}_{\mathrm{Cr}^{3+}}}{\mathrm{M}_{\mathrm{polymer}}}$

X4 - Exponent to be used for polymer component of gelation reaction.

Units: dimensionless

X14 - Exponent to be used for chromium component of gelation reaction.

Units: dimensionless

X16 - Exponent to be used for hydrogen ion component of gelation reaction.

Units: dimensionless

WM4 - Molecular weight of polymer.

Units: g/mole

4.4.96 AK1T, AK2T (This line is read only if NG>0 and IENG = 1)

AK1T - Parameter for calculating Kinetic rate coefficient for Cr^{3+} as a function of reservoir temperature.

Units: (•K)$^{-1}$

AK2T - Parameter for calculating Kinetic rate coefficient for gel as a function of reservoir temperature.

Units: (•K)$^{-1}$

Note: The kinetic rate coefficients as a function of temperature are computed from:

$$\mathrm{AK1} = \mathrm{AK1}_{\mathrm{ref}} \exp\left(\mathrm{AK1T}\left(\frac{1}{\mathrm{T}} \quad \frac{1}{\mathrm{T}_{\mathrm{ref}}} \right)\right)$$

$$\mathrm{AK2} = \mathrm{AK2}_{\mathrm{ref}} \exp\left(\mathrm{AK2T}\left(\frac{1}{\mathrm{T}} - \frac{1}{\mathrm{T}_{\mathrm{ref}}} \right)\right)$$

4.4.97 AG1, AG2, CRG, AGK, BGK (This line is read only if NG>0)

AG1 - Flory-Huggins parameter for gel viscosity, A_{g1}.

Units: cp ppm^{-1} = mPa.s ppm^{-1}

AG2 - Flory-Huggins parameter for gel viscosity, A_{g2}.

Units: cp ppm^{-2} = mPa.s ppm^{-2}

CRG - Constant, C_{δ}, in the dimensionless pore radius reduction group. This constant depends on the gel type.

Units: $\sqrt{\mathrm{darcy}}\,(\mathrm{wt\%})^{1/3} = \sqrt{\mu\mathrm{m}^{2}}\,(\mathrm{wt\%})^{1/3}$

AGK, BGK - Permeability reduction parameters, A_{15} and B_{15}, for Langmuir correlation with gel concentration.

Units: dimensionless

Note: Dimensionless pore radius reduction group:

$$N_\delta = C\delta \frac{[\mu]^{1/3}}{\left[\sqrt{k_x k_y}/\phi\right]^{1/2}}$$

$$C_\delta = 3.9 \times 10^{-3} N_g M_{\text{polymer}}^{1/3}$$

$$[\mu] = \lim_{\substack{C_{4\ell} \to 0 \\ \dot{\gamma} \to 0}} \left(\frac{\mu_p - \mu_w}{\mu_w C_{4\ell}} \right)$$

From this the permeability reduction factor for idealized case is expressed as:

$$RRF_{\max} = \frac{k_w\text{, before gel treatment}}{k_w\text{, after gel treatment}} = \left(1 - N_\delta\right)^{-4}$$

The "Langmuir-type" isotherm for permeability reduction as a function of gel concentration is:

$$RRF = 1 + \frac{\left(RRF_{\max} - 1\right) A_{15}\, C_{15,1}}{1 + B_{15}\, C_{15,1}}$$

Note: Gel viscosity is calculated from

$$\mu_{gel} = \mu_w \left[1 + A_{g1} C_{15,1} + A_{g2} C_{15,1}^2\right]$$

if there is flowing polymer concentration, add μ_{gel} to the μ_p calculation. See note for input line 4.4.62.

4.4.98 A15D, B15D, ICREX, A14D, B14D, CRNAK, HNAK, C160 (This line is read only if NG>0)

A15D, B15D - Gel adsorption parameters.

Units: vol. of water / ppm gel

ICREX - Flag indicating if Cr^{3+} will be allowed to exchange with clays.

Possible Values:

0 - Cr^{3+} exchange with clays is not allowed

1 - Cr^{3+} exchange with clays is allowed

A14D, B14D - Chromium adsorption parameters.

Units: vol. of water / ppm chromium

CRNAK - Chromium-sodium exchange reaction equilibrium constant.

HNAK - Hydrogen-sodium exchange reaction equilibrium constant.

C160 - Initial hydrogen ion concentration.

Units: meq/ml

Note: The "Langmuir-type" isotherm for chromium and gel adsorption is expressed as:

$$\overline{C}_\kappa = \frac{a_\kappa\, C_{\kappa,1}}{1 + b_\kappa\, C_{\kappa,1}}, \quad \kappa = \begin{cases} 14 \text{ for chromium} \\ 15 \text{ for gel} \end{cases}$$

The input values of CRNAK, HNAK, and C160 are ignored for IREACT=6

4.4.99 IP1, IP2 (This line is read only if NG>0, NY = 1 and NZ = 1)

IP1, IP2 - Gridblock locations where calculated pressure values should be printed to UNIT 19.

Note: These values are intended to be used for comparison with pressure tab data of 1-D experiments.

4.4.100 TEMPI (This line is read only if IENG = 1)
TEMPI- Constant initial reservoir temperature.
Units : •F (IUNIT=0) or •C (IUNIT=1)

4.4.101 DENS, CRTC, CVSPR, CVSPL(L), L=1,MXP (This line is read only if IENG = 1)
DENS - Reservoir rock density.
Units: lb/ft^3 (IUNIT=0) or g/cm^3 (IUNIT=1)
CRTC - Reservoir thermal conductivity.
Units: Btu (day-ft-•F)$^{-1}$ (IUNIT=0) or kJ (day-m-•K)$^{-1}$ (IUNIT=1)
CVSPR - Reservoir rock heat capacity.
Units: Btu (lb-•F)$^{-1}$ (IUNIT=0) or kJ (kg-•K)$^{-1}$ (IUNIT=1)
CVSPL(L) - Phase L heat capacity (MXP is equal to 3 (IGAS=0) or 4 (IGAS=1)).
Units: Btu (lb-•F)$^{-1}$ (IUNIT=0) or kJ (kg-•K)$^{-1}$ (IUNIT=1)

4.4.102 IHLOS, IANAL (This line is read only if IENG = 1)
IHLOS - Flag indicating if the heatloss calculation to overburden and underburden rock is considered or not. Heat flux into the reservoir from the overburden/underburden is calculated from the model of Vinsome and Westerveld [1980].
Possible Values:
0 - Heatloss is not considered
1 - Heatloss is considered
IANAL - Flag indicating if the temperature profile is calculated from analytical solution (only 1-D).
Possible Values:
0 - Analytical solution is not considered
1 - Analytical solution is considered

4.4.103 TCONO, DENO, CVSPO, TCONU, DENU, CVSPU (This line is read only if IENG = 1 and IHLOS = 1)
TCONO - Thermal conductivity of overburden rock.
Units: Btu (day-ft-•F)$^{-1}$ (IUNIT=0) or kJ (day-m-•K)$^{-1}$ (IUNIT=1)
DENO - Density of overburden rock.
Units: lb/ft^3 (IUNIT=0) or g/cm^3 (IUNIT=1)
CVSPO - Heat capacity of overburden rock.
Units: Btu (lb-•F)$^{-1}$ (IUNIT=0) or kJ (kg-•K)$^{-1}$ (IUNIT=1)
TCONU - Thermal conductivity of underburden rock.
Units: Btu (day-ft-•F)$^{-1}$ (IUNIT=0) or kJ (day-m-•K)$^{-1}$ (IUNIT=1)
DENU - Density of underburden rock.
Units: lb/ft^3 (IUNIT=0) or g/cm^3 (IUNIT=1)
CVSPU - Heat capacity of underburden rock.
Units: Btu (lb-•F)$^{-1}$ (IUNIT=0) or kJ (kg-•K)$^{-1}$ (IUNIT=1)

B.4.5 Physical Property Data for Geochemical Options

The fifth input section consists of physical property data that is read only if IREACT > 1. The data for this section is generated by a preprocessor program (EQBATCH) and does not have the same format as the rest of the input data for UTCHEM. This input section is not preceded by the usual seven comment lines and individual data lines are not preceded by three comment lines. Sections 6.6 through 6.9 of this appendix give a list of elements, fluid species, solid species, and adsorbed species for geochemical options.

4.5.1 IRSPS, IPHAD (This line is read only if IREACT > 1)

IRSPS - Flag indicating if the reactive species concentrations should be printed.

Possible Values:

0 - Reactive species concentrations will not be printed

1 - Independent aqueous reactive species, solid species, and sorbed species concentrations will be printed

2 - All aqueous species, solid species, and sorbed species concentrations will be printed

IPHAD - Flag indicating whether surfactant adsorption is pH dependent or not.

Possible Values:

0 - Surfactant adsorption is not pH dependent

1 - Surfactant adsorption is pH dependent

4.5.2 PHC, PHT, PHT1, HPHAD (This line is read only if IREACT > 1 and IPHAD > 0)

PHC - Critical pH above which surfactant adsorption is pH dependent.

PHT - Extrapolated pH value at zero surfactant adsorption.

PHT1 - pH value above which surfactant adsorption is constant.

HPHAD - Fraction of the low-pH adsorption plateau retained at a pH above PHT1.

4.5.3 CSELP, CSEUP (This line is read only if IREACT = 3 or 5)

CSELP - Lower optimum salinity limit for generated surfactant.

Units: meq/ml

CSEUP - Upper optimum salinity limit for generated surfactant.

Units: meq/ml

4.5.4 NELET, NFLD, NSLD, NSORB, NACAT, ICHRGE (This line is read only if IREACT > 1)

NELET - Total number of elements less non reacting element.

Maximum Value: 9

NFLD - Total number of fluid species.

NSLD - Total number of solid species.

NSORB - Total number of sorbed species.

NACAT - Total number of surfactant associated cations.

ICHRGE - Flag indicating whether an oxygen balance or a charge balance will be used.

Possible Values:

0 - Oxygen balance used

1 - Charge balance in solution used

Note: If solid SiO_2 is considered, the oxygen balance must be used.

4.5.5 NIAQ, NEX, NSLEL, NSURF1 (This line is read only if IREACT > 1)

NIAQ - Total number of independent fluid species.

NEX - Total number of insoluble exchangers.

NSLEL - Total number of elements comprising the solid species.

NSURF1 - Position number corresponding to the in situ generated surfactant anion in the fluid species array FLDSPS.

Note: NSURF1 is automatically set to 0 by the program if IREACT = 2 or 4.

4.5.6 NH, NNA, NCA, NMG, NCARB (This line is read only if IREACT > 1)

NH - Position number corresponding to the hydrogen element in the element array ELEMNT.

NNA - Position number corresponding to the sodium element in the element array ELEMNT.

NCA - Position number corresponding to the calcium element in the element array ELEMNT.

NMG - Position number corresponding to the magnesium element in the element array ELEMNT.

Note: If magnesium is not considered, NMG must be set equal to 0.

NCARB - Position number corresponding to the carbonate pseudo-element in the element array ELEMNT.

4.5.7 NALU, NSILI, NOXY (This line is read only if IREACT > 3)

NALU - Position number corresponding to the aluminum element in the element array ELEMNT.

NSILI - Position number corresponding to the silicon element in the element array ELEMNT.

NOXY - Position number corresponding to the oxygen element in the element array ELEMNT.

4.5.8 NACD (This line is read only if IREACT = 3 or 5)

NACD - Position number corresponding to the petroleum acid pseudo-element in the element array ELEMNT.

4.5.9 ELEMNT(I), for I = 1, NELET (This line is read only if IREACT > 1)

ELEMNT(I) - Name of the Ith element.

Note: The name of each element may not exceed 32 characters and each name must be on a separate line of the input file.

4.5.10 FLDSPS(I), for I = 1, NFLD (This line is read only if IREACT > 1)

FLDSPS(I) - Name of the Ith fluid species.

Note: The name of each fluid species may not exceed 32 characters and each name must be on a separate line of the input file. If IREACT = 3 or 5, the last fluid species must be HA_w (petroleum acid in water).

4.5.11 SLDSPS(I), for I = 1, NSLD (This line is read only if IREACT > 1 and NSLD > 0)

SLDSPS(I) - Name of the Ith solid species.

Note: The name of each solid may not exceed 32 characters and each name must be on a separate line of the input file.

4.5.12 SORBSP(I), for I = 1, NSORB (This line is read only if IREACT > 1 and NSORB > 0)

SORBSP(I) - Name of the Ith adsorbed cation.

Note: The name of each adsorbed cation may not exceed 32 characters and each name must be on a separate line of the input file.

4.5.13 ACATSP(I), for I = 1, NACAT (This line is read only if IREACT > 1 and NACAT > 0)

ACATSP(I) - Name of the Ith surfactant adsorbed cation.

Note: The name of each surfactant adsorbed cation may not exceed 32 characters and each name must be on a separate line of the input file.

4.5.14 NSORBX(I), for I = 1, NEX (This line is read only if IREACT > 1 and NSORB > 0)

NSORBX(I) - Number of cations for I^{th} exchanger.

4.5.15 AR(I,J), for J = 1, NFLD, for I = 1, NELET << or >>

AR(I,J), for J = 1, NFLD, for I = 1, NELET-1 (This line is read only if IREACT > 1)

AR(I,J) - Stoichiometric coefficient of I^{th} element in J^{th} fluid species.

Note: If ICHRGE = 0, then NFLD × NELET values are required by the program. If ICHRGE = 1, then NFLD × (NELET-1) values are required by the program.

4.5.16 BR(I,J), for J = 1, NSLD, for I = 1, NELET << or >>

BR(I,J), for J = 1, NSLD, for I = 1, NELET-1 (This line is read only if IREACT > 1 and NSLD > 0)

BR(I,J) - Stoichiometric coefficient of I^{th} element in J^{th} solid species.

Note: If ICHRGE = 0, then NSLD × NELET values are required by the program. If ICHRGE = 1, then NSLD × (NELET-1) values are required by the program.

4.5.17 DR(I,J), for J = 1, NSORB, for I = 1, NELET << or >>

DR(I,J), for J = 1, NSORB, for I = 1, NELET-1 (This line is read only if IREACT > 1 and NSORB > 1)

DR(I,J) - Stoichiometric coefficient of I^{th} element in J^{th} sorbed species.

Note: If ICHRGE = 0, then NSORB × NELET values are required by the program. If ICHRGE = 1, then NSORB × (NELET-1) values are required by the program.

4.5.18 ER(I,J), for J = 1, NACAT, for I = 1, NELET << or >>

ER(I,J), for J = 1, NACAT, for I = 1, NELET-1 (This line is read only if IREACT > 1 and NACAT > 1)

ER(I,J) - Stoichiometric coefficient of I^{th} element in J^{th} surfactant associated cation.

Note: If ICHRGE = 0, then NACAT × NELET values are required by the program. If ICHRGE = 1, then NACAT × (NELET-1) values are required by the program.

4.5.19 BB(I,J), for J = 1, NIAQ+NSORB+NACAT, for I = 1, NFLD+NSORB+NACAT (This line is read only if IREACT > 1)

BB(I,J) - Exponent of the J^{th} independent fluid species concentration when the I^{th} fluid species is expressed in terms of independent species concentrations.

4.5.20 EXSLD(I,J), for J = 1, NIAQ, for I = 1, NSLD (This line is read only if IREACT > 1 and NSLD • 1)

EXSLD(I,J) - Exponent of the Jth independent fluid species concentration in the solubility product definition of the Ith solid.

4.5.21 CHARGE(I), for I = 1, NFLD (This line is read only if IREACT > 1)

CHARGE(I) - Charge of the Ith fluid species.

4.5.22 SCHARG(I,J), for J = 1, NSORBX(I), for I = 1, NEX (This line is read only if IREACT > 1 and NSORB • 1)
SCHARG(I,J) - Charge of the Jth sorbed species on the Ith exchanger.

4.5.23 EQK(I), for I = 1, NFLD (This line is read only if IREACT > 1)
EQK(I) - Equilibrium constant for Ith fluid species when expressed in independent species concentrations only.

4.5.24 EXK(I,J), for J = 1, NSORBX(I)-1, for I = 1, NEX (This line is read only if IREACT > 1 and NEX > 0)
EXK(I,J) - Exchange equilibrium constant for Jth exchange equilibrium of the Ith insoluble exchanger.

4.5.25 EXEX(I,J,K), for K = 1, NIAQ+NSORB+NACAT, for J = 1, NSORBX(I)-1, for I = 1, NEX (This line is read only if IREACT > 1 and NEX > 0)
EXEX(I,J,K) - Exponent of Kth independent species in Jth equilibrium relation of the Ith exchanger.

4.5.26 REDUC(I,J), for J = 1, NSORBX(I)-1, for I = 1, NEX (This line is read only if IREACT > 1 and NEX > 0)
REDUC(I,J) - Valence difference of the two cations involved in the exchange reaction J on exchanger I.
Note: This value is positive if the higher valence cation bulk concentration has a positive exponent in EXEX(I,J) definition and is negative otherwise.

4.5.27 EXCAI(I), for I = 1, NEX (This line is read only if IREACT > 1 and NEX >0)
EXCAI(I) - Exchange capacity of Ith insoluble exchanger.
Units: meq/ml pore volume

4.5.28 SPK(I), for I = 1, NSLD (This line is read only if IREACT > 1 and NSLD • 1)
SPK(I) - Solubility product of Ith solid defined in terms of independent fluid species concentrations only.

4.5.29 CHACAT(I), for I = 1, NACAT (This line is read only if IREACT > 1 and NACAT • 1)
CHACAT(I) - Charge of Ith surfactant associated cation.

4.5.30 ACATK(I), for I = 1, NACAT-1 (This line is read only if IREACT > 1 and NACAT • 1)
ACATK(I) - Equilibrium constant for Ith exchange equilibrium for cation exchanges on surfactant.

4.5.31 EXACAT(I,J) for J = 1, NIAQ+NSORB+NACAT, for I = 1, NACAT-1 (This line is read only if IREACT > 1 and NACAT • 1)
EXACAT(I,J) - Exponent of Jth independent species in Ith equilibrium for cation exchange on surfactant.

4.5.32 CI(J), for J = 1, NACAT (This line is read only if IREACT > 1 and NACAT • 1)
CI(J) - Initial concentration of Jth surfactant associated cation.
Units: moles/liter pore volume

4.5.33 C5I, C6I (This line is read only if IREACT > 1)
C5I - Initial concentration of non reacting anions.
Units: equivalents/liter
C6I - Initial concentration of calcium in aqueous phase.
Units: equivalents/liter

4.5.34 CELAQI(J), for J = 1, N-NO6 (This line is read only if IREACT > 1)
CELAQI(J) - Initial concentrations of (J+11)th component.
Units: equivalents/liter
Note : NO6 = 11 for 1< IREACT<6
NO6 = 15 for IREACT = 6

4.5.35 CAC2I (This line is read only if IREACT = 3 or 5)
CAC2I - Initial concentration of acid in oil.
Units: moles/liter oil

4.5.36 CAQI(J), for J = 1, NIAQ (This line is read only if IREACT > 1)
CAQI(J) - Initial guesses for Jth independent species concentration.
Units: moles/liter water

4.5.37 CSLDI(I), for I = 1, NSLD (This line is read only if IREACT > 1 and NSLD • 1)
CSLDI(I) - Initial concentration of Ith solid.
Units: moles/liter pore volume

4.5.38 CSORBI(I), for I = 1, NSORB (This line is read only if IREACT > 1 and NSORB • 1)
CSORBI(I) - Initial concentration of Ith adsorbed cation.
Units: moles/liter pore volume

4.5.39 C1I, C2I (This line is read only if IREACT = 3 or 5)
C1I - Initial concentration of water in aqueous phase.
Units: volume fraction
C2I - Initial concentration of oil in oleic phase.
Units: volume fraction

4.5.40 ACIDIS, EQWPS (This line is read only if IREACT = 3 or 5)
ACIDIS - Dissociation constant of the petroleum acid, Ka.
EQWPS - Equivalent weight of petroleum acid.

B.4.6 Recurrent Injection/Production Data Set

The sixth input section consists of the recurrent injection/production well data. Please remember that there are seven comment lines at the beginning of this section and that each line is preceded by three comment lines.

4.6.1 IBOUND
IBOUND - The flag to specify if constant potential boundaries at the left and right sides of the simulation model are specified.

Possible Values:
- 0 : No boundary is specified
- 1 : Boundary is specified

4.6.2 IBL, IBR (This line is read only if IBOUND = 1)

IBL - The flag to specify if the left-hand side constant potential boundary is specified.

Possible Values:
- 0 : No boundary is specified
- 1 : Boundary is specified

IBR - The flag to specify if the right-hand side constant potential boundary is specified.

Possible Values:
- 0 : No boundary is specified
- 1 : Boundary is specified

4.6.3 PBL, C1BL, C5BL, C6BL (This line is read only if IBOUND = 1 and IBL = 1)

PBL- Pressure at the center of the top layer at the left boundary.
Units : psia (IUNIT=0) or kPa (IUNIT=1)

C1BL- Concentration of water in aqueous phase at the left boundary.
Units : volume fraction

C5BL - Concentration of chloride in aqueous phase at the left boundary.
Units : meq/ml

C6BL - Concentration of calcium in aqueous phase at the left boundary.
Units : meq/ml

4.6.4 PBR, C1BR, C5BR, C6BR (This line is read only if IBOUND = 1 and IBR = 1)

PBR - Pressure at the center of the top layer at the right boundary.
Units : psia (IUNIT=0) or kPa (IUNIT=1)

C1BR - Concentration of water in aqueous phase at the right boundary.
Units : volume fraction

C5BR - Concentration of chloride in aqueous phase at the right boundary.
Units : meq/ml

C6BR - Concentration of calcium in aqueous phase at the right boundary.
Units : meq/ml

4.6.5 NWELL, IRO, ITIME

NWELL - Maximum number of wells used for the simulation.

Note: If ICOORD = 2, NWELL must be equal to 1 and the MXW parameter in the source code must be set equal to 2.

IRO - Flag indicating the equivalent well radius model to be used.

Possible Values:
- 1 - Babu and Odeh model is used
  - Note: This model (IRO=1) does not work for ICOORD = 4.
- 2 - Peaceman model is used (this was the default in versions previous to UTCHEM-V-5.0)

Note: For information see Babu and Odeh [1989].

ITIME - Flag indicating the units to be used when specifying the minimum and maximum time step.

Possible Values:

0 - Minimum and maximum time steps are input in days

1 - Minimum and maximum time steps are input as Courant numbers

Note: This option is only used if IMES > 1 and is not a shut-in period. If IMES = 1, this flag is ignored. For a shut-in period you need to use ITIME = 0

Note: The Courant number is defined as:

• EMBED "Equation" "Word Object1" * mergeformat •••

The following values for minimum and maximum Courant numbers are recommended for different simulations as follows:

Process	Min. Courant #	Max. Courant #
Waterflood/tracer	0.04	0.4
Polymerflood	0.02	0.2
Surfactant/polymerflood	0.01	0.1
Geochemical process	0.01	0.1

4.6.6 The data on input lines 4.6.6.a through 4.6.6.d are repeated for M = 1 to NWELL times.

4.6.6.a IDW(M), IW(M), JW(M), IFLAG(M), RW(M), SWELL(M), IDIR(M), IFIRST(M), ILAST(M), IPRF(M)

IDW(M) - Well I.D. number for the Mth well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: This number is used by UTCHEM to keep track of which well is being described in the recurrent injection/production well section. The history profile data for the well indicated by IDW(M) will be written to FORTRAN UNIT number 18 + IDW(M).

IW(M) - First index of the reservoir gridblock containing the Mth well.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

Note: If the Mth well is completed parallel to the X-axis, IW(M) is the Y direction index—if the well is completed parallel to the Y- or Z-axis, IW(M) is the X direction index. See example below.
If ICOORD = 2, IW(1) = JW(1) = 1.

JW(M) - Second index of the reservoir gridblock containing the Mth well.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

Note: If the Mth well is completed parallel to the X- or Y-axis, JW(M) is the Z direction index—if the well is completed parallel to the Z-axis, JW(M) is the Y direction index. See example below.
If ICOORD = 2, IW(1) = JW(1) = 1.

IFLAG(M) - Flag indicating type of well constraint specification for Mth well.

Possible Values:

1 - Rate constrained injection well

2 - Pressure constrained production well (this option is available only if ICOORD = 1 or 3)

3 - Pressure constrained injection well (this option is available only if ICOORD = 1 or 3)
4 - Rate constrained production well

RW(M) - Radius of M^{th} well.
Units: feet (IUNIT=0) or m (IUNIT=1)

SWELL(M) - Skin factor for M^{th} well.
Units: dimensionless

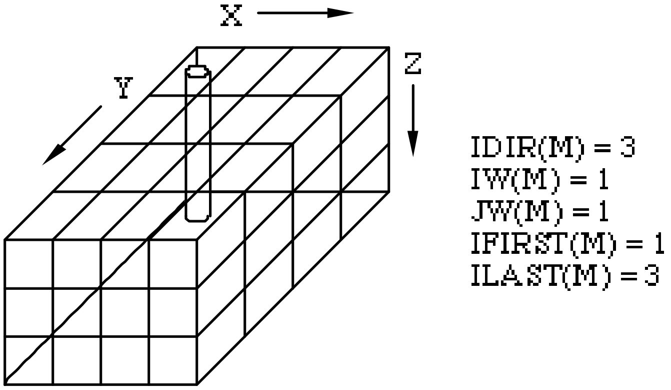
IDIR(M) - Flag indicating the direction in which the M^{th} well is completed.
Possible Values:
1 : Well completed parallel to the X-axis
2 : Well completed parallel to the Y-axis
3 : Well completed parallel to the Z-axis
Note: If ICOORD = 2, IDIR(1) must be equal to 3.

IFIRST(M) - Index of the first block in which the M^{th} well is completed.
Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

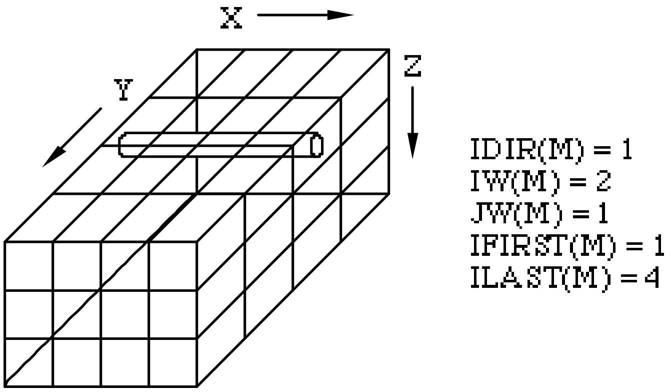
ILAST(M) - Index of the last block in which the M^{th} well is completed.
Possible Values: Between IFIRST(M) and the number of gridblocks in the pertinent direction, inclusive

IPRF(M) - Flag indicating if partial completion of the well is considered.
Possible Values:
0 - The well is fully completed
1 - The well is partially completed

Example: For a vertical well (completed through all the layers) as illustrated in the 4 × 4 × 3 example below, note the values of IDIR(M), IW(M), JW(M), IFIRST(M), and ILAST(M):



For a horizontal well (completed from the first to last gridblock in the X direction and parallel to the X-axis) as illustrated in the 4 × 4 × 3 example below, note the values of IDIR(M), IW(M), JW(M), IFIRST(M), and ILAST(M):



Note: Horizontal wells can be used for 2-D X-Y or 3-D simulations.

4.6.6.b KPRF(M,IWB), for IWB = 1, NWBC (This line is read only if IPRF = 1)

KPRF(M,IWB) - Flag indicating if the IWBth well block of the Mth well is perforated or not.

Possible Values:

0 - The well block is not perforated
1 - The well block is perforated

4.6.6.c WELNAM(M)

WELNAM(M) - Name of the Mth well.

Note: The name can consist of any combination of up to 18 alphanumeric characters. This information will be printed—along with the well I.D. number, IDW(M)—at the beginning of the history output files.

4.6.6.d ICHEK(M), PWFMIN(M), PWFMAX(M), QTMIN(M), QTMAX(M)

ICHEK(M) - The flag to specify whether to check the rate or pressure caps for the Mth well.

Possible Values:

0 - There will be no check on the rate or pressure limits and no automatic shut in for the pressure constraint injector
1 - There will be no automatic shut in for the pressure constraint injector but the pressure or rate limits are checked
2 - There will be both the automatic shut in and the check on the pressure or rate limits

PWFMIN(M) - Minimum flowing bottom hole pressure (specified at the top layer) for the Mth well.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

PWFMAX(M) - Maximum flowing bottom hole pressure (specified at the top layer) for the Mth well.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

QTMIN(M) - Minimum total flow rate (specified at the top layer) for the Mth well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

QTMAX(M) - Maximum total flow rate (specified at the top layer) for the Mth well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

Note: – PWFMIN(M) and PWFMAX(M) are the pressure caps for a rate constraint injector or producer well. QTMIN(M) and QTMAX(M) are the total rate caps for a pressure constraint injector or producer well. If the Mth pressure constraint injector or producer produces at total rate less than QTMIN(M), the Mth well will be switched to a rate constraint well with total rate of QTMIN(M) for the rest of the injector or production period. On the other hand, if the total rate is greater than the QTMAX(M), the Mth well then will be switched to a rate constraint well with the total rate of QTMAX(M). The similar concept is applied to a rate constraint injector or producer.

– The user can skip the well control calculation by specifying very small values for QTMIN(M) and PWFMIN(M) and very large values for QTMAX(M) and PWFMAX(M).

– The code still has the automatic option for shut in of a pressure constraint injector injecting at a rate of less than QTMIN(M).

4.6.7 The data on input lines 4.6.7.a, 4.6.7.b, 4.6.7.c, and 4.6.7.d are repeated for M = 1 to NWELL times.

Note 1: For injection wells that are on rate constraint only injection rates and concentrations for each phase are listed. For injection wells that are on pressure constraint the injection pressure is also specified. In this case the injection rates are treated as phase cuts in the injected fluid. For producer pressure constraint only the bottom hole pressure is specified. For producer rate constraint only the total production rate is specified.

Note 2: The user can shut in a pressure constraint well by specifying a negative bottom hole pressure or a rate constraint well by specifying a value of zero for rate (QI).

4.6.7.a ID(M), QI(M,L), (C(M,KC,L), for KC = 1, N), for L = 1, MXP (This set of data is read only if IFLAG(M) = 1 or 3)

ID(M) - Well I.D. number for the Mth well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: See note for IDW(M) on input line 4.6.6.a.

QI(M,L) - Injection rate of Lth phase in Mth well (see note).

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

C(M,KC,L) - Concentration of KCth component in Lth phase in Mth well.

Units: vary according to component (see note)

Note: The KC index changes the fastest, the L index changes the next fastest, and the M index changes the slowest. A separate data line should be in the input file for each phase - - that is, M × L lines will be read in. MXP is equal to 3 (IGAS = 0) or 4 (IGAS = 1).

– The following values for L correspond to the indicated phase:

1 - Aqueous phase
2 - Oleic phase
3 - Microemulsion phase
4 - Gas phase

– The following values for KC correspond to the indicated component (corresponding concentration units are in parentheses):

For all values of IREACT:

1 - Water (volume fraction)
2 - Oil (volume fraction)
3 - Surfactant (volume fraction)
4 - Polymer (weight percent)

    5 - Total nonsorbing anions concentration, assumed to all be chloride anions (meq/ml)
    6 - Divalent cations, assumed to all be calcium for IREACT<2 (meq/ml)
    7 - Alcohol 1 (volume fraction)
    8 - Alcohol 2 (volume fraction) or Gas (volume fraction)
    9 - Tracer 1
    10 - Tracer 2
    11 - Tracer 3
For IREACT = 0:
    12 - Tracer 4
    13 - Tracer 5
    …
    20 - Tracer 12
    21 - Tracer 13
For IREACT = 1:
    12 - $Na_2Cr_2O_7$ (ppm)
    13 - CSN_2H_4 (ppm)
    14 - Cr^{3+} (ppm)
    15 - Gel (ppm)
    16 - Hydrogen (meq/ml)
For IREACT = 2, 3, 4, 5, or 6:
    12 - Sodium (meq/ml)
    13 - Hydrogen (meq/ml)
    14 - Magnesium (meq/ml)
    15 - Carbonate (meq/ml)
For IREACT = 3:
    16 - Acid component of crude oil (meq/ml)
For IREACT = 4 , 5, or 6:
    16 - Aluminum (meq/ml)
    17 - Silica (meq/ml)
For IREACT = 5:
    18 - Acid component of crude oil (meq/ml)
For IREACT = 6
    18 - $Na_2Cr_2O_7$ (ppm)
    19 - CSN_2H_4 (ppm)
    20 - Cr^{3+} (ppm)
    21 - Gel (ppm)

4.6.7.b ID(M), PWF(M) (This line is read only if IFLAG(M) = 2 or 3)

ID(M) - Well I.D. number for the Mth well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: See note for IDW(M) on input line 4.6.6.a.

PWF(M) - Flowing bottom hole pressure for the Mth well.

Units: psia (IUNIT=0) or kPa (IUNIT=1)

4.6.7.c ID(M), TEMINJ(M) (This line is read only if IENG=1 and IFLAG(M) = 1 or 3)

ID(M) - Well I.D. number for the M^{th} well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: See note for IDW(M) on input line 4.6.6.a.

TEMINJ(M) - Injection temperature for M^{th} well.

Units: •F (IUNIT=0) or •C (IUNIT=1)

4.6.7.d ID(M), QI(M,1) (This line is read only if IFLAG(M) = 4)

ID(M) - Well I.D. number for the M^{th} well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: See note for IDW(M) on input line 4.6.6.a.

QI(L) - Total production rate for M^{th} well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

Note: This value needs to be input as a negative number

4.6.8 TINJ, CUMPR1, CUMHI1, CUMHI2, WRHPV, WRPRF, RSTC

TINJ - Cumulative injection time.

Units: days or pore volumes (dependent on value of ISTOP flag on input line 4.2.1)

CUMPR1 - Indicates interval at which profiles should be written to UNIT 4.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

CUMHI1 - Indicates interval at which production data should be written to UNIT 4.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

CUMHI2 - Indicates interval at which production data should be written to UNIT 3.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

WRHPV - Indicates interval at which production histories should be written to output file(s) for history plotting.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

Note: If WRHPV > total pore volume injected or maximum simulation time, the data will not be printed. The unit number of the file to be written to starts at 19 and continues upward. For example, for a run with three producers, UNITS 19, 20 and 21 would be used. The history of reservoir properties and overall rates from all the producing wells is written to UNIT 9.

WRPRF - Indicates interval at which concentration, pressure, saturation, tracer phase concentration, capacitance property, gel property, alkaline property , and temperature profiles should be written to UNITS 8, 11, 12, 13, 14, 10, 15, and 18 respectively.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

Note: If WRPRF > total pore volume injected or maximum simulation time, the data will not be written.

RSTC - Indicates the interval at which restart data should be written to UNIT 7.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

4.6.9 DT (This line is read only if IMES = 1 and ITIME = 0)

DT - Time step size for constant time step option.

Units: days

4.6.10 DT, DCLIM, DTMAX, DTMIN (This line is read only if IMES = 2 and ITIME = 0)

DT - Initial time step size, $\bullet t_i$.

Units: days

DCLIM - Tolerance for concentration change for the first three components, $\bullet C_{lim}$.

Units: volume fraction

DTMAX - Maximum time step size, $\bullet t_{max}$.

Units: days

DTMIN - Minimum time step size, $\bullet t_{min}$.

Units: days

Note: The time step selection is based on the method of relative changes for the first three components (water, oil, and surfactant) as:

$$\Delta t^{n+1} = \Delta t^{n} \min\left(\frac{\Delta C_{lim}}{\max\limits_{i=1}^{NBL} \left| \Delta C_{i,\kappa} \right|} \right) \qquad \kappa = 1, 2, 3$$

$\bullet t^{n+1}$ is limited to: $\bullet t_{min} \bullet \bullet t^{n+1} \bullet \bullet t_{max}$

4.6.11 DT, DCLIM, CNMAX, CNMIN (This line is read only if IMES = 2, ITIME = 1, and at least one well is not shut-in.)

DT - Initial time step size, $\bullet t_i$.

Units: days

DCLIM - Tolerance for concentration changes for the first three components.

Units: volume fraction

CNMAX - Maximum Courant number.

Units: dimensionless

CNMIN - Minimum Courant number.

Units: dimensionless

Note: The minimum and maximum time steps in days are computed based on the minimum and maximum Courant number as:

$$\Delta t_{min} = \frac{CNMIN}{\min\limits_{M=1}^{nwell} \left(\max\limits_{i=1}^{nwbc} \frac{Q_i}{\Delta x_i \; \Delta y_i \; \Delta z_i \; \phi_i} \right)}$$

and

$$\Delta t_{max} = \frac{CNMAX}{\min\limits_{M=1}^{nwell} \left(\max\limits_{i=1}^{nwbc} \frac{Q_i}{\Delta x_i \; \Delta y_i \; \Delta z_i \; \phi_i} \right)}$$

4.6.12 DT, (DCLIM(KC), for KC = 1, N), DTMAX, DTMIN (This line is read only if IMES = 3 or 4 and ITIME = 0)

DT - Initial time-step size, $\bullet t_i$.

Units: days

DCLIM(KC) - Tolerance for concentration change, $\bullet C_{lim,\kappa}$, of KCth component (IMES = 3) or relative tolerance for concentration change, $R_{lim,\kappa}$, of KCth component (IMES = 4).

Units: IMES = 3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 4.6.7.a)

IMES = 4: dimensionless

DTMAX - Maximum time step size, •t_{max}.

Units: days

DTMIN - Minimum time step size, •t_{min}.

Units: days

Note: For IMES = 3, the method of relative changes is applied to all the components in the simulation run:

$$\Delta t^{n+1} = \Delta t^{n} \min\left(\frac{\Delta C_{lim}}{\max\limits_{i=1}^{NBL} \left| \Delta C_{i,\kappa} \right|} \right) \qquad \kappa = 1, ..., n_c$$

•t^{n+1} is limited to: •t_{min} • •t^{n+1} • •t_{max}

•$C_{lim,\kappa}$ is a fraction of the initial or injected concentration (whichever is larger) of the KC^th^ component. For example: •$C_{lim,3} = 0.1 \times C_3$ where C_3 is the total concentration of component 3. If •$C_{lim,\kappa}$ of the KCth component is entered as zero, that component is not considered in the time-step size selection.

For IMES = 4, the new time-step size is calculated according to:

$$\Delta t^{n+1} = \Delta t^{n} \min\left(\frac{R_{lim,\kappa}}{\max\limits_{i=1}^{NBL} \left| \frac{\Delta C_{i,\kappa}}{C_{i,\kappa}} \right|} \right) \qquad \kappa = 1, ..., n_c$$

•t^{n+1} is limited to: •t_{min} • •t^{n+1} • •t_{max}

$R_{lim,\kappa}$ is the dimensionless relative change in concentration. For example: $R_{lim,3}$ = 0.1 indicates a 10% change in concentration of component 3.

4.6.13 DT, (DCLIM(KC), for KC = 1, N), CNMAX, CNMIN (This line is read only if IMES = 3 or 4, ITIME = 1, and reservoir is not shut-in.)

DT - Initial time step size, •t_i.

Units: days

DCLIM(KC) - Tolerance for concentration change, •$C_{lim,\kappa}$, of KCth component (IMES = 3) or relative tolerance for concentration change, $R_{lim,\kappa}$, of KCth component (IMES = 4).

Units: IMES = 3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 4.6.7.a)

IMES = 4: dimensionless

CNMAX - Maximum Courant number.

Units: dimensionless

CNMIN - Minimum Courant number.

Units: dimensionless

Note: See note for input lines 4.6.11 and 4.6.12 for time step calculation information.

IMPORTANT NOTE: The data on lines 4.6.14 through 4.6.23 describe the changes in boundary conditions and are repeated until the injected time (TINJ on input line 4.6.8) is greater than or equal to the maximum simulation time (TMAX on input line 4.3.1).

4.6.14 IRO, ITIME, IFLAG(M), M = 1, NWELL

IRO - Flag indicating the equivalent well radius model to be used.

Possible Values:

1 - Babu and Odeh model is used

2 - Peaceman model is used (this was the default in versions previous to UTCHEM-V-5.0)

Note: For information see Babu and Odeh [1989].

ITIME - Flag indicating the units to be used when specifying the minimum and maximum time step.

Possible Values:

0 - Minimum and maximum time steps are input in days

1 - Minimum and maximum time steps are input as Courant numbers

Note: This option is only used if IMES > 1 and it is not a shut-in period. If IMES = 1, this flag is ignored.

IFLAG(M) - Flag indicating type of well constraint specification for Mth well.

Possible Values:

1 - Rate constrained injection well

2 - Pressure constrained production well (this option is available only if ICOORD = 1 or 3)

3 - Pressure constrained injection well (this option is available only if ICOORD = 1 or 3)

4 - Rate constrained production well

4.6.15 NWEL1

NWEL1 - Number of wells with changes in location (IW(M), JW(M)), skin, direction, perforation, name, or minimum and maximum bottomhole pressure or minimum or maximum rate.

4.6.16 The data on input lines 4.6.16.a through 4.6.16.d are repeated for M = 1 to NWEL1 times.

4.6.16.a ID, IW(ID), JW(ID), RW(ID), SWELL(ID), IDIR(ID), IFIRST(ID), ILAST(ID), IPRF(ID)

ID - Well ID number with changes from the previous slug injection period.

IW(ID) - First index of the reservoir gridblock containing the IDth well.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

Note: See note for input line 4.6.6.a.

JW(ID) - Second index of the reservoir gridblock containing the IDth well.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

Note: See note for input line 4.6.6.a.

RW(ID) - Radius of IDth well.

Units: feet (IUNIT=0) or m (IUNIT=1)

SWELL(ID) - Skin factor for IDth well.

Units: dimensionless

IDIR(ID) - Flag indicating the direction in which the IDth well is completed.

Possible Values:

1 : Well completed parallel to the X-axis

2 : Well completed parallel to the Y-axis

3 : Well completed parallel to the Z-axis

Note: If ICOORD = 2, IDIR(1) must be equal to 3.

IFIRST(ID) - Index of the first block in which the IDth well is completed.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

ILAST(ID) - Index of the last block in which the IDth well is completed.

Possible Values: Between IFIRST(ID) and the number of gridblocks in the pertinent direction, inclusive

Note: At this time, UTCHEM assumes the well is completed continuously between IFIRST(ID) and ILAST(ID).

IPRF(ID) - Flag indicating if partial completion of the well is considered.

Possible Values:

0 - The well is fully completed
1 - The well is partially completed

4.6.16.b KPRF(ID,IWB), for IWB = 1, NWBC (This line is read only if IPRF = 1)

KPRF(ID,IWB) - Flag indicating if the IWBth well block of the IDth well is perforated or not.

Possible Values:

0 - The well block is not perforated
1 - The well block is perforated

4.6.16.c WELNAM(ID)

WELNAM(ID) - Name of the IDth well.

Note: The name can consist of any combination of up to 18 alphanumeric characters. This information will be printed—along with the well I.D. number, IDW(ID)—at the beginning of the history output files.

4.6.16.d ICHEK, PWFMIN(ID), PWFMAX(ID), QTMIN(ID), QTMAX(ID)

ICHEK(M) - The flag to specify whether to check the rate or pressure caps for the Mth well.

Possible Values:

0 - There will be no check on the rate or pressure limits and no automatic shut in for the pressure constraint injector
1 - There will be no automatic shut in for the pressure constraint injector but the user specified pressure or rate limits are checked
2 - There will be both the automatic shut in and the check on the user specified pressure or rate limits

PWFMIN(ID) - Minimum flowing bottom hole pressure (specified at the top layer) for the IDth well.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

PWFMAX(ID) - Maximum flowing bottom hole pressure (specified at the top layer) for the IDth well.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

QTMIN(ID) - Minimum total flow rate (specified at the top layer) for the IDth well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

QTMAX(ID) - Maximum total flow rate (specified at the top layer) for the IDth well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

Note: See the note for input line 4.6.6.d.

4.6.17 NWEL2, (ID(J), for J = 1, NWEL2)

NWEL2 - Number of wells with changes in rate, concentration or bottomhole pressure.

ID(J) - ID number for J^{th} well with changes.

4.6.18 The data on input lines 4.6.18.a through 4.6.18.d are repeated for M = 1 to NWEL2 times.

4.6.18.a ID, (QI(ID,L), for L = 1, MXP), (C(ID,KC,L), for KC = 1,N), for L =1, MXP (This set of data is read only if IFLAG(ID) =1 or 3)

ID - Well ID number with changes from the previous slug injection period.

QI(ID,L) - Injection rate of L^{th} phase in ID^{th} well (see note for input line 4.6.7.a).

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

C(ID,KC,L) - Concentration of KCth component in Lth phase for IDth well.

Units: vary according to component (see note for line 4.6.7.a)

Note: If IGAS = 0, then MXP = 3. If IGAS = 1, then MXP = 4.

4.6.18.b ID(ID), PWF(ID) (This line is read only if IFLAG(ID) = 2 or 3)

ID(ID) - Well ID number with changes from the previous slug injection period.

PWF(ID) - Flowing bottom hole pressure for the ID^{th} well.

Units: psia (IUNIT=0) or kPa (IUNIT=1)

4.6.18.c ID(ID), TEMINJ(ID) (This line is read only if IENG = 1 and IFLAG(ID) = 1or 3)

ID(ID) - Well ID number with changes from the previous slug injection period.

TEMINJ(ID) - Injection temperature for the ID^{th} well.

Units: •F (IUNIT=0) or •C (IUNIT=1)

4.6.18.d ID(ID), QI(ID,1) (This line is read only if IFLAG(ID) = 4)

ID(ID) - Well ID number with changes from the previous slug injection period.

QI(ID,1) - Total production rate for ID^{th} well.

Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

Note: This value needs to be input as a negative number.

4.6.19 TINJ, CUMPR1, CUMHI1, CUMHI2, WRHPV, WRPRF, RSTC

TINJ - Cumulative injection time.

Units: days or pore volumes (dependent on value of ISTOP flag on input line 4.2.1)

CUMPR1 - Indicates interval at which profiles should be written to UNIT 4.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

CUMHI1 - Indicates interval at which production data should be written to UNIT 4.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

CUMHI2 - Indicates interval at which production data should be written to UNIT 3.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

WRHPV - Indicates interval at which production histories should be written to output file(s) for history plotting.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

Note: If WRHPV > total pore volume injected or maximum simulation time, the data will not be printed. The unit number of the file to be written to starts at 19 and continues upward. For example, for a run with three producers, UNITS 19, 20, and 21 would be used. The history of reservoir properties and the total rate from all the producing wells is written to UNIT 9.

WRPRF - Indicates interval at which concentration, pressure, saturation, tracer phase concentration, capacitance property, pressure difference, gel property, alkaline property , and temperature profiles should be written to UNITS 8, 11, 12, 13, 14, 10, 15 and 18 respectively.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

Note: If WRPRF > total pore volume injected or maximum simulation time, the data will not be written.

RSTC - Indicates the interval at which restart data should be written to UNIT 7.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 4.2.1)

4.6.20 DT (This line is read only if IMES = 1 and ITIME = 0)

DT - Time step size for constant time step option.

Units: days

4.6.21 DT, DCLIM, DTMAX, DTMIN (This line is read only if IMES = 2 and ITIME = 0)

DT - Initial time step size, •t_i.

Units: days

DCLIM - Tolerance for concentration change for the first three components, •C_{lim}.

Units: volume fraction

DTMAX - Maximum time step size, •t_{max}.

Units: days

DTMIN - Minimum time step size, •t_{min}.

Units: days

Note: See note for input line 4.6.10.

4.6.22 DT, DCLIM, CNMAX, CNMIN (This line is read only if IMES = 2, ITIME = 1, and at least one well is not shut-in.)

DT - Initial time step size, •t_i.

Units: days

DCLIM - Tolerance for concentration changes for the first three components.

Units: volume fraction

CNMAX - Maximum Courant number.

Units: dimensionless

CNMIN - Minimum Courant number.

Units: dimensionless

Note: See note for input line 4.6.11.

4.6.23 DT, (DCLIM(KC), for KC = 1, N), DTMAX, DTMIN (This line is read only if IMES = 3 or 4 and ITIME = 0)

DT - Initial time-step size, •t_i.

Units: days

DCLIM(KC) - Tolerance for concentration change, •$C_{lim,\kappa}$, of KCth component (IMES = 3) or relative tolerance for concentration change, $R_{lim,\kappa}$, of KCth component (IMES = 4).

Units: IMES = 3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 4.6.7.a)
IMES = 4: dimensionless

DTMAX - Maximum time step size, •t_{max}.
Units: days

DTMIN - Minimum time step size, •t_{min}.
Units: days

Note: See note for input line 4.6.12.

4.6.24 DT, (DCLIM(KC), for KC = 1, N), CNMAX, CNMIN (This line is read only if IMES = 3 or 4, ITIME = 1, and reservoir is not shut-in.)

DT - Initial time step size, •t_i.
Units: days

DCLIM(KC) - Tolerance for concentration change, •$C_{lim,\kappa}$, of KCth component (IMES = 3) or relative tolerance for concentration change, $R_{lim,\kappa}$, of KCth component (IMES = 4).
Units: IMES = 3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 4.6.7.a)
IMES = 4: dimensionless

CNMAX - Maximum Courant number.
Units: dimensionless

CNMIN - Minimum Courant number.
Units: dimensionless

Note: See note for input lines 4.6.11 and 4.6.12 for time step calculation information.

B.5 NOMENCLATURE

The nomenclature consists of the names of the variables as they appear in equations in this text (and related reports) and descriptions of those variables. FORTRAN names of the variables as they appear in the UTCHEM simulator appear in parenthesis where applicable.

a_T = Adsorbed tracer amount per unit mass of rock.
a_3 = Surfactant adsorption parameter
a_{31} = Surfactant adsorption parameter (AD31)
a_{32} = Surfactant adsorption parameter (AD32)
a_4 = Polymer adsorption parameter
a_{41} = Surfactant adsorption parameter (AD41)
a_{42} = Polymer adsorption parameter (AD42)
a_κ = Adsorption parameter for κ^{th} component (A14D, A15D)
A_{p1} = Polymer viscosity parameter (AP1)
A_{p2} = Polymer viscosity parameter (AP2)
A_{p3} = Polymer viscosity parameter (AP3)
A_{15} = Permeability reduction parameter for Langmuir correlation with gel concentration (AGK)
B_{15} = Permeability reduction parameter for Langmuir correlation with gel concentration (BGK)
b_3 = Surfactant adsorption parameter (B3D)
b_4 = Polymer adsorption parameter (B4D)
b_κ = Adsorption parameter for κ^{th} component (B14D, B15D)
c_{pc} = Capillary pressure parameter (CPC)
C = Shear rate coefficient
$C_{i,\kappa}$ = Total concentration of component κ in gridblock i

$\Delta C_{i,\kappa}$ = Change in total concentration of component κ in gridblock i over the current time-step
$\Delta C_{lim,\kappa}$ = Tolerance for concentration change of component κ
C_o = Initial condition for tracer used in radioactive decay equation
C_{SE} = Effective salinity for phase behavior and surfactant adsorption
C_{SEL} = Type II(–)/III phase boundary or effective salinity limit (CSEL7 for Alcohol 1—Component 7 and CSEL8 for Alcohol 2—Component 8)
C_{SEP} = Effective salinity (ion strength) for polymer properties
C_{SEU} = Type III/II(+) phase boundary or effective salinity limit (CSEU7 for Alcohol 2—Component 7 and CSEU8 for Alcohol 2—Component 8)
C_{T1} = Concentration of tracer in phase 1
C_6^{o} = Concentration of free calcium cations
C_9^{o} = Concentration of free sodium cations
C_δ = Permeability reduction parameter for gel (CRG)
C_κ = Overall concentration of component κ in the mobile phases
C_κ = Adsorbed concentration of component κ
$C_{\kappa o}$ = Concentration of tracer component κ in oil
$C_{\kappa w}$ = Concentration of tracer component κ in water
$\tilde{C}_\kappa$ = Overall concentration of component κ in the mobile and stationary phases
$C_{\kappa\ell}$ = Concentration of component κ in phase ℓ
CNMAX = Maximum Courant number
CNMIN = Minimum Courant number
D_S = Retardation factor for tracer (RET)
e_ℓ = Relative permeability exponent for phase ℓ
$e_{\ell c}$ = Relative permeability exponent for phase ℓ at low interfacial tension (E13C, E23C, and E31C)
$e_{\ell w}$ = Relative permeability exponent for phase ℓ at high interfacial tension (E1W, E2W, and E3W)
f_κ^s = Amount of component κ associated with surfactant
k = Permeability at 100% brine saturation
k_a = Apparent permeability used in capillary pressure calculations
$k_{r\ell}$ = Relative permeability of phase ℓ
$k_{r\ell}^{o}$ = End point relative permeability of phase ℓ
$k_{r\ell c}^{o}$ = End point relative permeability of phase ℓ at low interfacial tension (P1RC for phase 1, P2RC for phase 2, and P3RC for phase 3)
$k_{r\ell w}^{o}$ = End point relative permeability of phase ℓ at high interfacial tension (P1RW for phase 1, P2RW for phase 2, and P3RW for phase 3)
k_x = Absolute permeability in the x-direction (PERMX)
k_y = Absolute permeability in the y-direction (PERMY)
k_z = Absolute permeability in the z-direction (PERMZ)
K_κ = Tracer κ partition coefficient (TK)
L = Length of the core, or reservoir length
$M_{Cr^{3+}}$ = Molecular weight of chromium component
$M_{polymer}$ = Molecular weight of polymer component
n = Cr^{3+}/polymer mass stoichiometric ratio
n_{pc} = Capillary pressure exponent (EPC)
$N_{c\ell}$ = Capillary number of phase ℓ
N_v = Viscosity number

N_δ = Dimensionless number representing the reduction of the pore radius due to adsorption of gel
$P_{C\ell\ell'}$ = Capillary pressure between phases ℓ and ℓ'
P_α = Exponent for calculating shear rate dependence of polymer viscosity (POWN)
Q_i = Maximum injection/production flow rate in well block i
Q_v = Cation exchange capacity of clay (QV)
R_k = Permeability reduction factor
RRF = Residual resistance factor for gel
RRF_{max} = Maximum residual resistance factor for gel
$S_{n\ell}$ = Normalized mobile saturation of phase ℓ used in relative permeability and capillary pressure calculations
S_p = Exponent for calculating salinity dependence of polymer viscosity (SSLOPE)
S_ℓ = Saturation of phase ℓ
$S_{\ell r}$ = Residual saturation of phase ℓ
$S_{\ell' rc}$ = Residual saturation of phase ℓ' at low interfacial tension (S1RWC, S2RWC, and S3RWC for phases 1, 2 and 3)
$S_{\ell' rw}$ = Residual saturation of phase ℓ' at high interfacial tension (S1RW, S2RW, and S3RW for phases 1, 2 and 3)
SCR = Stoichiometric ratio between Cr^{3+} and polymer
t = A time variable in the radioactive decay of tracer equation
Δt_i = Initial time-step size (DT)
Δt_{max} = Maximum time-step size (DTMAX)
Δt_{min} = Minimum time-step size (DTMIN)
Δt^n = Time-step size at nth time level
Δt^{n+1} = Time-step size at n+1th time level
t_o = An initial time at which the tracer concentration C_o is known; used in the radioactive decay equation
T_1 = Capillary desaturation parameter for aqueous phase (T11)
T_2 = Capillary desaturation parameter for oleic phase (T22)
T_3 = Capillary desaturation parameter for microemulsion phase (T33)

T_4 = Capillary desaturation parameter for gas phase (T44)
u = Flux
V_t = Tracer velocity
•x_i = Size of gridblock i in x direction
x_4 = Exponent used in gelation reaction
x_{14} = Exponent used in gelation reaction
x_{16} = Exponent used in gelation reaction
•y_i = Size of gridblock i in y direction
•z_i = Size of gridblock i in z direction

Greek Symbols

α_1 = Compositional microemulsion phase viscosity parameter (ALPHA1)
α_2 = Compositional microemulsion phase viscosity parameter (ALPHA2)
α_3 = Compositional microemulsion phase viscosity parameter (ALPHA3)
α_4 = Compositional microemulsion phase viscosity parameter (ALPHA4)
α_5 = Compositional microemulsion phase viscosity parameter (ALPHA5)
β^C = Cation exchange constant for clay (XKC)
β_P = Effective salinity parameter for polymer viscosity (BETAP)

β^S = Cation exchange constant for surfactant (XKS)

β_6 = Effective salinity parameter for calcium—Component 6 (BETA6)

β_7 = Effective salinity parameter for Alcohol 1—Component 7 (BETA7)

β_8 = Effective salinity parameter for Alcohol 2—Component 8 (BETA8)

$\dot{\gamma}_{eq}$ = Equivalent shear rate for porous medium

$\dot{\gamma}_c$ = Coefficient in equivalent shear rate equation (GAMMAC)

$\dot{\gamma}_{1/2}$ = Shear rate at which polymer viscosity is one-half the polymer viscosity at zero shear rate (GAMHF)

γ_1 = Specific weight of brine—Component 1 (DEN1)

γ_2 = Specific weight of oil—Component 2 (DEN2)

γ_3 = Specific weight of surfactant—Component 3 (DEN3)

γ_7 = Specific weight of Alcohol 1—Component 7 (DEN7)

γ_8 = Specific weight of Alcohol 2 or gas—Component 8 (DEN8)

λ_κ = Radioactive decay coefficient for κ^{th} tracer (RDC)

$[\mu]$ = Intrinsic viscosity of a gel solution

μ_o = Polymer viscosity at zero shear rate

μ_p = Polymer viscosity

μ_w = Water viscosity

μ_ℓ = Viscosity of phase ℓ (VIS1 for phase 1, VIS2 for phase 2, and VIS4 for phase 4)

$\mu_{4,ref}$ = Viscosity of gas phase at reference pressure

$\mu_{4,s}$ = Slope of gas viscosity function

μ_∞ = Viscosity at infinite shear rate

ρ_g = Rock density

ρ_s = Solution density

ρ_ℓ = Density of phase ℓ

σ_{wo} = Interfacial tension between oil and water

$\sigma_{\ell\ell'}$ = Interfacial tension between phases ℓ and ℓ'

ϕ = Porosity (POR)

ϕ_i = Porosity of gridblock i

Φ = Potential

Θ_o = Relaxation time coefficient

Subscripts

κ = Component number

For all values of IREACT:

1 = Water

2 = Oil

3 = Surfactant

4 = Polymer

5 = Chloride

6 = Calcium

7 = Alcohol 1

8 = Alcohol 2 or Gas

9 = Tracer 1

10 = Tracer 2

11 = Tracer 3

For IREACT = 0:

12 = Tracer 4

13 = Tracer 5
.
.
.
20 = Tracer 12
21 = Tracer 13

For IREACT = 1:
12 = Sodium dichromate ($Na_2Cr_2O_7$)
13 = Thiourea (CSN_2H_4)
14 = Trivalent chromium (Cr^{3+})
15 = Gel
16 = Hydrogen

For IREACT = 2, 3, 4, 5, or 6:
12 = Sodium
13 = Hydrogen
14 = Magnesium
15 = Carbonate

For IREACT = 3:
16 = Acid component of crude oil

For IREACT = 4, 5, or 6:
16 = Aluminum
17 = Silica

For IREACT = 5:
18 = Acid component of crude oil

For IREACT = 6
18 = Sodium dichromate ($Na_2Cr_2O_7$)
19 = Thiourea (CSN_2H_4)
20 = Trivalent chromium (Cr^{3+})
21 = Gel

ℓ = Phase number
1 = Aqueous
2 = Oleic
3 = Microemulsion
4 = Gas

r = Residual
w = Low capillary number values
c = High capillary number values

B.6 OUTPUT FILES AND REACTIONS

The following sections describe: (1) data that is automatically written to the profile data file, (2) restart run procedure, (3) data written to stored restart data file, (4) data written to history files for each well, (5) data written to history of reservoir properties and overall injection and production rates from all the wells, (6) data written to aqueous phase tracer concentration data files, (7) list of elements and reactions for IREACT=2, (8) list of elements and reactions for IREACT=3, (9) list of elements and reactions for IREACT=4 or 6, and (10) list of elements and reactions for IREACT=5.

B.6.1 Default Data Written to Profile Data File

The information in the following lists is always written to the profile data file (PROFIL) and is not controlled by the various print control flags in the input files.

Printed at each CUMHI1 interval:

- Time, number of time steps
- Time step size
- Courant number
- Cumulative pore volume injected
- Original in place for each component
- Cumulative injection for each component
- Cumulative production for each component
- Amount retained for each component
- Relative error for each component
- Fraction of oil recovered
- If IREACT • 2:
  - Average number of iterations, computation time
- For each well:
  - Position of the well, first and last well block completed
  - Cumulative injection/production
  - Bottomhole pressure for each well block
  - All well related information (such as pressure for each phase, phase concentration, phase cut, etc.)
  - Producer wellbore temperature and phase cut and concentration

Printed at each CUMPR1 interval:

- Reservoir temperature if IENG = 1
- Phase saturation profile for each phase
- Aqueous phase pressure profile
- Concentration of each component in the fluid
- If tracers are present and ICAP•0:
  - Flowing concentration
  - Dendiritic concentration
  - Flowing saturation
  - Dendiritic saturation

B.6.2 Restart Run Procedure

The restart procedure is available with UTCHEM. This enables a user to continue a run past the initial time period or to break a large run up into smaller segments. Each time you run UTCHEM, a file called RESTAR is created. This file (described in section 6.3 of this appendix) contains all the information necessary to continue the run at a later time. In order to do so, the user needs to:

1.- Rename the output file RESTAR from the previous run to INPUT2
2.- Set the variable IMODE equal to 2 on line 4.1.3 of input file INPUT
3.- Change the value of TMAX on input line 4.3.1 of file INPUT to the new injection period being simulated in the restart run

4.- Change the value of TINJ on input line 4.5.8 of file INPUT if appropriate

5.- Add additional information for input lines 4.5.14 through 4.5.24 of file INPUT if the well conditions are different for the new injection period

Note: Make sure the source code you run the restart problem (IMODE=2) has the same values for the array sizes in the parameter statement as the one used in original run (IMODE=1).

B.6.3 Data Written to Stored Restart Run Data File

The information in the following list is always written to the stored restart data file (RESTAR). If the user is running a RESTART run, this data file needs to be renamed to correspond to the INPUT2 input file. The values in parentheses are the FORTRAN variable names as they appear in the code.

Printed at the end of each run:

Time (T), injection time (TINJ), time step size (DT), number of time steps (ICNT)

New slug injection or restart flag (IINJ), number of time step reduction (INEC), cumulative pore volume injection (CUMPV), number of blocks in X-direction minus 1 (NXM1)

Cumulative injection (CUMI), cumulative production (CUMP), original in place (OIP) for each component

Cumulative injection/production (CUMQ) for each well

Phase concentration (C), phase saturation (S), effective salinity (CSE), overall concentration (CTOT), number of phases (NPHASE)

If ICOORD=2:

Boundary concentration (CE), boundary pressure (PE)

Viscosity (VIS), relative permeability (RPERM), injection rate (QI), total rate for each well (QT), phase rate (Q), bottomhole pressure (PWF)

Pressure (P)

Surfactant adsorption (C3ADSS), surfactant adsorption parameter (A3DS), polymer adsorption (C4ADSS)

Permeability reduction factor (RKF), calcium concentration (C6JO), calcium adsorbed by clay (C6ADSS), calcium adsorbed by surfactant (C6HATS)

Alcohol 7 partitioning coefficient (X7OLD), alcohol 8 partitioning coefficient (X8OLD)

Variables for writing profiles to UNIT 4 (CUMPRO), histories to UNIT 4 (CUMHIS), histories to UNIT 3 (CUMHCP)

Oil breakthrough (BTO), tracer breakthrough (TBT), tracer injection concentration (CINJT), tracer retardation factor (TRD)

Lower effective salinity (CSEL), upper effective salinity (CSEU)

Density (DEN), capillary pressure (PRC)

Total surfactant (TSURF)

If ICAP>0:

Dendiritic concentration (CD), dendiritic saturation (SD), flowing saturation (SF), total flowing concentration (CTF)

If NG•0:

Chromium adsorption (C14ADS), gel adsorption (C15ADS), cation exchange capacity of clay (QW)

If IENG = 1

Cum. heat inj. (CUMHI), cum. heat prod. (CUMHP), temperature (TEM), total volumetric heat capacity (TVHC)

If IENG = 1 and IHLOS = 1
    Cum. heat loss (TQLOS), integral for overburden and underburden heatloss calculations (RINO, RINU), time of change of overburden temp. from the reservoir block (TTCHG), overburden temperature (TEMPOB), underburden temperature (TEMPUB)
If IENG =1 and ICOORD =2
    Boundary enthalpy (ENTHE)
If IREACT >1 :
    Solid concentration (CSLDT), adsorbed concentration (CSORBT), species concentration (CAQSP), surf. associated cation concentration (CACATT), cation concentration (CACAT)
    Cumulative no. of iteration for geochem option (ITCUM)

B.6.4 Data Written to Well History Plotting Data File(s)

The information in the following list is always written to the well history plotting data files (HIST01-HISTℓ) for each production well.

Printed at each WRHPV interval:

Cumulative pore volume, time in days, cumulative production (ft^3, m^3, or STB), water oil ratio, cumulative oil recovery, total production rate (ft^3/day, m^3/day, or STB/day)
Water cut, oil cut, microemulsion cut, gas cut (only if IGAS = 1)
Wellbore pressure for each well block (psi or kPa)
Wellbore temperature (•F or •C) (only if IENG=1)
For I = 1, N:
    If ICF(I) = 1: phase concentration for component N (C(I,L), L=1,MXP), total concentration of component N (CTOT(I))
Lower effective salinity, upper effective salinity, effective salinity (only if ICSE = 1)
For IREACT >1
    Independent species concentration, mole/liter of water (CAQSP(KK), KK = 1, NIAQ)
    Dependent species concentration, mole/liter of water (CAQSP(KK), KK = NIAQ+1,NFLD) (only if IRSPS>0)
    Phase Concentration of (inj.+genereated) surfactant (PSURF(I,L), L = 1,3), total concentration of (inj.+ generated) surfactant (TSURF) (only if IREACT = 3 or 5)
    Concentration of solid components, mole/liter of pore volume (CSLDT(KK), KK = 1, NSLD) (only if NSLD>0)
    Log_{10} of interfacial tension between water/microemulsion and oil/microemulsion (XIFT1, XIFT2) (only if ICNM>0) (dyne/cm)

The information in the following list is always written to the well history plotting data files for each injection well.

Printed at each WRHPV interval:

Cumulative pore volume, time in days, cumulative injection (ft^3, m^3, or STB), injection rate (ft^3/day, m^3/day, or STB/day)
Wellbore pressure for each well block (psi or kPa)

Pressure drop between the wells (for the specific case of one injector and one producer only) or pressure drop between the pressure tabs (when NG>0, NY=1, NZ=1, see line 4.4.93) (psi or kPa)

B.6.5 Data Written to Overall History Plotting Data File

The information in the following list is always written to the overall history plotting data file (OVERAL).

Printed at each WRHPV interval:

Cumulative pore volume, time in days, volumetric averaged reservoir pressure (psi or kPa), cumulative oil produced (%OOIP), cumulative oil produced (bbls or m^3), volumetric averaged reservoir temperature (•F or •C) (only if IENG=1)

Total injection rate (B/D or m^3/day), total production rate (B/D or m^3/day), total fluid injected (1000 bbls or m^3), total fluid produced (1000 bbls or m^3)

Overall production rate for each phase (QBAR(L) for L = 1, MXP where MXP=3 if IGAS=0 and MXP=4 if IGAS =1) (B/D or m^3/day)

Average cut for each phase (FBAR(L) for L = 1, MXP where MXP=3 if IGAS=0 and MXP=4 if IGAS =1)

Average saturation for each phase (SBAR(L) for L = 1, MXP where MXP=3 if IGAS=0 and MXP=4 if IGAS =1)

If ICF(3) = 1: Cumulative surfactant injected (bbls or m^3), Cumulative surfactant produced (bbls or m^3), adsorbed surfactant (bbls or m^3), retained surfactant (bbls or m^3)

If ICF(4) = 1: Cumulative polymer injected (wt%), Cumulative polymer produced (wt%), adsorbed polymer (wt%), retained polymer (wt%)

B.6.6 List of Elements and Reactive Species for IREACT = 2

Elements or pseudo-element:	Hydrogen (reactive), Sodium, Calcium, Magnesium, Carbonate, Chlorine, Oxygen, S (inj. surfactant)
Independent aqueous or oleic species:	H^+, Na^+,Ca^{2+}, Mg^{2+},CO_3^{2-} , Cl^-, S^-, H_2O
Dependent aqueous or oleic species:	$Ca(OH)^+$, $Mg(OH)^+$, $Ca(HCO_3)^+$, $Mg(HCO_3)^+$, OH^-, HCO_3^- , H_2CO_3, $CaCO_3^o$, $MgCO_3^o$
Solid species:	$CaCO_3$ (Calcite), $Ca(OH)_2$ (Calcium hydroxide), $MgCO_3$ (Magnesite), $Mg(OH)_2$ (Magnesium hydroxide)
Adsorbed cations:	$\overline{H}^{+}$, $\overline{Na}^{+}$, $\overline{Ca}^{2+}$, $\overline{Mg}^{2+}$
Adsorbed cations on micelles:	$\overline{\overline{Na}}^{+}$, $\overline{\overline{Ca}}^{2+}$, $\overline{\overline{Mg}}^{2+}$

Aqueous reactions	Equilibrium constant
$H_2O \overset{K_1^{eq}}{\rightleftharpoons} H^+ + OH^-$	$K_1^{eq} = [H^+]\ [OH^-]$
$H^+ + CO_3^{2-} \overset{K_2^{eq}}{\rightleftharpoons} HCO_3^-$	$K_2^{eq} = \dfrac{\left[HCO_3^-\right]}{[H^+]\left[CO_3^{2-}\right]}$
$Ca^{2+} + H_2O \overset{K_3^{eq}}{\rightleftharpoons} Ca(OH)^+ + H^+$	$K_3^{eq} = \dfrac{[Ca(OH)^+]\ [H^+]}{[Ca^{2+}]}$
$Mg^{2+} + H_2O \overset{K_4^{eq}}{\rightleftharpoons} Mg(OH)^+ + H^+$	$K_4^{eq} = \dfrac{[Mg(OH)^+]\ [H^+]}{[Mg^{2+}]}$
$Ca^{2+} + H^+ + CO_3^{2-} \overset{K_5^{eq}}{\rightleftharpoons} Ca(HCO_3)^+$	$K_5^{eq} = \dfrac{\left[Ca(HCO_3)^+\right]}{[Ca^{2+}]\left[CO_3^{2-}\right][H^+]}$
$Mg^{2+} + H^+ + CO_3^{2-} \overset{K_6^{eq}}{\rightleftharpoons} Mg(HCO_3)^+$	$K_6^{eq} = \dfrac{\left[Mg(HCO_3)^+\right]}{[Mg^{2+}]\left[CO_3^{2-}\right][H^+]}$
$2H^+ + CO_3^{2-} \overset{K_7^{eq}}{\rightleftharpoons} H_2CO_3$	$K_7^{eq} = \dfrac{[H_2CO_3]}{\left[CO_3^{2-}\right][H^+]^2}$
$Ca^{2+} + CO_3^{2-} \overset{K_8^{eq}}{\rightleftharpoons} CaCO_3^o$	$K_8^{eq} = \dfrac{\left[CaCO_3^o\right]}{[Ca^{2+}]\left[CO_3^{2-}\right]}$
$Mg^{2+} + CO_3^{2-} \overset{K_9^{eq}}{\rightleftharpoons} MgCO_3^o$	$K_9^{eq} = \dfrac{\left[MgCO_3^o\right]}{[Mg^{2+}]\left[CO_3^{2-}\right]}$

Dissolution reactions	Solubility product
$CaCO_3 \overset{K_1^{sp}}{\rightleftharpoons} Ca^{2+} + CO_3^{2-}$	$K_1^{sp} = [Ca^{2+}]\left[CO_3^{2-}\right]$

$MgCO_3 \overset{K_2^{sp}}{\rightleftharpoons} Mg^{2+} + CO_3^{2-}$	$K_2^{sp} = [Mg^{2+}]\left[CO_3^{2-}\right]$
$Ca(OH)_2 \overset{K_3^{sp}}{\rightleftharpoons} Ca^{2+} + 2OH^-$	$K_3^{sp} = [Ca^{2+}][H^+]^{-2}$
$Mg(OH)_2 \overset{K_4^{sp}}{\rightleftharpoons} Mg^{2+} + 2OH^-$	$K_4^{sp} = [Mg^{2+}][H^+]^{-2}$
<u>Exchange reactions (on clay)</u>	<u>Exchange equilibrium constant</u>
$2\overline{Na}^+ + Ca^{2+} \overset{K_1^{ex}}{\rightleftharpoons} 2Na^+ + \overline{Ca}^{2+}$	$K_1^{ex} = \dfrac{\left[\overline{Ca}^{2+}\right][Na^+]^2}{[Ca^{2+}]\left[\overline{Na}^+\right]^2}$
$2\overline{Na}^+ + Mg^{2+} \overset{K_2^{ex}}{\rightleftharpoons} 2Na^+ + \overline{Mg}^{2+}$	$K_2^{ex} = \dfrac{\left[\overline{Mg}^{2+}\right][Na^+]^2}{[Mg^{2+}]\left[\overline{Na}^+\right]^2}$
$\overline{H}^+ + Na^+ + OH^- \overset{K_3^{ex}}{\rightleftharpoons} \overline{Na}^+ + H_2O$	$K_3^{ex} = \dfrac{[Na^+]\left[\overline{H}^+\right]}{\left[\overline{Na}^+\right][H^+]}$
<u>Exchange reactions (on micelle)</u>	<u>Exchange equilibrium constant</u>
$2\overline{\overline{Na}}^+ + Ca^{2+} \overset{K_1^{exm}}{\rightleftharpoons} 2Na^+ + \overline{\overline{Ca}}^{2+}$	$K_1^{exm} = \dfrac{\left[\overline{\overline{Ca}}^{2+}\right][Na^+]^2}{\left[\overline{\overline{Na}}^+\right]^2[Ca^{2+}]}$
	where $K_1^{exm} = \beta_1^{exm}\ [S^-]$
$2\overline{\overline{Na}}^+ + Mg^{2+} \overset{K_2^{exm}}{\rightleftharpoons} 2Na^+ + \overline{\overline{Mg}}^{2+}$	$K_2^{exm} = \dfrac{\left[\overline{\overline{Mg}}^{2+}\right][Na^+]^2}{\left[\overline{\overline{Na}}^+\right]^2[Mg^{2+}]}$
	where $K_2^{exm} = \beta_2^{exm}\ [S^-]$

B.6.7 List of Elements and Reactive Species for IREACT = 3

Elements or pseudo-element: Hydrogen (reactive), Sodium, Calcium, Magnesium, Carbonate, A (from acid HA), Oxygen, Chlorine, S (Injected surfactant)

Independent aqueous or oleic species: H^+, Na^+,Ca^{2+}, Mg^{2+},CO_3^{2-} , HA_o, Cl^-, S^-, H_2O

Dependent aqueous or oleic species: $Ca(OH)^+$, $Mg(OH)^+$, $Ca(HCO_3)^+$, HA_w, $Mg(HCO_3)^+$, OH^-, HCO_3^- , A^-, H_2CO_3, $CaCO_3^o$, $MgCO_3^o$

Solid species: $CaCO_3$ (Calcite), $Ca(OH)_2$ (Calcium hydroxide), $MgCO_3$ (Magnesite), $Mg(OH)_2$ (Magnesium hydroxide)

Adsorbed cations: $\overline{H}^+$, $\overline{Na}^+$, $\overline{Ca}^{2+}$, $\overline{Mg}^{2+}$

Adsorbed cations on micelles: $\overline{\overline{Na}}^+$, $\overline{\overline{Ca}}^{2+}$, $\overline{\overline{Mg}}^{2+}$

Aqueous reactions	Equilibrium constant
$H_2O \overset{K_1^{eq}}{\rightleftharpoons} H^+ + OH^-$	$K_1^{eq} = [H^+]\ [OH^-]$
$HA_w + OH^- \overset{K_2^{eq}}{\rightleftharpoons} A^- + H_2O$	$K_2^{eq} = \dfrac{[A^-]\ [H^+]}{[HA_w]}$
$H^+ + CO_3^{2-} \overset{K_3^{eq}}{\rightleftharpoons} HCO_3^-$	$K_3^{eq} = \dfrac{\left[HCO_3^-\right]}{[H^+]\left[CO_3^{2-}\right]}$
$Ca^{2+} + H_2O \overset{K_4^{eq}}{\rightleftharpoons} Ca(OH)^+ + H^+$	$K_4^{eq} = \dfrac{[Ca(OH)^+]\ [H^+]}{[Ca^{2+}]}$
$Mg^{2+} + H_2O \overset{K_5^{eq}}{\rightleftharpoons} Mg(OH)^+ + H^+$	$K_5^{eq} = \dfrac{[Mg(OH)^+]\ [H^+]}{[Mg^{2+}]}$
$Ca^{2+} + H^+ + CO_3^{2-} \overset{K_6^{eq}}{\rightleftharpoons} Ca(HCO_3)^+$	$K_6^{eq} = \dfrac{\left[Ca(HCO_3)^+\right]}{[Ca^{2+}]\left[CO_3^{2-}\right][H^+]}$
$Mg^{2+} + H^+ + CO_3^{2-} \overset{K_7^{eq}}{\rightleftharpoons} Mg(HCO_3)^+$	$K_7^{eq} = \dfrac{\left[Mg(HCO_3)^+\right]}{[Mg^{2+}]\left[CO_3^{2-}\right][H^+]}$

$2H^+ + CO_3^{2-} \overset{K_8^{eq}}{\rightleftharpoons} H_2CO_3$	$K_8^{eq} = \dfrac{[H_2CO_3]}{\left[CO_3^{2-}\right][H^+]^2}$
$Ca^{2+} + CO_3^{2-} \overset{K_9^{eq}}{\rightleftharpoons} CaCO_3^o$	$K_9^{eq} = \dfrac{\left[CaCO_3^o\right]}{[Ca^{2+}]\left[CO_3^{2-}\right]}$
$Mg^{2+} + CO_3^{2-} \overset{K_{10}^{eq}}{\rightleftharpoons} MgCO_3^o$	$K_{10}^{eq} = \dfrac{\left[MgCO_3^o\right]}{[Mg^{2+}]\left[CO_3^{2-}\right]}$
<u>Partitioning of HA</u>	<u>Partition coefficient</u>
$HA_o \overset{K_D}{\rightleftharpoons} HA_w$	$K_D = \dfrac{[HA_w]_{water}}{[HA_o]_{oil}}$
<u>Dissolution reactions</u>	<u>Solubility product</u>
$CaCO_3 \overset{K_1^{sp}}{\rightleftharpoons} Ca^{2+} + CO_3^{2-}$	$K_1^{sp} = [Ca^{2+}]\left[CO_3^{2-}\right]$
$MgCO_3 \overset{K_2^{sp}}{\rightleftharpoons} Mg^{2+} + CO_3^{2-}$	$K_2^{sp} = [Mg^{2+}]\left[CO_3^{2-}\right]$
$Ca(OH)_2 \overset{K_3^{sp}}{\rightleftharpoons} Ca^{2+} + 2OH^-$	$K_3^{sp} = [Ca^{2+}][H^+]^{-2}$
$Mg(OH)_2 \overset{K_4^{sp}}{\rightleftharpoons} Mg^{2+} + 2OH^-$	$K_4^{sp} = [Mg^{2+}][H^+]^{-2}$
<u>Exchange reactions (on matrix)</u>	<u>Exchange equilibrium constant</u>
$2\overline{Na}^+ + Ca^{2+} \overset{K_1^{ex}}{\rightleftharpoons} 2Na^+ + \overline{Ca}^{2+}$	$K_1^{ex} = \dfrac{\left[\overline{Ca}^{2+}\right][Na^+]^2}{[Ca^{2+}]\left[\overline{Na}^+\right]^2}$
$2\overline{Na}^+ + Mg^{2+} \overset{K_2^{ex}}{\rightleftharpoons} 2Na^+ + \overline{Mg}^{2+}$	$K_2^{ex} = \dfrac{\left[\overline{Mg}^{2+}\right][Na^+]^2}{[Mg^{2+}]\left[\overline{Na}^+\right]^2}$

$\overline{H}^{+} + Na^{+} + OH^{-} \underset{\blacklozenge}{\overset{K_3^{ex}}{\varnothing}} \overline{Na}^{+} + H_2O$ $\qquad K_3^{ex} = \frac{[Na^{+}]\left[\overline{H}^{+}\right]}{\left[\overline{Na}^{+}\right][H^{+}]}$

Exchange reactions (on micelle) Exchange equilibrium constant

$2\overline{\overline{Na}}^{+} + Ca^{2+} \underset{\blacklozenge}{\overset{K_1^{exm}}{\varnothing}} 2Na^{+} + \overline{\overline{Ca}}^{2+}$ $\qquad K_1^{exm} = \frac{\left[\overline{\overline{Ca}}^{2+}\right][Na^{+}]^2}{\left[\overline{\overline{Na}}^{+}\right]^2[Ca^{2+}]}$

where $K_1^{exm} = \beta_1^{exm}\{[A^-]+[S^-]\}$

$2\overline{\overline{Na}}^{+} + Mg^{2+} \underset{\blacklozenge}{\overset{K_2^{exm}}{\varnothing}} 2Na^{+} + \overline{\overline{Mg}}^{2+}$ $\qquad K_2^{exm} = \frac{\left[\overline{\overline{Mg}}^{2+}\right][Na^{+}]^2}{\left[\overline{\overline{Na}}^{+}\right]^2[Mg^{2+}]}$

where $K_2^{exm} = \beta_2^{exm}\{[A^-]+[S^-]\}$

B.6.8 List of Elements and Reactive Species for IREACT = 4 or 6

Elements or pseudo-element:	Hydrogen (reactive), Sodium, Calcium, Magnesium, Carbonate, Aluminum, Silicon, Oxygen, Chlorine, S (Injected surfactant)
Independent aqueous or oleic species:	H^+, Na^+,Ca^{2+}, Mg^{2+}, Al^{3+}, CO_3^{2-} , Cl^-, S^-, H_4SiO_4, H_2O
Dependent aqueous or oleic species:	$Ca(OH)^+$, $Mg(OH)^+$, $Al(OH)^{2-}$,$Al(OH)_2^-$, $Ca(HCO_3)^+$, $Mg(HCO_3)^+$, OH^-, HCO_3^- , $H_3SiO_4^-$, $H_2SiO_4^{2-}$, $HSi_2O_6^{3-}$, $Si_2O_5^{2-}$, $Al(OH)_4^-$, H_2CO_3, $CaCO_3^o$, $MgCO_3^o$
Solid species:	$CaCO_3$ (Calcite), $Al_2Si_2O_5(OH)_4$ (Kaolinite), $MgCO_3$ (Magnesite), $NaAlSi_2O_6.H_2O$ (Analcite), SiO_2 (Silica), $Mg(OH)_2$ (Magnesium Hydroxide)
Adsorbed cations on rock surface:	$\overline{H}^{+}$, $\overline{Na}^{+}$, $\overline{Ca}^{2+}$, $\overline{Mg}^{2+}$
Adsorbed cations on micelles:	$\overline{\overline{Na}}^{+}$, $\overline{\overline{Ca}}^{2+}$, $\overline{\overline{Mg}}^{2+}$

Aqueous reactions	Equilibrium constant
$H_2O \overset{K_1^{eq}}{\rightleftharpoons} H^+ + OH^-$	$K_1^{eq} = [H^+]\ [OH^-]$
$H^+ + CO_3^{2-} \overset{K_2^{eq}}{\rightleftharpoons} HCO_3^-$	$K_2^{eq} = \dfrac{\left[HCO_3^-\right]}{[H^+]\left[CO_3^{2-}\right]}$
$Ca^{2+} + H_2O \overset{K_3^{eq}}{\rightleftharpoons} Ca(OH)^+ + H^+$	$K_3^{eq} = \dfrac{[Ca(OH)^+]\ [H^+]}{[Ca^{2+}]}$
$Mg^{2+} + H_2O \overset{K_4^{eq}}{\rightleftharpoons} Mg(OH)^+ + H^+$	$K_4^{eq} = \dfrac{[Mg(OH)^+]\ [H^+]}{[Mg^{2+}]}$
$Al^{3+} + H_2O \overset{K_5^{eq}}{\rightleftharpoons} Al(OH)^{2+} + H^+$	$K_5^{eq} = \dfrac{[Al(OH)^{2+}][H^+]}{[Al^{3+}]}$
$Al^{3+} + 2H_2O \overset{K_6^{eq}}{\rightleftharpoons} Al(OH)_2^+ + 2H^+$	$K_6^{eq} = \dfrac{[Al(OH)_2^+][H^+]^2}{[Al^{3+}]}$
$Al^{3+} + 4H_2O \overset{K_7^{eq}}{\rightleftharpoons} Al(OH)_4^- + 4H^+$	$K_7^{eq} = \dfrac{[Al(OH)_4^-][H^+]^4}{[Al^{3+}]}$
$H_4SiO_4 \overset{K_8^{eq}}{\rightleftharpoons} H^+ + H_3SiO_4^-$	$K_8^{eq} = \dfrac{[H^+][H_3SiO_4^-]}{[H_4SiO_4]}$
$H_4SiO_4 \overset{K_9^{eq}}{\rightleftharpoons} 2H^+ + H_2SiO_4^{2-}$	$K_9^{eq} = \dfrac{[H^+]^2[H_2SiO_4^{2-}]}{[H_4SiO_4]}$
$Ca^{2+} + H^+ + CO_3^{2-} \overset{K_{10}^{eq}}{\rightleftharpoons} Ca(HCO_3)^+$	$K_{10}^{eq} = \dfrac{\left[Ca(HCO_3)^+\right]}{[Ca^{2+}]\left[CO_3^{2-}\right][H^+]}$
$Mg^{2+} + H^+ + CO_3^{2-} \overset{K_{11}^{eq}}{\rightleftharpoons} Mg(HCO_3)^+$	$K_{11}^{eq} = \dfrac{\left[Mg(HCO_3)^+\right]}{[Mg^{2+}]\left[CO_3^{2-}\right][H^+]}$

$2H^{+} + CO_3^{2-} \overset{K_{12}^{eq}}{\underset{\blacklozenge}{\varnothing}} H_2CO_3$

$$K_{12}^{eq} = \frac{[H_2CO_3]}{\left[CO_3^{2-}\right][H^{+}]^{2}}$$

$2H_4SiO_4 \overset{K_{13}^{eq}}{\underset{\blacklozenge}{\varnothing}} 2H_2O + 3H^{+} + HSi_2O_6^{3-}$

$$K_{13}^{eq} = \frac{[H^{+}]^{3}[HSi_2O_6^{3-}]}{[H_4SiO_4]^{2}}$$

$2H_4SiO_4 \overset{K_{14}^{eq}}{\underset{\blacklozenge}{\varnothing}} 2H^{+} + 3H_2O + Si_2O_5^{2-}$

$$K_{14}^{eq} = \frac{[H^{+}]^{2}[Si_2O_5^{2-}]}{[H_4SiO_4]^{2}}$$

Solid species	Solubility product
$CaCO_3$	$K_1^{sp} = [Ca^{2+}]\left[CO_3^{2-}\right]$
$MgCO_3$	$K_2^{sp} = [Mg^{2+}]\left[CO_3^{2-}\right]$
SiO_2	$K_3^{sp} = [H_4SiO_4]$
$Al_2Si_2O_5(OH)_4$	$K_4^{sp} = [H^{+}]^{-6}[Al^{3+}]^{2}[H_4SiO_4]^{2}$
$NaAlSi_2O_6.H_2O$	$K_5^{sp} = [H^{+}]^{-4}[Na^{+}][Al^{3+}][H_4SiO_4]$ 2
$Mg(OH)_2$	$K_6^{sp} = [Mg^{2+}][H^{+}]^{-2}$

Exchange reactions (on matrix)	Exchange equilibrium constant
$2\overline{Na}^{+} + Ca^{2+} \overset{K_1^{ex}}{\underset{\blacklozenge}{\varnothing}} 2Na^{+} + \overline{Ca}^{2+}$	$K_1^{ex} = \frac{\left[\overline{Ca}^{2+}\right][Na^{+}]^{2}}{[Ca^{2+}]\left[\overline{Na}^{+}\right]^{2}}$
$2\overline{Na}^{+} + Mg^{2+} \overset{K_2^{ex}}{\underset{\blacklozenge}{\varnothing}} 2Na^{+} + \overline{Mg}^{2+}$	$K_2^{ex} = \frac{\left[\overline{Mg}^{2+}\right][Na^{+}]^{2}}{[Mg^{2+}]\left[\overline{Na}^{+}\right]^{2}}$

$$\overline{H}^{+} + Na^{+} + OH^{-} \overset{K_3^{ex}}{\rightleftharpoons} \overline{Na}^{+} + H_2O \qquad K_3^{ex} = \frac{[Na^{+}]\left[\overline{H}^{+}\right]}{\left[\overline{Na}^{+}\right][H^{+}]}$$

<u>Exchange reactions (on micelle)</u> — <u>Exchange equilibrium constant</u>

$$2\overline{\overline{Na}}^{+} + Ca^{2+} \overset{K_1^{exm}}{\rightleftharpoons} 2Na^{+} + \overline{\overline{Ca}}^{2+} \qquad K_1^{exm} = \frac{\left[\overline{\overline{Ca}}^{2+}\right][Na^{+}]^2}{\left[\overline{\overline{Na}}^{+}\right]^2[Ca^{2+}]}$$

where $K_1^{exm} = \beta_1^{exm}\ [S^{-}]$

$$2\overline{\overline{Na}}^{+} + Mg^{2+} \overset{K_2^{exm}}{\rightleftharpoons} 2Na^{+} + \overline{\overline{Mg}}^{2+} \qquad K_2^{exm} = \frac{\left[\overline{\overline{Mg}}^{2+}\right][Na^{+}]^2}{\left[\overline{\overline{Na}}^{+}\right]^2[Mg^{2+}]}$$

where $K_2^{exm} = \beta_2^{exm}\ [S^{-}]$

B.6.9 List of Elements and Reactive Species for IREACT = 5

Elements or pseudo-element:	Hydrogen (reactive), Sodium, Calcium, Magnesium, Carbonate, Aluminum, Silicon, A (from acid HA), Oxygen, Chlorine, S (InjectedSurfactant)
Independent aqueous or oleic species:	H^{+}, Na^{+}, Ca^{2+}, Mg^{2+}, Al^{3+}, CO_3^{2-} , H_4SiO_4, HA_o, H_2O
Dependent aqueous species:	$Ca(OH)^{+}$, $Mg(OH)^{+}$, $Al(OH)^{2-}$, $Al(OH)_2^{-}$, $Ca(HCO_3)^{+}$, $Mg(HCO_3)^{+}$, A^{-}, OH^{-}, HCO_3^{-} , $H_3SiO_4^{-}$, $H_2SiO_4^{2-}$, $HSi_2O_6^{3-}$, $Si_2O_5^{2-}$, $Al(OH)_4^{-}$, H_2CO_3, HA_w
Solid species:	$CaCO_3$ (Calcite), $Al_2Si_2O_5(OH)_4$ (Kaolinite), $MgCO_3$ (Magnesite), $NaAlSi_2O_6{\cdot}H_2O$ (Analcite), SiO_2 (Silica), $Mg(OH)_2$, (Magnesium Hydroxide)
Adsorbed cations on rock surface:	$\overline{H}^{+}$, $\overline{Na}^{+}$, $\overline{Ca}^{2+}$, $\overline{Mg}^{2+}$
Adsorbed cations on micelles:	$\overline{\overline{Na}}^{+}$, $\overline{\overline{Ca}}^{2+}$, $\overline{\overline{Mg}}^{2+}$

Aqueous reactions	Equilibrium constant
$H_2O \overset{K_1^{eq}}{\rightleftharpoons} H^+ + OH^-$	$K_1^{eq} = [H^+]\ [OH^-]$
$HA_w + OH^- \overset{K_2^{eq}}{\rightleftharpoons} A^- + H_2O$	$K_2^{eq} = \frac{[A^-]\ [H^+]}{[HA_w]}$
$H^+ + CO_3^{2-} \overset{K_3^{eq}}{\rightleftharpoons} HCO_3^-$	$K_3^{eq} = \frac{\left[HCO_3^-\right]}{[H^+]\left[CO_3^{2-}\right]}$
$Ca^{2+} + H_2O \overset{K_4^{eq}}{\rightleftharpoons} Ca(OH)^+ + H^+$	$K_4^{eq} = \frac{[Ca(OH)^+]\ [H^+]}{[Ca^{2+}]}$
$Mg^{2+} + H_2O \overset{K_5^{eq}}{\rightleftharpoons} Mg(OH)^+ + H^+$	$K_5^{eq} = \frac{[Mg(OH)^+]\ [H^+]}{[Mg^{2+}]}$
$Al^{3+} + H_2O \overset{K_6^{eq}}{\rightleftharpoons} Al(OH)^{2+} + H^+$	$K_6^{eq} = \frac{[Al(OH)^{2+}][H^+]}{[Al^{3+}]}$
$Al^{3+} + 2H_2O \overset{K_7^{eq}}{\rightleftharpoons} Al(OH)_2^+ + 2H^+$	$K_7^{eq} = \frac{[Al(OH)_2^+][H^+]^2}{[Al^{3+}]}$
$Al^{3+} + 4H_2O \overset{K_8^{eq}}{\rightleftharpoons} Al(OH)_4^- + 4H^+$	$K_8^{eq} = \frac{[Al(OH)_4^-][H^+]^4}{[Al^{3+}]}$
$H_4SiO_4 \overset{K_9^{eq}}{\rightleftharpoons} H^+ + H_3SiO_4^-$	$K_9^{eq} = \frac{[H^+][H_3SiO_4^-]}{[H_4SiO_4]}$
$H_4SiO_4 \overset{K_{10}^{eq}}{\rightleftharpoons} 2H^+ + H_2SiO_4^{2-}$	$K_{10}^{eq} = \frac{[H^+]^2[H_2SiO_4^{2-}]}{[H_4SiO_4]}$
$Ca^{2+} + H^+ + CO_3^{2-} \overset{K_{11}^{eq}}{\rightleftharpoons} Ca(HCO_3)^+$	$K_{11}^{eq} = \frac{\left[Ca(HCO_3)^+\right]}{[Ca^{2+}]\left[CO_3^{2-}\right][H^+]}$

$$Mg^{2+} + H^{+} + CO_3^{2-} \overset{K_{12}^{eq}}{\rightleftharpoons} Mg(HCO_3)^{+} \qquad K_{12}^{eq} = \frac{\left[Mg(HCO_3)^{+}\right]}{[Mg^{2+}]\left[CO_3^{2-}\right][H^{+}]}$$

$$2H^{+} + CO_3^{2-} \overset{K_{13}^{eq}}{\rightleftharpoons} H_2CO_3 \qquad K_{13}^{eq} = \frac{[H_2CO_3]}{\left[CO_3^{2-}\right][H^{+}]^{2}}$$

$$2H_4SiO_4 \overset{K_{14}^{eq}}{\rightleftharpoons} 2H_2O + 3H^{+} + HSi_2O_6^{3-} \qquad K_{14}^{eq} = \frac{[H^{+}]^{3}[HSi_2O_6^{3-}]}{[H_4SiO_4]^{2}}$$

$$2H_4SiO_4 \overset{K_{15}^{eq}}{\rightleftharpoons} 2H^{+} + 3H_2O + Si_2O_5^{2-} \qquad K_{15}^{eq} = \frac{[H^{+}]^{2}[Si_2O_5^{2-}]}{[H_4SiO_4]^{2}}$$

Partitioning of HA	Partition coefficient
$HA_o \overset{K_D}{\rightleftharpoons} HA_w$	$K_D = \frac{[HA_w]\,water}{[HA_o]\,oil}$

Solid species	Solubility product
$CaCO_3$	$K_1^{sp} = [Ca^{2+}]\left[CO_3^{2-}\right]$
$MgCO_3$	$K_2^{sp} = [Mg^{2+}]\left[CO_3^{2-}\right]$
SiO_2	$K_3^{sp} = [H_4SiO_4]$
$Al_2Si_2O_5(OH)_4$	$K_4^{sp} = [H^{+}]^{-6}[Al^{3+}]^{2}[H_4SiO_4]^{2}$
$NaAlSi_2O_6.H_2O$	$K_5^{sp} = [H^{+}]^{-4}[Na^{+}][Al^{3+}][H_4SiO_4]^{2}$
$Mg(OH)_2$	$K_6^{sp} = [Mg^{2+}][H^{+}]^{-2}$

Exchange reactions (on matrix) Exchange equilibrium constant

$$2\overline{\mathrm{Na}}^{+} + \mathrm{Ca}^{2+} \overset{K_1^{ex}}{\rightleftharpoons} 2\mathrm{Na}^{+} + \overline{\mathrm{Ca}}^{2+}$$

$$K_1^{ex} = \frac{\left[\overline{\mathrm{Ca}}^{2+}\right][\mathrm{Na}^{+}]^{2}}{[\mathrm{Ca}^{2+}]\left[\overline{\mathrm{Na}}^{+}\right]^{2}}$$

$$2\overline{\mathrm{Na}}^{+} + \mathrm{Mg}^{2+} \overset{K_2^{ex}}{\rightleftharpoons} 2\mathrm{Na}^{+} + \overline{\mathrm{Mg}}^{2+}$$

$$K_2^{ex} = \frac{\left[\overline{\mathrm{Mg}}^{2+}\right][\mathrm{Na}^{+}]^{2}}{[\mathrm{Mg}^{2+}]\left[\overline{\mathrm{Na}}^{+}\right]^{2}}$$

$$\overline{\mathrm{H}}^{+} + \mathrm{Na}^{+} + \mathrm{OH}^{-} \overset{K_3^{ex}}{\rightleftharpoons} \overline{\mathrm{Na}}^{+} + \mathrm{H_2O}$$

$$K_3^{ex} = \frac{[\mathrm{Na}^{+}]\left[\overline{\mathrm{H}}^{+}\right]}{\left[\overline{\mathrm{Na}}^{+}\right][\mathrm{H}^{+}]}$$

Exchange reactions (on micelle) Exchange equilibrium constant

$$2\overline{\overline{\mathrm{Na}}}^{+} + \mathrm{Ca}^{2+} \overset{K_1^{exm}}{\rightleftharpoons} 2\mathrm{Na}^{+} + \overline{\overline{\mathrm{Ca}}}^{2+}$$

$$K_1^{exm} = \frac{\left[\overline{\overline{\mathrm{Ca}}}^{2+}\right][\mathrm{Na}^{+}]^{2}}{\left[\overline{\overline{\mathrm{Na}}}^{+}\right]^{2}[\mathrm{Ca}^{2+}]}$$

where $K_1^{exm} = \beta_1^{exm}\,\{[\mathrm{A}^-] + [\mathrm{S}^-]\}$

$$2\overline{\overline{\mathrm{Na}}}^{+} + \mathrm{Mg}^{2+} \overset{K_2^{exm}}{\rightleftharpoons} 2\mathrm{Na}^{+} + \overline{\overline{\mathrm{Mg}}}^{2+}$$

$$K_2^{exm} = \frac{\left[\overline{\overline{\mathrm{Mg}}}^{2+}\right][\mathrm{Na}^{+}]^{2}}{\left[\overline{\overline{\mathrm{Na}}}^{+}\right]^{2}[\mathrm{Mg}^{2+}]}$$

where $K_2^{exm} = \beta_2^{exm}\,\{[\mathrm{A}^-] + [\mathrm{S}^-]\}$

Appendix C
Discretized Flow Equations

The coordinate system can be either cartesian, radial, or curvilinear. The discretized equations presented here are for the cartesian coordinate system referred to as (x, y, z). The finite-difference grid is block-centered and numbered from 1 to $N_xN_yN_z$, where N_x, N_y, and N_z correspond to the number of gridblocks in the x, y, and z directions, respectively. The volume of the m^th block (i, j, k) is $\Delta V_m=\Delta x_m \Delta y_m \Delta z_m$ where i, j, and k correspond to the x, y, and z coordinate directions, respectively. The time increment δt is from timestep n to timestep n+1. The delta operator δ denotes discrete differences:

$$\begin{aligned}
&\delta_t f^n = f^{n+1} - f^n \\
&\delta_x f_m = f_m - f_{m-1}, \delta_x f_i = f_i - f_{i-1} \\
&\delta_y f_m = f_m - f_{m-Nx}, \delta_y f_j = f_j - f_{j-1} \\
&\delta_z f_m = f_m - f_{m-NxNy}, \delta_z f_k = f_k - f_{k-1}
\end{aligned} \tag{C.1}$$

Most variables, including pressure, concentrations, adsorbed concentrations, saturations, capillary pressures, phase properties such as density, viscosity, interfacial tension, and relative permeabilities are calculated and stored at gridblock centers. Some variables, such as transmissibilities and phase velocities, are evaluated at the faces between gridblocks. Applying the finite-difference approximations to the species conservation equations (Eq. C.1) and the pressure equation (Eq. C.10), we obtain a system of finite-difference equations. For the purpose of simplicity, the system of equations is illustrated for a two-dimensional problem even though the code is three-dimensional.

The species conservation equation for species κ at gridpoint m is

$$\left(F_{a\kappa}\right)_m^{n+1} = \left(F_{a\kappa}\right)_m^n + \delta_t t^n \left(F_{t\kappa} + F_{q\kappa}\right)_m^{\bar{n}} \tag{C.2}$$

The superscript $\bar{n}$ indicates that the variables are evaluated using both old timestep (n) variables and new timestep (n+1) variables.

$F_{a\kappa}$ is the accumulation term

$$\left(F_{a\kappa}\right)_m = \left\{\phi_R \Delta V \tilde{C}_\kappa \left[1 + \left(C_f + C_\kappa^0\right)\left(P_R - P_{R0}\right)\right]\right\}_m \tag{C.3}$$

$F_{t\kappa}$ is the transport term as

$$
\begin{aligned}
(F_{t\kappa})_m^{\bar{n}} = -\delta_x & \left[1 + C_\kappa^0 (P_R - P_{R0})\right]_m^{n+1} \sum_{\ell=1}^{n_p} \Big\{ (C_{x\kappa\ell})_m^n (\bar{T}_{x\ell})_m^n \\
& \cdot \left[\delta_x \left(P_R^{n+1} + P_{c\ell R}^n \right)_{m+1} - \left(\bar{\gamma}_{x\ell}^n \right)_m \delta_x (D)_{m+1} \right] \\
& + \left(\bar{K}_{xx\kappa\ell}^{\bar{n}} \right)_m \delta_x \left(C_{\kappa\ell}^n \right)_{m+1} + \left(\bar{K}_{xy\kappa\ell}^{\bar{n}} \right)_m \delta_y \left[\left(C_{\kappa\ell}^n \right)_m + \left(C_{\kappa\ell}^n \right)_{m+Nx} \right] \Big\} \\
-\delta_x & \left[1 + C_\kappa^0 (P_R - P_{R0})\right]_m^{n+1} \sum_{\ell=1}^{n_p} \Big\{ (C_{y\kappa\ell})_m (\bar{T}_{y\ell})_m \\
& \cdot \left[\delta_y \left(P_R^{n+1} + P_{c\ell R}^n \right)_{m+Nx} - \left(\bar{\gamma}_{y\ell}^n \right)_m \delta_y (D)_{m+Nx} \right] \\
& + \left(\bar{K}_{yy\kappa\ell}^{\bar{n}} \right)_m \delta_y \left(C_{\kappa\ell}^n \right)_{m+Nx} + \left(\bar{K}_{yx\kappa\ell}^{\bar{n}} \right)_m \delta_x \left[\left(C_{\kappa\ell}^n \right)_m + \left(C_{\kappa\ell}^n \right)_{m+1} \right] \Big\}
\end{aligned}
\tag{C.4}
$$

where $C_{x\kappa\ell}$, $C_{y\kappa\ell}$, $\bar{T}_{x\ell}$, and $\bar{T}_{y\ell}$ are defined by

$$
\begin{aligned}
(C_{x\kappa\ell})_m &= (C_{\kappa\ell})_m + \varphi_m \left\{ r_{xm} \left[(C_{\kappa\ell})_m \right] \right\} \delta_x (C_{\kappa\ell})_{m+1} / 2 \\
(C_{y\kappa\ell})_m &= (C_{\kappa\ell})_m + \varphi_m \left\{ r_{ym} \left[(C_{\kappa\ell})_m \right] \right\} \delta_y (C_{\kappa\ell})_{m+Nx} / 2
\end{aligned}
\tag{C.5}
$$

$$
\begin{aligned}
(\bar{T}_{x\ell})_m &= \left\{ (k_{r\ell})_m \varphi_m \left\{ r_{xm} \left[(k_{r\ell})_m \right] \right\} \delta_x (k_{r\ell})_{m+1} / 2 \right\} (T_x / \mu_\ell)_m \\
(\bar{T}_{y\ell})_m &= \left\{ (k_{r\ell})_m \varphi_m \left\{ r_{ym} \left[(k_{r\ell})_m \right] \right\} \delta_y (k_{r\ell})_{m+Nx} / 2 \right\} (T_y / \mu_\ell)_m
\end{aligned}
\tag{C.6}
$$

$(T_x)_m$ and $(T_y)_m$, given by

$$
\begin{aligned}
(T_x)_m &= 2(\Delta y \Delta z)_m / (\Delta x_m / k_m + \Delta x_{m+1} / k_{m+1}) \\
(T_y)_m &= 2(\Delta x \Delta z)_m / (\Delta y_m / k_m + \Delta y_{m+Nx} / k_{m+Nx})
\end{aligned}
\tag{C.7}
$$

are transmissibilities.

φ_m is the flux limiter function defined as follows (Liu *et al.*, 1994):

$$
\varphi_m = \frac{2\left(f_{m+1/2} - f_m\right)}{f_{m+1} - f_m}
\tag{C.8}
$$

The magnitude of the limiting depends on the smoothness of the data, measured by the ratio of consecutive cell gradients r:

$$
r_m = \frac{f_m - f_{m-1}}{f_{m+1} - f_m}
\tag{C.9}
$$

and $\varphi(r) = \max\left(0, \min\left(\varphi_b, \frac{2 + r}{3} \right) \right)$.

$$\begin{aligned}
r_{xm}\left[\left(C_{\kappa\ell}\right)_m\right] &= \delta_x\left(C_{\kappa\ell}\right)_m \Big/ \delta_x\left(C_{\kappa\ell}\right)_{m+1}\\
r_{ym}\left[\left(C_{\kappa\ell}\right)_m\right] &= \delta_y\left(C_{\kappa\ell}\right)_m \Big/ \delta_y\left(C_{\kappa\ell}\right)_{m+Nx}\\
r_{xm}\left[\left(k_{r\ell}\right)_m\right] &= \delta_x\left(k_{r\ell}\right)_m \Big/ \delta_x\left(k_{r\ell}\right)_{m+1}\\
r_{ym}\left[\left(k_{r\ell}\right)_m\right] &= \delta_y\left(k_{r\ell}\right)_m \Big/ \delta_y\left(k_{r\ell}\right)_{m+Nx}
\end{aligned} \tag{C.10}$$

$\overline{K}_{xx\kappa\ell}, \overline{K}_{yy\kappa\ell}, \overline{K}_{xy\kappa\ell}$, and $\overline{K}_{yx\kappa\ell}$ are the dispersion coefficients defined by

$$\begin{aligned}
\left(\overline{K}_{xx\kappa\ell}\right)_m &= \Delta y_m \Delta z_m \Big/ \left[\left(\Delta x_m + \Delta x_{m+1}\right)/2\right]\left(\phi_R S_\ell K_{xx\kappa\ell} + \delta_t t^n u_{x\ell}^2 / \phi_R\right)_m\\
\left(\overline{K}_{xy\kappa\ell}\right)_m &= \Delta y_m \Delta z_m \Big/ \left[\Delta y_m + \left(\Delta y_{m-Nx} + \Delta y_{m+Nx}\right)/2\right]\left(\phi_R S_\ell K_{xy\kappa\ell} + \delta_t t^n u_{y\ell} / \phi_R\right)_m\\
\left(\overline{K}_{yy\kappa\ell}\right)_m &= \Delta x_m \Delta z_m \Big/ \left[\left(\Delta y_m + \Delta y_{m+Nx}\right)/2\right]\left(\phi_R S_\ell K_{yy\kappa\ell} + \delta_t t^n u_{y\ell}^2 / \phi_R\right)_m\\
\left(\overline{K}_{yx\kappa\ell}\right)_m &= \Delta y_m \Delta z_m \Big/ \left[\Delta x_m + \left(\Delta x_{m-1} + \Delta x_{m+1}\right)/2\right]\left(\phi_R S_\ell K_{yx\kappa\ell} + \delta_t t^n u_{y\ell} u_{x\ell} / \phi_R\right)_m
\end{aligned} \tag{C.11}$$

The average specific weight of phase ℓ is calculated from

$$\begin{aligned}
\left(\overline{\gamma}_{x\ell}\right)_m &= \left[\left(\gamma_\ell E_\ell \Delta x\right)_m + \left(\gamma_\ell E_\ell \Delta x\right)_{m+1}\right] \Big/ \left[\left(E_\ell \Delta x\right)_m + \left(E_\ell \Delta x\right)_{m+1}\right]\\
\left(\overline{\gamma}_{y\ell}\right)_m &= \left[\left(\gamma_\ell E_\ell \Delta y\right)_m + \left(\gamma_\ell E_\ell \Delta x\right)_{m+Nx}\right] \Big/ \left[\left(E_\ell \Delta y\right)_m + \left(E_\ell \Delta y\right)_{m+Nx}\right]
\end{aligned} \tag{C.12}$$

where E_ℓ is the existence index of phase ℓ and is defined as

$$\left(E_\ell\right)_m = \begin{cases} 0 & \left(S_\ell\right)_m = 0 \\ 1 & \left(S_\ell\right)_m > 0 \end{cases} \tag{C.13}$$

$F_{q\kappa}$ is the source and sink term:

$$\begin{aligned}
\left(F_{q\kappa}\right)_m^{\bar{n}} = \Bigg\{ &\sum_{\ell=1}^{n_p}\left[Q_\ell^n + (PI)_\ell^n\left(P_{wf} - P_R^{n+1} - P_{c\ell R}^n\right)\right]C_{\kappa\ell}^n\\
&+\phi_R \Delta V\left[1 + \left(C_f + C_\kappa^0\right)\left(P_R^{n+1} - P_{R0}\right)\right]\left(\sum_{\ell=1}^{n_p} S_\ell^n r_{\kappa\ell} + r_{\kappa s}\right)\Bigg\}_m
\end{aligned} \tag{C.14}$$

which includes wells constrained by either rate or pressure and the production from chemical reactions.

The pressure equation at gridpoint m is

$$\left(F_a^{n+1} - F_{t1}^{\bar{n}}\right)_m = \left(F_a\right)_m^n + \delta_t t^n\left(F_{t2} + F_q\right)_m^n \tag{C.15}$$

F_a is the total accumulation

$$\left(F_a\right)_m = \left(\phi_R \Delta V C_t P_R\right)_m \tag{C.16}$$

F_{t1} is the total transport as a function of reference phase pressure:

$$\begin{aligned}\left(F_{t1}^{\bar{n}}\right)_m = & -\delta_x\left\{\sum_{\ell=1}^{n_p}\left(\bar{T}_{x\ell}\right)_m^n\left[1+\left(P_R-P_{R0}\right)\sum_{\kappa=1}^{n_{cv}}C_\kappa^0 C_{\kappa\ell}\right]_m^n \delta_x\left(P_R^{n+1}\right)_{m+1}\right\} \\ & -\delta_y\left\{\sum_{\ell=1}^{n_p}\left(\bar{T}_{y\ell}\right)_m^n\left[1+\left(P_R-P_{R0}\right)\sum_{\kappa=1}^{n_{cv}}C_\kappa^0 C_{\kappa\ell}\right]_m^n \delta_y\left(P_R^{n+1}\right)_{m+Nx}\right\}\end{aligned} \tag{C.17}$$

Both F_{t2}, the total transport as a function of capillary pressure and gravity, and F_q, the total source or sink, are evaluated using values of the old timestep:

$$\begin{aligned}\left(F_{t2}\right)_m = & -\delta_x\left\{\sum_{\ell=1}^{n_p}\left(\bar{T}_{x\ell}\right)_m\left[1+\left(P_R-P_{R0}\right)\sum_{\kappa=1}^{n_{cv}}C_\kappa^0 C_{\kappa\ell}\right]_m \cdot\left[\delta_x\left(P_{c\ell R}\right)_{m+1}-\left(\bar{\gamma}_{x\ell}\right)_m\delta_x\left(D\right)_{m+1}\right]\right\} \\ & -\delta_y\left\{\sum_{\ell=1}^{n_p}\left(\bar{T}_{y\ell}\right)_m\left[1+\left(P_R-P_{R0}\right)\sum_{\kappa=1}^{n_{cv}}C_\kappa^0 C_{\kappa\ell}\right]_m \cdot\left[\delta_y\left(P_{c\ell R}\right)_{m+Nx}-\left(\bar{\gamma}_{y\ell}\right)_m\delta_y\left(D\right)_{m+Nx}\right]\right\}\end{aligned} \tag{C.18}$$

$$\left(F_q\right)_m = \sum_{\kappa=1}^{n_{cv}}\sum_{\ell=1}^{n_p}\left\{\left[Q_\ell + \left(PI\right)_\ell\left(P_{wf}-P_R-P_{c\ell R}\right)\right]C_{\kappa\ell}\right\}_m \tag{C.19}$$

Coefficients of reference phase pressure P_R on the left-hand side of Eq. C.15 are concentration-dependent and are evaluated using values at the old timestep. The equation written for all gridblocks in the spatial domain results in a system of equations with reference phase pressure P_R as the only unknown and is solved implicitly. The conservation equations (Eq. C.2) are then solved explicitly for overall concentrations. Phase concentrations and saturations are obtained by phase equilibria calculations. Other phase pressures are obtained using capillary pressure relations.

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