Report as of FY2006 for 2006CT105B: "GIM3 - A visual and interactive contaminant transport simulator for regulatory and educational applications"

Publications

- Other Publications:
  - Luo, Y. and X. Yang, 2006. Dynamics of chemicals at watershed scale: a geo-referenced multimedia modeling approach. ASABE Paper No. 062034. ASABE, St. Joseph, MI
- Articles in Refereed Scientific Journals:
  - Luo, Y. Q. Gao and X. Yang, 2007. Dynamic modeling of chemical fate and transport in multimedia environment at watershed scale, Part II. Trichloroethylene test case. Environmental Management 83: 56-65
- unclassified:
  - Luo, Y. Q. Gao and X. Yang, 2007. Dynamic modeling of chemical fate and transport in multimedia environment at watershed scale, Part I. Theoretical considerations and model implementation. Environmental Management 83: 44-55
  - Luo Y. and X. Yang, 2007. A multimedia environmental model of chemical distribution: fate, transport and uncertainty analysis. Chemosphere 66: 1396-1407

Report Follows

GIM3 - A Visual and Interactive Simulator of Contaminant Transport for Regulatory and Educational Applications

A Technical Report to Connecticut Water Resources Institute

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1 Introduction
1.1 Background Information

Pollutants released to the environment are distributed into various environmental compartments, such as water, soil, and biota, as a result of complex physical, chemical, and biological processes (Cohen *et al.*, 1990; Coulibaly *et al.*, 1998). Environmental-impact analysis of water quality in surface water and groundwater depends upon clear understanding of the source-receptor relations, which demand holistic modeling of the transport and transformation of the materials in multimedia arena. These models for water quality are traditionally based on a single environmental pathway, or loosely coupled with related pathways by considering the inter-media mass fluxes as inputs or outputs. A new multimedia modeling framework is in demand for the sake of a true integration of the contaminant transport processes in all the environmental components. To implement the model in regulatory and educational applications, a user-friendly interface has to be developed for the sophisticated mathematic algorithms and data analyses in the model.

As an attempt to track chemical dynamics with spatial variation in multimedia environment, a geo-referenced environmental fate model was developed at the University of Connecticut (Luo and Yang, 2003a, 2003b, 2004a, 2004b, 2005, 2005a, 2005b). This model relied on fugacity to describe the mass potential of chemical species in an Eulerian approach, in which the region of interest was divided into a number of connected boxes representing connected environmental system. Chemical fate and transport in seven major environmental media of air, plant foliage, ground soil, root zone, vadose zone, surface water, and sediment were incorporated in the modeling framework. The model started with inter-media physical and biological processes, representing a unique way in multimedia modeling (Most of the existing "multimedia models" start with uni-medium models and try to couple them by manipulating "boundary conditions" or "driving functions"). The numerical solution used a finite differential method in implicit scheme to solve the set of partial differential equations. The core algorithm is implemented using MATLAB code in IBM PC platform. Our model has been calibrated and tested for nitrogen species in the lower Connecticut River basin, CT and MA, and the Lamprey River basin, NH (Luo and Yang, 2003a, 2003b, 2004a, 2004b). The results showed that the model can simulate the nitrogen flux and load in the surface water and soil layers with acceptable accuracy in the comparison of USGS monitoring data and the field measurement from the Connecticut River Airshed-Watershed Consortium. The model was also applied to the field condition of the Connecticut River basin to simulate the transport of VOCs by using TCE as a test agent (Luo and Yang, 2005; Luo *et al.*, 2006). The predicted concentration and distribution in various environmental media were compared to published field data or predictions by well-validated models.

Over the years a number of simulation models has been developed for bulk flow and contaminant transport in the multi-media environment. Some of these applications are quite sophisticated with impressive capabilities (Devillers *et al.*, 1995; Van Dam, 1997; Woodbury, 2000). However, most of these simulators are designed for professional purpose, and not easy for students to use or for daily regulatory purposes. In this project,

we developed a user-friendly simulator of contaminant transport and transformation in a multimedia environment, GIM^3, representing GIS-integrated multimedia model at watershed scale. This computer program was based on our current studies at the University of Connecticut. We foresee a potential of our software in regulatory and educational applications, provided a user-friendly (visual and interactive) interface be developed.

With the capacity of simulating the source-receptor relationships and predicting geographic distribution of pollutants, the software developed in this study can be a practical tool for government agencies to evaluate and regulate various contamination sources in agricultural and industrial activities. The integration of transport processes, visual interactivity, and seamless communication features make the model possible for user to focus on critical conceptual issues, to quickly and iteratively examine hypotheses and system responses, to identify dominant processes, and to assess key parameters. Additionally, as an educational application, this software environment allows student to visually examine the dynamics of the bulk flow, contaminant transport, and biochemical transformation. Therefore, the proposed software can be used to enhance teaching and learning in number of courses across environmental engineering and water resources curriculum at graduate and undergraduate levels, such as Environmental Biophysics, Transport Phenomena, Groundwater modeling, and Small Watershed Analysis.

1.2   Program Overview

GIM^3 is aimed to provide a meaningful computer-based platform for the simulation, analysis, visualization, and presentation of chemical fate and distribution in the multimedia environment. Shown in **Figure 1** are the modules proposed in GIM^3, including (1) multimedia transport simulator, (2) site definition, (3) data management, and (4) Graphic User Interface (GUI). The multimedia transport model in our previous study was the core simulator. Site definition module conducts data preparation and spatial allocation for the sequent core multimedia simulation processor. Data management module was designed to collect, acquire, and share data within the whole simulation system. GUI provided an interactive platform for users to design simulation scenario and view the results. The computer program was developed following the procedures below.
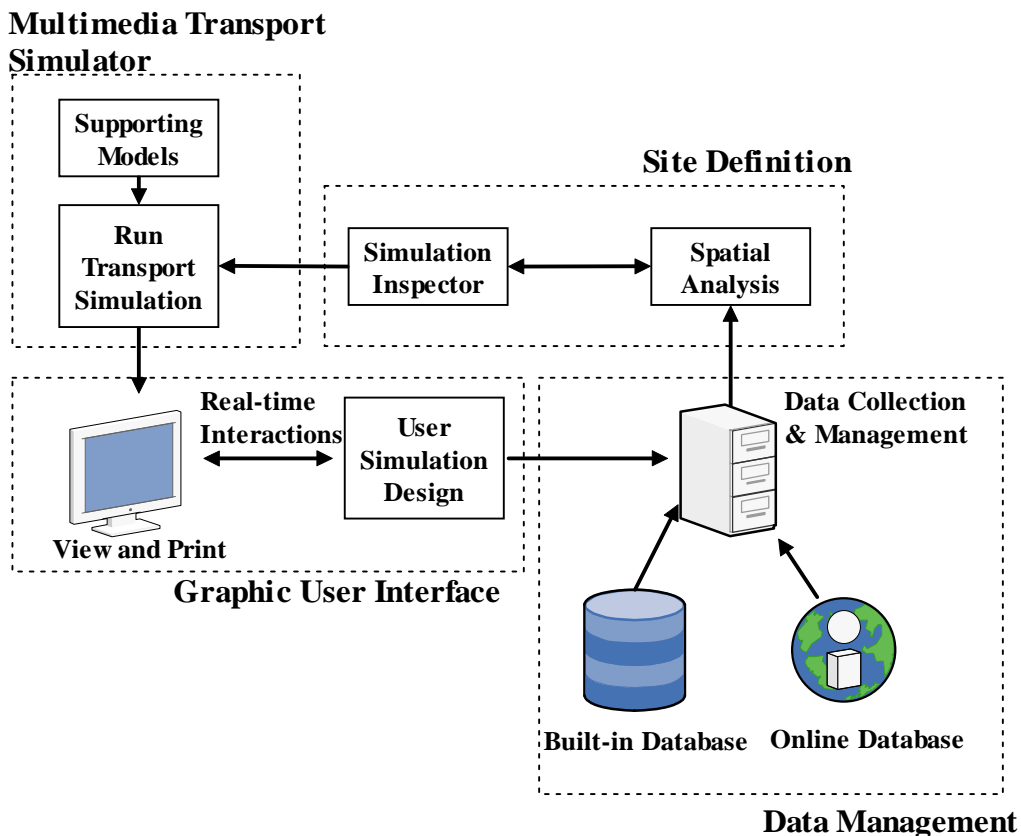
Figure 1. Structure of GIM^3 modules

(1) Restructure the multimedia transport simulator

Designed for research purpose, the multimedia environmental model in our previous studies treated the multimedia transport simulation and other supporting procedures (e.g., data preparation and results presentation) in separate sequential processes. As we elaborate further on, however, GIM^3 is expected to significantly advance the state of regulatory and educational computing in the field of environmental and water resources engineering by bringing decision-makers and students much closer to the process of scientific investigation, discovery, and design. Therefore, the original codes of multimedia fate and transport were restructured to dynamically and intelligently treat scenario design, site definition, analysis and visualization. The simulation algorithm was rebuilt as reusable components that can be manipulated visually in a simulation scenario design. Users start with a collection of such components, and wire them together to form multimedia transport simulation without actually writing any new codes. Typical components include,

- initialization components for input data formatting, global data inspection, and variable declaration,
- parameterization components for calculating the model parameters of fugacity capacity, bulk diffusivity, and mass transport coefficients,
- simulation components for handling initial and boundary conditions, generating numerical grids, and solving partial differential equations, and

- output components for presenting simulation results and preparing data for visualizations.

The revised model code was built in MATLAB Builder for COM (Common Object Model) to be embedded in the overall program (Ledin, 2004). Although GIM[3] involves essentially the same modeling components, the same amount of numerical and geographic computations and processing as in our multimedia transport model, they are restructured and integrated into a single application program, which makes it possible to perform real-time interactive multimedia modeling, real-time analysis, and real-time presentation.

(2) Develop GUIs for simulation design and real-time interaction
Decision-makers and students would naturally want to interact with modeling process in real-time. The real-time interactive capability was achieved by writing the graphical user interface via an object-oriented paradigm using Microsoft Visual Basic that calls a number of external model modules.

The GUI for simulation design was developed to assist users with the time-consuming chore of data compilation and specification of model parameters. Supported by the GUI, the users are established at the center of the system during the simulation design. The simulation design begins by specifying the study region, the time and length of the simulation, chemical information (properties, emission, and background concentration), compartments and inter-media transport processes to be included, initial and boundary conditions, and result output options. A similar interface is also developed for real-time interaction to change original configurations, and view the intermediate results. Users can pause at any time, during the simulation or analysis, to interact with most aspects of the modeling processes and modify parameters without having to restart the whole simulation. Once a simulation design or a real-time interaction has been completed, a simulation inspector automatically checks the setup parameters before the simulation execution. Areas of deficiency or inconsistence will be identified, thus enabling the users to quick provide the missing information or modify the incompatible inputs.

(3) Prepare input data and apply GIS technology in site definition
The meaningful real-world problem solving for regulatory and educational purposes may involve the use of national-wide environmental databases. The input information required for the model simulation comprised regional properties (landscape parameters, hydrologic conditions, and meteorological data) and pollutant information (chemical properties, emission rate, and background concentrations). GIM[3] will include a built-in chemical property database for most common contaminants and nutrients. In addition, users can add or edit entries in the database. Most of other input data are available in the on-line databases hosted by EPA, USGS, or other agents (**Table 15**). In GIM[3], GIS-based spatial analysis provides model input data by making use of very comprehensive landscape and chemical release data available form the different agencies. A number of data processing functions were designed in this study for such spatial analyses of watershed delineation, coordinate conversion, soil properties extraction, and parameter

aggregation. These functions were developed by specifying classes in the ESRI ArcObjects (Chang, 2004).

2   Environmental Description and Transport Formulations
2.1   Environmental Description

The simulation domain of this study was an entire river basin. It included basic elements of atmosphere, terrestrial and aquatic biota, unsaturated soil, surface water, and sediment, with the top of the troposphere as upper boundary, and the bottom of vadose-zone soil as lower boundary. The simulation domain was horizontally segmented into n small regions depending on the size of the domain. The segmentation of regions followed the delineation of watersheds to minimize technical complexity in handling water flows between adjacent watersheds. The threshold areas in the watershed delineation were in the range of $10^2 \sim 10^4$ km^2. This spatial resolution was used to ascertain that a chemical was likely to spend enough time in each watershed to allow reactions and inter-media transport to occur. The environment in each watershed was divided into a number of boxes or compartments linked by a variety of inter-media transport processes. Seven major compartments, including the atmosphere, plant canopy, surface soil, root-zone soil, vadose-zone soil, surface water, and sediment, were considered in each watershed (Figure 2). The total number of compartments was $m = 7n$ where n is the number of watersheds delineated in the simulation domain. These environmental compartments were considered well-mixed and homogeneous, in terms of environmental properties and chemical concentration. Each compartment included different sub-compartments characterized by their physical properties. For example, the surface water compartment has three sub-compartments of pure water, suspended particles, and aquatic biota.
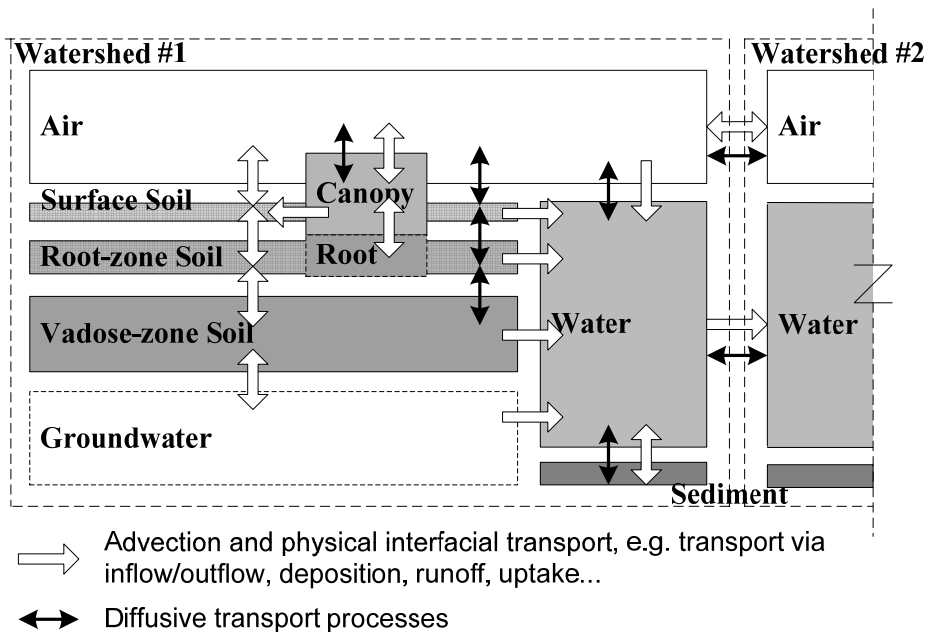
Figure 2. Environmental description with primary inter-media mass transfer processes (details in Table 2)

The air compartment horizontally covered the area of the corresponding watershed and vertically extended from the ground surface to the top of the troposphere. This compartment consisted of pure air and suspended aerosol particles. The plant canopy compartment was separately set over the soil and comprised forest, cropland and pasture. Characterized by the coverage and the mass of plant canopy, this compartment included only the above-ground portion of plant. The portion of plants below the ground was considered in the root-zone soil compartment.

The archetypal structure of soil layers was aggregated into three well-mixed soil compartments. In the absence of tilling, particles deposited from the atmosphere were accumulated in and resuspended from a thin surface soil layer (0.1~1 cm). The root-zone soil was below the surface and encompassed the region capturing the plant-rooting zone and the maximum diffusion depth. The root-zone soil layer must be thick enough to act as an effective non-escape barrier for contaminant diffusion to the vadose zone. According to McKone and Bennett (2003), the thickness of the root-zone soil (h_s, m) was estimated as the steady-state penetration depth derived from a unit value of the Damkoehler Number (Jury, 1990; McKone and Bennett, 2003),

$$\frac{M_{Rs} \cdot h_s}{D_{ts}/h_s + u_{infil}} = 1 \qquad (1)$$

where M_{Rs} (day^{-1}) is the chemical degradation rate constant in root-zone soil, D_{ts} (m^2 day^{-1}) is the bulk diffusivity of chemical in root-zone soil, and u_{infil} (m day^{-1}) is the average infiltration velocity. The vadose-zone soil compartment was defined from the bottom of the root-zone soil to the top of the groundwater table. All soil compartments consisted of air, water, and particles in soil. The root-zone soil contained plant roots as well. Transport parameters in soil were derived by matching compartment inventories to those obtained from analytical solution (McKone, 1993, 1996; Bennett et $al.$, 1998).

The surface water compartment was the surface water bodies in a watershed. This compartment comprised pure water, suspended solids, and aquatic biota. The sediment compartment, with area extent equal to that of surface water compartment, consisted of pure water and particles in the top active layer of sediment (2~5 cm) where active contaminants exchange occurred with overlying water column.

The current version of the model did not consider the upper layer atmosphere (the stratosphere) and coastal aquatic environment. The chemical flux across the troposphere-stratosphere was neglected by assuming that the bi-directional fluxes are balanced by each other. The migration and dilution of chemicals in groundwater was not explicitly simulated. Instead, the contaminant leaching from the vadose-zone soil was considered as an input to the groundwater. Due to the complexity in describing the structure of fractured permeable media, we neglected the bulk transport from air to soil resulting from barometric fluctuations (Nilson et $al.$, 1991; William et $al.$, 1997). Snow melting and snow scavenging were considered in the model. The influence of snow pack on the air-ground interactions, however, was neglected in the current phase of the study.

The connectivities of environmental compartments were defined in the model simulation design. Watershed delineation and water compartment connectivity was based on the

surface hydrologic analysis developed by Jenson and Domingue (1988). Using the National Hydrography Dataset (NHD) as a reference, watersheds were delineated from digital elevation data (DEM) in the simulation domain. The connection relations from upper to lower river segments were given by calculating the flow accumulation in the watersheds. Lakes were incorporated into the river-networking system as a special river segment. Digital maps of ground and soil characteristics were overlapped in this function to aggregate hydrologic parameters on a watershed basis. The resultant topological relations and derived environmental properties enabled the evaluations of spatial and temporal variations in the simulations of hydrology and chemical transport.

With watershed segmentation, soil and plant canopy compartments were considered to be isolated from the neighborhood, *i.e.*, there was no direct chemical transport between the soil or canopy compartments in any two adjacent watersheds.

The connectivity structures in water, soil, and canopy compartment were considered to be invariant with time. However, the connectivity of air compartments is time dependent, and changes with wind direction. The current segmentation of air compartments based on watershed delineation (Figure 2) was not suitable for horizontal transport of chemicals in the atmosphere. Based on wind direction, advective air outflows from one watershed may affect more than one downwind watershed. Therefore, the atmosphere was re-segmented as interconnected grid cells (Figure 3a). The grid size can be set to user-defined values, and different cell size can be used for a nesting area. GIS functions were used to generate the grid system, and to calculate the projective area between the grid cells and the underlying compartments of soil, canopy, and surface water. Calculations of the horizontal transport and air-ground interactions were conducted in the following procedures:

(1) Input meteorological data was interpolated and assigned to each grid cell by Ordinary Kriging (Jarvis and Stuart, 2001; Bai and Feng, 2003);

(2) Daily averages of the meteorological data was used to estimate the advective and diffusive transport parameters using the effective velocity strategy (Strand and Hov, 1993). The transport parameters then were used to calculated the advective and diffusive transport between adjacent air grid cells;

(3) For each of the patches (*e.g.*, A, B, C, and D in Figure 3b) intercepted by air grid cell and ground compartments, inter-media transport fluxes were calculated by the equations (8) to (10);

(4) The fluxes from (2) and (3) were incorporated with chemical transformation and emission into the mass balance equation, Eq. **(17)**, to calculated the chemical inventories in each air grid cell;

(5) Chemical inventories in air and inter-media fluxes between air and ground were reported on a watershed basis. These values are calculated based on the projective area of air grid cells on the ground compartments in a watershed (Figure 3b).

(a)

Sub-watershed   Air grid cell

(b)

A   B

D   C

Air Column
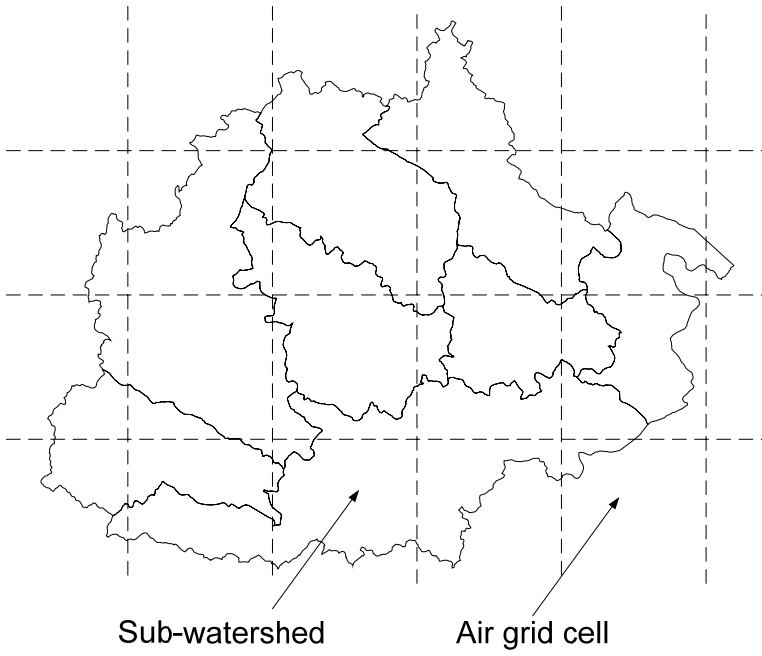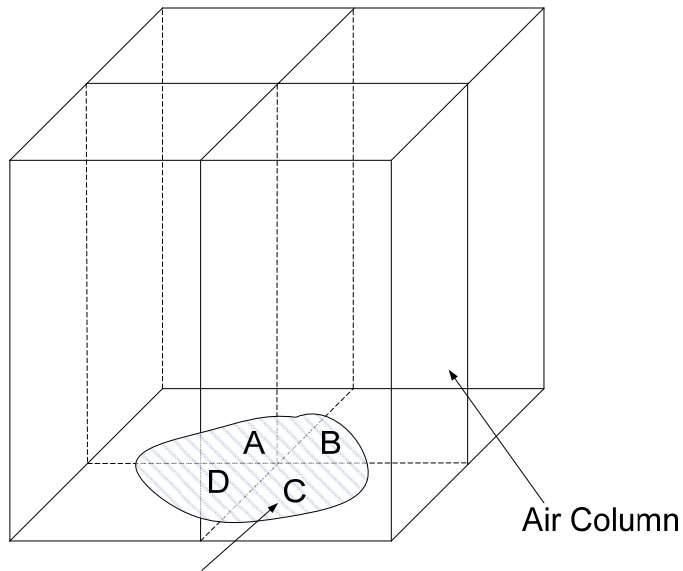
Interactive surface of
soil, canopy, or water

Figure 3. Schematics of (a) air connectivity design, and (b) inter-media transport calculation based on projective areas between air grid cell and compartments at ground.

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2.2   Fugacity Approach

The concept of fugacity was introduced by Lewis (1908). In thermodynamics, the fugacity is a state function of matter at fixed temperature. The fugacity, which has units of pressure, represents the tendency of a fluid to escape or expand isothermally. For gases at low pressure where the ideal gas is a good approximation, fugacity is nearly equal to pressure. The ratio $\Phi = f/P$ between fugacity f and pressure P is called the fugacity coefficient. For an ideal gas, $\Phi = 1$.

In mass balance model, the relation between the fugacity (F, Pa) and concentration (C, mol/m^3) in phase i can be expressed as

$$f_i = \frac{C_i}{Z_i} \tag{2}$$

where Z is the so-called fugacity capacity in mol/Pa/m^3 (Table 1). When equilibrium is established between two adjacent phases or environmental compartments, their fugacities will be equal. This concept is useful to simplify the formulation since the equilibrium is assumed to be established instantaneously between two phases within one medium. This relationship was given by Mackay (2001).

In a multimedia system of M compartments at equilibrium, the equality of the chemical fugacities in various compartments (for a given chemical and stand-state reference chemical potential) requires that the following condition holds:

$$f_1 = f_2 = f_3 = \cdots = f_i = f_j; i, j = 1,...,M; i \neq j \tag{3}$$

or using Eq. (2)

$$\frac{C_i}{Z_i} = \frac{C_j}{Z_j}; i \neq j \tag{4}$$

Since the fugacity capacity for a given chemical in a specific phase is only a function of the nature of the chemical and density of the phase, Eq. (4) can be rearranged to obtain a simple definition for the environmental partition coefficients (H):

$$H_{ij=} \frac{C_i}{C_j} = \frac{Z_i}{Z_j}; i \neq j \tag{5}$$

Table 1. Formulations of fugacity capacity (McKone, 1993; Coulibaly, 2000; Cohen and Cooter, 2002a)

Media	Fugacity capacity
Sub-compartments	
Pure air	$Z_{air} = 1/RT$
Pure water	$Z_{water} = 1/H$
Aerosol particles	$Z_{ap} = 3 \times 10^6 /(VP \cdot RT)$
Particles in soils, water, and sediment	$Z_{ip} = \rho_{ip} \cdot K_{OC} \cdot f_{OCip} / H$ subscript *i* denotes ground soil (g), root-zone soil (s), vadose-zone soil (v), surface water (w), or sediment (d)
Aquatic biota	$Z_{wf} = \rho_w BCF / H$
Plant root	$Z_{pr} = \dfrac{K_{ps}(f_{sa}Z_{air} + f_{sw}Z_{water} + f_{sp}Z_{sp})\rho_p}{\rho_{sp}f_{sp}}$
Compartments	
Atmosphere	$Z_a = (1 - f_{ap})Z_{air} + f_{ap}Z_{ap}$
Plant	$Z_{pf} = \rho_p(K_{fa}Z_{air} + K_{fx}Z_{ap} \cdot f_{ap})$ $K_{fa} = \dfrac{0.5 + (0.4 + 0.01K_{OW})RT}{\rho_p H}$
Ground soil	$Z_g = f_{ga}Z_{air} + f_{gw}Z_{water} + f_{gp}Z_{gp}$
Root-zone soil	$Z_s = f_{sa}Z_{air} + f_{sw}Z_{water} + f_{sp}Z_{sp} + f_{sr}Z_{pr}$
Vadose-zone soil	$Z_v = f_{va}Z_{air} + f_{vw}Z_{water} + f_{vp}Z_{vp}$
Surface water	$Z_w = (1 - f_{wp} - f_{wf})Z_{water} + f_{wp}Z_{wp} + f_{wf}Z_{wf}$
Sediment	$Z_d = f_{dw}Z_{water} + f_{dp}Z_{dp}$

Note:

Z_{air}	fugacity capacity in pure air (mol Pa^{-1} m^{-3})
Z_{water}	fugacity capacity in pure water (mol Pa^{-1} m^{-3})
Z_{ap}	fugacity capacity in aerosol particle (mol Pa^{-1} m^{-3})
Z_{gp}	fugacity capacity in ground soil particle (mol Pa^{-1} m^{-3})
Z_{sp}	fugacity capacity in root-zone soil particle (mol Pa^{-1} m^{-3})
Z_{vp}	fugacity capacity in vadose-zone soil particle (mol Pa^{-1} m^{-3})
Z_{wp}	fugacity capacity in suspended sediment particle (mol Pa^{-1} m^{-3})
Z_{dp}	fugacity capacity in sediment particle (mol Pa^{-1} m^{-3})
Z_{wf}	fugacity capacity in aquatic biota (mol Pa^{-1} m^{-3})
Z_{pr}	fugacity capacity in plant root (mol Pa^{-1} m^{-3})
Z_a	fugacity capacity in atmosphere compartment (mol Pa^{-1} m^{-3})
Z_{pf}	fugacity capacity in plant compartment (mol Pa^{-1} m^{-3})
Z_g	fugacity capacity in ground soil compartment (mol Pa^{-1} m^{-3})
Z_s	fugacity capacity in root-zone soil compartment (mol Pa^{-1} m^{-3})
Z_v	fugacity capacity in vadose-zone soil compartment (mol Pa^{-1} m^{-3})
Z_w	fugacity capacity in surface water compartment (mol Pa^{-1} m^{-3})

Z_d	fugacity capacity in sediment compartment (mol Pa^{-1} m^{-3})
T	ambient temperature (K)
R	gas constant (8.31 Pa m^3 mol^{-1} K^{-1})
ρ_{gp}	density of ground soil particle (kg m^{-3}[particle])
ρ_{sp}	density of root-zone soil particle (kg m^{-3}[particle])
ρ_{vp}	density of vadose-zone soil particle (kg m^{-3}[particle])
ρ_{wp}	density of suspended sediment particle (kg m^{-3}[particle])
ρ_{dp}	density of sediment particle (kg m^{-3}[particle])
ρ_w	water density (kg m^{-3})
ρ_p	density of fresh plant (kg m^{-3})
f_{OCgp}	organic content in ground soil (-)
f_{OCsp}	organic content in root-zone soil (-)
f_{OCvp}	organic content in vadose-zone soil (-)
f_{OCwp}	organic content in surface water (-)
f_{OCdp}	organic content in sediment (-)
BCF	bio-cumulation factor (m^3 kg^{-1})
K_{ps}	partition ratio of plant-root and soil (mol kg^{-1}[plant] per mol kg^{-1}[soil])
K_{fa}	partition ratio between plant and air-vapor (mol kg^{-1}[plant])
K_{fx}	partition ratio between plant and air-particle (mol kg^{-1}[plant])
f_{ap}	volume fraction of aerosol particle in atmosphere (-)
f_{gp}	volume fraction of particle in ground soil (-)
f_{sp}	volume fraction of particle in root-zone soil (-)
f_{vp}	volume fraction of particle in vadose-zone soil (-)
f_{wp}	volume fraction of particle in surface water (-)
f_{dp}	volume fraction of particle in sediment (-)
f_{ga}	volume fraction of air in ground soil (-)
f_{sa}	volume fraction of air in root-zone soil (-)
f_{va}	volume fraction of air in vadose-zone soil (-)
f_{gw}	volume fraction of water in ground soil (-)
f_{sw}	volume fraction of water in root-zone soil (-)
f_{vw}	volume fraction of water in vadose-zone soil (-)
f_{dw}	volume fraction of water in sediment (-)
f_{wf}	volume fraction of aquatic biota in water (-)
f_{sr}	volume fraction of plant root in root-zone soil (-)

Under the assumption of homogenous composition of the environmental compartments, the following transport and transformation mechanisms were considered in developing mass balance equations for multimedia chemical dynamics.

(1) Mass exchange between species, *i.e.*, chemical degradation or mass gain from parent compounds,

(2) Mass exchange between compartments within a watershed, *i.e.*, inter-media mass transport,

(3) Mass exchange between watersheds resulting from the advective flows of air and water,

(4) Mass exchange between the simulation domain and the external environment, including distant chemical inputs and outputs by advective flows of air and water, sediment burial, and chemical loss with groundwater recharge, and

(5) Source emission of chemicals.

By considering all these processes, a general unsteady-state mass balance can be described with the following differential equation,

$$\frac{dN_i}{dt} = S_i + \sum_{j=1}^{m}(Q_{ji} - Q_{ij}) - (Q_{ix} + Q_{Ri}) \text{ , } i = 1, 2, \ldots, m \tag{6}$$

where N_i (mol) is the chemical inventory in the compartment i at time t, m is the total number of compartments defined in the simulation domain, S_i (mol s^{-1}) is the total chemical source in this compartment, Q_{ij} and Q_{ji} (mol s^{-1}) are the rates of unidirectional chemical flux from compartment i to j, and vice versa, and Q_{Ri} (mol s^{-1}) is the chemical degradation rate in i. For a compartment located on the boundary of the simulation domain, Q_{ix} (mol s^{-1}) is the chemical loss rate from i to a hypothetical receptor compartment, x, in the external environment outside of the simulation domain. All these transport and transformation processes were represented mathematically as first-order equations based on the fugacity concept discussed in the following section.

2.3 Inter-media Mass Transport

Transport equations for various media were coupled through the formulation of inter-media transport processes, including advective, diffusive, and physical interfacial processes (Table 2).

Table 2. Inter-media mass transport processes recognized and formulated in this study

Interface	Transport processes
Air – canopy, and	Diffusion
Air – surface soil	Dry deposition
	Wet deposition by rain and snow
	Wind resuspension
Air - water	Dry deposition [a]
	Dry deposition
	Wet deposition by rain and snow
Surface soil - vadose zone	Diffusion
	Infiltration
Surface soil - surface water	Overland flow
	Soil erosion
Root zone - vegetation	Plant uptake
	Phloem flow
Root zone - vadose zone	Infiltration
	Flow form vadose zone to root zone
Vadose zone - groundwater	Recharge
Vadose zone - surface water	Interflow
Surface water - bottom sediment	Diffusion
	Sedimentation
	Resuspension

[a] Dry deposition was defined for aerosol particles only. The dry deposition of gases was formulated as a diffusion process.

Based on the fugacity concept, the overall inter-media flux from compartment i to j was quantified by the D values that were described in detail by Mackay (2001)

$$Q_{ij} = D_{ij} \cdot f_i = (D_{Dij} + D_{Aij} + D_{Pij}) \cdot f_i \qquad (7)$$

where D_{ij} (mol Pa^{-1} s^{-1}) is the overall transport coefficient from compartment i to j, and D_{Dij}, D_{Aij}, and D_{Pij} (mol Pa^{-1} s^{-1}) are the transport coefficients for advective, diffusive, and physical interfacial transport processes from i to j, respectively. In addition to the D values defined by Mackay (2001), this model also included transport mechanisms in plant canopy and soil layers. It was noteworthy that Q_{ij} presented only the unidirectional flux rate from i to j, while the net mass exchange by the inter-media diffusion was given by the algebraic sum of Q_{ij} and Q_{ji}.

The D value of the inter-media diffusion was formulated based on the two-film theory (Whitman, 1923; Lewis and Whitman, 1924)

$$D_{Dij} = A_{ij} \left(\frac{\delta_{ij\_i}}{Z_i D_{ti}} + \frac{\delta_{ij\_j}}{Z_j D_{tj}} \right)^{-1} \qquad (8)$$

where A_{ij} (m^2) is the interface area between compartment i and j, δ's (m) are the boundary layer depths of the two compartments at the interface, and D_t's (m^2 s^{-1}) are the bulk diffusivities of the chemical in the respective compartments. The boundary layer depth of each compartment in the diffusive transport was estimated using empirical or semi-theoretical equations from the literature (Jury, 1983; McKone, 1993; Thibodeaux, 1995; Bennett *et al.*, 1998; Meyers *et al.*, 1998; Mackay, 2001; Cohen and Cooter, 2002a, 2002b). Based on the volume fractions of air and water in a compartment, the bulk diffusivity can be calculated from the diffusivities of the chemical in pure air and water (Coulibaly, 2000).

The inter-media advection was driven by hydrologic flows and plant-soil interactions (plant uptake and phloem flow). The D value of the inter-media advection was calculated as

$$D_{Aij} = A_{ij} \cdot Z_c \cdot u_{ij} \qquad (9)$$

where Z_c (mol Pa^{-1} m^{-3}) is the fugacity capacity of the chemical in the carrying media (water or phloem fluid), and u_{ij} (m s^{-1}) is the flow velocity. Eq. (9) was also valid in simulating the advective chemical fluxes between two connected watersheds by air/water flows. For calculating the advective chemical fluxes, Z_c denotes the fugacity capacity of the chemical in air or water, and u_{ij} is the advective flow velocity of air or water across the watershed boundaries.

The physical interfacial processes involve chemical transport by particles in air or in water, and cannot be categorized as either advection or diffusion. In this study, these processes included chemical transports by atmospheric dry deposition of aerosol particles, wind resuspension of particles from surface soil and plant foliage, soil erosion, sedimentation and resuspension of solids in water bodies (Cohen *et al.*, 1990; Cohen and Cooter, 2002a). The general formulation of the D values for these transport processes can be expressed as

$$D_{Pij} = A_{ij} \cdot (\gamma_{ip} Z_{ip}) \cdot u'_{ij} \qquad (10)$$

where the index i represents the originating compartment from which chemicals are removed, including air (for atmospheric deposition), surface soil (for wind resuspension and soil erosion), or sediment (for sediment resuspension and burial), γ_{ip} (dimensionless)

is the volume fraction of particles in compartment i, Z_{ip} (mol Pa^{-1} m^{-3}) is the fugacity capacity of the chemical in particles in compartment i, and u'_{ij} (m s^{-1}) is the velocity of the corresponding interfacial transport. These velocities were estimated based upon empirical and semi-theoretical methods from the literature (Ackers and White, 1975; Cowherd *et al.*, 1985; Hicks *et al.*, 1987; Meyers and Baldocchi, 1988; Meyers *et al.*, 1998).

For computational convenience, the mass balance was formulated in term of chemical inventory by introducing an overall transfer rate constant. Eq. (7) was rearranged as
$Q_{ij} = M_{ij} N_i$, with

$$N_i = Z_i \cdot V_i \cdot f_i \text{, and } M_{ij} = D_{ij} / (Z_i V_i) \tag{11}$$

where M_{ij} (s^{-1}) is the overall transfer rate constant of the inter-media chemical flows from compartment i to j. Similarly, M_{ji} (s^{-1}) was defined as the overall transfer rate constant of Q_{ji}. The transfer rate constant for an individual transport processes was given by

$$M_{Dij} = D_{Dij} / (Z_i V_i), M_{Aij} = D_{Aij} / (Z_i V_i), \text{ or } M_{Pij} = D_{Pij} / (Z_i V_i) \tag{12}$$

where M_{Dij}, M_{Aij}, and M_{Pij} are the transfer rate constants for diffusive, advective, and physical interfacial processes, respectively. The transfer rate constant indicated the fraction of the chemicals in the originating compartment that was removed by the corresponding transport process per unit time. For example, if a transfer rate constant of a dry particulate deposition was found to have the value of 0.1 s^{-1}, then 10% of the chemical in aerosol particles would be deposited per second. The transfer rate constants of inter-media transport processes were summarized in Table 3. The reciprocal of the transfer rate constant (M^{-1}) was the characteristic time of the corresponding transport process, *i.e.*, the time required for the transport process to reduce the fugacity to e^{-1} of the original fugacity of a chemical in a compartment.

Table 3. Overall transfer rate constants for inter-media transport processes

Inter-media transport	Overall transport rate constant
Air to canopy	$$M_{ap} = \frac{LAI \cdot D_{Dap} + A_p I_w u_{\text{rain}}(Z_{water} + \gamma_{ap} Z_{ap} Q) + A_p I_d \gamma_{ap} u_{\text{depo}} Z_{ap}}{Z_a V_a}$$
Air to surface soil	$$M_{ag} = \frac{D_{Dag} + A_g u_{\text{rain}}(Z_{water} + \gamma_{ap} Z_{ap} Q) + A_g \gamma_{ap} u_{\text{depo}} Z_{ap}}{Z_a V_a}$$
Air to water	$$M_{aw} = \frac{D_{Daw} + A_w u_{\text{rain}}(Z_{water} + \gamma_{ap} Z_{ap} Q) + A_w \gamma_{ap} u_{\text{depo}} Z_{ap}}{Z_a V_a}$$
Canopy to air	$$M_{pa} = \frac{LAI \cdot D_{Dap} + A_p \gamma_{ap} u_{\text{windres}} Z_{ap}}{Z_p V_p}$$
Canopy to root zone	$M_{ps} = A_p u_{\text{phlm}} Z_{phlm} / (Z_p V_p)$
Canopy to surface soil	$M_{pg} = A_p u_{\text{litter}} Z_p / (Z_p V_p)$
Surface soil to air	$$M_{ga} = \frac{D_{Dag} + A_g \gamma_{gp} u_{\text{windres}} Z_{gp}}{Z_g V_g}$$
Surface soil to root zone	$$M_{gs} = \frac{D_{Dgs} + A_g u_{\text{infil}} Z_{water}}{Z_g V_g}$$
Surface soil to water	$$M_{gw} = \frac{A_g (u_{\text{runoff}} Z_{water} + \gamma_{gp} u_{\text{erosion}} Z_{gp})}{Z_g V_g}$$
Root zone to canopy	$M_{sp} = A_g u_{\text{uptake}} Z_{water} / (Z_s V_s)$
Root zone to surface water	$M_{sg} = D_{Dsg} / (Z_s V_s)$
Root zone to vadose zone	$$M_{sv} = \frac{D_{Dsv} + A_g u_{\text{perc}} Z_{water}}{Z_s V_s}$$
Vadose zone to root zone	$M_{vs} = D_{Dsv} / (Z_v V_v)$
Vadose zone to water	$M_{vw} = A_g u_{\text{inter}} Z_{water} / (Z_v V_v)$
Vadose zone to groundwater	$M_{vq} = A_g u_{\text{rech}} Z_{water} / (Z_v V_v)$
Water to air	$M_{wa} = D_{Dwa} / (Z_w V_w)$
Water to sediment	$$M_{wd} = \frac{D_{Dwd} + A_w \gamma_{wp} u_{\text{sedmt}} Z_{wp}}{Z_w V_w}$$
Sediment to water	$$M_{dw} = \frac{D_{Dwd} + A_w \gamma_{dp} u_{\text{resus}} Z_{dp}}{Z_d V_d}$$
Burial to deep sediment	$M_{dx} = A_w \gamma_{dp} u_{\text{burial}} Z_{dp} / (Z_d V_d)$

Note:

LAI (-): Leaf area index

I_w and I_d (-): Canopy interception fractions of wet and dry deposition

Z_{water} (mol Pa^{-1} m^{-3}): Fugacity capacity of the chemical in pure water

Z_{ap}, Z_{gp}, Z_{wp}, and Z_{dp} (mol Pa^{-1} m^{-3}): Fugacity capacity of the chemical in aerosol particles, in surface soil solids, in suspended particles of water, and in sediment solids, respectively

γ_{ap}, γ_{gp}, γ_{wp}, and γ_{dp} (-): Volume fraction of particles/soilds in air, in surface soil, in water, and in sediment, respectively

Q (-):   Particle scavenging ratio for rain or snow

u_{rain} (m s^{-1}):   Precipitation rate

u_{depo} (m s^{-1}):   Dry deposition velocity of aerosol particles

$u_{windres}$ (m s^{-1}):   Wind resuspension velocity of particles from canopy and surface soil

u_{phlm} (m s^{-1}):   Velocity of fluid that moves from canopy tissues down into the roots through the phloem tubes

u_{litter} (m s^{-1}):   Velocity of leaf litterfall

u_{infil} (m s^{-1}):   Infiltration rate

u_{runoff} (m s^{-1}):   Surface runoff rate

u_{uptake} (m s^{-1}):   Velocity of water that moves from soil into the roots and up through the plant as a result of transpiration

u_{perc} (m s^{-1}):   Percolation rate, from root zone to vadose zone

u_{inter} (m s^{-1}):   Lateral inter-flow rate, from vadose zone to water

u_{rech} (m s^{-1}):   Groundwater recharge rate

u_{sedmt} (m s^{-1}):   Velocity of particle sedimentation

u_{resus} (m s^{-1}):   Velocity of resuspension of sediment solids

u_{bural} (m s^{-1}):   Velocity of sediment burial

Indices a, p, g, s, v, w, and d denote the compartment of air, plant canopy, ground surface soil, root-zone soil, vadose-zone soil, surface water, and sediment, respectively, M's (s^{-1}) and D's (mol Pa^{-1} s^{-1}) are the transfer rate constants and Mackay D values of transport processes, respectively, A's (m^2) are the horizontal projective areas of compartments, V's (m^3) are the compartment volumes, and Z's are the fugacity capacities of chemical in compartments or sub-compartments. The areas of surface soil, root-zone soil, and vadose-zone soil were assumed to be the same and denoted as A_p. Similarly, the areas of surface water and sediment were assumed to taken the same value of A_w.

Chemical losses to the external environment outside of the simulation domain were formulated in a similar way. These processes included chemical burial in sediment, and advective/diffusive transport in air or water compartments located on the boundaries of the simulation domain. The overall rate constant (M_{ix}) of the chemical loss from compartment i to an external sink was defined as

$$M_{ix} = \frac{D_{Dix} + D_{Aix} + D_{Pix}}{Z_i V_i}$$ (13)

where the subscript x denotes a hypothetical receptor compartment in the external environment connected to i, and D_{Dix}, D_{Aix} and D_{Pix} are the corresponding D values for diffusion, advection, and sediment burial, respectively.

2.4   Mass Balance Equations

The rates of transformation or degradation of the chemical were estimated via first-order kinetics, which implied that the substrate concentration was the primary factor in affecting the decomposition rate, and the microbial biomass was always present in high enough concentrations not to be rate limiting. As for reactions that do not follow first

order kinetics, a pseudo first order reaction was assumed. The degradation flux of a chemical in specific compartment i, Q_{Ri} (mol s^{-1}), was calculated by

$$Q_{Ri} = M_{Ri} \cdot Z_i \cdot V_i \cdot f_i \tag{14}$$

where M_{Ri} (s^{-1}) is the degradation rate of a chemical in compartment i. If transformations between inter-converting species were applicable for the modeled species, the mass gain (Q_{Ti}, mol s^{-1}) from a parent compound was

$$Q_{Ti} = M'_{Ri} \cdot Z'_i \cdot V_i \cdot f'_i \tag{15}$$

where, f'_i and Z'_i are the fugacity and fugacity capacity of the parent species in compartment i, respectively, and M'_{Ri} (s^{-1}) is the degradation rate of the parent species.

For watersheds on the boundary of the simulation domain, chemical inputs by advective flows of air or water from external environment were taken as distant sources (Q_{Ii}, mol s^{-1}). In a compartment, a total source term (S_i, mol s^{-1}) was defined as the sum of the chemical inputs from transformation (Q_{Ti}), distant transport (Q_{Ii}), and emission source (Q_{Si}),

$$S_i = Q_{Ti} + Q_{Si} + Q_{Ii} \tag{16}$$

Substituting Q's in terms of N and M, the mass balance equation in (6) was rearranged as

$$\frac{dN_i}{dt} = S_i + \sum_{j=1}^{m}(M_{ji}N_j) - (\sum_{j=1}^{m}M_{ij} + M_{ix} + M_{Ri})N_i$$

$$= S_i + \sum_{j=1}^{m}(M_{ji}N_j) - M_{Oi}N_i \tag{17}$$

where M_{Oi} (s^{-1}) is the total loss rate of the chemical in compartment i. For the whole simulation domain, Eq. (17) was written for m compartments to solve for the time-dependent chemical inventories. Each of these equations was re-written in implicit forms with the finite difference method and solved for N's by

$$(1/\Delta t + M_{Oi})N_i\big|_{t+1} - \sum_{j=1}^{m}(M_{ji}N_j)\big|_{t+1} = (S_i + N_i/\Delta t)\big|_t, \; i = 1, 2, \ldots, m \tag{18}$$

The model was implemented with both capabilities for providing steady-state and time-dependent solutions. At steady state, sources were in balance with sinks and there was no chemical accumulation in each compartment. Consequently, the set of ordinary differential equations were transformed to a set of linear equations expresses in matrix form. The numerical solution was implemented with MATLAB codes in IBM PC platform.

3 Spatial Characterization in ArcObjects
3.1 Spatial Analysis Overview

The purpose of the landscape characterization is to provide an appropriate way of reallocating spatial data from geographic information system to environmental compartments defined by the user and devised for simulating chemicals transport and distribution in the complex multimedia system. The total number of media (NM) is defined as the maximal number of medium types in the system. The total number of compartments in the simulation domain (NC) hence is NG*NM, where NG is the total number of watersheds. Chemical concentrations in each compartment in the system can be indicated here by two indices of the watershed index (G) and medium index (M): $[C]_{G,M}$. For the convenience in describing the topological structure, a one-dimensional vector is used to describe the chemical distribution in each compartment: $[C]_{(G-1)*NM+M}$.

The appropriate topologic structure of environmental compartments was developed in this study to reduce the otherwise complex processes associated to multimedia mass exchange in the real world. Since watersheds are devised in the spatial allocation to relate the mass transport with the geographical data, two types of topologic mapping were designed for the in-watershed and between-between structures. In each watershed, a compartment does not connect with all other compartments. Within an adjacent pair of compartments, inter-media mass transport might be unidirectional. In the current model approach, for example, the advective mass exchanges between soil and canopy are only from soil water to plant root by uptake. The topological structure of the environmental compartments in this model is illustrated in Figure 4.

1→2; 1→3; 1→4
Particulate deposition
2→1; 3→1 Particle resuspension
3→2 Plant uptake
3→4 Interflow and soil erosion
3→6 Leaching
4→5 Sedimentation
5→4 Resuspension
6→4 Baseflow
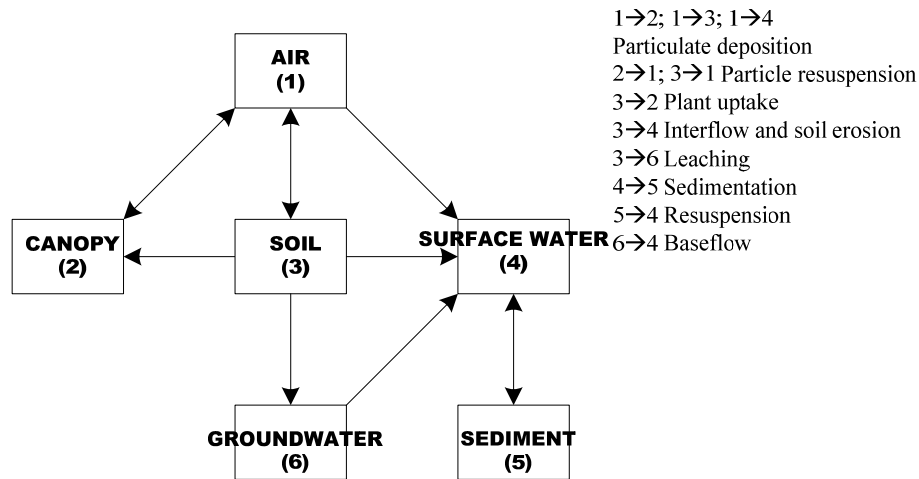
Note: The arrows indicate the directions of advective flows between adjacent compartments, where the diffusive flows are supposed to be bidirectional.

Figure 4. Topological structure of the inter-media mass transport pathways across environmental compartments within one watershed.

Based on the topological structure shown in Figure 4, a binary mapping matrix is developed for determining if contaminants are possibly exchanged between two compartments within one grid, according to the mass exchange shown below:

$$[E_{ij}(t)]_{NM \times NM} = \begin{bmatrix} 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix} \tag{19}$$

where E is a Boolean value. If the IMT occurs between compartments i and j, E=1 (TURE); otherwise E=0 (FALSE). And by default E_{ii}=0 since inter-media mass transport does not take place within a single medium. Generally, above matrix is symmetric, indicating the IMT processes are two-directional between the adjacent compartments, unless some one-directional or nonreversible transfers are specified, *e.g.*, in Coulibaly (2000) the advective processes between surface soil to water bodies are regarded as one-directional. Similar method is used to establish the topological structure of all watersheds in the simulation domain. The transport matrix for the whole domain is extended from (19) as,

$$[E_{ij}(t)]_{NC \times NC} \tag{20}$$

3.2 Spatial Data Layers

Five spatial data layers were characterized in this study as follows,
(1) Air cells. Air cells were defined based on the geographic extension of the watershed layer. The grid size can be set to user-defined values, with a default value of 12km by 12 km (Xu *et al.*, 2000a, 2000b). As defined in the environmental description, the atmospheric compartment extents from the ground surface to the top of mixing layer. Currently, atmosphere was considered to be homogenous in the mixing layer as respect to the long-term average of chemical distribution. Therefore, only one layer was taken with height of about 1000km.
(2) Ground surface layer. Ground surface layer was defined by the GIRAS land use dataset and surface soil (top 20cm) dataset extracted from STATSGO (State Soil Geographic Database) or SSURGO (Soil Survey Geographic Database). The layer was designed to estimate model parameters (e.g., compartmental area, CN, and erosion factor) for simulations of surface hydrology and chemical transport.
(3) Watershed layer. Watershed layer was delineated from national elevation data (NED). Stream networks (Reach File or National Hydrography Dataset) and/or watershed boundaries might be also applied; otherwise, synthetic streams and watershed boundaries would be generated by the surface hydrologic analysis in ArcGIS (Maidment, 1993; Maidment, 2002).
(4) Soil layer. Soil layer extends from surface soil to ground water table. This layer was parameterized by STATSGO or SSURGO dataset. Three soil layers were defined as surface/ground soil (0.5cm), root-zone soil (capturing both rooting depth and maximal diffusion depth), and vadose-zone soil (to the ground water table). Spatially, the depths of ground water table are interpolated from USGS NWIS (national water information

system) measurements. Temporally, the depths are taken as annual averages and assumed to be constant over the whole simulation period for each location.

3.3   Landscape Analysis

The primary digital maps as inputs for the landscape analysis included (1) watershed boundaries generated from drainage delineation, (2) GIRAS land use maps, 1:250,000 digital map with Anderson land use code (Anderson *et al.*, 1976), and (3) STATSGO and SSURGO spatial data for spatial information of soil map units. This spatial analysis generated grid cells for air compartments and landscape analysis reports, including the projective relationships of air cells, land use type, and soil map units grouped by watersheds. The general procedures for the landscape characterization for environmental properties were described as follows.

(1) Generating air grid
Air grid was defined based on the geographic extension of the watershed layer. The grid size can be set to user-defined values, with a default value of 12km by 12 km Connecticut (Xu *et al.*, 2000a, 2000b). The major steps in generating air grids are shown in Table 4.

Table 4. Procedures in generating air grid

Step	Description	ArcGIS interface
1	Get spatial extent from watershed coverage	*IEnvelope*
2	Create a grid to cover the extent (all cells have value of unit)	*IRasterWorkspace2*
3	Convert the grid in (2) to points (points are assigned with unique IDs)	*IConversionOp*
4	Convert the point in (3) back to grid (cells have the same ID as the corresponding points)	*IConversionOp*
5	Convert the grid in (4) into vector format	*IConversionOp*

(2) Preparing GIRAS land use map for the simulation domain
GIRAS land use maps are originally designed to be used by quadrangle (100*100 mi^2). The maps were cropped and combined to match the spatial coverage of the simulation domain. Level 2 of the Anderson land use code was used to simplify the spatial analysis (Table 5).

Table 5. The Anderson land use codes

Level 1	Level 2	Description
1		Urban or built-up land
	11	Residential
	12	Commercial and services
	13	Industrial
	14	Transportation, communication, utilities
	15	Industrial and commercial complexes
	16	Mixed urban or built-up land
	17	Other urban or built-up land
2		Agricultural land
	21	Cropland and pasture
	22	Orchards, groves, vineyards, nurseries, and ornamental horticultural
	23	Confined feeding operations
	24	Other agricultural land
3		Rangeland
	31	Herbaceous rangeland
	32	Shrub and brush rangeland
	33	Mixed rangeland
4		Forest land
	41	Deciduous forest land
	42	Evergreen forest land
	43	Mixed forest land
5		Water
	51	Streams and canals
	52	Lakes
	53	Reservoirs
	54	Bays and estuaries
6		Wetland
	61	Forested wetland
	62	Nonforested wetland
7		Barren land
	71	Dry salt flats
	72	Beaches
	73	Sandy areas not beaches
	74	Bare exposed rock
	75	Strip mines, quarries, gravel pits
	76	Transitional areas
8		Tundra
	81	Shrub and brush tundra
	82	Herbaceous tundra
	83	Bare ground
	84	Wet tundra
	85	Mixed tundra
9		Perennial snow or ice
	91	Perennial snowfields
	92	Glaciers

(3) Preparing soil map for the simulation domain

The preparation of soil unit map was similar to that for the land use map. To make it work in grid format, the soil unit ID was converted to pure-numeric formation based on ASCII standards. For example, the soil ID of "CT001" was converted as 6784001 (67 and 84 are ASCII values for "C" and "T", respectively).

(4) Generating landscape analysis report

The vector maps of watershed (identified by watershed ID), air cells (by air cell ID), land use (by the Anderson code), and soil (by soil unit code) were converted into 100*100 m^2 grids with the same extent and spatial reference. The method of "*Sample*" in the "*IExtractionOp*" interface of ArcGIS was used to generate the landscape analysis report by extracting cells of air grid, land use, and soil map based on the watershed delineation (Figure 5).

Watershed	Latitude	Longitude	Air Cell	Land use	Soil Unit
3	1882032.54	982793.95	2	5	8684055
3	1883032.54	982793.95	2	5	8684056
1	1895032.54	982793.95	3	5	7872022
3	1882032.54	981793.95	2	5	8684055
3	1883032.54	981793.95	2	5	8684056
1	1893032.54	981793.95	3	5	7872022
1	1894032.54	981793.95	3	5	7872022
1	1895032.54	981793.95	3	5	7872022
1	1896032.54	981793.95	3	5	7872022
3	1881032.54	980793.95	2	5	8684055
3	1882032.54	980793.95	2	5	8684055

Figure 5. Data structure in the landscape analysis report

3.4 Soil Database

A soil database was developed in this study to characterize the soil properties aggregated by layer depths of 0-8 inch, 8-40 inch, and 40-80 inch (Table 6). The parameter estimations of soil properties in this study were currently based on the STATSGO database (USDA, 2006b). There is a new soil database of SSURGO with finer spatial resolution of soil properties. This database is still under development and not all areas in the United States are available in digital format.

Table 6. Soil properties aggregated in the soil database created in this study

Soil properties	Descriptions
Soil texture	Presented in soil texture class and percentage of sand, silt, and clay. Soil texture is determined by the soil composition in the soil fraction which passes a No. 10 (2 mm) sieve. As an alternative, soil texture classes could be defined from the ranges of sand, silt, and clay based on the USDA soil texture triangle, or estimated from Table 7
KFFACT	USLE Erodibility factor
OC	Organic carbon content (g[OC in soil]/g[soil particles]), derived from organic material content (OM) as OC=0.58OM
PERM	Permeability (in/hr)
AWC	Available water content.
pH	pH value
HYDGRP	Hydrologic group (USDA, 1993). In the data aggregation, numeric-equivalent hydrologic group was assigned as A=1, B=2, C=3, and D=4. the average numeric groups are then converted back to letters using the following criteria: (0, 1.5] for A, (1.5, 2.5] for B, (2.5, 3.5] for C, and (3.5, 4] for D

3.4.1   Summary of soil databases

The 1:250,000 STATSGO database is designed to be used for broad planning and management uses covering state, regional, and multi-state areas. This database is being updated and renamed to the Digital General Soil Map of the United States. The STATSGO database has similar data structure as that in the SSURGO database (Figure 6).
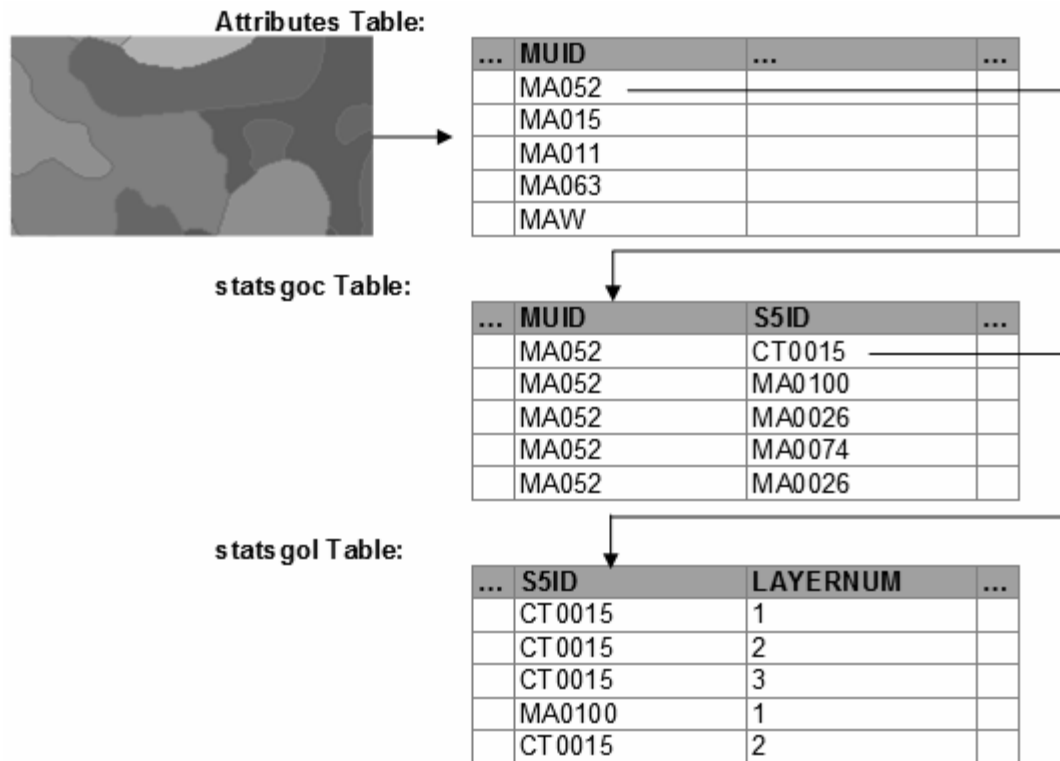
Figure 6. Data structure in the STATSGO database

3.4.2 Procedures in processing soil properties

The STATSGO soil databases contain soil properties up to 2 meters (about 80 inch) with 3-5 sampling layers below the ground surface. These data was aggregated for representing the physical conditions in the compartments of surface soil, root-zone soil, and vadose-zone soil. Since the depth of these soil compartments vary with different watersheds, a multi-layer soil characteristics database was constructed for the parameter estimations in this study. The determination of soil layers in the multi-layer soil database represented a balance between the desires to provide structural information for transport simulation while avoiding the error by introducing large number of layers. Most of the components in the STATSGO database were sampled as three layers from the ground surface to up to 80 inch below. Therefore, three standard soil layers were defined in the multi-layer soil database in this study. Soil properties in this database were grouped by the soil map unit and aggregated in three soil layers: layer 1 from 0 to 20 cm (8 inch), layer 2 from 20 to 100 cm (40 inch), and layer 3 from 100 cm to 200 cm (80 inch) (Figure 7). Data in layer 1 was used to estimate the environmental properties on the ground surface, *e.g.*, SCS curve number and USLE erodibility factors. Data in layers 2 and 3 represented the general physical properties in root-zone soil and vadose-zone soil, respectively. When the depth of plant rooting depth and ground water table were specified, the soil properties for root-zone and vadose-zone soil compartments were interpolated from layers 2 and 3.

S5ID	CT0014	MA0024	MI0045	NY0244
LAYER1	2	7	2	2
LAYER2	18	8	8	25
LAYER3	45	50	16	45
LAYER4	bedrock	bedrock	34	bedrock

	CT0014	MA0024	MI0045	NY0244
LAYER1	8	8	8	8
LAYER2	32	32	32	32
LAYER3	40	40	40	40
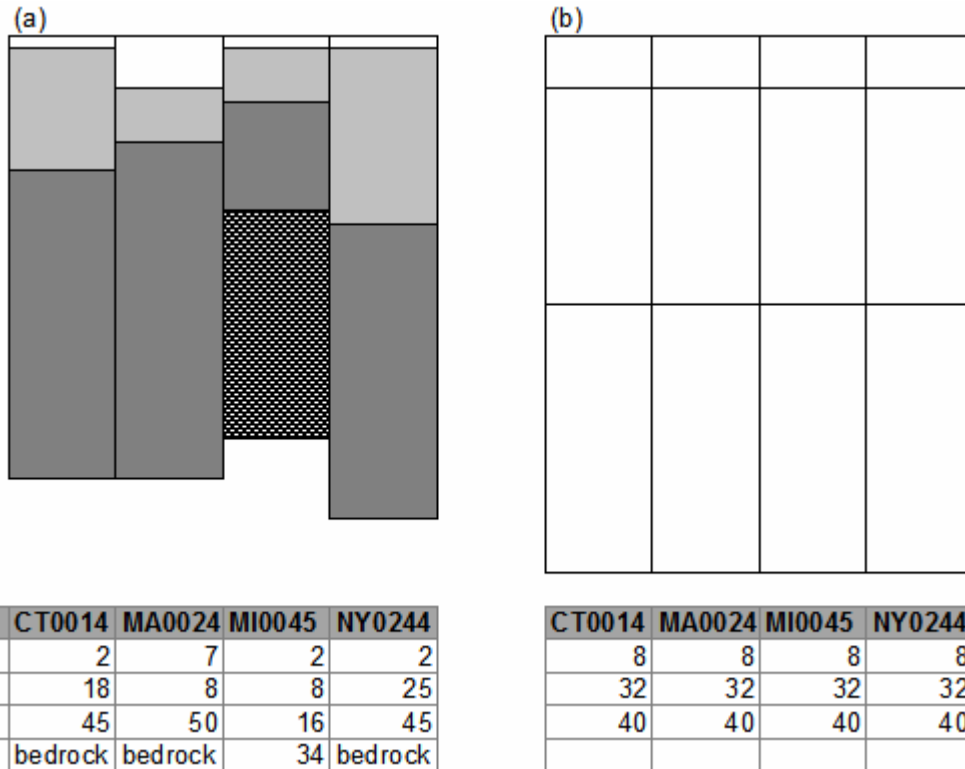
Figure 7. Diagram of soil layers in the STATSGO database and in the multi-layer soil database created in this study (soil layer depth in inch)

The aggregation of soil properties followed the approaches used in creating CONUS-SOIL database (Miller and White, 1998). The data values in each layer for the STATSGO database were discretized at the interval of 1 inch. The average values of the data were obtained for each standard layer in the multi-layer soil database. For soil texture class as a categorical variable, representative category was assigned by matching the soil texture class to the relative amount of sand, silt, and clay based on a least square method (Table 7). In this study, the deepest soil layer in the STASGO database was assumed to extent down to bedrock. If the depth-to-bedrock in the STATSGO and SSURGO database was above the deepest standard layer 200 cm (80 in), the portion of this standard layer below the bedrock was considered as solid rock.

Table 7. Soil texture classes and relative amounts of sand, silt, and clay in the < 2 mm fraction of soil (Miller and White, 1998)

Class No	Soil texture	Class abbr.	% sand	% silt	% clay
1	Sand	S	92	5	3
2	Loamy loam	LS	82	12	6
3	Sandy loam	SL	58	32	10
4	Silty loam	SiL	17	70	13
5	Silt	Si	10	85	5
6	Loam	L	43	39	18
7	Sandy clay loam	SCL	58	15	27
8	Silty clay loam	SiCL	10	56	34
9	Clay loam	CL	32	34	34
10	Sandy clay	SC	52	6	42
11	Silty clay	SiC	6	47	47
12	Clay	C	22	20	58
13	Organic materials	OM	0	0	0
14	Water	W	0	0	0
15	Bedrock	BR	0	0	0
16	Other	O	0	0	0

For each soil map unit, the average values of the physical and hydraulic variables were calculated by weighting the values for each component by the area percentages. The soil texture class was obtained by the same method used in data aggregation for soil layers. The average soil hydrological group was first converted to the numeric-equivalent values (Table 6), and assigned as area-weighted values for each soil unit. The resultant soil database was arranged in Microsoft ACCESS (MDB) format and included two tables of "Unit" and "Component" for soil unit and soil components, respectively. Currently, 26 variables are defined for each soil map unit (Table 8).

Table 8. Fields in the soil database created in this study

Field ID	Field Name in		Description
	Unit Table	Component Table	
0	MUID	S5ID	IDs for soil unit or component
1	Sand8	Sand8	% sand in layer1 (0-8 inch)
2	Silt8	Silt8	% silt in layer 1
3	Clay8	Clay8	% clay in layer 1
4	Sand40	Sand40	% sand in layer 2 (8-40 inch)
5	Silt40	Silt40	% silt in layer 2
6	Clay40	Clay40	% clay in layer 2
7	Sand80	Sand80	% sand in layer 3 (40-80 inch)
8	Silt80	Silt80	% silt in layer 3
9	Clay80	Clay80	% clay in layer 3
10	KFFACT8	KFFACT8	USLE Erodibility factor in layer 1
11	OC8	OC8	Organic carbon content in layer 1
12	OC40	OC40	Organic carbon content in layer 2
13	OC80	OC80	Organic carbon content in layer 3
14	PERM8	PERM8	Permeability in layer 1
15	PERM40	PERM40	Permeability in layer 2
16	PERM80	PERM80	Permeability in layer 3
17	AWC8	AWC8	Available water content in layer 1
18	AWC40	AWC40	Available water content in layer 2
19	AWC80	AWC80	Available water content in layer 3
20	PH8	PH8	pH value in layer 1
21	PH40	PH40	pH value in layer 2
22	PH80	PH80	pH value in layer 3
23-40	reserved	N/A	Blank fields
41	HYDGRP	N/A	Hydrologic soil group
42	SEQNUMs	N/A	Number of components in the unit
43	TEXTURE8	N/A	Surface soil texture
44	WTDEP	N/A	Ground water table in STATSGO

Note: This table shows fields in a database derived from STATSGO as an example, and databases derived from SSURGO has similar fields

3.5   Derived Landscape Parameters

(1) Percentage of land use area in each watershed was calculated directed from the landscape analysis report (Figure 5).
(2) Root-zone soil depth was estimated base on the land use type and the soil texture for the top 20 cm (Table 9)

Table 9. Root-zone soil depth, adapted from (Dunne and Leopold, 1978; USEPA, 2003a)

Anderson Code [1]	Assumed vegetation	Root-zone depth for the soil texture of [2]				
		S	LS, SL	L, OM, SI, SIL	CL, SCL, SICL	C, SC, SIC
11~17, 22	orchards	1.5	1.67	1.5	1	0.67
21, 24	Moderately deep-rooted crops	0.75	1	1	0.8	0.5
23	Shallow-rooted crops	0.5	0.5	0.62	0.4	0.25
31, 32, 33, 81, 82, 84, 85	Deep-rooted crops	1	1	1.25	1	0.67
41, 42, 43, 61	Mature forest	2.5	2	2	1.6	1.17
71~76	No vegetation	0	0	0	0	0

[1] the Anderson land use code is in Table 5

[2] the soil texture class is in Table 7

(3) Vadose-zone soil depth was determined by the root-zone soil depth and the ground water table, and

(4) SCS curve number was estimated based on the land use type and the soil hydrologic group (Table 10).

Table 10. SCS curve number values (USDA, 1986)

Anderson Code [1]	Assumed cover type	SCS CNs for the soil hydrologic group of			
		A	B	C	D
11- residential	residential (averaged over different lot sizes)	58	73	82	86
12 - commercial and services	commercial and business	89	92	94	95
13, 15 - industrial/commercial services	industrial	81	88	91	93
14 -transportation, communication, utilities	paved roads, open ditches (with right of way)	83	89	92	83
16 - mixed urban or builtup land	commercial and business, industrial, residential – one-fourth acre or less (average)	80	97	91	93
17 - other urban or builtup land	urban open space (fair)	49	69	79	84
21 - cropland and pasture	mean cropland and pasture – fair (average)	57	72	80	85
22 - orchards, groves, vineyards, nurseries, and ornamental horticultural land	woods – grass combination (fair)	43	65	76	82
23, 24 - confined feeding operations/ other agricultural land	farmsteads	59	74	82	86
31 - herbaceous rangeland	herbaceous and pasture/ grassland/ range (average)	49	70	80	87
32 - shrub and brush rangeland	oak-aspen, desert shrub, sagebrush, brush – fair (average)	45	57	68	74
33 - mixed rangeland	31, 32 (average)	47	64	74	81
41, 42, 43 - deciduous/evergreen/ mixed forestland	woods (fair)	36	60	73	79
71, 72, 73, 76 - barren land	bare ground/newly graded areas	77	86	91	84
74 - bare exposed rock	paved parking lots/bare rock	98	98	98	98
75 - strip mines, quarries, gravel pits	gravel roads	76	85	89	91

4   User's Manual
4.1   Program Installation

Before installing the GIM3 program, please make sure the hardware and software environment in the target computer has meet the system requirements as shown in **Table 11**.

Table 11. System requirements for GIM3

	Required system	Recommended system
Processor and CPU Speed	Intel Pentium or Intel Xeon Processors 1.0 GHz	2.0 GHz
Memory/RAM	512 MB	1.0 GB
Disk Space	500 MB	1.2 GB
Operation System	Microsoft Windows XP	
Software Environment	Microsoft .NET Framework 2.0 ESRI ArcGIS 9.x	MATLAB R14 MATLAB COM Builder 4.x Microsoft Visual Basic 2005 Microsoft Access Any C++ Compiler

The complied program was published by Microsoft Visual Basic 2005. The script of "install.bat" will install the MATLAB Component Runtime (MCR) and the GIM3 program in the target computer. The installation directory of MCR could be specified by users, while the GIM3 program will be installed in a default folder by the .NET framework. Usually, the folder is located in
\Documents and Settings\[use account name]\Local Settings\Apps\2.0\.

During installation, a program shortcut will be generated in the Windows Start menu as Microsoft-GIM3. The program could be uninstalled from the "Add/Remove Programs" option in the Windows Control Panel.

4.2   Input Data
4.2.1   Built-in Data

(1) "1.bmp"
To develop a raster workspace in the ArcObjects spatial analysis, an image file is required in the folder for the raster workspace. The small image file "1.bmp" will be copied to the targeted folder during the program execution.

(2) "SysData.mdb"
This database in Access format includes parameters required for the spatial analysis and transport simulation. The tables in the database are shown in **Table 12**.

Table 12. Tables in the "SysData.mdb" as built-in data

Table Name	Description	Reference
BDTABLE	Soil bulk density	Carsel and Parrish (1988), USEPA (1996)
CNTable	SCS curve number values	Table 10
RootDep	Root-zone soil depth	Table 9
SSCTable	Soil texture	Table 7
ChemBase	Chemical properties	CEPA (1993)
Grid	Template for grid database	
MTC	Template for mass transport coefficient database	
SysPara	Template for model initialization database	

(3) "soil.mdb"

The database is used to save intermediate output of soil properties extracted from STATSGO database. Soil properties are stored in this database once a MUID in the STATSGO is processed. If the same MUID is found in the future simulation, its soil properties would be retrieved from this database rather than be calculated again, which saves CPU time greatly in the spatial analysis.

4.2.2   User Input Data

The following data are required as use inputs: (1) spatial data, (2) hydrometeorological data for each sub-watershed, and (3) chemical data of sources, initial conditions, and boundary conditions.

Spatial data of includes geographic information of sub-watershed boundaries, landuse types, and soil properties, in ESRI Shapefile format (ESRI, 1998). EPA BASINS database provides all required spatial data for GIM3 program. These data are available in http://www.epa.gov/waterscience/ftp/basins/gis_data/huc, organized by the 8-digitial HUC codes. For the sub-watershed delineation, the attribute table includes at least two fields, "GRIDCODE" for the sub-watershed ID, and "GRIDCODE1" for the downstream sub-watershed ID. For soil properties, the current version of GIM3 program uses STATSGO database. The minimal inputs include (1) STATSGO index shapefile (statsgo.shp) with a field of "MUID" for map unit identification symbols, (2) soil layers data ("statsgol.dbf"), and (3) soil components data ("statsgoc.dbf"). More details for the STATSGO database was described in Section 3.4 of this report. As mentioned before, the new soil database of SSURGO provides soil properties with higher spatial resolution. When the construction of the SSURGO database is completed, it might be used in the next version of the GIM3 program. The landuse data is based on 1:250,000 scale quadrangles of landuse/land cover GIRAS spatial data in the conterminous United States. The required input files include (1) GIRAS index shapefile ("lulcndx.shp") with a field of "COVNAME" for quadrangle indices, and (2) landuse data in a sub-folder of "landuse" for all quadrangles in the simulation domain.

The inputs for hydrometeorological data and chemical data should be organized in a single file in Microsoft Access format (*.mdb). The required datasets and the

corresponding table names are shown in **Table 13**. Data structures for the datasets are described as follows.

Table 13. Required datasets for the inputs of hydrometeorological data and chemical data

Table Name in the Access database file	Description
Hydrological data	
AGWO	Base flow rate (m/day)
FLOW	watershed flow discharge (m/day)
IFWO	Inter flow rate (m/day)
INFL	Infiltration rate (m/day)
PREC	Precipitation rate (m/day)
SAET	Actual evaporation (m/day)
SURO	Overland flow rate (m/day)
Meteorological data	
DRCT	Wind direction (degree)
TEMP	Ambient temperature (K)
WIND	Wind speed (m/s)
Chemical data	
TRI	Chemical emissions (g/day)
IC	Initial concentrations (g/m3)
BC	Boundary air concentrations (g/m3)

In all tables, the first field is reserved for automatic numbering. The second and third fields are text fields used for description, units or other uses. Data inputs start from the fourth field (**Table 14**). For hydrological and meteorological data, input data was organized as a table of N rows and M columns, where N is the total number of records in the time interval which is specified in the model initialization, and M is the total number of sub-watersheds. For chemical emissions and initial conditions, input data was tabulated for each environmental compartment in each sub-watershed. For boundary conditions, GIM3 program only requires chemical concentrations in air for the area adjacent to the simulation domain in north, east, south, and west direction.

Table 14. Data structure for the (a) hydrometeorological data, (b) chemical emission and initial conditions, and (c) chemical boundary conditions

(a)

ID	Description	Unit	Watershed1	Watershed2	…
1					
2				Input data	
3					
…					

(b)

ID	Description	Unit	Watershed1	Watershed2	…
1	Air				
2	Plant				
3	Surface soil				
4	Root zone			Input data	
5	Vadose zone				
6	Surface water				
7	Sediment				

(c)

ID	Description	Unit	Air conc.
1	North to domain		
2	East to domain		Input data
3	South to domain		
4	West to domain		

4.2.3 Sample Inputs

Sample input files could be found in the "tutorial" folder for program tutorial. The sample files describe the simulation scenario for the transport of trichloroethylene (TCE) in the Connecticut River Basin (CTRB) during 2000. The spatial Shapefile and geographic database for the simulation domain were saved in the sub-folder of "feature", with sub-watershed delineation file as "CTRB.shp". Hydrometeorological data and chemical data (CTRB.mdb) could be found in the sub-folder of "data".

4.3 User Interfaces and Simulation Guidance

The key procedures in applying the GIM3 program include,
- Prepare use input data for hydrometeorological conditions and chemical data
- Spatial analyses for land and soil characterization
- Generate landscape parameters
- Define the chemical species
- (Optional) Edit the program-generated and default input data
- Run GIM3 program, and
- (Optional) Analyze, plot and graph GIM3 output using MATLAB

4.3.1　Launch the Program

Before running the program, input data should be prepared well following the requirements,

    (1) Built-in data and user input data should be placed in the same folder,

    (2) Following the file structures in EPA BASINS spatial data, the sub-watershed delineation Shapefile, the GIRAS landuse index Shapefile (lulcndx.shp), all files for STATSGO database (statsgo.shp, statsgol.dbf, and statsgoc.dbf) should be in the same folder, while the GIRAS quadrangle tables are in a sub-folder of "landuse".

Once installed in a computer, the GIM3 program could be launched by the shortcut in Windows Start menu. **Figure 8** shows the main user interface of the program.
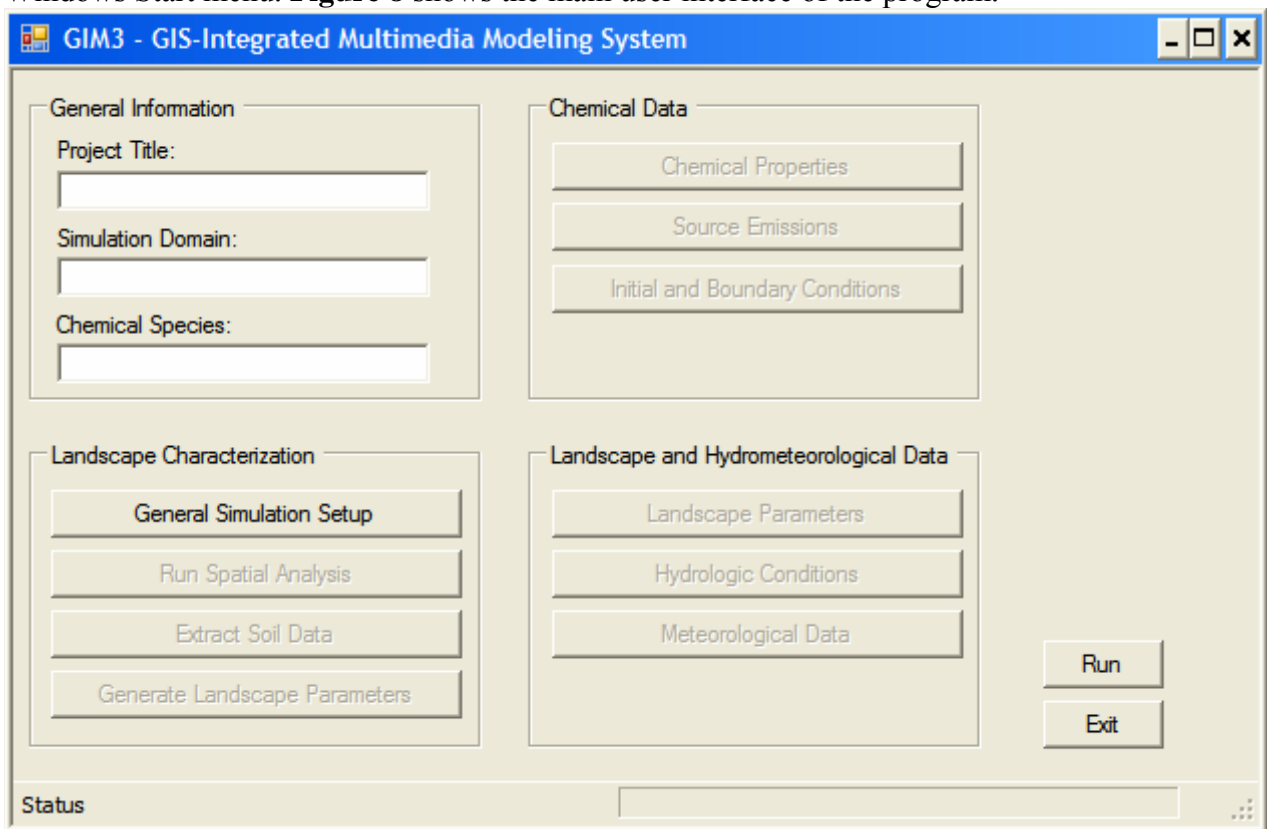
Figure 8. Main user interface of the GIM3 program

4.3.2　Initialize the Simulation

In the function of "General Simulation Setup", the program asks user to specify some basic information for the model simulation (**Figure 9**). The required information includes

    (1) Path and Shapefile name of the sub-watershed delineation. The path specified here is also used for the landuse and soil databases,

    (2) Path and Access file name for hydrometeorological data and chemical data. The path specified here is also used for built-in data,

(3) Temporary folder is used to store intermediate outputs in the spatial analysis. The program identifies the system temporary folder automatically, while user could change the folder,

(4) Sizes of land cell and air cell specify the sampling interval for landscape spatial analysis and air-ground interactions,

(5) The program accounts the total numbers of hydrometeorological input data, while user could request for transport simulation based on annual average of these data, and

(6) Options for time-dependent and steady-state simulation are provided in the program.
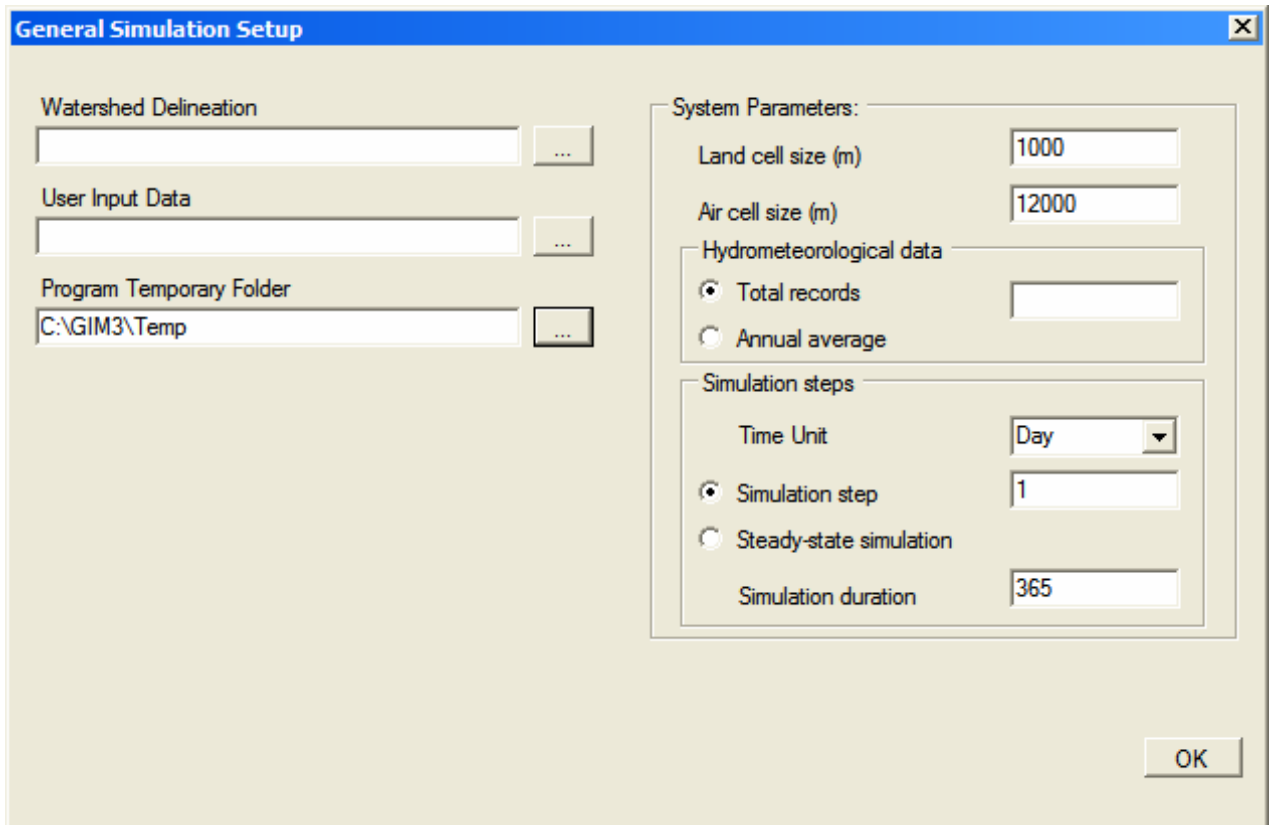
Figure 9. Interface for "General Simulation Setup"

4.3.3 Execute Spatial Analysis and Extract Soil Properties

No user interfaces are designed for these functions. The technical details for these functions were described in sections 3.3 and 3.4.

4.3.4 Generate Landscape Parameters

Based on the GIS sampling results, landscape parameters are generated in a database, and the mass transport coefficients are also copied into this database. The parameters to be generated include compartment areas, depths of soil layers, organic carbon contents of soil layers, and air and water contents of soil layers. Based on the built-in data of "SysData.mdb", the program provides defaults values for mass transport coefficients and

some landscape parameters. Options are available for user to change and save their own values for these parameters (**Figure 10**).
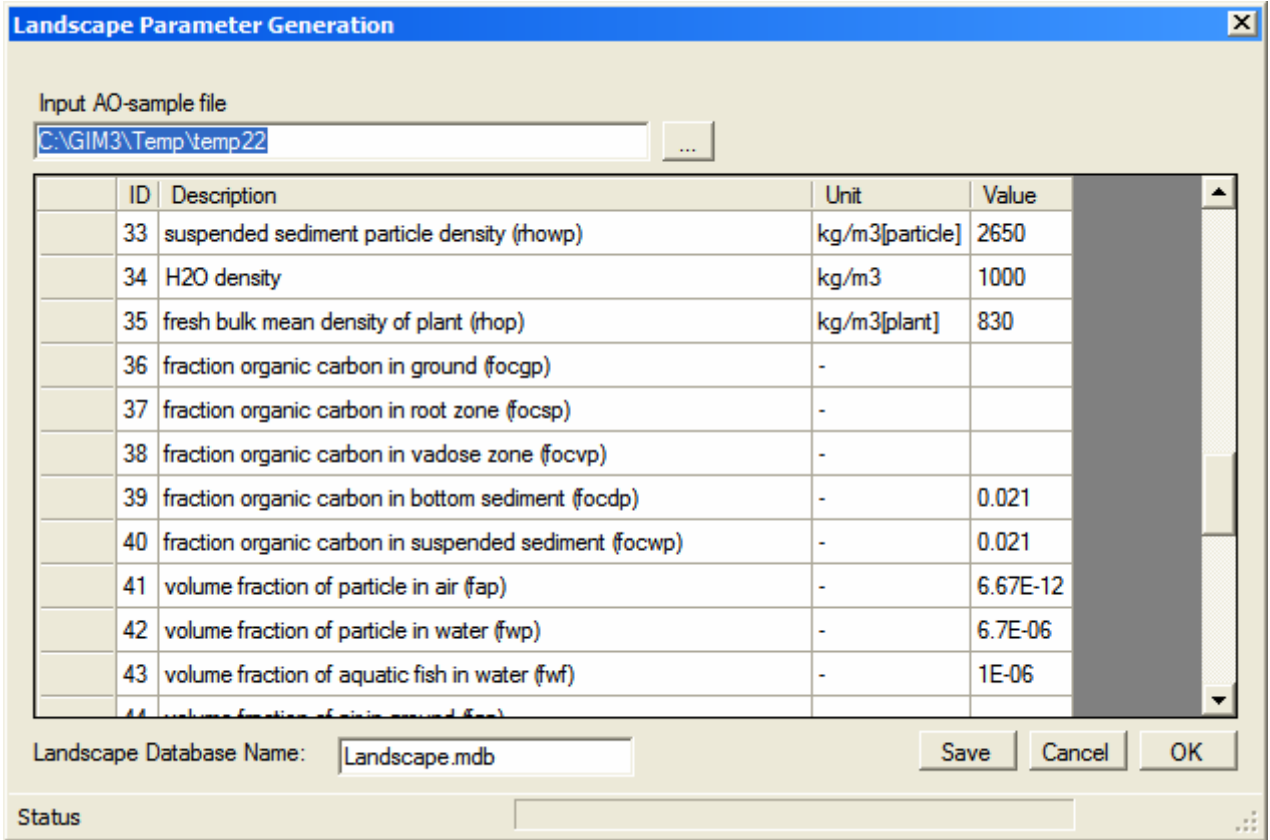
Figure 10. Interface for "Generate Landscape Parameters"

4.3.5   Prepare Chemical Properties

The built-in database of "SysData.mdb" includes chemical properties and associate uncertainties for 78 chemicals. User could select a chemical in the database as a test agent in the transport simulation (**Figure 11**). To avoid inappropriate operations on the chemical properties database, this interface does not provide options for revising the database. Any revision, such as changing values, adding or deleting a chemical, should be done directed in the database file of "SysData.mdb".
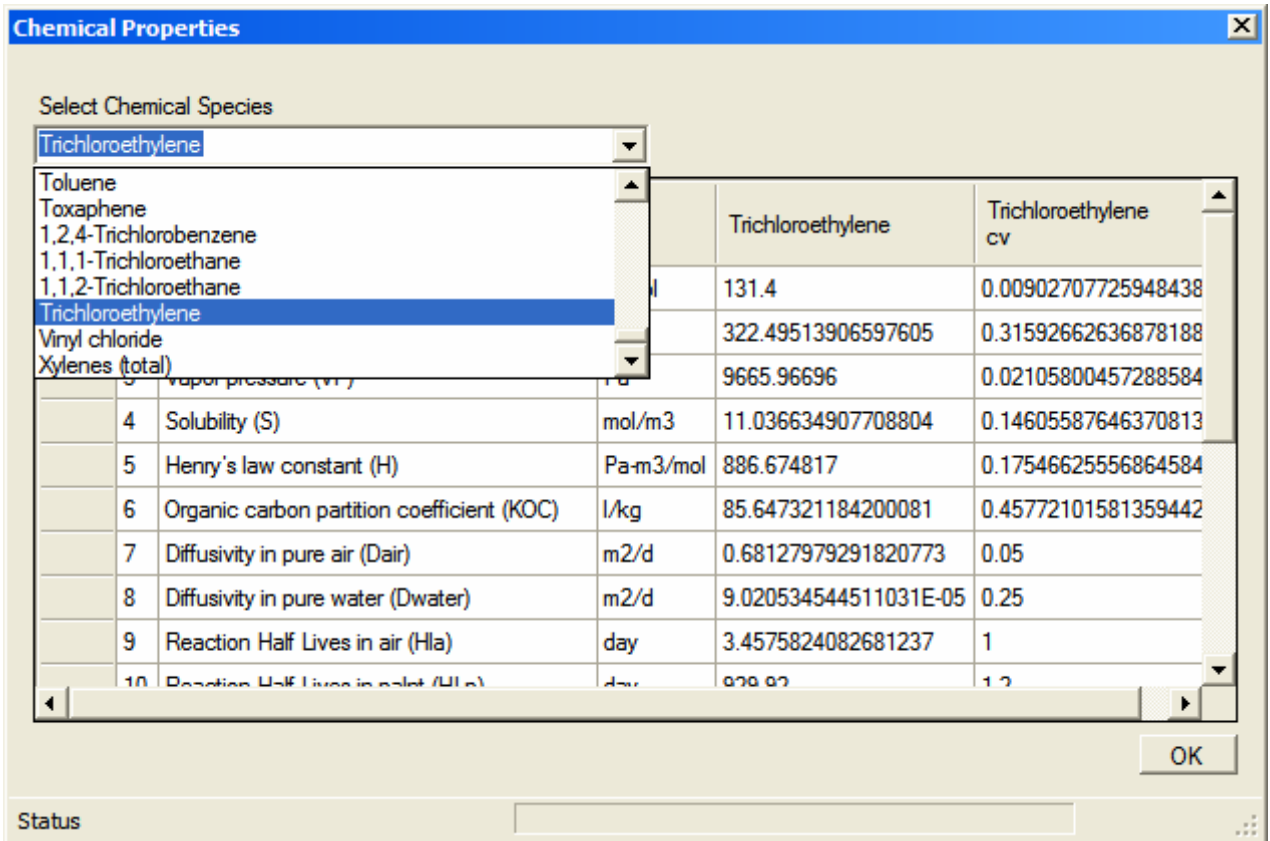
Figure 11. Interface for "Chemical Properties"

4.3.6 View and adjust user input data

User input data could be viewed and adjusted before used in the model simulation (**Figure 12**).

Input Data Viewer

Parameter Databases

AGWO - Base flow rate (m/day)

ID	De	Watershed1	Watershed2	Watershed3	Watershed4	Watershed5	Watersh
1		0.00084328	0.0010947	0.0010947	0.0010439	0.0011049	0.001483
2		0.00083058	0.001077	0.001077	0.0010262	0.0010871	0.001458
3		0.00081534	0.0010592	0.0010592	0.0010084	0.0010693	0.001432
4		0.00080264	0.0010414	0.0010414	0.0009906	0.0010516	0.001409
5		0.0007874	0.0010211	0.0010211	0.00097282	0.0010312	0.001381
6		0.00077216	0.0010033	0.0010033	0.00095504	0.0010109	0.001358
7		0.00075692	0.00098298	0.00098298	0.00093472	0.0009906	0.001331
8		0.00074168	0.00096266	0.00096266	0.00091694	0.00097282	0.001308
9		0.00072898	0.00094742	0.00094742	0.00089916	0.00095504	0.001282
10		0.00071628	0.00092964	0.00092964	0.00088392	0.00093726	0.001255
11		0.00070358	0.00091694	0.00091694	0.00087122	0.00092456	0.001244

Save   OK

Status

Figure 12. Interface for input data viewer, base flow data as example

4.4   Output Data

Outputs from the spatial analysis are saved as Shapefile format or raster format in the program temporal folder. These files could be displayed and operated with ArcGIS or other GIS software.

Outputs from the transport simulation are saved as MATLAB matrix format in the program data folder (the same folder with user input data). Data in this file ("results.mat") are compatible with all functions and programs in MATLAB and its associated applications. The sophisticated MATLAB functions and toolboxes could be used for output data analysis. To reduce the complexity in program development, therefore, the GIM3 program does not include modules for data visualization and statistical analysis. The descriptions of output variables in the file of "results.mat" are shown in Table 16.

5   Conclusions and Suggestions

This project produced a user-friendly software which can be used to test and analyze multimedia environmental problems associated with contaminant transport and transformation, such as the movement of pesticides through the hydrologic cycle, or the response of solute concentrations in groundwater and surface water to nutrient input changes. With the capacity of simulating the source-receptor relationships and predicting

geographic distribution of pollutants, the software developed in this study can be a practical tool for government agencies to evaluate and regulate various contamination sources in agricultural and industrial activities. The integration of transport processes, visual interactivity, and seamless communication features make the model possible for user to focus on critical conceptual issues, to quickly and iteratively examine hypotheses and system responses, to identify dominant processes, and to assess key parameters. Additionally, as an educational application, this software environment allows student to visually examine the dynamics of the bulk flow, contaminant transport, and biochemical transformation. Therefore, the proposed software can be used to enhance teaching and learning in number of courses across environmental engineering and water resources curriculum at graduate and undergraduate levels, such as Environmental Biophysics, Transport Phenomena, Groundwater modeling, and Small Watershed Analysis.

The integration of Graphic User Interface (GUI) and real-time interaction capabilities will make the software an ideal tool for regulatory and education applications. Supported by the GUI, the users are established at the center of the system during the simulation design. The simulation design begins by specifying the study region, the time and length of the simulation, chemical information, compartments and inter-media transport processes to be included, initial and boundary conditions, and result output options. A similar interface is also developed for real-time interaction to change original configurations, and view the intermediate results. This software can be used by government agencies to evaluate and regulate various pollution sources in agricultural and industrial activities. As an educational tool, it can be used for teaching and learning in classroom by visually examining the dynamics of the bulk flow, contaminant transport, and biochemical transformation

Efforts to refine and improve the newly developed model in this study should initially be directed toward evaluating the model's description of the air compartment and air flows between regions. Transport in air is the most likely route for long-range migration of contaminants. Therefore, accurate model results will depend on having a realistic description of the air compartment and relevant flows. Multiply layers for the air cells should be created for presenting the veridical variation in chemical distribution in the atmosphere. The seasonal variation in mixing layer height should also be introduced. In addition, the interaction between air boundary layer and the upper air layers may be also significant for fate and transport of some species (Zhang *et al.*, 2003). An air quality model compatible with current EPA supported model systems is suggested to be integrated into the modeling framework for supporting the estimation of atmospheric deposition and air-surface interaction.

In the current version of the multimedia environmental fate model, some transport pathways were largely simplified. For example, the migration and dilution of chemicals in groundwater was not explicitly simulated. Instead, the contaminant leaching from the vadose-zone soil was considered as an input to the groundwater. In constructing an algorithm for contaminant transport in the saturate zone, we take the perspective that the mathematical formulation is not necessary to be complex. The reason is that, relative to the mathematical algorithm, the greatest degree of uncertainty in applying the model

enters through geologic heterogeneity, such as the values used for the crucial parameters of dispersivity. In addition, the groundwater algorithm developed here for a multimedia environmental fate model is not intended to compete with numerical groundwater models. Based on the database of regional aquifer properties developed in the spatial characterization, a contaminate plume analysis may be an appropriate for a simple module for groundwater compartment. This model will account for groundwater transport with quantitative uncertainty, so this pathway can be compared with other pathways (McKone *et al.*, 1997).

6 Appendix
6.1 Available Databases

Table 15. Data sources for GIM3 program simulation

ID	Name of Database	Parameters	Software	Comments	Reference
1	USDA ARS Pesticide Properties Database (PPD)	Pesticide Properties		The ARS PPD is a compendium of chemical and physical properties of 334 widely used pesticides. Information included in the database focuses on 16 of the most important properties that affect pesticide transport and degradation characteristics http://www.ars.usda.gov/Services/docs.htm?docid=6433	(USDA, 2005)
2	USDA-NASS Agricultural Statistics Data Base	Pesticide Emissions		NASS publishes U.S., State, and County level agricultural statistics for many commodities and data series. Quick Stats offers the ability to query by commodity, state(s) and year(s). The query dataset can be downloaded for easy use in your database or spreadsheet. http://151.121.3.33:8080/QuickStats/	
3	Clean Air Status and Trends Network (CASTNET)	Atmospheric Deposition; Wind Data; Air Concentration		CASTNET is the nation's primary source for data on dry acidic deposition and rural, ground-level ozone. Operating since 1987, CASTNET is used in conjunction with other national monitoring networks to provide information for evaluating the effectiveness of national emission control strategies. CASTNET consists of over 80 sites across the eastern and western United States and is cooperatively operated and funded with the National Park Service. http://www.epa.gov/castnet/	(USEPA, 2002b)
4	NH GRANIT	GIS for New Hampshire	ArcGIS	This site offers you access to a range of resources, including: (1) search and retrieval of GRANIT data descriptions (metadata); (2) retrieval of primary GRANIT data layers posting of news related to database developments; (3) announcements of upcoming meetings and events; (4) mapping of core data sets; (5) access to a catalog listing of photography covering various geographic units of New Hampshire. http://www.granit.sr.unh.edu/	

ID	Name of Database	Parameters	Software	Comments	Reference
5	EPA BASINS Supporting Database	Basin Core Data, DEM, NED, GIRAS, NHD	BASINS, HSPF	http://www.epa.gov/waterscience/basins/metadata.htm http://www.epa.gov/waterscience/ftp/basins/gis_data/huc	(USEPA, 2001)
6	WDM Weather Data	Precipitation, Temperature, Wind Speed, Radiation…	HSPF, WDMUtil	http://www.epa.gov/waterscience/ftp/basins/wdm_data/	
7	SSURGO database	Soil properties	ArcGIS, ArcView	see spatial characterization section for more details on data description and processing http://www.ncgc.nrcs.usda.gov/products/datasets/statsgo/	(USDA, 2006b)
8	SSURGO database	Soil properties	ArcGIS, ArcView	see spatial characterization section for more details on data description and processing Http://www.ncgc.nrcs.usda.gov/products/datasets/ssurgo/	(USDA, 2006a)
9	USGS NWISWeb Data	realtime and historical data for hydrology and water quality	BASINS, HSPF, ArcGIS	The USGS investigates the occurrence, quantity, quality, distribution, and movement of surface and underground waters and disseminates the data to the public, State and local governments, public and private utilities, and other Federal agencies involved with managing our water resources. http://waterdata.usgs.gov/nwis	
10	CalTox 4.0 Database	Chemical Properties, typical landscape data	CalTox, Excel	CalTOX is a risk assessment model that calculates the emissions of a chemical, the concentration of a chemical in soil, and the risk of an adverse health effect due to a chemical. It consists of two parts: a multimedia environmental fate model, which evaluates the distribution of a chemical among different environmental compartments (air, surface water, etc.), and a multiple pathway exposure model, which calculates how much of a chemical reaches the body using environmental concentration and contact factors (e.g. breathing rate). CalTOX is a spreadsheet model. Different model versions of CalTOX have been used for different purposes and in various publications. http://eetd.lbl.gov/ied/ERA/caltox/index.html	(McKone and Enoch, 2002)

ID	Name of Database	Parameters	Software	Comments	Reference
11	CalTox 2.x Database	Chemical Properties, typical landscape data	CalTox, Excel	CalTOX is an innovative spreadsheet model that relates the concentration of a chemical in soil to the risk of an adverse health effect for a person living or working on or near the contaminated soil. CalTOX computes site-specific health-based soil clean-up concentrations given target risk levels or human health risks given soil concentrations at the site. http://www.dtsc.ca.gov/AssessingRisk/caltox.cfm	(McKone, 1993)
12	Interagency Monitoring of Protected Visual Environments Program (IMPROVE)	aerosol		Summary of optical measurements the haze aerosol composition, spatial distribution and trends and from the IMPROVE monitoring network. http://vista.cira.colostate.edu/improve/	(IMPROVE, 2002)
13	EPA AirData	Air pollution data		AirData presents annual summaries of air pollution data from two EPA databases: · AQS (Air Quality System) database provides air monitoring data - ambient concentrations of criteria and hazardous air pollutants at monitoring sites, primarily in cities and towns. · NEI (National Emission Inventory) database provides estimates of annual emissions of criteria and hazardous air pollutants from all types of sources. The NEI database in 2002 replaced two separate EPA databases for emissions of criteria air pollutants (National Emission Trends, or NET) and hazardous air pollutants (National Toxics Inventory, or NTI). http://www.epa.gov/air/data/	(USEPA, 2004)
14	NASA LAI data	LAI		About 1000 LAI values from 0.1-0.18 (minimum; desert and tundra) to 47.0 (maximum; a peculiarity of one allometric method for estimating all-sided LAI in coniferous tree stands). Units are m2/m2 or dimensionless. However, only 14% of the records have LAI greater than 8.0 (a more typical maximum value for one-sided or projected LAI, unlikely to be exceeded except with peculiar conditions or methodology.) http://www.daac.ornl.gov/VEGETATION/lai_des.html	(Scurlock *et al.*, 2001)
15	EPA Toxics Release Inventory (TRI)	TRI		The Toxics Release Inventory (TRI) is a publicly available EPA database that contains information on toxic chemical releases and other waste management activities reported annually by certain covered industry groups as well as federal facilities. This inventory was established under the Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA) and	(USEPA, 2003b)

ID	Name of Database	Parameters	Software	Comments	Reference
				expanded by the Pollution Prevention Act of 1990. http://www.epa.gov/tri/	
16	1996 National Air Toxics Assessment by ASPEN model	Model ambient air concentration		As part of EPA's National Air Toxics Assessment activities, EPA conducted a national-scale assessment of 33 air pollutants (a subset of 32 air toxics on the Clean Air Act's list of 188 air toxics plus diesel particulate matter (diesel PM)). The assessment includes four steps that look at the year 1996. (1) Model (ASPEN) and Data: http://www.epa.gov/ttn/atw/nata/natsa2.html (2) 1996 National Air Toxics Assessment: http://www.epa.gov/ttn/atw/nata/	(USEPA, 2002a)
17	NOAA National Weather Service	Weather and Metorology data		http://www.nws.noaa.gov/	
18	Forest Inventory and Analysis National Program (FIA)	Forest Inventory		FIA reports on status and trends in forest area and location; in the species, size, and health of trees; in total tree growth, mortality, and removals by harvest in wood production and utilization rates by various products; and in forest land ownership. http://www.fia.fs.fed.us/	(USDA, 2004)

6.2 Core Transport Simulation Codes in MATLAB

The following MATLAB code is the core simulation function in the GIM3 simulation. It calculates transport parameters, allocate sources and inter-media fluxes among compartments, and simulate chemical inventories at each time step.

```
function Ct=GIM34sim(paraLand,paraChem,paraSource,N0,datapath)

load([datapath 'HydroMet.mat'])

sim_step=syspara(7);
sim_end=syspara(8);
basins=syspara(9);
medias=syspara(10);
taircells=syspara(11);
airrows=syspara(12);
aircols=syspara(13);
chkwater=syspara(14);
Wac=syspara(15);Aac=Wac*Wac;        %Wac=cell width
HMrecords=syspara(16);
Cin=zeros(1,4);
Cin(1)=syspara(17);
Cin(2)=syspara(18);
Cin(3)=syspara(19);
Cin(4)=syspara(20);


PI=3.14159;
R=8.31;           %univeral gas constant (Pa*m3/mol/K)
Kfx=3000;         %partition coeff b/w foliage - aerosol, mol/kg (plant) per mol/m3 (air)
             %in-dependent of chemicals, see CalTOX modifaction, p14
kTRI=1;          %TRI adjust factor
kED=0;           %Eddy dofussivity=kED*1e6*Dair;

%****************************
%chemical properties
%****************************
MW=paraChem(1);        %molecular weight (g/mol)
Kow=paraChem(2);
PKow=-log10(Kow);      %octanol-water (p)artition (c)oefficient (pc) (L[water]/L[octanol]
VP=paraChem(3);          %vapor pressure (pa), from L. Coulibaly, or 69mmHg at 298K
H=paraChem(5);          %Henry Law constant (Pa*m3/mol) at 298K, follow CalTox
Koc=paraChem(6);         %sorption coefficient (l/kg), follow CalTox
Dair=paraChem(7);        % diffusion coefficient in air phase, m2/d, CalTox
Dwater=paraChem(8);       % diffusion coefficient in water phase, m2/d, CalTox
Tm=paraChem(16);
BCF=paraChem(17);


%**************************************
%half life, HL(day); T valus (R) =ln2/HL (1/day)
%**************************************
HLa=paraChem(9); HLp=paraChem(10);
HLg=paraChem(11);HLs=paraChem(12);
HLv=paraChem(13);HLw=paraChem(14); HLd=paraChem(15);
Ra=0.693/HLa;Rw=0.693/HLw;Rg=0.693/HLg;Rp=0.693/HLp;
```

```
%*****************************************
%Land, Hydro, Climate/Met property;
%*****************************************
rhogp=paraLand(29,:);         %soil particle density in ground (kg/m3particle)
rhosp=paraLand(30,:);         %soil particle density in root zone
rhovp=paraLand(31,:);         %soil particle density in vadose zone
rhodp=paraLand(32,:);         %bottom sediment particle density
rhowp=paraLand(33,:);          %suspended sediment particle density
rhow=paraLand(34,:);          %H2O density
rhop=paraLand(35,:);          %fresh bulk mean density of plant


focgp=paraLand(36,:);          %fraction organic carbon in ground (-); 0.029 in L.C. but CalTox uses
focsp=focgp
focsp=paraLand(37,:);          %in root zone. 0.01 in CalTox
focvp=paraLand(38,:);          %in vadose zone, 2e-3 in CalTox
focdp=paraLand(39,:);          %in bottom sendiment; 0.02 in CalTox
focwp=paraLand(40,:);           %in suspended sendiment, 0.2 in L.C>, but CalTix use focwp=focdp


fap=paraLand(41,:);          %volume fraction of particle in air
fwp=paraLand(42,:);           %vf of particle in water
fwf=paraLand(43,:);           %vf of aquatic biota/fish in water
fga=paraLand(44,:);           %vf of air in ground;
fgw=paraLand(45,:);           %vf of water in ground, or water content
fgp=1-fga-fgw;          %vf of particle in ground
fsa=paraLand(46,:);
fsw=paraLand(47,:);
fsp=1-fsa-fsw;
fva=paraLand(48,:);
fvw=paraLand(49,:);
fvp=1-fva-fvw;
fdw=paraLand(50,:);
fdp=1-fdw;


LAI=paraLand(21,:);
vdp=paraLand(1,:);                %atmos dry depo velocity of particle, m/d
vsp=paraLand(2,:);                %sedimentation velocity of suspended particle. m/d, LC
Q=paraLand(3,:);                %scavenging ratio, L.C., CHEMGL, and Mackay 1992
resus=paraLand(4,:);            %resuspension rate, LC


%*****************************************
%matrix calculation begins: geo parameters
%*****************************************
Aa=paraLand(17,:);          %area of atmosphere, or total area, m2, GIM3B
da=paraLand(22,:);
%algorithm2. for Aa<600km2, da=0.22*Aa^0.4, else da=700

Va=Aa.*da;          %mixing layer volume, m3
Ap=paraLand(18,:);   %plant area
dp=paraLand(23,:);Vp=LAI.*Ap.*dp;
%dp value from (above-ground) plant dry biomass inventory, and dp for
%foliage part only, root part is inserted into root zone.

Ag=paraLand(19,:);dg=paraLand(24,:);Vg=Ag.*dg;                %land area
As=Ag;ds=paraLand(25,:);Vs=As.*ds;
Av=Ag;dv=paraLand(26,:);Vv=Av.*dv;
```

```
Aw=paraLand(20,:);
dw=paraLand(27,:);
Vw=Aw.*dw;
Ad=Aw;dd=paraLand(28,:);Vd=Ad.*dd;
Vt=[];
for i=1:basins
    Vt=[Vt;Va(i);Vp(i);Vg(i);Vs(i);Vv(i);Vw(i);Vd(i)];
end

TOPOw=[1:1:basins
    paraLand(63,:)]';%water flows from basins i to j

%yearly mean ratio of infil (root->vadose) to infil (ground->root)
kinfil2_1=sum(AGWO+IFWO)./sum(INFL+SAET);

%****************************************
%air diffusion and vertical loss
%****************************************
%air diffusion
Ta_d=kED*1e6*Dair/Aac*3600*24;

%****************************************
%source term, no external distant input
%****************************************
TRI=kTRI*TRI;

%****************************************
%initial condition
%****************************************
NB=[];
for ibasin=1:basins
    NB=[NB;N0((ibasin-1)*7+2:(ibasin-1)*7+7)];
end

ConnectivityFields=size(Connectivity,2);
LandCell=Connectivity(:,1:basins);
WaterCell=zeros(taircells,basins);
if (chkwater==1);
    WaterCell=WaterCell+Connectivity(:,basins+1:2*basins);
end

%allocate air inventory as IC
NA=zeros(taircells,1);
for icell=1:taircells
    if sum(Connectivity(icell,:))==0; continue; end    %this aircell is not overlaid with any basin
    iAir =icell;
    for ibasin=1:basins
        NA(iAir)=NA(iAir)+N0((ibasin-
1)*7+1)*(LandCell(icell,ibasin)+WaterCell(icell,ibasin))/sum(Connectivity(icell,:));
    end
end
NBx=NB;NAx=NA;

%****************************************
%level 4 simulation begins
%****************************************
```

```
for year=1:sim_end

for day=1:HMrecords

vw=WIND(day,:);                    %m/s
drct=(270-DRCT(day,:))*(PI/180);
currentw=5.17e-2*vw;               %m/s
T=TEMP(day,:);                     %K
inter=IFWO(day,:);                 %interflow from vadose zone to surface water
rain=PREC(day,:);                  %rain in m/d to the whole basin
runoff=SURO(day,:);                %overland flow in m/d to land
erosion=runoff/3e4;                %ground erosion, m/d for land area
infil=INFL(day,:)+SAET(day,:);     %infiltration: (1)ground->root zone, from flows.m
perc=kinfil2_1.*infil;             %infiltration: (2)root zone->vadose zone
uptake=zeros(1,basins);            %always 0 in annual simulation

%negtive infil2 considered as plant uptake water from vadose zone to root zone,
for col=1:basins;
   if perc(col)<0; uptake(col)=-perc(col);perc(col)=0;end
end

rech=AGWO(day,:);
et=abs(SAET(day,:));
transp=4.8e-3*LAI;                 %Paterson and Mackay (1994), xylem~transp=2e-4 m3/hour /m2 foliage
%algorithm2: transp=1.5*et;
%algorithm3: rough estimation=.43*et*bio_inv(3.5 kg/m2)

phlm=transp/10;                    %caltox 2.3
outflow=FLOW(day,:);               %outflow, m/d in Aa (chkwater=0) or Aw (chkwater=1)

%****************************************
% phase fugucity capacity
%****************************************
Zair=1/R./T;                       %fc of pure air
Zwater=1/H;                        %fc of pur water
Zap=3e6*Zair/VP;
%algorithm2. for T<Tm, Zap=exp(6.81*(1-Tm./T))*3e6.*Zair/VP;

Zgp=Zwater*rhogp/1000*Koc.*focgp;      %fc of particle in ground
Zsp=Zwater*rhosp/1000*Koc.*focsp;      %fc of particle in root zone
Zvp=Zwater*rhovp/1000*Koc.*focvp;      %fc of particle in vadose zone
Zwp=Zwater*rhowp/1000*Koc.*focwp;      %fc of particle in suspended sedment
Zdp=Zwater*rhodp/1000*Koc.*focdp;      %fc of particle in bottom sediment
Zwf=BCF/H;
%algorithm2: Zwf=rhow*BCF/H;

Krs=0.82+0.03*PKow*Zwater;             %partition coeff b/w root tissue and soil solid
Kfa=(0.5+(0.4+0.01*Kow)*R*T*Zwater)/rhop;   %b/w foliage - air

%****************************************
%bulk fugacity capacity
%****************************************
Za=(1-fap).*Zair+fap.*Zap;             %bulk fc of iar
Zg=fga.*Zair+fgw.*Zwater+fgp.*Zgp;     %bulk fc of ground
Zs=fsa.*Zair+fsw.*Zwater+fsp.*Zsp;     %bulk fc of root zone
Zv=fva.*Zair+fvw.*Zwater+fvp.*Zvp;     %bulk fc of vadose zone
```

```
Zp=(Za+Zs)/2;                      %bulk fc of plant
Zw=(1-fwp-fwf).*Zwater+fwp.*Zwp+fwf.*Zwf;   %bulk fc of water
Zd=fdw.*Zwater+fdp.*Zdp;                    %bulk fc of sediment
Zpr=Krs.*Zs.*rhop./rhosp./fsp;          %CalTox 2.3 revised following LC
Zpf=Kfa.*rhop.*Zair+Kfx.*rhop.*Zap.*fap;
Zp=Zpf;                           %CalTox2.3 assume Zp=Zpf, and insert Zpr into root zone

%*****************************************
%bulk diffusion coefficient
%*****************************************
Da=Dair.*(Zair./Za);              %bulk dc in air
Dg=Dair.*(Zair./Zg).*(fga.^3.33./(fga+fgw).^2)+Dwater.*(Zwater./Zg).*(fgw.^3.33./(fga+fgw).^2);
Ds=Dair.*(Zair./Zs).*(fsa.^3.33./(fsa+fsw).^2)+Dwater.*(Zwater./Zs).*(fsw.^3.33./(fsa+fsw).^2);
Dv=Dair*(Zair./Zv).*(fva.^3.33./(fva+fvw).^2)+Dwater.*(Zwater./Zv).*(fvw.^3.33./(fva+fvw).^2);
Dp=(Da+Ds)/2;
Dw=Dwater.*(Zwater./Zw);          %bulk dc in water
Dd=Dwater.*(Zwater./Zd).*fdw.^1.33;    %bulk dc in sediment, water is the only fluid

%*****************************************
%A/W diffusion formulation based on CalTox
%*****************************************
if (vw+currentw)>0.5
   Uaw_a=273*(vw+currentw)*sqrt(18/MW);
else
   Uaw_a=140*sqrt(18/MW)*ones(1,basins);
end

if vw>1.9
   %air-water diffusion, water-side MTC, same comment as Uaw_a
   Uaw_w=5.64*(currentw.^0.969./dw.^0.673).*sqrt(32/MW).*exp(0.526*(vw-1.9));
else
   Uaw_w=5.64*(currentw.^0.969./dw.^0.673).*sqrt(32/MW);
end

%diffusion - fugacity-based MTC, Y (mol/m2/Pa/d), and all D in m2/d, delta in m
Yaw_a=Za.*Uaw_a;                  %air-water diffusion, air-side fugacity-based MTC
Yaw_w=Zw.*Uaw_w;                  %air-water diffusion, water-side fugacity-based MTC
Yaw=1./(1./Yaw_a+1./Yaw_w);       %bulk air-water diffusion fugacity-based MTC

deltaag_a=paraLand(8,:);          %(b)oundary (l)ayer (d)epth of air-ground diffusion in air side
Yag_a=Za*Dair/deltaag_a;          %air-ground diffusion, air-side MTC
deltaag_g=0.108*Dg.^0.229;        %bld of air-ground diffusion in ground side
Yag_g=Zg.*Dg./deltaag_g;          %air-ground diffusion, ground-side MTC
Yag=1./(1./Yag_a+1./Yag_g);       %bulk air-ground diffusion MTC
Ygs_g=Zg.*Dg./deltaag_g;
deltags_s=318*Ds.^0.683;
Ygs_s=Zs.*Ds./deltags_s;
Ygs=1./(1./Ygs_g+1./Ygs_s);
deltawd_w=0.002;                  %L.C.
deltawd_d=318*Dd.^0.683;
Ywd_w=Zw*Dwater/deltawd_w;
Ywd_d=Zd.*Dd./deltawd_d;
Ywd=1./(1./Ywd_w+1./Ywd_d);       %bulk water-sediment diffusin MTC
deltaap_a=0.005;                  %L.C.
deltaap_p=5e-6;
Yap_a=Zair*Dair/deltaap_a;
```

```matlab
Yap_p=Zs.*Ds./deltaap_p;
Dwv_a=2.1;                  %water vapor diffusivity in air, m2/d
rwv_stom=0.0027;            %stomata resistance to water vapor, d/m
rstom=Dwv_a*rwv_stom/Dair;      %stomata resistence to chemical, m/d
Ystom=Zair/rstom;            %change confirmed, by CalTox 2.3
Yap=1./(1./Yap_a+1./Yap_p)+Ystom;   %L.C. and urban model

%*****************************************
%calulate T values, 1/d
%*****************************************
Rv=0.693/HLv*Zwater*fvw/Zv;
Rs=0.693/HLs*Zwater*fsw/Zs;
Rd=0.693/HLd*Zwater*fdw/Zd;

Idp=1-exp(-2.8*rhop.*Vp./Ap);      %intercept factor of dry deposition to plant
if (chkwater==1)
   Tap=(Ap./Ag).*(LAI.*Yap+Idp.*fap.*vdp.*Zap)./(Za.*da);
else
    Tap=(Ap./Aa).*(LAI.*Yap+Idp.*fap.*vdp.*Zap)./(Za.*da);
end

Tpa=(LAI.*Yap+fap.*vdp.*Zap)./(Zp.*dp);
Tsp=(Ap./Ag).*transp.*Zwater./(Zs.*ds);
Zphlm=0.9*Zwater;
Tps=phlm.*Zphlm./(Zp.*dp);

Tpg=1/180*ones(1,basins);Tgp=0*ones(1,basins);        %caltox 2.3
Tpx=Tpa+Tps+Tpg+Rp;            %TOTAL export rate of plant

Idg=1-Ap./Ag.*Idp; %intercept factor of dry deposition to grpud
if (chkwater==1)
   Tag=(Yag+rain.*Zwater+fap.*Zap.*(rain.*Q+Idg.*vdp))./(Za.*da);
else
    Tag=(Ag./Aa).*(Yag+rain.*Zwater+fap.*Zap.*(rain.*Q+Idg.*vdp))./(Za.*da);
end

if (chkwater==1)
   Taw=(Yaw+rain.*Zwater+fap.*Zap.*(rain.*Q+vdp))./(Za.*da);
else
    Taw=(Aw./Aa).*(Yaw+rain.*Zwater+fap.*Zap.*(rain.*Q+vdp))./(Za.*da);
end

Tga=(Yag+fap.*Zap.*vdp)./(Zg.*dg);  %particle dry depo=resuspension
Tgs=(Ygs+infil.*Zwater)./(Zg.*dg);
Tgw=(runoff.*Zwater+erosion.*Zgp.*fgp)./(Zg.*dg);  %runoff and erosion
Tgx=Tga+Tgs+Tgw+Rg;
Tsg=Ygs./(Zs.*ds);
Tsv=perc.*Zwater./(Zs.*ds);
Tsx=Tsp+Tsg+Tsv+Rs;
Tvq=rech.*Zwater./(Zv.*dv);        %percolation
Tvw=(inter.*Zwater)./(Zv.*dv);     %interflow
Tvs=(uptake.*Zwater)./(Zv.*dv);     %uptake
Tvx=Tvq+Tvw+Tvs+Rv;                 %diffusion b/w root-vadose zone neglected

Twa=Yaw./(Zw.*dw);
Twd=(Ywd+vsp.*Zwp.*fwp)./(Zw.*dw);
```

```
Two=outflow./dw;
Twx=Twa+Twd+Two+Rw;


Tdw=(Ywd+resus.*Zdp.*fdp)./(Zd.*dd);
Tdx=2*Tdw+Rd;                %burial rate=resus rate


TB=zeros(basins*6,basins*6);
for col=1:basins;
   Tij=zeros(6,6);               %here 1=plant,2=grond,... NO air
   Tij(1,3)=Tsp(col);Tij(3,1)=Tps(col);
   Tij(2,1)=Tpg(col);Tij(1,2)=Tgp(col);
   Tij(2,3)=Tsg(col);Tij(3,2)=Tgs(col);
   Tij(3,4)=Tvs(col);Tij(4,3)=Tsv(col);
   Tij(5,2)=Tgw(col);
   Tij(5,6)=Tdw(col);Tij(6,5)=Twd(col);
   Tij(5,4)=Tvw(col)+Tvq(col);     %soil->groundwater flow to surface water eventually

   Tix=[Tpx(col) Tgx(col) Tsx(col) Tvx(col) Twx(col) Tdx(col)]';
   Tij=Tij-diag(Tix);

   idx=(col-1)*6;
   TB(idx+1:idx+6,idx+1:idx+6)=Tij;
end


%*****************************************
%surface water connectivity
%*****************************************
for ibasin=1:basins
   ibasin_fr=TOPOw(ibasin,1);ibasin_to=TOPOw(ibasin,2);
   if ibasin_to>0;                  %j=0 marks the outlet
      TB((ibasin_to-1)*6+(6-1),(ibasin_fr-1)*6+(6-1))=Two(i);
      %1st 6=media-1; 2nd 6=water,
   end
end


%*****************************************
%allocate WIND and DRCT from basin scale to aircell scale
%*****************************************
gdrct=mean(drct)*ones(taircells,1);
gvw=mean(vw)*ones(taircells,1);
for icell=1:taircells
   if sum(Connectivity(icell,:))==0; continue;end
   gdrct(icell)=(LandCell(icell,:)+WaterCell(icell,:))*drct'/sum(Connectivity(icell,:));
   gvw(icell)=(LandCell(icell,:)+WaterCell(icell,:))*vw'/sum(Connectivity(icell,:));
end


%*****************************************
%air connectivity
%*****************************************
TA=zeros(taircells,taircells);
%cell w/o interaction w/ land has a fixed loss rate, and advections
for icell=1:taircells
   %loss
   Ta_ay=(0.23*(gvw(icell)*3600*24)/Wac)*abs(sin(gdrct(icell)));
   Ta_ax=(0.23*(gvw(icell)*3600*24)/Wac)*abs(cos(gdrct(icell)));
   TA(icell,icell)=-(Ta_ay+Ta_ax+4*Ta_d+Ta_az+Ra);
```

```
   %gain
   %(1) gain from the neighbor cell north to icell (diffusion)
   icell_n=icell-aircols;
   if icell_n>0
      Ta_ay=(0.23*(gvw(icell_n)*3600*24)/Wac)*sin(gdrct(icell_n));
      if (Ta_ay<0)
         %wind in -y direction, and transport mass to icell from north
         TA(icell,icell_n)=Ta_d+(-Ta_ay);
      else
         TA(icell,icell_n)=Ta_d;
      end
   end

   %(2) gain from the neighbor cell south to icell (diffusion and advection)
   icell_n=icell+aircols;
   if icell_n<=taircells;
      Ta_ay=(0.23*(gvw(icell_n)*3600*24)/Wac)*sin(gdrct(icell_n));
      if (Ta_ay>0)
         TA(icell,icell_n)=Ta_d+Ta_ay;
      else
         TA(icell,icell_n)=Ta_d;
      end
   end

   %(3) gain from the neighbor cell west to icell (diffusion)
   icell_n=icell-1;
   if mod(icell_n,aircols)~=0;
      Ta_ax=(0.23*(gvw(icell_n)*3600*24)/Wac)*abs(cos(gdrct(icell_n)));
      if (Ta_ax>0)
         TA(icell,icell_n)=Ta_d+Ta_ax;
      else
         TA(icell,icell_n)=Ta_d;
      end
   end

   %(4) gain from the neighbor cell east to icell (diffusion)
   icell_n=icell+1;
   if mod(icell_n,aircols)~=1;
      Ta_ax=(0.23*(gvw(icell_n)*3600*24)/Wac)*abs(cos(gdrct(icell_n)));
      if (Ta_ax<0)
         TA(icell,icell_n)=Ta_d+(-Ta_ax);
      else
         TA(icell,icell_n)=Ta_d;
      end
   end
end

%cell w/ interaction w/ land has intermdia fluxes
for icell=1:taircells
   if sum(Connectivity(icell,:))==0; continue; end     %no air-ground interaction
   iAir =icell;
   if (chkwater==1)
      if sum(LandCell(icell,:))~=0
         TA(iAir,iAir)=TA(iAir,iAir)-sum(LandCell(icell,:).*(Tap+Tag))/sum(LandCell(icell,:));
      end
```

```matlab
    if sum(WaterCell(icell,:))~=0
        TA(iAir,iAir)=TA(iAir,iAir)-sum(WaterCell(icell,:).*Taw)/sum(WaterCell(icell,:));
    end

  else
     TA(iAir,iAir)=TA(iAir,iAir)-sum(LandCell(icell,:).*(Tap+Tag+Taw))/sum(LandCell(icell,:));
  end
end


%***************************************
%source terms1: air-land interaction
%***************************************
%source term for basins
SB=zeros(basins*(medias-1),1);
%source term for air cells
SA=zeros(taircells,1);

%calculate source for air cells
for icell=1:taircells
   if sum(Connectivity(icell,:))==0; continue; end     %no air-ground interaction
   iAir =icell;

   for ibasin=1:basins
     iRowWater=(ibasin-1)*6+(6-1);        %6 for water
     iRowPlant=(ibasin-1)*6+(2-1);       %2 for foliage
     IRowGround=(ibasin-1)*6+(3-1);       %3 for ground surface soil

     %mass flux from air to ground
     SB(iRowPlant)=SB(iRowPlant)+(LandCell(icell,ibasin)/Aac)*NA(iAir)*Tap(ibasin);
     SB(IRowGround)=SB(IRowGround)+(LandCell(icell,ibasin)/Aac)*NA(iAir)*Tag(ibasin);

     if (chkwater==1)
        SB(iRowWater)=SB(iRowWater)+(WaterCell(icell,ibasin)/Aac)*NA(iAir)*Taw(ibasin);
     else
        SB(iRowWater)=SB(iRowWater)+(LandCell(icell,ibasin)/Aac)*NA(iAir)*Taw(ibasin);
     end

     %mass flux from groud to air
     if (chkwater==1)
        SA(icell)=SA(icell)+(LandCell(icell,ibasin)/Ag(ibasin))*(NB(iRowPlant)*Tpa(ibasin)...
           +NB(IRowGround)*Tga(ibasin)+TRI(1,ibasin)/MW)...
           +(WaterCell(icell,ibasin)/Aw(ibasin))*(NB(iRowWater)*Twa(ibasin));
     else
        SA(icell)=SA(icell)+(LandCell(icell,ibasin)/Aa(ibasin))*(NB(iRowPlant)*Tpa(ibasin)...
           +NB(IRowGround)*Tga(ibasin)+TRI(1,ibasin)/MW+NB(iRowWater)*Twa(ibasin));
     end

   end %basin

end %aircell

%***************************************
%source terms2: TRI in water and soil
%***************************************
for ibasin=1:basins
```

```matlab
    for imedia=2:medias        %for all compartments except air
        iRowMedia=(ibasin-1)*6+(imedia-1);
        SB(iRowMedia)=SB(iRowMedia)+TRI(imedia,ibasin)/MW;
    end

end

%****************************************
%source terms3: inflow-bound chemicals (boundary condition)
%****************************************
for icell=1:aircols %north to the study area

    Ta_ay=(0.23*(gvw(icell)*3600*24)/Wac)*sin(gdrct(icell));
    if (Ta_ay<0);
        SA(icell)=SA(icell)+Cin(1)/MW*(700*Aac)*(-Ta_ay);
    end

end
for icell=taircells-aircols+1:taircells %south to the study area
    Ta_ay=(0.23*(gvw(icell)*3600*24)/Wac)*sin(gdrct(icell));
    if (Ta_ay>0);SA(icell)=SA(icell)+Cin(3)/MW*(700*Aac)*Ta_ay;end
end
for icell=1:aircols:taircells-aircols+1 %east to the study area
    Ta_ax=(0.23*(gvw(icell)*3600*24)/Wac)*abs(cos(gdrct(icell)));
    if (Ta_ax>0);SA(icell)=SA(icell)+Cin(4)/MW*(700*Aac)*Ta_ax;end
end
for icell=aircols:aircols:taircells %south to the study area
    Ta_ax=(0.23*(gvw(icell)*3600*24)/Wac)*abs(cos(gdrct(icell)));
    if (Ta_ax<0);SA(icell)=SA(icell)+Cin(2)/MW*(700*Aac)*(-Ta_ax);end
end

%****************************************
%simulation for next time step
%****************************************
%for basin
NB=FDMsolver(TB, SB, NB,sim_step);
NBx=[NBx NB];

%for air
NA=FDMsolver(TA, SA, NA,sim_step);
NAx=[NAx NA];

end %day
end %sim_end

%****************************************
%post processing
%****************************************

NAB=zeros(1,basins); %air mass accumulated at basin
for icell=1:taircells
    iAir=icell;
    for ibasin=1:basins

        NAB(ibasin)=NAB(ibasin)+LandCell(icell,ibasin)/Aac*NA(iAir);
```

```
    if (chkwater==1)
        NAB(ibasin)=NAB(ibasin)+WaterCell(icell,ibasin)/Aac*NA(iAir);
    end
  end
end

Nt=[];NTt=[]; %Nt: current compartment inventory, NTt=basin(air+land) inventory
for iBasin=1:basins
  %%%%%%Ct=[Ct;[NAB(iBasin) NB((iBasin-1)*6+1:iBasin*6)']'./Vt((iBasin-1)*7+1:iBasin*7)*MW] ;
  Nt=[Nt; [NAB(iBasin) NB((iBasin-1)*6+1:iBasin*6)']'];
  NTt=[NTt; sum([NAB(iBasin) NB((iBasin-1)*6+1:iBasin*6)']')];
end

if min(Nt)<0||isreal(Nt)==0;    %negative or complex inventory
   disp('negative concentration found');beep;
   pause;
end
%report as compartment concentration
Ct=Nt./Vt*MW;  %final concentration for all media, (7*5,1)
%report as basin (air+land) mass
%Ct=NTt;

CAmatrix=[];
for irow=airrows:-1:1
   CAmatrix=[CAmatrix; NA((irow-1)*aircols+1:irow*aircols)'/(Aac*da(1))*MW];
end

end %function
```

Table 16. Variables used in the GIM3 simulation codes

Parameters	Format	Description
datapath	string	The directory where input data files are saved
sim_step	scalar	Time step in ODE numerical solution (day)
sim_end	scalar	Total periods in the simulation
basins	scalar	Total # of basins/watersheds in the simulation
medias	scalar	Total # of compartments in one basin/watershed (default=7)
taircells	scalar	Total # of the air grid cells
airrows	scalar	Total # of rows in the air grid cells
aircols	scalar	Total # of columns in the air grid cells
chkwater	boolean	If water bodies are simulated separately from watersheds
Wac	scalar	Width of an air grid cell (m)
Aac	scalar	Area if an air grid cell (m2)
HMrecords	scalar	Total # of hydrological input data recorders (day)
Cin	Vector	Background concentrations in the areas adjacent to the simulation domain (1 for north, 2 for east, 3 for south, and 4 for west)
PI	constant	the ratio of the circumference of a circle (3.14159)
R	constant	univeral gas constant (8.31 Pa*m3/mol/K)
Kfx	constant	partition coeff b/w foliage and aerosol (3000 mol/kg [plant] per mol/m3 [air])
kTRI	scalar	TRI adjust factor
kED	scalar	Eddy difussivity
MW	scalar	molecular weight (g/mol)
Kow	Scalar	octanol-water partition coefficient (L[water]/L[octanol]
VP	Scalar	vapor pressure (pa)

Parameters	Format	Description
H	Scalar	Henry Law constant (Pa*m3/mol) at 298K
KOC	Scalar	soil organic carbon-water partition coefficient (l/kg)
Dair	Scalar	diffusion coefficient in air phase, m2/d
Dwater	Scalar	diffusion coefficient in water phase, m2/d
Tm	Scalar	Melting point (K)
BCF	Scalar	Bio-concentration factor
HL[]	Scalar	Chemical half-lives for compartments of air [a], plant foliage [p], ground surface soil [g], root zone [s], vadose zone [v], surface water [w], and sediment [d]. (day)
R[]	Scalar	Chemical reaction constants for compartments of air [a], plant foliage [p], ground surface soil [g], root zone [s], vadose zone [v], surface water [w], and sediment [d]. (day-1)
rho[]p	Scalar	Densities of particles in compartments of ground surface soil [g], root zone [s], vadose zone [v], surface water [w], and sediment [d]. (kg/m3[particle])
rhow	Scalar	Density of water (kg/m3)
rhop	Scalar	fresh bulk mean density of plant (kg/m3[plant])
foc[]p	Scalar	Mass fraction of organic carbon in compartments of air [a], plant foliage [p], ground surface soil [g], root zone [s], vadose zone [v], surface water [w], and sediment [d].
f[]()	Scalar	Volume fraction of particle (p), air (a), water (w), and aquatic biota (f) in compartments of air [a], plant foliage [p], ground surface soil [g], root zone [s], vadose zone [v], surface water [w], and sediment [d].
LAI	Scalar	Leaf area index
vdp	Scalar	Atmospheric dry deposition velocity of particles (m/d). Note: here vdp is the real velocity of particle, not an effective velocity across the air-ground interface. When calculating bulk inter-media flux, fap will be applied as in Tap correlation. Same to vsp, and erosion.
vsp	Scalar	Sedimentation velocity of suspended particles (m/d)
Q	Scalar	Scavenging ratio
resus	Scalar	Sediment resuspension rate
A[]	Scalar	Projection area of air [a], plant foliage [p], ground surface soil [g], root zone [s], vadose zone [v], surface water [w], and sediment [d]. (m2)
d[]	Scalar	Depth/thickness of air [a], plant foliage [p], ground surface soil [g], root zone [s], vadose zone [v], surface water [w], and sediment [d]. (m)
TOPOw	Scalar	Connection relationship between the watersheds
kinfil2_1	Scalar	Long-term mean ratio of infiltration to percolation
Ta_d	scalar	Rate constant for air diffusion
TRI	Vector	Chemical source emissions (g/d)
N[]	Vector	Instantaneous chemical inventories in compartments [B] and in air grid cells [A]. (mol)
N[]x	Matrix	Collection of instantaneous inventories for every time step. (mol)
vw	Vector	Wind speed at basin scale (m/s)
drct	Vecto	Wind direction at basin scale (0 from north, 90 from east, 180 from south, and 270 from west (degree)
currentw	Vector	Water current velocity (m/s)
T	Vector	Temperature (K)
inter	Vector	Inter flow rate from vadose zone to surface water (m/d)
rain	Vector	Precipitation rate (m/d)
runoff	Vector	Overland runoff rate from ground soil to surface water (m/d)
erosion	Vector	Soil erosion rate from ground soil to surface water (m/d)
infil	Vector	Infiltration rate from ground soil to root zone (m/d)
perc	Vector	Percolation rate from root zone to vadose zone (m/d)
uptake	Vector	Plant uptake rate from root zone to plant (m/d)
rech	Vector	Groundwater recharge rate from vadose zone to groundwater,

Parameters	Format	Description
		estimated as base flow rate from groundwater to surface water (m/d)
et	Vector	Evapotranspiration rate (m/d)
transp	Vector	Plant transpiration rate, estimated as xylem flow rate from root zone to plant (m/d)
phlm	Vector	Phloem fluid flow rate from plant to root zone (m/d)
outflow	Vector	Watershed discharge (m/d)
Zair	Vector	Fugacity capacity of air phase (mol/Pa/m3)
Zwater	Vector	Fugacity capacity of water phase (mol/Pa/m3)
Z[]p	Vector	Fugacity capacities of particles in air [a], plant foliage [p], ground surface soil [g], root zone [s], vadose zone [v], surface water [w], and sediment [d]. (mol/Pa/m3)
Zwf	Vector	Fugacity capacity of aquatic biota (mol/Pa/m3)
Krs	Vector	Partition coefficient between root tissue and soil solid
Kfa	Vector	Partition coefficient between root tissue and soil solid
Zp[]	Vector	Fugacity capacities of root [r] and foliage [f] of plant
Z[]	Vector	Fugacity capacities of bulk compartments of air [a], plant foliage [p], ground surface soil [g], root zone [s], vadose zone [v], surface water [w], and sediment [d]. (mol/Pa/m3)
Zphlm	Vector	Fugacity capacity of phloem fluid (mol/Pa/m3)
D[]	Vector	Chemical diffusivities of bulk compartments of air [a], plant foliage [p], ground surface soil [g], root zone [s], vadose zone [v], surface water [w], and sediment [d]. (m2/d)
Uaw_a	Vector	Air-side, air-water diffusion MTC, concentration based (m/d)
Uaw_w	Vector	Water-side, air-water diffusion MTC, concentration based (m/d)
Y[][]_[]	Vector	Interface diffusion MTC at each side, fugacity based (mol/m2/Pa/d)
Y[][]	Vector	Overall diffusion MTC, fugacity based (mol/m2/Pa/d)
Delta[][]_[]	Vector	Interface boundary layer depth at each side (m)
rwv_stom	Vector	Stomata resistance to water vapor, d/m
rstom	Vector	Stomata resistance to chemical, m/d
Ystom	Vector	Overall diffusion MTC at stomata-air interface, fugacity based (mol/m2/Pa/d)
Idp	Vector	intercept factor of dry deposition to plant
Idg	Vector	intercept factor of dry deposition to ground
T[][]	Vector	Rate constant of interface mass transport (day-1)
T[]x	Vector	Rate constant of total loss from a compartment (day-1)
T[]o	Vector	Rate constant of loss to downstream water body [w] or downwind air grid cell [a] (day-1)
TB	Matrix	Rate constant matrix for landscape compartments (day-1)
TA	Matrix	Rate constant matrix for air grid cells (day-1)
gvw	Vector	Wind speed at grid scale (m/s)
gdrct	Vector	Wind direction at grid scale (degree)
Ta_a[]	Scalar	Rate constant of horizontal air advective loss, [x] and [y] (day-1)
SB	Vector	Overall source term for landscape compartments (mol/day)
SA	Vector	Overall source term for air grid cells (mol/day-1)
NAB	Vector	Chemical inventory in air aggregated at basin scale (mol)
Nt	Vector	Chemical inventory for compartments at basin scale (mol)
NTt	Vector	Chemical inventory for basins/watersheds (mol)
CAmatrix	Matrix	Chemical concentration in air grid cells (g/m3)

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