

Criteria for Selection of Environmental Data Sets Decision Support Software Demonstration

One objective of the demonstration program is to test the capability of the selected Decision Support Software (DSS) to visualize contamination data and provide guidance on where to sample to define the region which is contaminated. A series of test cases is being developed. These test cases will, to the extent possible, be taken from existing environmental contamination problems. To test the capabilities of the DSS over a wide range of conditions a suite of test cases will be developed. The developers of the DSS will be asked to solve as many of the verification problems as they can during the demonstration to be held in the summer of 1998. The test cases will be designed to examine different aspects of the definition of the nature and extent of contamination with increasing levels of complexity. The following lists the criteria and data needs for selecting environmental data sets for use as test cases.

Contamination Zone Thoroughly Characterized

The data that will be used for testing will be from actual sites. Every effort will be made to keep the sites anonymous. As a benchmark for testing decision support tools, the data set must be complete enough to accurately define the location and extent of the contamination zone. The data should delineate the three-dimensional boundary of the contaminated zone. Detailed characterization of the contamination is the most important criteria for selection of a data set. If possible, data measurements over a period of time would be useful in developing test problems.

Contaminants

To test the range of capabilities in the Decision Support Software a number of contaminants with different transport characteristics should be tested. Contamination originating from the same source with multiple contaminants having significantly different transport characteristics would prove useful for testing. The types of contaminants needed include:

- ☐ non-aqueous phase liquids (NAPL): generally they are soluble in water up to a few parts per thousand, below this limit they will travel in the aqueous phase, above this limit they will travel as a separate phase. It is felt that most DSS will not address the movement of non-aqueous phase contaminants traveling as a separate phase. Therefore, the demonstration will focus on NAPL contamination that moves with the groundwater.
- ☐ heavy metals: often characterized by high degree of sorption and low mobility.
- ☐ radioactive: their unique characteristic is radioactive decay. Some radionuclides are mobile and relatively rapidly in the groundwater phase while others exhibit low-mobility and are predominantly found in the solid phase.

Phase

There are three phases in which the contaminant can reside, liquid, solid, or gas. For the demonstration problems, emphasis is placed on soil and groundwater contamination. For this

reason and because of the difficulty in predicting non-aqueous phase transport, problems with non-aqueous phase contamination existing as a separate phase should not be included. Gas phase contamination of volatile organic compounds is typically much less of a problem than liquid phase contamination and therefore will not be considered. Solid phase contamination is often a large problem for heavy metals and certain radionuclides (e.g., Cs-137) and will be considered for inclusion in the suite of test problems.

Performing a detailed calculation of water flow is an important but a time-consuming task. The demonstration is scheduled to last approximately two-weeks. It is felt that it is not possible to calibrate a water flow field in this time frame. Therefore, groundwater contamination problems will be developed for cases in which the flow is well behaved and can be adequately described using a simplification over the approach requiring calibration of the flow field. Water flow problems will be simplified by supplying a hydraulic potential map and hydraulic conductivities, or by supplying average flow rates over the problem domain.

Site History

The history of the site often provides important information pertaining to the nature and extent of contamination. The location and history of the facilities use of contaminated materials will be needed to help in the data evaluation.

An important piece of information for defining the plume is the history of potential sources. For example, the signature of a continuous source with relatively uniform release over time is a plume with highest concentrations near the source which will decrease as one moves away from the source region. In contrast, if the source resulted from a one-time event or a short-duration event, the maximum concentration is located away from the source and the leading and trailing edges of the plume depend on the source and transport characteristics. Both types of problems should be tested if possible.

Site Characterization

Knowledge pertaining to the local geohydrology and stratigraphic units may be needed to supply data for the analysis. General information such as the average groundwater flow rate and direction, porosity, sorption characteristics (K_d), thickness of the unsaturated zone, thickness of the aquifer, etc., may also be needed to define the problem.

Contamination in fractured media is characterized by regions of high concentration in the fractures and low concentrations outside of the fractures. The regions of high concentration are extremely variable and may change markedly on the order of a few inches or feet. These sites are difficult to characterize and most likely their analysis is beyond the scope of existing DSS. For this reason, data from fractured sites will have to be carefully reviewed prior to inclusion in the final suite of test problems. It may not be possible to define a problem from a fractured site for the demonstration.

Types of Problems:

The preceding sections present the general requirements for data to define problems for testing of DSS. The next three sections, Types of Problems, Data Set Requirements, and Data, provide a more detailed description of the data needs and the format in which they are needed. When selecting a problem for consideration, the following information is needed.

For the demonstration data for the following types of problems is desired:

- ☐ a two-dimensional surface soil contamination problem (5-10 acres in size)
- ☐ a three-dimensional surface/subsurface soil contamination problem (5-10 acres in size)
- ☐ a groundwater contamination problem - flow adequately represented as one-dimensional (horizontal flow)
- ☐ a groundwater contamination problem - flow adequately represented in two-dimensions (horizontal and vertical flow)
- ☐ A groundwater contamination problem - multiple flow paths, layered geologic media with a fully three-dimensional flow field).
- ☐ soil and groundwater contamination - simple flow field, one or two-dimensional.

Examples with multiple contaminants are preferred. However, single contaminant problems are also desirable. It is desired to have a wide range of contaminants for testing. As a minimum, data containing VOC contamination in groundwater and metal/radionuclide contamination in soils should be obtained.

Data Sets Requirements (narrative):

For each problem a narrative description of the site and operational history relative to the contaminant(s) of concern is needed. The narrative should describe the general characteristics of the problem and any special circumstances that are known. The following example provides the level of detail requested: TCA was used at this facility from 1970 - 1995. Operational records indicate that less than 50 gallons of TCA was spilled per year.. However, in 1982, a spill of approximately 325 gallons occurred.. Other spills of approximately 100 gallons occurred in 1975, 1980, and 1991. For groundwater contamination problems, general information on the site hydrogeology is needed. This is discussed further in data needs.

Data - electronic format only

The following provides a list of the major types and categories of data needed to develop the test problems.

- ☐ Contaminants
x,y,z coordinates and contaminant concentration for all sample locations. If the time history is available this may be useful for groundwater contamination problems.
- ☐ Site
Graphic files (gif or tif format) of site, buildings, roads, etc.
2-dimensional and/or 3-dimensional visualizations of site

- Geology, hydrogeology
Hydraulic potential maps (only groundwater contamination problems)
2D or 3D visualizations of geology, hydrogeology
- Transport parameters (only groundwater contamination problems)
Hydraulic conductivities for each stratigraphic unit
Hydraulic gradients over the flow domain
Average flow rates through each stratigraphic unit (if possible to define an average).
Dispersion parameters for each dimension in the problem (i.e. for a two-dimensional problem, dispersion parameters are needed for two directions.)
First order degradation rate parameters (biodegradation and radioactive decay rates)
Sorption parameters, distribution coefficient for each contaminant of concern for each stratigraphic unit.

Data should be provided by either e-mail, or downloaded from an FTP site. If it is possible to download data directly from a data base this is acceptable. If the data already exists in a GIS format (for example, Arcinfo), it would be helpful to have these files. We will need the data used to visualize the site, geology and hydrogeology in tabular as well as the visual format.. The tabular data will be used to define dimensions for problem definition.

Points of Contact

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