CHEMICAL OXIDATION REACTIVE TRANSPORT IN 3-D (CORT3D)

COMPUTER MODELING CODE

Version 2.01

USER DOCUMENTATION

Developed by:
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In partial completion of Ph.D. at the Colorado School of Mines

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3. Introduction to CORT3D

CORT3D (Chemical Oxidation Reactive Transport in 3-Dimensions) provides for simulation of three-dimensional, in situ chemical oxidation reactive transport in

groundwater aquifers. CORT3D is based on a modified form of RT3D (Reactive Transport in 3-Dimensions) version 2.5 (Clement 1997 and 2001, Clement et al. 1998, Clement et al., 2000, Clement and Johnson 2002, Johnson et al. 2006) and MODFLOW 2000 (McDonald and Harbaugh 1988, Harbaugh and McDonald 1996a and 1996b, Harbaugh et al. 2000).

RT3D is a finite difference numerical code for simulation of three dimensional, multi-species, reactive transport in groundwater aquifers. RT3D is based on MT3D (Zheng 1990) and was developed at the Pacific Northwest National Laboratory (PNNL) for use in design of accelerated in situ bioremediation systems and for evaluation of natural attenuation, but is not limited to those scenarios. Indeed, RT3D provides the flexibility to simulate reaction kinetics for any chemical system of interest (including a mixture of mobile and immobile components) via the user-defined reaction package feature. CORT3D utilizes this feature to incorporate an oxidation-specific reaction package. Additionally, a number of executables are utilized by CORT3D to incorporate changing permeability and DNAPL dissolution as the simulation progresses.

Because dissolution and oxidation are transient processes where DNAPL saturation decreases with time and manganese oxide solids (a byproduct of the chemical oxidation process when using permanganate) increase with time (i.e. effective porosity and permeability change), the groundwater flow pattern needs to be updated over time. The more frequent the update of the flow solution (through changes of effective hydraulic conductivity, porosity, DNAPL saturation, and manganese oxide volume), the closer the simulation approaches a transient solution.

CORT3D offers a great deal of flexibility incorporating subsurface processes. It includes DNAPL dissolution, equilibrium or rate-limited sorption, 2nd order kinetic contaminant oxidation, kinetic oxidation of natural oxidant demand (NOD)—both a fast kinetic portion and a slow kinetic portion, and different diffusion coefficients for each aqueous species. The code tracks aqueous contaminant, aqueous chloride, and aqueous oxidant as well as DNAPL, sorbed contaminant, manganese oxide, fast NOD, and slow NOD.

4. Installation

To install CORT3D simply execute the install file (CORT3D_SETUP.EXE). This will create a sub-directory called CORT3D within the "Program Files" sub-directory of your system drive and place all related files within that sub-directory. As a minimum, the CORT3D executables, documentation, source code, and examples will be installed. Additionally, a "CORT3D" folder will be created in your Windows Start Menu structure under "All Programs" containing a link to run the C3DI front-end program.

During installation, you will also be given the option to install a very useful, free text editor called "Crimson Editor." This text editor can be used for creating/editing simulation input text files. You will also be given the option to install the free "Model Viewer" from the U.S. Geological Survey—it is useful for viewing the output from your simulations.

5. Model Formulation

The formulation of each process represented in the model code follows. The code does not incorporate oxidant auto-decomposition as it is yet to be determined whether this results in a significant reduction in oxidant concentrations. This type of auto-catalytic decomposition of permanganate was suggested by Urynowicz (2000) based on research results indicating that more oxidant mass was consumed in destruction of a given mass of TCE when initial oxidant concentration was increased.

5.1. DNAPL Dissolution

Mass transfer or dissolution of the DNAPL into the aqueous phase is implemented using the well-known stagnant film model (Sherwood et al. 1975) utilizing a first-order linear driving force

$$\frac{dX_{napl}}{dt} = -\frac{\phi_{eff}}{\rho_B} k_{La} \left(C^*_{cont} - C_{cont} \right) \tag{5.1}$$

where X_{napl} is the mass fraction of DNAPL in soil (MM^{-1}), ϕ_{eff} is the effective soil porosity available for water flow, ρ_B is the soil bulk density (L^3T^{-1}), C^*_{cont} is the maximum solubility limit of the contaminant (ML^{-3}), C_{cont} is the aqueous concentration of the contaminant (ML^{-3}), and k_{La} is the DNAPL dissolution rate or lumped mass transfer

coefficient (T^{-1}). The lumped mass transfer coefficient is the product of the intrinsic mass transfer coefficient, k_L, (LT^{-1}) times the DNAPL-water interfacial area, A_{nw}, (L^2), divided by the porous media volume of interest, V, (L^3). The lumped mass transfer coefficient is used because the complex architecture of DNAPL sources makes A_{nw} virtually impossible to estimate. However, k_{La} is dependent on a number of system parameters, such as pore size and the DNAPL saturation which affect the specific interfacial surface area for dissolution. As a result, mass transfer is a system dependent process, and estimation of k_{La} is system specific and must be done empirically using measurable system parameters (Ewing 1996, Imhoff et al. 1994, Miller et al. 1990, Nambi 1999, Powers et al. 1994a, Powers et al. 1994b, Saba and Illangasekare 2000). A general approach is to utilize an empirically determined Gilland-Sherwood correlation (Welty et al. 1976)

$$Sh = a + b \, Re^c \, Sc^d \tag{5.2}$$

to estimate the modified Sherwood number (Sh) from other dimensionless numbers describing the system (e.g. Reynolds number, Re, and Schmidt number, Sc), where a, b, c, and d are empirically determined constants. The modified Sherwood number relates the mass transport in a system to the diffusive forces, the Reynolds number relates system inertial forces to viscous forces, and the Schmidt number relates viscous forces to diffusive forces. Mathematical equations for these three dimensionless numbers are

$$Sh = \frac{k_{La} d_{50}^2}{D_m} \tag{5.3}$$

$$Re = \frac{\rho_w \bar{v} d_{50}}{\mu_w} \tag{5.4}$$

$$Sc = \frac{\mu_w}{\rho_w D_m} \tag{5.5}$$

where d_{50} is the representative (median) grain size (L), D_m is the molecular diffusion coefficient for a bulk solution of the solute (at an infinitely dilute concentration) (L^2T^{-1}), ρ_w is the aqueous phase density (ML^{-3}), $\bar{v}$ is the average linear groundwater velocity (LT^{-1}), and μ_w is the aqueous phase dynamic viscosity ($ML^{-1}T^{-1}$). The Sherwood number determined from the empirical correlation (Equation 5.2) is then used in Equation 5.3 to estimate the lumped mass transfer coefficient, k_{La}. Most correlations incorporate

volumetric DNAPL content (θ_n) in some form to account for the changing DNAPL-water interfacial area as dissolution proceeds (Miller et al. 1990, Powers et al. 1994b).

Differences in empirical coefficients and formulations are at least partly due to differences in experimental conditions. For example Powers et al. (1994a) used a 1-D system with spherical dissolving organic media and Powers et al. (1994b) used a 1-D homogeneous system, while Saba and Illangasekare (2000) were considering a 2-D system with heterogeneity-induced flow-bypassing. Miller et al. (1990) and Imhoff et al. (1994) both used 1-D systems. Ewing (1996) and Saba et al. (2001) considered a 2-D system with surfactant flushing. Nambi and Powers (2003) further expanded the available choices by looking at 2-D systems with high DNAPL saturations resulting in slower mass transfer characterized by a significantly increased exponent on the DNAPL saturation term. Clement at al. (2004b) utilized a slightly simplified correlation of the same form, where a single parameter (P_p) replaced bSc^d from equation 5.2, to model DNAPL dissolution in 3-D systems.

The CORT3D utilizes a general form of the mass transfer correlation of Saba and Illangasekare (2000). This correlation was used by Saenton (2003) for intermediate-scale 2D PCE natural dissolution as well as surfactant enhanced dissolution experiments, and was found to be flexible and effective. The generic correlation is

$$Sh = \alpha_1 \, \text{Re}^{\alpha_2} \, Sc^{\alpha_3} \left(\frac{\theta_n d_m}{\tau L} \right)^{\alpha_4} \tag{5.6}$$

where the empirical coefficients α_1, α_2, α_3, α_4, τ are unique for a given system, and are determined through calibration or inverse modeling.

The model code does not directly account for potential ISCO effects on mass transfer when calculating the lumped mass transfer coefficient because doing so requires knowledge of the intrinsic mass transfer coefficient without chemical reaction, k_L, which cannot be determined for DNAPL dissolution in porous media because it is not possible to know the DNAPL-water interfacial area needed to obtain k_L from the lumped mass transfer coefficient, k_{La}, which is determined empirically. Further, the change in interfacial area resulting from manganese oxide formation during ISCO using permanganate further precludes any possibility of knowing the interfacial area, so determining the resulting change in k_{La}, does not appear possible. On the other hand, the $MnO_{2\,(s)}$ formation at the

DNAPL surface is indirectly captured in the calculation of k_{La} by the changing Reynolds number which changes as a result of decreasing porosity. As currently implemented, if the intrinsic mass transfer coefficient is expected to increase due to fast chemical reaction, the Gilland-Sherwood parameters need to be estimated for dissolution during chemical reaction thru inverse modeling. A forward simulation is then run in phases, using the appropriate Gilland-Sherwood parameters for each phase.

5.2.   Contaminant Diffusion

Numerical finite difference model codes tend to introduce artificial numerical dispersion under highly diffusion-dominated conditions. Contaminant that enters a model cell during a transport time step is considered to be at the center of the model cell at the start of the next time step, artificially increasing mobile species transport further than it would have diffused in a given time step. However, models using these codes can still be useful for comparing different scenarios. To that end, the original RT3D version 2.5 computer model code has been modified to allow different effective diffusion coefficients to be simulated for each mobile species. Further, the effective diffusion coefficient for each species varies spatially based on soil properties. This modification is important for simulating diffusive transport of permanganate into LPM, where transport is dominated by diffusion (Siegrist et al. 1999, Struse et al. 2002). The original RT3D code used a single effective diffusion coefficient for all species, thereby limiting its effectiveness at simulating diffusion-dominated transport. In CORT3D, effective diffusion coefficients, D_e, (L^2T^{-1}) are estimated using a modified Millington-Quirk relationship (Jury et al. 1991), relating effective diffusion to water content (θ_w) as well as effective porosity.

$$D_e = D_m \frac{\theta_w^{10/3}}{\phi_{eff^2}} \tag{5.7}$$

In the fully water-saturated case, the water content is equal to effective porosity and Equation 5.7 simplifies to the Millington-Quirk relation (1959, 1961)

$$D_e = D_m \phi_{eff}^{4/3} \tag{5.8}$$

Use of the modified Millington-Quirk relation has been shown effective for a variety of soils. Tidwell et al. (2000) researched the effect of porosity on diffusion of potassium iodide into Culebra dolomite slabs using x-ray absorption imaging at the

centimeter-scale. They found that diffusion rates within the slabs indeed varied spatially, and depended on the magnitude of porosity at each location. Conversely, Itakura et al. (2003) performed diffusion experiments using three different organic contaminants, including TCE and three soil configurations (reconstituted and intact kaolin clay as well as reconstituted sandy silt), and determined the relation

$$D_e = D_m \phi_{eff}$$ (5.9)

inadequately fit a combination of their data (19 points) and that from four other studies (6 points). Subsequently, they concluded "there is little correlation between tortuosity and porosity." However, from the data they present (and excluding only two of the six data points from other studies, keeping 23 of 25 data points), it appears that the modified Millington-Quirk relation of Equation 5.7 fits the data to some degree with an R^2 of 0.65 compared to an R^2 of 0.40 for Equation 5.8.

5.3. *Contaminant Oxidation*

A new chemical oxidation reaction package or module has been developed for use with the modified RT3D code. The new package tracks a number of mobile and immobile species. The mobile species are: aqueous phase contaminant (cont), permanganate (MnO_4^-), and chloride (Cl^-). Contaminant concentrations (resulting from the oxidation reaction) are calculated using the second order reaction (Huang et al. 1999, Siegrist et al. 2001),

$$\frac{dC_{cont}}{dt} = -k_2 C_{cont} C_{MnO_4^-}$$ (5.10)

where C_i is the concentration of component i (ML^{-3}), dC_i/dt is the rate of change in concentration of component i with time, and k_2 is the 2nd-order reaction coefficient for degradation of the contaminant by MnO_4^- ($L^3M^{-1}T^{-1}$).

MnO_4^-, and Cl^- concentrations are calculated based on the reaction stoichiometry, but the MnO_4^- equation also includes NOD terms. Although the reaction package was written so the stoichiometric ratios are adjustable to accommodate modeling oxidation of different contaminants, for oxidation of PCE the stoichiometric reaction given by Equation 5.11 applies. This reaction has been shown to represent the oxidation of PCE by permanganate over the pH range of 3.5-10 expected to be found in the subsurface (Huang

et al. 2002, Siegrist et al. 2001, Yan and Schwartz 1999). The reaction equations for permanganate and chloride are shown in Equations 5.12 and 5.13,

$$4MnO_4^- + 3C_2Cl_4 + 4H_2O \rightarrow 6CO_2 + 4MnO_{2\ (s)} + 8H^+ + 12Cl^- \tag{5.11}$$
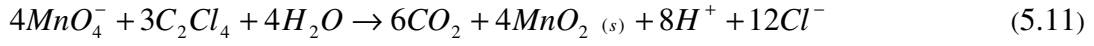
$$\frac{dC_{MnO_4^-}}{dt} = Y_{MnO_4^-/cont} \frac{dC_{cont}}{dt} - \left(k_{NOD_f} X_{NOD_f} + k_{NOD_s} X_{NODs}\right)\frac{\rho_B}{\phi} \tag{5.12}$$

$$\frac{dC_{Cl^-}}{dt} = -Y_{Cl^-/cont}\left(k_2 C_{cont} C_{MnO_4^-}\right) \tag{5.13}$$

where $Y_{i/j}$ is the stoichiometric molar mass ratio of component i to component j from Equation 5.11 and the component molecular weights. In Equation 5.12, X_{NOD_f} is the mass fraction of NOD sites with a faster oxidation rate (MM^{-1}), X_{NOD_s} is the mass fraction of NOD sites with a slower oxidation rate (MM^{-1}), k_{NOD_f} is the first-order oxidation rate for fast NOD sites (T^{-1}), and k_{NOD_s} is the first-order oxidation rate for slow NOD sites (T^{-1}).

In addition to the specified mobile species, the reaction package also tracks a number of immobile species, including: DNAPL phase contaminant, sorbed contaminant, MnO$_{2\ (s)}$, and natural oxidant demand (NOD). Generation of MnO$_{2\ (s)}$ occurs via Equation 5.14,

$$\frac{dX_{MnO_2}}{dt} = \frac{\phi}{\rho_B}\left[Y_{MnO_2/MnO_4^-}\left(-\frac{dC_{MnO_4^-}}{dt}\right)\right] \tag{5.14}$$

where, X_{MnO2} is the mass fraction of MnO$_2$(s) precipitates in the soil (MM^{-1}) and dX_i/dt is the rate of change in mass fraction for component i with time. The MnO$_{2\ (s)}$ precipitates are assumed to be immobile and remain at the location they are generated. Treating all the generated MnO$_{2\ (s)}$ as immobile provides a worst-case simulation of generated solids filling pore-space and potentially altering permeability will be discussed shortly. The MnO$_{2\ (s)}$ formed during oxidation using permanganate may take different forms depending on soil and water conditions as well as where it forms. Much of it is likely to form within the pore space as an amorphous, hydrous, porous form reducing effective porosity available for water flow. The amorphous, hydrous particles of MnO$_{2\ (s)}$ that form within the pore space may also become lodged in pore throats blocking flow. Additionally, some may form as a more structured and solid film on soil particle surfaces where it can reduce the pore throat

diameter. MnO_2 (s) can also form as a film at the DNAPL-water interface reducing the interfacial area for mass transfer from the DNAPL to the aqueous phase (Urynowicz 2000). It is unlikely that MnO_2 (s) will form in the same combination of these mechanisms for all conditions.

5.4. Sorption

The reaction package can also simulate either equilibrium or rate-limited sorption of contaminant through the following equation (Haggerty and Gorelick 1994),

$$\frac{dX_{sorb}}{dt} = \frac{\phi}{\rho_B} \xi \left(C_{cont} - \frac{X_{sorb}}{\lambda_{cont}} \right) \tag{5.15}$$

where ξ is the rate-limited sorption mass transfer coefficient (T^{-1}), X_{sorb} is the mass fraction of sorbed contaminant in the soil (MM^{-1}), and λ_{cont} is the linear sorption coefficient ($L^3 M^{-1}$). As ξ gets larger, the non-equilibrium sorption approaches equilibrium sorption; on the other hand, as ξ gets very small sorption becomes negligible. Clement et al. (2004a) utilized and verified the functionality of this formulation in their modeling study of the coupling of DNAPL dissolution with rate-limited sorption and kinetic biological degradation.

5.5. Natural Oxidant Demand

Field soils and aquifer sediments typically contain natural organic matter (NOM), reduced metals, and other reductants that can be readily oxidized. These soil constituents are referred to collectively as natural oxidant demand (NOD), or sometimes soil oxidant demand (SOD), and compete with target contaminants for available oxidant. Zhang and Schwartz (2000) proposed that components comprising the NOD have a much faster reaction rate with MnO_4^- than do chlorinated contaminants, in order to explain delayed breakthrough of MnO_4^- in column experiments by Schnarr et al. (1998). This conceptual model of NOD oxidation corresponds to an instantaneous sink. Under this concept, all of the NOD must be oxidized before any PCE oxidation occurs; thus, in order to oxidize a

given mass of PCE, the mass of MnO_4^- needed will be equal to the NOD plus the mass determined from the reaction stoichiometry.

Conversely, there is evidence that not all NOD components are oxidized faster than the contaminant (Mumford et al. 2002, Mumford et al. 2005, Siegrist et al. 1999, Struse et al. 2002, Yan and Schwartz 1999). Because NOD is generally a complex mixture of components whose surface area available for oxidant contact varies, it is appropriate to treat NOD oxidation as a kinetic process. This means that oxidation of NOD and PCE occur simultaneously, with relative rates of oxidation controlling depletion of each.

Because NOD results from a mixture of constituents, the kinetic rate for oxidation of NOD can vary widely for different soils. While the kinetic rates for some NOD constituents of a particular soil are often higher than that of the target contaminant, preliminary results related to this research, and that of others, suggests NOD frequently consists of at least two components with markedly different oxidation rates (Crimi and Siegrist 2004, Jackson 2004, Mumford et al. 2005). As an example, Chambers et al. (2000) found two distinct NOD oxidation rates for each of three different field soils in batch tests. The rate during the first 24 hours was 10 – 20 times faster than the rate during the next 13 days. They also found that the slower rate for the three soils was virtually the same, while the initial fast rate varied by soil type with silt and clay being about twice that of sand.

Mumford et al. (2005) considered the possibility that the multiple rates could be a result of organic carbon located within soil grain micropores being more difficult for oxidant to access. They performed batch NOD studies on native coarse sand from the Borden test site (grain size greater than 0.42mm), as well as on coarse Borden sand that had first been crushed (grain size less than 0.074mm). Results from the one week NOD tests showed no significant difference, suggesting that either the proposed geometric configuration is not a rate-limiting factor or that reduced species in micropores are still unavailable even after crushing (Mumford et al. 2005).

The results from the studies already mentioned suggest that the reaction order is first-order with respect to NOD, but do not elucidate what the reaction order is with respect to permanganate. However, recent research by Urynowicz et al. (2008) confirm the

applicability of modeling NOD using first-order kinetics for both fast and slow NOD fractions.

In CORT3D, NOD is assumed to be immobile, because batch studies so far have suggested the soil NOD is typically far greater than any NOD exerted by dissolved constituents in the groundwater. Further, the volume of NOD oxidized is assumed to be negligible compared to the pore space so that removal of NOD does not increase permeability; however, the oxidation of NOD does consume permanganate generating MnO_2 (s) which in turn reduces permeability. At locations where oxidant is present, changes to the mass fraction of fast and slow NOD are calculated using first-order Equations 5.15 and 5.16, respectively.

$$\frac{dX_{nod_f}}{dt} = -k_{nod_f} X_{nod_f} \qquad (5.16)$$

$$\frac{dX_{nod_s}}{dt} = -k_{nod_s} X_{nod_s} \qquad (5.17)$$

5.6.   *Permeability Effects*

Research has shown that oxidation of a high DNAPL saturation source using permanganate may result in permeability reductions due to precipitation of manganese oxides (Lee et al. 2003, Schroth et al. 2001, Siegrist et al. 2002). However, research into permeability effects from permanganate oxidation of DNAPL source zones at lower saturations is more ambiguous. Nelson et al. (2001) concluded that the manganese oxides produced during oxidation of a PCE DNAPL present at approximately 4-7% saturation had negligible effect on the permeability, despite the system remaining at a neutral pH due to natural buffering from the carbonate mineral-containing sands. On the contrary, Lee et al. (2003) found that permanganate oxidation of a TCE DNAPL source zone at 8% saturation resulted in generation of up to 4900mg MnO_2 (s)/kg porous media, in an unbuffered silica sand system utilizing de-ionized water. Further, they witnessed a six-fold decrease in velocity of the oxidation front over the two-month experiment, attributing this decrease to reductions in permeability. This is especially interesting because less MnO_2 (s) is expected to precipitate at low pH where the reaction favors generation of Mn^{2+} instead of MnO_2 (s) (Stewart 1965, Yan and Schwartz 1999).

There are various methods to relate permeability changes to changes in porosity resulting from immobile components in porous media pore spaces, such as a power law model as in Equation 5.18 (Wyllie 1962) or capillary-tube model like the Kozeny-Carman equation in Equation 5.19 (Bear 1972)

$$k_{r,w} = \left(\frac{1 - S_n - S_{r,w}}{1 - S_{r,w}} \right)^3 \tag{5.18}$$

$$k_{r,w} = \frac{\phi_{eff}^3}{K_s (1 - \phi_{eff})^2} \left(\frac{d_m^2}{180} \right) \tag{5.19}$$

where $k_{r,w}$ is the relative water permeability, S_n is the saturation of immobile component in the pore space, $S_{r,w}$ is the residual water saturation for the porous media and K_s is the saturated hydraulic conductivity.

Saenton (2003) found Equation 5.18 to provide good agreement to experimentally derived permeability data (Saba 1999) for DNAPL in silica sands like those that are being used in this research. Additionally, Clement et al. (1996) proposed a form of Equation 5.18 for pore-clogging due to microbial growth. These power law and Kozeny-Carman equations may not be perfectly suited to permeability reduction following chemical precipitation in porous media because they significantly under-predict permeability reductions, especially at high levels of plugging (Reis and Acock 1994). However, application of the CORT3D model code is done at a much larger scale than the pore-scale. Although Equations 5.18 and 5.19 may not be applicable to estimating pore-scale permeability reduction due to chemical precipitation, they may be adequate at the much larger modeling scale. For example, Equation 5.18 may estimate a 10% permeability reduction. In reality pores with the smallest throats may see a nearly 100% reduction, while pores with large throats may see virtually no reduction. Because the large throat pores are initially responsible for the greatest transport of water, plugging of the smallest pores has relatively little impact, and the overall change (at a modeling scale) may be well represented by the estimate of Equation 5.18.

Along these lines, CORT3D incorporates Equation 5.20, which is a version of Equation 5.18, to estimate permeability changes

$$k_{r,w} = \left(\frac{1 - S_{mno2} - S_n - S_{r,w}}{1 - S_{r,w}} \right)^3 \tag{5.20}$$

where S_{mno2} is a pseudo-saturation representing the volume of total pore space filled with manganese oxide solids. This pseudo-saturation is estimated by converting the mass fraction of solids produced to a volume using an effective manganese oxide precipitate density. The effective density is essentially a fitting parameter, and not an actual density of manganese oxide particles generated. This is because $MnO_{2\ (s)}$ formed during oxidation using permanganate may take different forms depending on soil and water conditions as well as where it forms. Much of it is likely to form within the pore space as an amorphous, hydrous, porous form reducing effective porosity available for water flow; this form is expected to have an undetermined density that is lower than that of dry, solid $MnO_{2\ (s)}$. Additionally, the amorphous, hydrous particles of $MnO_{2\ (s)}$ that form within the pore space may also become lodged in pore throats blocking flow. Further, some may form as a more structured and solid film on soil particle surfaces where it can reduce the pore throat diameter. The effective density parameter accounts for permeability reductions resulting from all three of these mechanisms. The magnitude of permeability reduction occurring as a result of each mechanism is expected to be site specific, depending on soil and water conditions. As a result, it is expected that the effective density parameter may vary between simulations of different site conditions, but should be a constant for all similar conditions within a single simulation. It should also be noted that the relation represented by Equation 5.20 was generated for unconsolidated sand with well-sorted grains and non-wetting DNAPL (Wyllie 1962). If significantly different conditions are to be modeled, a different relation may be necessary. For example, the exponent is changed from 3 to 4 for cemented sandstone (Wyllie 1962).

Because dissolution and oxidation are transient processes where DNAPL saturation decreases with time and manganese oxide solids increase with time (i.e. effective porosity and permeability change), the groundwater flow pattern needs to be updated periodically. The more frequent the update of the flow solution (through changes of effective hydraulic conductivity, porosity, DNAPL saturation, and manganese oxide volume) the closer the simulation approaches the transient solution. Because the flow and transport solutions are not coupled in this model code, long (time) simulations are broken down to a number of short steady-state flow and transient transport runs that are executed in sequence.

Similar to the model code of Saenton (2003) for simulating surfactant enhanced aquifer remediation, effective hydraulic conductivities are used within MODFLOW to generate the velocity field. This velocity field is then used in estimating the DNAPL dissolution mass transfer coefficient. Then the transport model code simulates the DNAPL dissolution, oxidation, and other relevant reactions over a relatively short time interval. If overall simulation time is not over, the transport results are used to generate new porosities and hydraulic conductivities and the process is repeated.

6.   Overview of CORT3D Operation

Simulations are broken down to a number of short steady-state runs that are executed in sequence. The CORT3D.PL perl script automates the execution of individual programs in the sequence shown in Table 6.1, through the desired number of iterations, to arrive at the target simulation time. Table 6.2 lists the executables and briefly describes what each one is used for and Table 6.3 lists the required input files for each executable program. Table 6.4 lists files generated by various modules or executables, and subsequently used by another module during a simulation. The 'fort.yxxx' files each pertain to a specific simulation parameter, as described in Table 6.4, with one such file for each model layer (described in more detail later).

Table 6.1: Overall Program Sequence

c_modk.exe
mf2k.exe
c_dss.exe
c_rt3d.exe
pm.exe
c_record.exe
c_updt.exe
c_mass.exe
c_post.exe

Loop for specified number of iterations
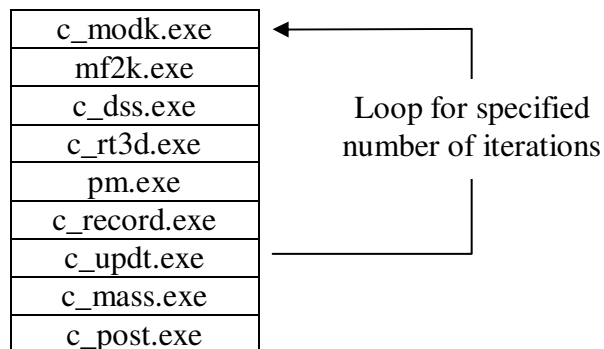
As will be described later in greater detail, input files can be created manually using your favorite text editor or they can be created using the C3DI.EXE (CORT3D Input) program. Once all the input files are created, the simulation can be executed from

the command prompt after opening a command window or it can be executed from within the C3DI.EXE program.

Table 6.2: Executable Files and Their Functions.

Program	Function(s)
c3di.exe	CORT3D Input program – optionally provides a user-friendly method for setting up simulation input files and executing simulation
perl.exe & perl58.dll	Perl interpreter that processes CORT3D script
cort3d.pl	Script file that automates the iterative running of the model
file_gen.exe	Generates a series of input files (e.g. concentration) containing a single value for all cells of all layers of the model
c_modk.exe	Reads saturated K, DNAPL saturation, and residual saturation, and outputs effective K (Fort.6xxx series) for MODFLOW simulation
mf2k.exe	MODFLOW 2000 executable – generates flow solution
c_dss.exe	Reads initial porosity, soil median grain size, DNAPL saturation, manganese oxide mass fraction, and layer thickness, and returns input parameters for CORT3D simulation (see Table 4)
c_rt3d.exe	Modified RT3D executable, including chemical oxidation package – generates transport/reaction solution
pm.exe	Processes output from C_RT3D by reading unformatted concentration results and writing as text files.
c_record.exe	Reads C_RT3D outputs from current iteration and records them in master data files for entire simulation, to be read using Model Viewer from USGS and/or GMS from US Army Corps of Engineers
c_update.exe	Calculates new DNAPL saturation and mass based on outputs from pm.exe, and extracts observations (i.e. concentrations) at specified locations
c_mass.exe	Reads C_RT3D outputs for final iteration and calculates total mass of aqueous and nonaqueous components in domain
c_post.exe	Reads simulation input files and creates properly formatted files necessary so GMS can be used to facilitate simulation post-processing

The 'file_gen.y000' files of Table 6.3 are necessary to ensure initial concentrations (or mass fractions for immobile components) are established for each component, except DNAPL contaminant, at every model cell; generally these will be used to set initial concentrations and mass fractions to zero. The 'y' in the 'file_gen.y000' filenames represents the series number of the parameter or component (see Table 6.4). The FILE_GEN program sets the initial concentration (or mass fraction) for the given component to the same value at every model location. As an example, if the background chloride concentration in an aquifer was 30 mg/L you could use the 'file_gen.9000' to set an initial value for chloride of 30 mg/L within every model cell.

Alternately, if the initial concentration (or mass fraction) of one or more components vary spatially, this is accommodated by creating 'fort.yxxx.ini' files. It is only necessary to create 'fort.yxxx.ini' files for those components whose initial concentration (or mass fraction) varies spatially, and only for those layers within which the initial concentration (or mass fraction) varies. In the 'fort.yxxx.ini' filenames, the 'y' again represents the series number of the parameter or component (see Table 6.4), and 'xxx' represents the model layer number with preceding zeros. For example, if the initial concentration of chloride is not uniform throughout layer 1, the initial chloride concentrations in layer 1 are specified using the 'fort.9001.ini' file. If no 'fort.9xxx.ini' files exist for the other layers, initial chloride values will be set in those layers to the value defined in the 'file_gen.9000' file. In short, if a 'fort.yxxx.ini' file exists it will be used to set the initial value for the associated parameter in all cells of the specified layer, whereas all other cells will be set to the initial parameter values specified in 'file_gen.y000' files.

The 'cort3d.inp' file contains the filenames of input files for the various executable modules, as well as a switch to indicate if a particular simulation is a continuation of a previous simulation. This is useful, for example, if it is desired to change a stress (e.g., turn on/off an injection well) at some point within a simulation. In this event, a simulation is run for the period during which stresses remain constant. Then, a new (continuation) simulation is run for the next time period during which a different set of stresses are applied. For example, an initial run might employ oxidant injection for three weeks. The continuation run (of whatever duration is desired) would utilize the final conditions from run one as inputs to simulate the post-injection phase. In addition to input files, the 'cort3d.inp' file lists names to be used for the various output files: (1) aqueous species concentrations and non-aqueous species mass fractions; (2) total mass of non-aqueous or immobile species remaining in system at the end of each iteration; (3) observation locations; and (4) mobile species concentrations, immobile species mass fractions, and hydraulic heads at each observation point at the end of each iteration. The 'cort3d.inp' file also contains the parameter values for the Gilland-Sherwood correlation defining the natural dissolution of DNAPL within the system, as well as the average soil grain density.

Table 6.3: Input Files Required By Executables.

Program	Required Input Filename
cort3d.pl	cort3d.inp sn.inp.ini fort.yyxxx.ini (*for any component that varies within or between 1 or more layers as described following Table 2*)
file_gen.exe	file_gen.7000 file_gen.8000 file_gen.9000 file_gen.10000 file_gen.12000 file_gen.13000 file_gen.14000
c_modk.exe	cort3d.inp phi0.inp init_k.inp srw.inp
c_dss.exe	cort3d.inp phi0.inp d50.inp
c_update.exe	cort3d.inp phi0.inp
pm.exe	pm.conc7 pm.conc8 pm.conc9 pm.mfrac10 pm.mfrac11 pm.mfrac12 pm.mfrac13 pm.mfrac14

Note: see text following Table 6.2 for explanation of when to change these files from default.

Note: these input files should not be changed under normal use

Initial DNAPL contaminant distribution is designated using the 'sn.inp.ini' file; this file contains the initial DNAPL saturation value for each cell in the model. Similarly, the initial mass fraction distribution of manganese oxide (mass of manganese oxide per mass of dry soil) present in porespace (if any) is designated using the fort.10xxx.ini files.

The 'phi0.inp', 'init_k.inp', 'srw.inp', and 'd50.inp' files are used to define initial properties of the subsurface aquifer material. Specifically, the 'phi0.inp' is used to define the initial total porosity (available to contain water, DNAPL, and/or $MnO_{2\ (s)}$) of each cell within the system. The 'init_k.inp' file is used to define the initial (fully water-saturated),

horizontal hydraulic conductivity of each cell (i.e., the hydraulic conductivity when none of the porespace is containing DNAPL or $MnO_{2 (s)}$). The 'srw.inp' file is used to define the residual water saturation of each cell within the system. The 'd50.inp' file is used to describe the soil particle size; specifically, the median soil grain size diameter within each cell is entered in this file.

The 'pm.xxxxy' files tell the PM.EXE executable what data to extract from the binary RT3D output concentration files after each iteration, with 'xxxx' being either "conc" or 'mfrac' and 'y' representing the component being processed just as in the 'file_gen.y000' files. The extracted information is then used by other modules in preparing input files for the next iteration and to update the cumulative output files. In normal use, these files should not need to be changed. The only foreseeable reason to change the values in these files is if the source code is modified to utilize different RT3D output filenames instead of the default 'RT3D00y.UCN' where 'y' is the species.

Table 6.4 summarizes the various input/output files created and/or updated during a simulation. The volumetric flow rate, Darcy flux, and current iteration concentration/mass fraction files ('q_.tmp', 'flux__. tmp', 'RT3D00_.ucn', respectively) are temporary in nature. They are updated within an iteration, and created anew with the next iteration. The 'MV*.ucn' files are used for post-processing with the USGS Model Viewer 1.2 software. The 'GMS*.*' files (except 'GMS*.out') are used for post-processing using the US Army Corps of Engineers Groundwater Modeling System (GMS) software (version 6.5 has been tested, but version 5.0 and later are expected to work as well). The 'MV*.out' and 'GMS*.out' files are text files of cumulative concentration and mass fraction for each species (y), mirroring the Model Viewer and GMS UCN files, respectively.

Output files ('mass.out', 'obs_c.out', 'obs_m.ou't, and 'obs_h.out') will contain the remaining mass in the model domain for each immobile species, concentration of mobile species at each observation point and effluent, mass fraction of immobile species at each observation point, and hydraulic head at each observation point, respectively. These files contain an entry for each iteration, and can be easily imported into Microsoft Excel for data analysis. Another output file ('mass_final.out') is created containing a summary of the total final mass remaining within the model domain of each mobile and immobile species.

Table 6.4: Program Generated Input/Output Files

File Type /Name	Description [units]	Generated by Program
fort.1xxx	Cell thickness, Δz [L]	c_dss
fort.2xxx	Soil Bulk density, ρ_B [ML^{-3}]	
fort.3xxx	Lumped mass transfer coefficient, k_{La} [T^{-1}]	
fort.4xxx	Effective porosity, ϕ [-]	
fort.5xxx	Initial porosity, ϕ_0 [-]	
fort.6xxx	Effective hydraulic conductivity, K [LT^{-1}]	c_modk
fort.7xxx	Concentration of aqueous contaminant [ML^{-3}]	file_gen c_update
fort.8xxx	Concentration of oxidant (MnO$_4^-$) [ML^{-3}]	
fort.9xxx	Concentration of chloride (Cl$^-$) [ML^{-3}]	
fort.10xxx	Mass fraction of manganese oxide solids (MnO$_{2\,(s)}$) [MM^{-1}]	
fort.11xxx	Mass fraction of DNAPL contaminant [MM^{-1}]	
fort.12xxx	Mass fraction of sorbed contaminant [MM^{-1}]	
fort.13xxx	Mass fraction of fast natural oxidant demand (NOD) [MM^{-1}]	
fort.14xxx	Mass fraction of slow NOD [MM^{-1}]	
qx.tmp	Volumetric flow rate through each cell in x-direction [L^{3}T$^-$]	c_dss
qy.tmp	Volumetric flow rate through each cell in y-direction [L^{3}T$^-$]	
qz.tmp	Volumetric flow rate through each cell in z-direction [L^{3}T$^-$]	
flux_x.tmp	Darcy flux through each cell in x-direction [LT^{-1}]	
flux_y.tmp	Darcy flux through each cell in y-direction [LT^{-1}]	
flux_z.tmp	Darcy flux through each cell in z-direction [LT^{-1}]	
mass.out	Total mass of each immobile component in simulated aquifer at end of each iteration [M]	c_update
obs_c.out	Concentration of each mobile component at designated observation points and effluent, along with total aqueous flow rate at effluent, at end of each iteration [ML^{-3}]	
obs_m.out	Mass fraction of each immobile component at designated observation points at end of each iteration [MM^{-1}]	
obs_h.out	Hydraulic head at each observation point at end of each iteration [L]	
RT3D00x.ucn	Current iteration concentration and mass fraction for each species (y), used by CORT3D modules for further processing	c_rt3d
MV00x.ucn	Cumulative concentration and mass fraction for each species (y), for post-processing using Model Viewer	c_record
GMS00x.ucn	Cumulative concentration and mass fraction for each species (y), for post-processing using GMS	
MV00x.out	Text file of cumulative concentration and mass fraction for each species (y), mirroring Model Viewer UCN files	
GMS00x.out	Cumulative concentration and mass fraction for each species (y), mirroring GMS UCN files	
GMS.zzz	Input files for post-processing with GMS	c_post

7. User Instructions

To begin with, it is important to point out the need to be consistent on the use of units. Previous users of MODFLOW and RT3D will be used to the need to specify and utilize consistent Time, Length, and Mass units when setting up the input files. However, standard RT3D simulations do not always require concentrations to be input in units that are consistent with the specified Mass and Length units. With CORT3D, the oxidation reactions are non-linear and the movement of data between modules requires standardization. Consequently, **it is imperative that concentrations be entered in units consistent with the Mass and Length units being utilized**. For example, if the Mass unit is kg and the Length unit is m, the concentrations must be equivalent to kg/m^3 (e.g., g/L or mg/mL).

7.1. *Manual Setup of Simulation Files*

Manual setup of simulation files is performed by created a number of text files containing all the parameters needed for the simulation. The number of files needed depends on the dimensions of the model and the processes to be simulated. The text files can be created with your favorite text editor. Although Notepad.exe (that may already be on your computer) works, something with a little more capability is recommended. The Crimson Editor distributed with CORT3D is freeware and makes setting up the simulation input files a bit easier.

7.1.1 *Setup MODFLOW 2000 Flow Model Input Files*

The first step in setting up a CORT3D simulation is to develop a steady-state flow model in MODFLOW 2000, using the layer property flow (LPF) package. However, horizontal hydraulic conductivities need to be entered to be read free-format from external files with one file per layer. Below is an example entry for layer 1.

OPEN/CLOSE fort.6001   1.0 (free) 0 HK layer 1

Subsequent layers are entered in the same manner, except that 6001 is incremented for each layer so it becomes 6002 for layer 2, 6003 for layer 3, and so on. This modification allows MODFLOW to read the hydraulic conductivities calculated by the "c_modk" module of CORT3D. The "c_modk" module calculates the effective hydraulic

conductivity as a result of DNAPL and manganese oxide within the pore space using a modification of Wyllie's (1962) power law relation for estimating relative permeability (Equation 5.20).

7.1.1   Setup RT3D Transport Model Input Files

Next, the transport simulation is set up just as if setting up an RT3D simulation, except that the BTN file is modified to specify external files for cell thickness, effective porosity, starting concentrations of mobile aqueous components, and starting mass fractions of immobile components as shown in bold in Figure 7.1. The number in the first column (e.g., 1001) specifies the external 'fort.yxxx' file corresponding to the appropriate parameter and model layer (see Table 6.4 for descriptions); for 2D and 3D simulations, enter a line for each layer, for each parameter. The length of the transport simulation (PERLEN) should be set to the desired length of one CORT3D iteration, so the number of iterations times the period length is equal to the simulation length.

```
GMS MT3D Simulation                                    COMMENT1
08 November 2004                                       COMMENT2
        1         1        40         1         8         3   NLAY,NROW,NCOL,NPER,NCOMP,MCOMP
 hr  cm  mg                                            TUNIT,LUNIT,MUNIT
 T T T T T F F F F                                     TRNOP(ADV,DSP,SSM,RCT,GCG,NA,NA,NA,NA,NA)
 1                                                     LAYCON
        0 1.0000000                                    DELR
        0 4.5000000                                    DELC
        0 4.5000000                                    HTOP
     1001       1.0                                0   DZ(K)
     4001       1.0                                0   PRSTY_EFF
        0         1                                    DELR
     7001       1.0                                0   CONC FOR CONT (M/L3)
     8001       1.0                                0   CONC FOR MNO4 (M/L3)
     9001       1.0                                0   CONC FOR CL (M/L3)
    10001       1.0                                0   MASSFRAC FOR MNO2 (M/M)
    11001       1.0                                0   MASSFRAC FOR DNAPL CONT (M/M)
    12001       1.0                                0   MASSFRAC FOR SORBED CONT (M/M)
    13001       1.0                                0   MASSFRAC FOR FAST NOD (M/M)
    14001       1.0                                0   MASSFRAC FOR SLOW NOD (M/M)
    -999.0      0.01                                   CINACT, THKMIN
        1         0         0         0         T   IFMTCN,IFMTNP,IFMTRF,IFMTDP,SAVUCN
        0                                              NPRS {save results at end}
        0         1                                    NOBS, NPROBS
        T         1                                    CHKMAS, NPRMAS
  6.00000         1 1.000000                           PERLEN,NSTP,TSMULT
     0.0      1000 1.000000         0.0                DT0,MXSTRN,TTSMULT,TTSMAX
```

Figure 7.1: BTN Input File Structure (differences from traditional RT3D input shown in bold).

The RCT reaction package input file is set up as shown in Figure 7.2, following RT3D instructions, for a user-defined reaction. Specifically, the second entry in row 1 is set to 10 (for user-defined reaction), the third item in row 1 is set to 15 (15 constant reaction data), and the fourth item in row 1 is set to 2 (two variable reaction data). Row 2 specifies the external file(s) containing soil dry bulk density (enter as many lines as model layers). Reaction data entered are shown in bold in Figure 7.2, although values will vary according to the conditions being simulated. Just as in the BTN file, variable reaction parameters are read from external files with the number in the first column (e.g., 3001) specifying the external 'fort.yxxx' file corresponding to the appropriate parameter and model layer. For 2D and 3D simulations, enter a line for each layer, for each parameter. See Table 7.1 for a description of each of the reaction parameters.

Note that you can effectively turn off simulation of decreasing permeability due to manganese oxide formation, by setting the effective density of manganese oxide solids (rho_mno2) in the RCT file to a very high value (e.g., 99,999 g/cm^3). Similarly, simulation of increasing permeability as DNAPL dissolves can be effectively turned off by setting the contaminant density (rho_cont) to a very high value (e.g., 99,999 g/cm^3).

```
       0      10      15       2       1       2
    2001      1.0                      2   RHOB (M/M)
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
0.03132                              rc(1):Dm_cont   (L2/T)
0.0588                               rc(1):Dm_mno4   (L2/T)
0.07308                              rc(1):Dm_cl     (L2/T)
1.3333                               rc(1):Y_mno4_cont (mol/mol)
4.0                                  rc(1):Y_cl_cont   (mol/mol)
1.0                                  rc(1):Y_mno2_mno4 (mol/mol)
3000.0                               rc(1):rho_mno2 (M/L3)
165830.0                             rc(1):MW_cont   (M/mol)
1630.0                               rc(1):rho_cont (M/L3)
262000.0                             rc(1):k2_cont (L3/mol-T)
0.200                                rc(1):C_c_star (M/L3)
0.0                                  rc(1):xi        (1/T)
150.0                                rc(1):lambda_c (L3/M)
52152.35                             rc(1):k_nod_f   (1/T)
3.36e-005                            rc(1):k_nod_s   (1/T)
    3001      1.0                      2   vrc(1):k_La (1/T)
    5001      1.0                      2   vrc(2):initial porosity
```

Figure 7.2: RCT Input File Structure (CORT3D-specific items shown in bold).

Table 7.1: Reaction Variables for RCT Input File

Parameter	Type	Description[1]
Dm_cont	Constant	Molecular diffusion coefficient for aqueous contaminant (L^2T^{-1})
Dm_mno4	Constant	Molecular diffusion coefficient for permanganate (L^2T^{-1})
Dm_cl	Constant	Molecular diffusion coefficient for chloride (L^2T^{-1})
Y_mno4_cont	Constant	Stoichiometric mole ratio, moles permanganate consumed to destroy one mole of contaminant ($MolMol^{-1}$)
Y_cl_cont	Constant	Stoichiometric mole ratio, moles chloride created by destroying one mole of contaminant ($MolMol^{-1}$)
Y_mno2_mno4	Constant	Stoichiometric mole ratio, moles manganese oxide created from consumption of one mole permanganate ($MolMol^{-1}$)
rho_mno2	Constant	Effective density of manganese oxide solids (ML^{-3})
MW_cont	Constant	Molecular weight of contaminant ($MMol^{-1}$)
rho_cont	Constant	Density of contaminant (ML^{-3})
k2_cont	Constant	Second-order kinetic rate constant for oxidation of contaminant by permanganate ($L^3Mol^{-1}T^{-1}$)
C_c_star	Constant	Aqueous solubility limit for contaminant (ML^{-3})
xi	Constant	Rate-limited sorption mass transfer coefficient (T^{-1})
lambda_c	Constant	Linear sorption coefficient (L^3M^{-1})
k_nod_f	Constant	First-order kinetic rate constant for oxidation of the fraction of NOD with a faster rate (T^{-1})
k_nod_s	Constant	First-order kinetic rate constant for oxidation of the fraction of NOD with a slower rate (T^{-1})
k_La	Variable	Lumped mass transfer coefficient (T^{-1})
porosity	Variable	Effective porosity of porous media (-)

[1]Variables M, L, T, and Mol shown as units for these parameters denote mass, length, time, and moles, respectively

7.1.1 Setup Component Initial Concentration and Mass Fraction Files

The next step is to specify the initial concentration of each component except DNAPL. This is accomplished using either the 'fort.yxxx.ini' method (when the value in every cell is the same) and/or 'file_gen.yxxx' method when (at least one layer contains values that vary by cell).

The 'fort.yxxx.ini' files are free format, and any number of values can be entered on each line. The only requirements are that the correct number of values be entered, that the values be entered in the proper order, and that at least one space and/or line return separate values. Values can also be entered as multiples (**unless the file will be opened with the C3DI.EXE front-end program; the C3DI.EXE program does not allow multiples—each value must be entered individually in the input file**). For example,

250 consecutive cells containing the value 0.0070 can be entered as 250 numbers separated by spaces and/or line returns, or as a multiple (e.g., 250*0.0070). The files must be built sequentially such that values for all the columns (x=1...j) in model row 1 are entered first, followed by columns of row 2, then columns of row 3...j for the layer 'xxx' the file is being built for.

Note that you can effectively turn off simulation of NOD affects on oxidation by simply setting the initial mass fraction of both NOD components to zero in all model cells.

7.1.1 Setup CORT3D.INP File

Next, the CORT3D-specific input file <u>CORT3D.INP</u> needs to be constructed as shown in the example of Figure 7.3. This file is used by each of the CORT3D modules (CORT3D.PL, FILE_GEN.EXE, C_MODK.EXE, C_DSS.EXE, C_RECORD.EXE, C_UPDT.EXE, C_MASS.EXE, and C_POST.EXE) in carrying out the simulation.

```
ex2.mfn       / MODFLOW name (NAM or MFN) file
ex2.rts       / MODFLOW RT3D super (RTS) file
56            / number of iterations to perform
n             / is this a continuation of another run (Y/N)?
init_K.inp    / input file containing hydraulic conductivity for all layers
phi0.inp      / input file containing porosity for all layers (w/ no DNAPL)
d50.inp       / input file containing d50 for all layers
srw.inp       / input file containing residual water saturation for all layers
sn.inp        / input file containing DNAPL saturation for all layers
smn.inp       / input file containing MnO2 pseudo-saturation for all layers
conc7.out     / output file containing contaminant concentration
conc8.out     / output file containing permanganate concentration
conc9.out     / output file containing chloride concentration
mfrac10.out   / output file containing MnO2 mass fraction
mfrac11.out   / output file containing DNAPL mass fraction
mfrac12.out   / output file containing Sorbed contaminant mass fraction
mfrac13.out   / output file containing Fast NOD mass fraction
mfrac14.out   / output file containing Slow NOD mass fraction
mass.out      / output file containing mass of immobile species within model
obs_c.out     / output file containing mobile species conc. at obs. points
obs_m.out     / output file containing immobile species mass frac. at obs points
obs_h.out     / output file containing heads at observation points
4200.0        / density of the solid phase (M/L3)
1.008801779   / tortuosity factor (tau)
75.50161425   / alpha_1 - empirical parameter for natural dissolution
.6878052435   / alpha_2 - empirical parameter for natural dissolution
1.991786E-4   / alpha_3 - empirical parameter for natural dissolution
.5942657302   / alpha_4 - empirical parameter for natural dissolution
3             / number of obs pts.
30  1   1     / col row lay (j,i,k) for obs. pts.
35  1   1
40  1   1
39            / effluent concentration measured at this column
```

Figure 7.3: Example <u>CORT3D.INP</u> Input File

Input instructions for <u>CORT3D.INP</u> are listed below. Each record refers to a line of the input file. A comment can be included on the line, following the required input, by preceding the comment with a "/" and a space.

Record #1:   File name of MODFLOW Name (NAM or MFN) file

Record #2:   File name of RT3D Super (RTS) file

Record #3:   Number of iterations the simulation time has been broken down into

Record #4:   Indicate whether this is a continuation of a previous run. This is used when the simulation is divided up into phases to accommodate different boundary conditions or stresses.

Record #5:   File name of input file containing initial (saturated) hydraulic conductivity for all layers

Record #6:   File name of input file containing initial (fully) water saturated porosity for all layers (with no DNAPL or manganese oxide)

Record #7:   File name of input file containing median soil grain size (d50)

Record #8:   File name of input file containing residual water saturation

Record #9:   File name of input file containing DNAPL saturation

Record #10:   File name of input file containing $MnO_{2\,(s)}$ pseudo-saturation

Record #11:   File name of output file to write contaminant concentration

Record #12:   File name of output file to write permanganate concentration

Record #13:   File name of output file to write chloride concentration

Record #14:   File name of output file to write $MnO_{2\,(s)}$ mass fraction

Record #15:   File name of output file to write DNAPL mass fraction

Record #16:   File name of output file to write Sorbed contaminant mass fraction

Record #17:   File name of output file to write Fast NOD mass fraction

Record #18:   File name of output file to write Slow NOD mass fraction

Record #19:   File name of output file to write mass of immobile species remaining within model

Record #20:   File name of output file to write mobile species concentrations, at observation points

Record #21:   File name of output file to write immobile species mass fraction, at observation points

Record #22:   File name of output file to write hydraulic heads at observation points

Record #23:   Density of the solid phase (soil grain density)

Record #24:   Soil tortuosity factor (τ); used in Gilland-Sherwood relationship for natural dissolution

Record #25:   Pre-multiplier (α_1) in Gilland-Sherwood relationship for natural dissolution

Record #26:   Exponent (α_2) of Reynolds number in Gilland-Sherwood relationship for natural dissolution

Record #27:   Exponent (α_3) of Schmidt number in Gilland-Sherwood relationship for natural dissolution

Record #28:   Exponent (α_4) of $\left(\dfrac{\theta_n d_{50}}{\tau L} \right)$ term in Gilland-Sherwood relationship for natural dissolution

Record #29:   Number of observations points at which to record concentration, mass fraction, and hydraulic head for each iteration

Record #30:   column, row, layer (j,i,k) of each observation point. Enter one observation point per line. Enter as many lines as there are observation points specified in Record #29.

Record #31:   Enter column number to use for calculating and recording effluent concentrations and flow rate

7.1.1   Setup Oxidation Initial Aquifer Property & DNAPL Saturation Files

Additionally, input files are needed to define several additional simulation parameters. These are: <u>D50.INP</u>, <u>INIT_K.INP</u>, <u>PHI0.INP</u>, <u>SRW.INP</u>, and <u>SN.INP.INI</u>. These text files contain an entry for every model cell. Just as described for building the 'fort.yxxx' files, values can be specified using free format. The files are built sequentially such that all of the model columns (x=1…j) in model row 1 of model layer 1 are first, followed by all the columns of row 2 of layer 1, and then the columns of layers 3…j in layer 1. The same sequence is then repeated for layers 2 through k.

7.1.1   Execute Simulation

After preparing all required input files, open a "Command Prompt" window and change to the folder containing all the input files and the "CORT3D.PL" file. Ensure all executable files (including "PERL.EXE" and "PERL58.DLL") are either in a location included in the PATH environment variable of your computer, or located in the same folder as the input files. Then type "PERL CORT3D.PL" to start the simulation.

Alternately, you can load the input files into (or create them with) the C3DI front-end program and then execute the simulation from within C3DI.

7.2. Using C3DI (CORT3D Input) for Setting Up Simulation Files

You will quickly realize that manual generation of input files for simulation problems can become quite a burden. Consequently, the C3DI front-end program was developed for CORT3D to provide an interactive program that helps prepare model-input data. C3DI prompts for the required data, checks for errors, and ensures that files are created with the proper structure. C3DI works by displaying screens on which you enter data or make choices.

7.2.1 Design Decisions

In designing C3DI, several design decisions were made. They are:

1. First, as pointed out earlier, multipliers are not allowed in any of the input files. This means you cannot enter an array containing 250 entries of the value 0.10 as 250*0.10.

2. When defining point stresses for the Transport model, all Point Stresses (even for those where all components are at zero concentration) must be included in the SSM input file. This becomes important if you manually generate the SSM input file and later try to read the simulation into C3DI.

3. Spatial data is entered into C3DI using grid coordinates rather than arbitrary geographic coordinates that require transformation in order to determine grid coordinates. Also, data values for the grid must be entered for all locations required by the underlying MODFLOW-2000 and RT3D programs (i.e., C3DI does not interpolate missing values).

4. Parameters, Zone files, and Multiplier files are not used for any data entry.

5. Every attempt was made so that defining a simulation will be intuitive; guiding the user through the process while maintaining the terminology defined in the MODFLOW-2000, RT3D, and MT3DMS manuals. A notable benefit of using C3DI is elimination of the need to enter redundant data. For example, once the model dimensions (number of rows, columns, and layers) is defined, it goes into both the Flow model and Transport model input files—you do not have to enter it twice.

7.2.2 Starting C3DI

When you start C3DI, either by clicking on it in Windows Explorer or by choosing it from the "All Programs" structure in Windows, you will see the following splash screen before the initial or "Main" data entry screen appears as shown in Figure 7.5.
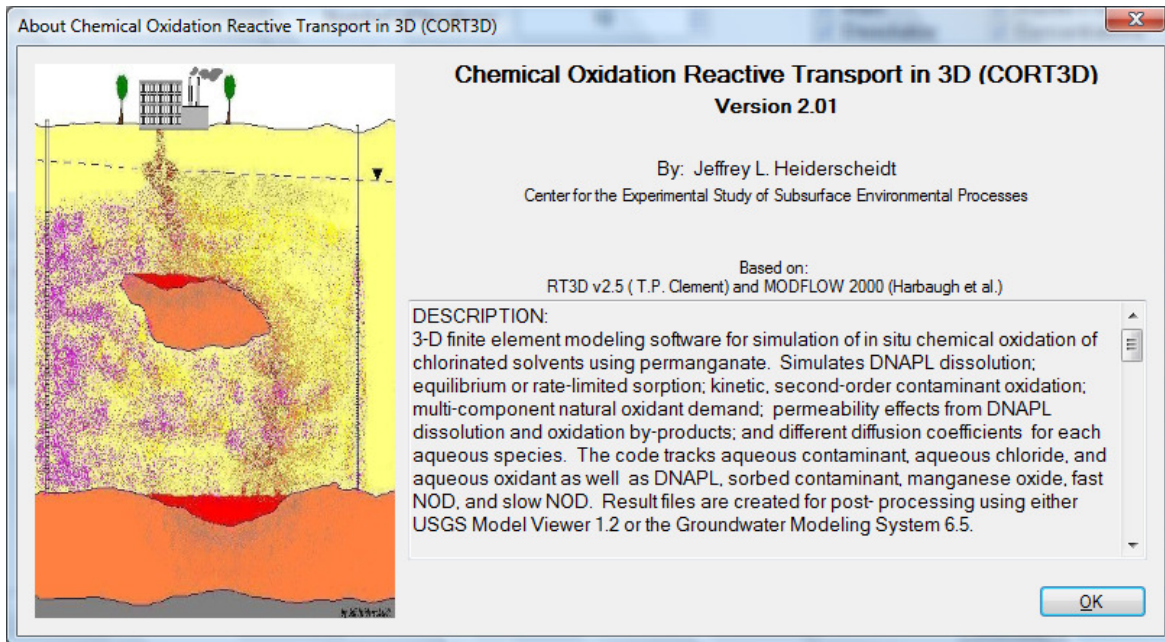
Figure 7.4: Opening C3DI Splash Screen

7.2.3 Main Screen

The Main screen is where you begin setting up the simulation dimensions, load an existing simulation, save the current simulation, choose other data entry screens, view what data entry has been completed, and execute a simulation. You must define the dimensions of your model (number of rows, columns, and layers) before you can select one of the other input screens listed down the left side. Once you define the dimensions and select one of the other screens, the dimensions become read-only so that you cannot change them. This is necessary because many of the inputs entered on the other screens are dependent upon the model dimensions. If you were allowed to change model dimensions after entering other inputs, the model setup files would no longer work.

While C3DI is a small program, as a simulation is defined, the many arrays containing the simulation data can require fairly substantial amounts of memory. In the

title bar at the top of the Main screen, you will see an estimate of the maximum sum of Rows * Columns * Layers * Stress Periods that will fit into available memory. The value is determined based on the available physical memory in your computer. As you enter values for number of rows, columns, layers, or stress periods (on the "Define Flow Model" screen), the number will update to display the estimated maximum sum of remaining dimension values.
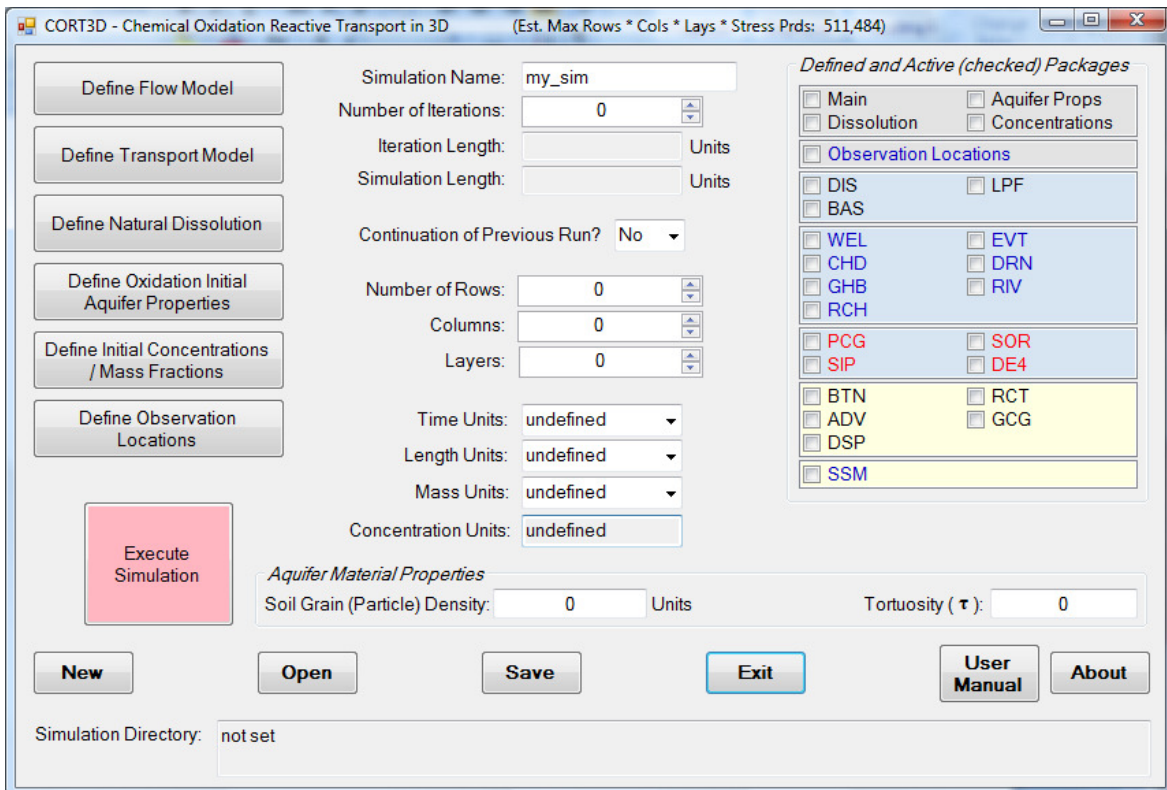
Figure 7.5: Main Screen

The Main screen is also where you enter the desired units for time, length, mass, and concentration. The available choices for concentration units will be determined based upon the inputs for length and mass. Other items to input on this screen include the name of the simulation, the number of iterations (flow model execution followed by transport model execution) that make up the entire simulation length, the soil grain particle density (this is NOT the soil bulk density, which includes soil pore space), and the soil tortuosity. The tortuosity value is used in determining the mass transfer rate for DNAPL dissolution,

and is typically determined via calibration like the other DNAPL dissolution parameters. Unlike the dimensions (rows, columns, and layers) these other entries can be entered, or changed, at any time.

The list of checkboxes on the upper-right side of the Main screen indicates which packages of the Flow and Transport models have been activated by completing data entry. If a package is active, a check will be displayed in the box. The packages listed inside gray boxes are part of the overall simulation definition, packages listed inside blue boxes are part of the Flow model definition, and packages listed inside the yellow boxes are part of the Transport model definition. Packages whose name is listed in black text are always required before a simulation can be executed. Conversely, those listed in blue text are optional; they only need to be entered if you want to include the process represented by that package in your model. Finally, one of the packages listed in red text must be active in order to execute the simulation—these packages are mutually exclusive, so that the last one you entered data for is the one that will be active.

Once a simulation has been saved, or opened from existing files, the current sub-directory is displayed along the bottom of the screen.

In addition to the buttons down the left side of the screen that are used to access the data entry screens, there are several other buttons that should be pointed out. As the name implies, the "Execute Simulation" button is used to execute the CORT3D model code using the currently loaded simulation data files. When you begin defining a simulation, the "Execute Simulation" button is red in color and does nothing when clicked. Once all required data are entered for a simulation, the button turns green and if clicked will open a command window and execute the model code.

The "Open" button will bring up a familiar Windows file dialog box as shown in Figure 7.6. You can navigate to the desired sub-directory and select an existing "CORT3D.INP" file, which will completely overwrite the currently loaded simulation with the one you select. Alternately, you can select a MODFLOW Name file (*.MFN), which will load the selected flow simulation and replace existing flow simulation data in the currently loaded simulation. You can also select an RT3D Super file (*.RTS), which will load the selected transport simulation and replace the existing transport simulation data in the currently loaded simulation. Because a goal of developing the C3DI software was to

eliminate redundant data entry, the flow simulation data should be entered (and must agree with that defined in the transport input files) before choosing to load an RTS file.
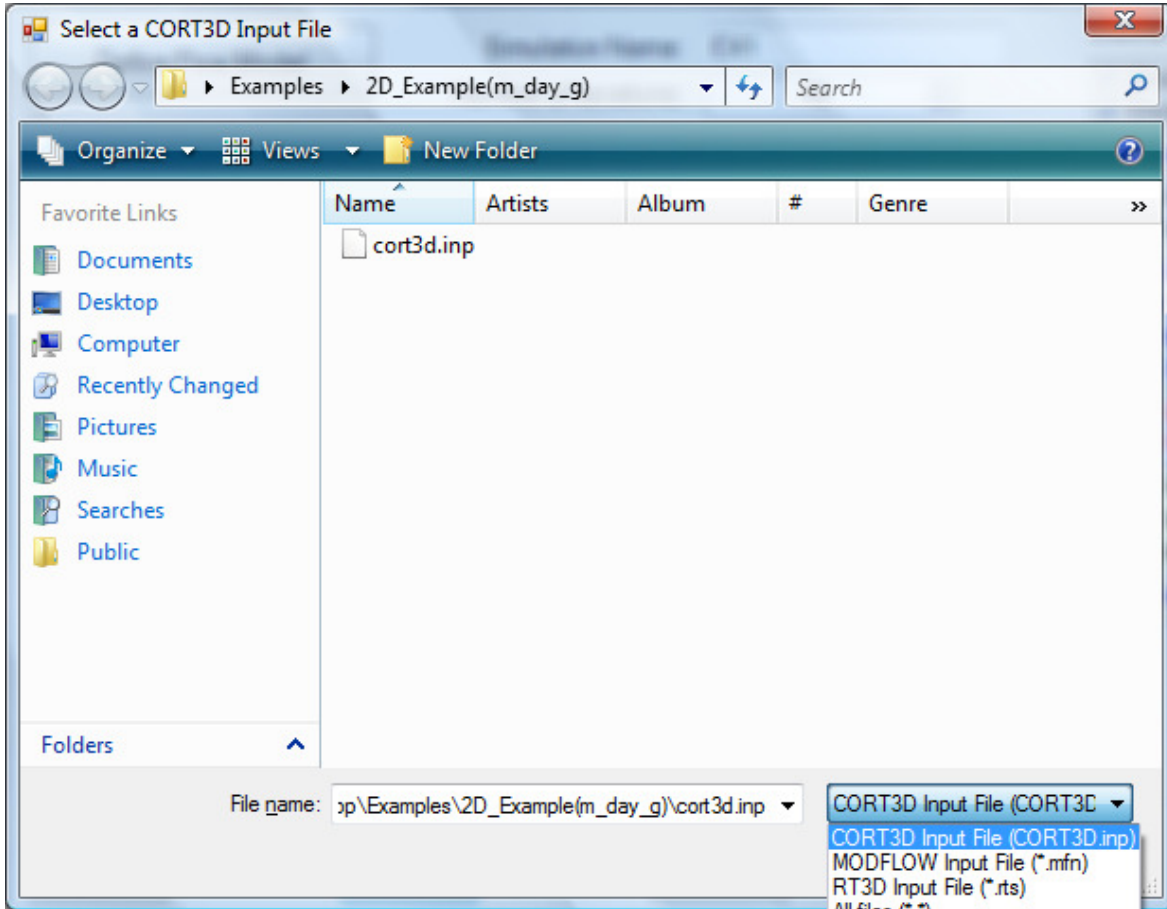
Figure 7.6: Open File Dialog Box

As the name suggests, the "Save" button will bring up a Windows file dialog box, where you can choose an existing or create a new sub-directory to save the simulation into. If there is an existing simulation stored in the selected sub-directory, you will be asked if you want to overwrite it. All files that have currently been completed (as indicated by a check next to the package name on the Main screen as shown in Figure 7.7) will be saved.

The "New" button will completely clear the currently loaded simulation from memory and allow you to begin defining a new simulation. The "Exit" button will prompt you to save the current simulation, if you have started defining one, before closing the C3DI program. The "User Manual" button will open the CORT3D manual using

Microsoft Word, Adobe Acrobat Reader, or Windows WordPad if one of them exists. The "About" button will bring up the C3DI opening splash screen to provide information about the C3DI program.
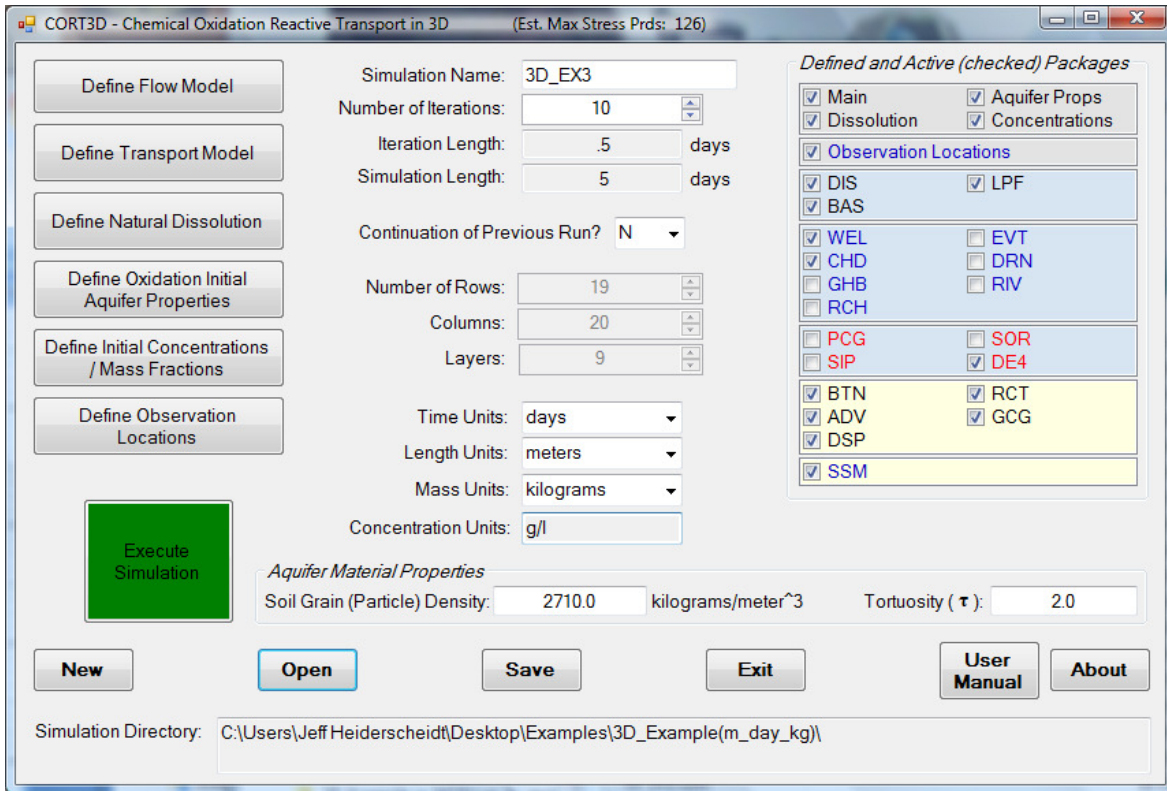
Figure 7.7: Main Screen Showing Complete/Active Packages

7.2.4 *Defining Flow Model*

Clicking on the "Define Flow Model" button of the Main screen will bring you to a tabbed screen where data for the flow model input files are entered. Clicking "Close" on any of the tabbed input screens will return you to the Main screen.

Figure 7.8 displays the Discretization tab (corresponding to the Flow Model DIS package). On this tab (and many of the other tabs) there are array grids used to enter 1-D, 2-D, or 3-D data. Often these grids will include a "Set…" button and a "Multiply…" button. You can set all values in the grid to the same value by entering a value in the adjacent space and clicking the "Set…" button. Similarly, you can change all values in the grid by the same factor by entering a value in the adjacent space and the clicking "Multiply…" button. The grids also support "cut and paste" operations. You can select cells of the grid and press "Ctrl-C" to copy the values to the clipboard. Similarly, you can copy cells from a text file (tab-delimited) or spreadsheet file. The values can be pasted into the grid by selecting a cell and pressing "Ctrl-V." Pasting places the values into cells in the same spatial pattern as they were copied, beginning at the top-left cell you have highlighted (if you have multiple cells highlighted). Pasting does not repeat the copied cells; that is, you cannot copy one cell and then highlight and paste into ten cells in one operation.
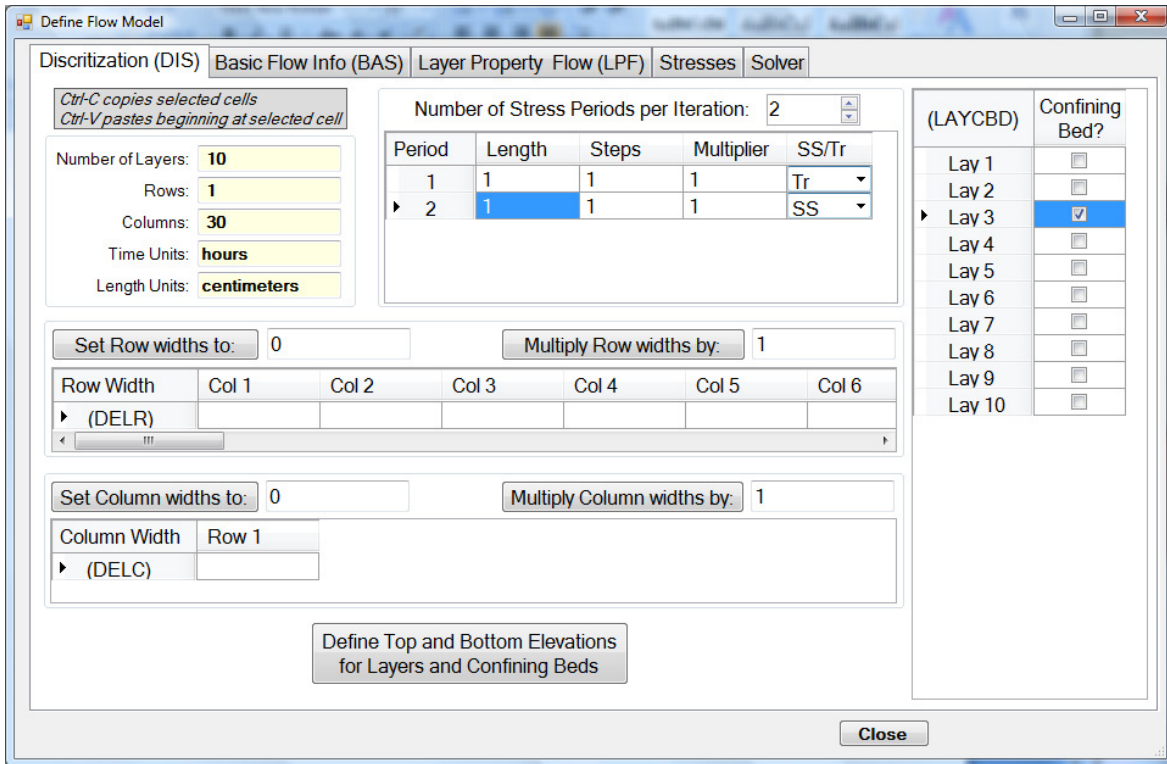
Figure 7.8: Flow Model Definition—Discretization (DIS Package) Tab

DELR is cell width along rows.   Enter one value for each of the NCOL columns.

DELC is cell width along columns. Enter one value for each of the NROW rows.

LAYCBD indicates whether or not a layer has a Quasi-3D confining bed below it. Checked indicates a confining bed and unchecked indicates no confining bed. As required by the MODFLOW program, LAYCBD for the bottom layer cannot be checked.

Stress Periods:

"Number of Stress Periods" is the number of stress periods in each iteration of the
overall simulation (variable NPER).

"Length" is the length of a stress period (variable PERLEN).

"Steps" is the number of time steps in a stress period (variable NSTP).

"Multiplier" is the multiplier for the length of successive time steps (variable
TSMULT). The length of a time step is calculated by multiplying the length
of the previous time step by TSMULT. The length of the first time step,
Δt1, is related to PERLEN, NSTP, and TSMULT by the relation:

$$\Delta t1 = PERLEN\ (TSMULT-1)/(TSMULT^{NSTP}-1)$$

SS/Tr is a selection variable indicating whether the stress period is transient or
steady state. Select the appropriate choice.
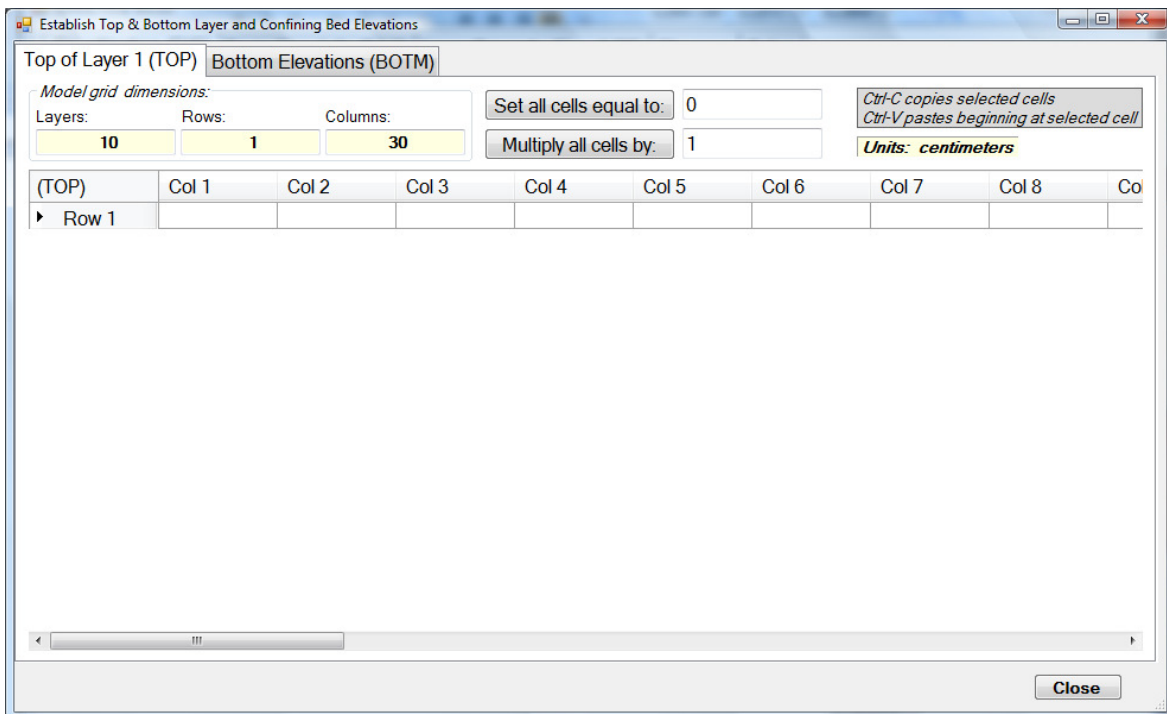
Figure 7.9: Flow Model Definition—Defining Layer 1 Top Elevations

TOP is the top elevation of layer 1 (the uppermost layer). For the common situation in which the top layer represents a water-table aquifer, setting Top equal to land-surface elevation may be reasonable.
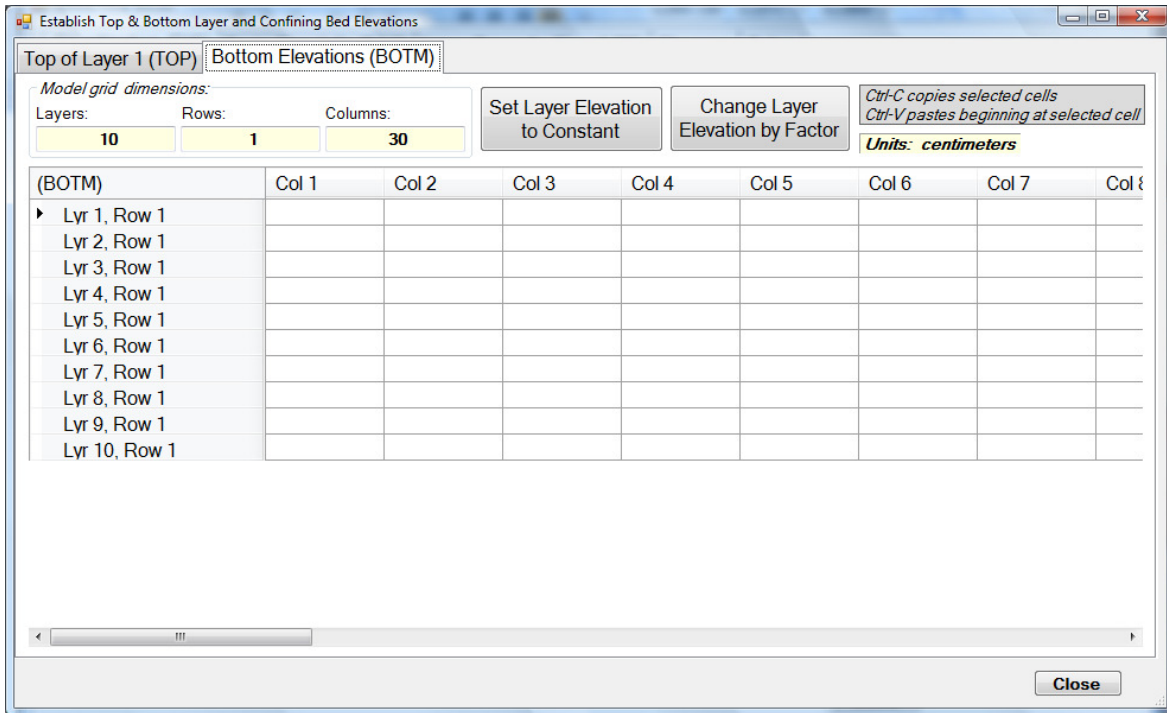
Figure 7.10: Flow Model Definition—Defining Layer Bottom Elevations

BOTM is the bottom elevation of a model layer or a Quasi-3D confining bed (for layers where LAYCBD was checked on the DIS tab). The "Set…" and "Change…" buttons bring up screens as shown in Figures 7.11 and 7.12, respectively, where values can be entered or changed layer-by-layer. Selecting a layer, entering a value, and clicking the "Set…" or "Multiply…" button will return to the Defining Layer Bottom Elevations screen and update the BOTM grid. Pressing "Cancel" will return to the Defining Layer Bottom Elevations screen without changing values in the BOTM grid.
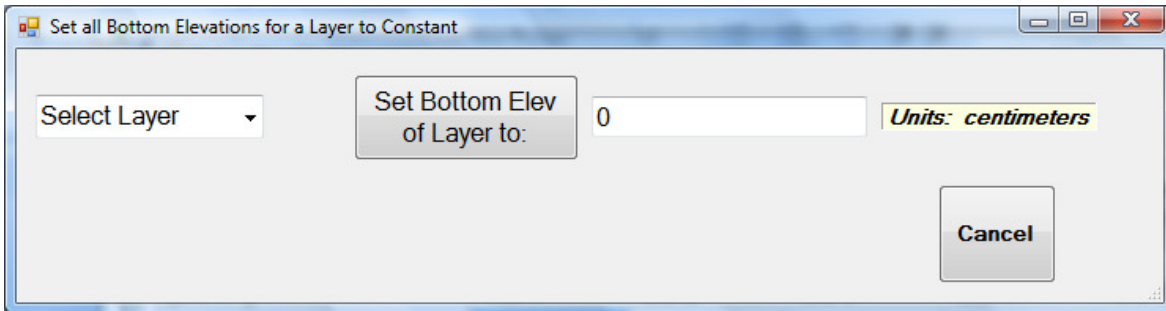
Figure 7.11: Flow Model Definition—Setting Layer Bottom Elevations to Constant
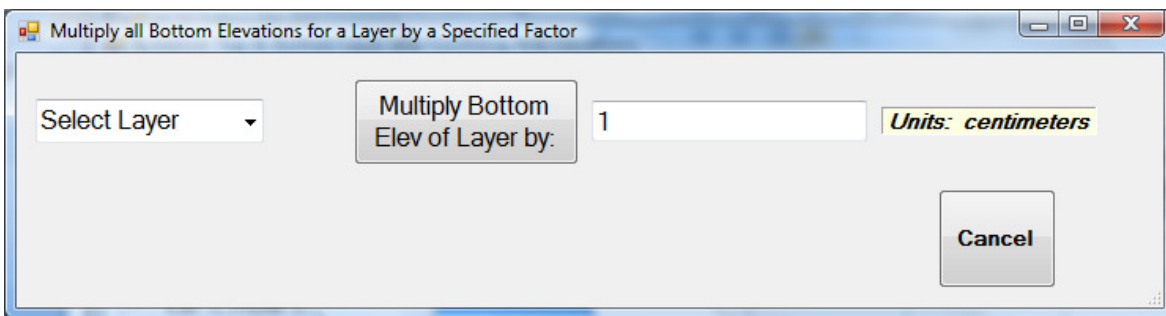
Figure 7.12: Flow Model Definition—Multiplying Layer Bottom Elevations by Constant

Figure 7.13 shows the Basic Flow Information tab (corresponding to the Flow Model BAS6 package).
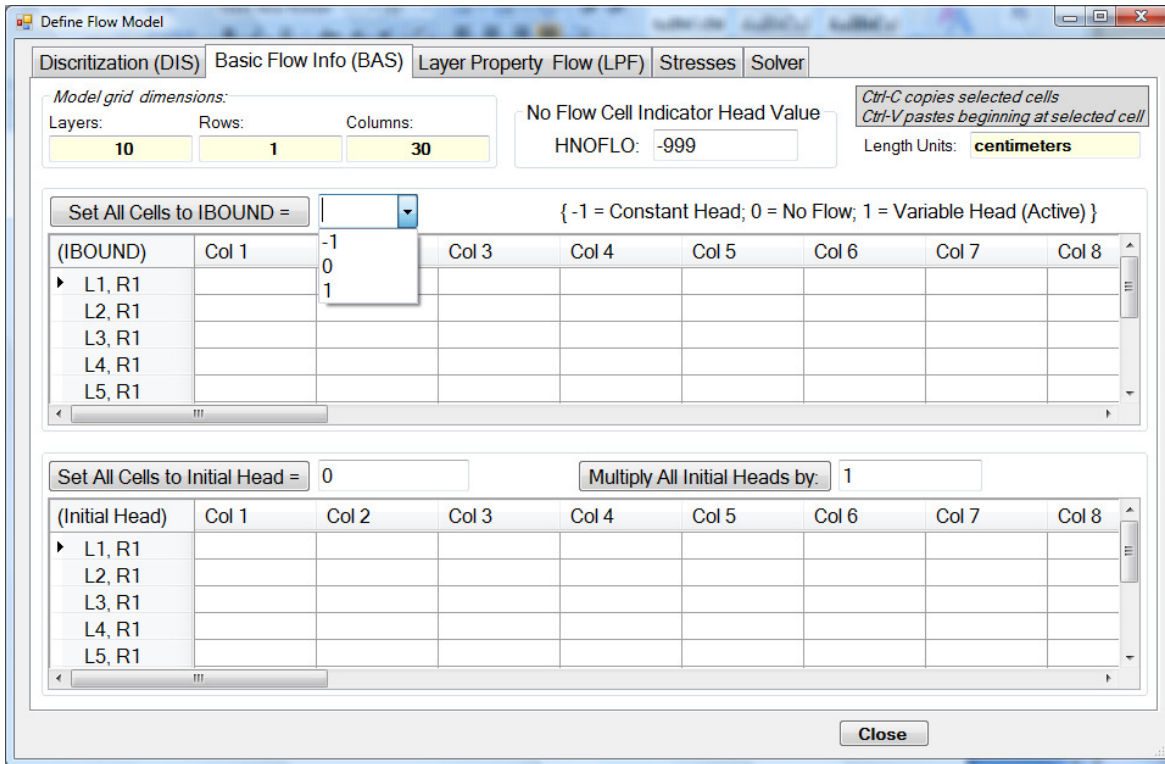
Figure 7.13: Flow Model Definition—Basic Flow Info (BAS6 Package) Tab

HNOFLO is the value of head to be assigned to all inactive (no flow) cells (cells where IBOUND = 0) throughout the simulation. Inactive cells are not used in model calculations, so this does not affect model results but serves to identify inactive cells when head is printed. Even if the user does not anticipate having inactive cells, a value for HNOFLO must be entered.

IBOUND is the boundary condition variable. One value is read for every model cell. An IBOUND value of -1 means the cell has a constant head. A value of 0 means the cell is inactive (there is no flow). A value of 1 means the cell is active (the head can change).

Initial Head (variable STRT) is the head at the beginning of the simulation. STRT must be specified for all simulations, including steady-state simulations, and a value is needed for every model cell. For simulations in which the first

stress period is steady state, the values used for STRT generally do not affect the simulation [though exceptions may occur if cells go dry and/or rewet]. However, the execution time will be less if STRT includes hydraulic heads that are close to the steady-state solution.

Figure 7.14 shows the Layer Property Flow tab (corresponding to the Flow Model LPF package).
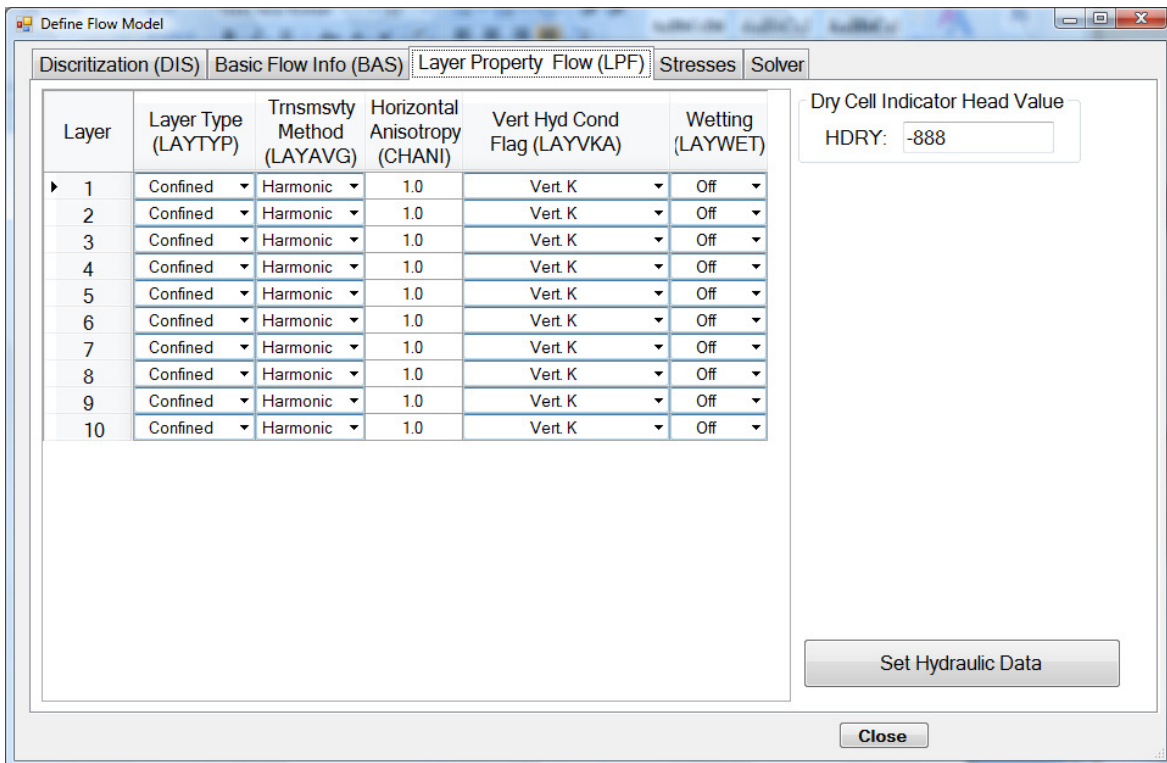
Figure 7.14: Flow Model Definition—Layer Property Flow (LPF Package) Tab

Dry Cell Indicator Head Value (variable HDRY) is the head that is printed or saved at cells that have converted to dry during a simulation. Although this value is not used in the model calculations, it is useful as an indicator when looking at the resulting heads that are output from the model. HDRY is, thus, similar to HNOFLO in the Basic Package, which is the value assigned to cells that are no-flow cells at the start of a model simulation.

LAYTYP is the layer type. Select either confined or convertible. The choice determines what variables will be defined on the "Set Hydraulic Data" screen for each layer of the model grid:

- Confined—Transmissivity and storage coefficient of the layer are constant for the entire simulation (LAYTYP = 0).
- Convertible—Transmissivity of the layer varies, and the storage coefficient may alternate between confined and unconfined values (LAYTYP ≠ 0). Transmissivity is calculated from the saturated thickness and hydraulic conductivity. Vertical flow from above is limited if the layer de-saturates. For the water table, specify convertible and be sure that the top elevation is higher than the computed head.

LAYAVG defines the method of calculating interblock transmissivity. The methods are described in the MODFLOW manual

- Harmonic (LAYAVG = 0)—Harmonic mean (method used in MODFLOW-88)
- Logarithmic (LAYAVG = 1)—Logarithmic mean
- Arith-log (LAYAVG = 2)—Arithmetic mean of saturated thickness and logarithmic-mean hydraulic conductivity

CHANI (horizontal anisotropy) is the ratio of hydraulic conductivity in the Y direction (along a column) to hydraulic conductivity in the X direction (along a row). A nonzero value here applies to all cells in the layer. Specify 1.0 for isotropic layers. Specify 0.0 in order to use array HANI to specify individual values for every cell in the layer through the Set Hydraulic Data screen.

LAYVKA is a flag indicating whether array VKA (entered on the Set Hydraulic Data screen) is vertical hydraulic conductivity or the ratio of horizontal to vertical hydraulic conductivity.

LAYWET is the wetting flag. Wetting can be on or off for each layer. Wetting cannot be on for a confined layer. If wetting is turned on for at least one layer, additional variables will appear on the right side of the screen as shown in Figure 7.15.
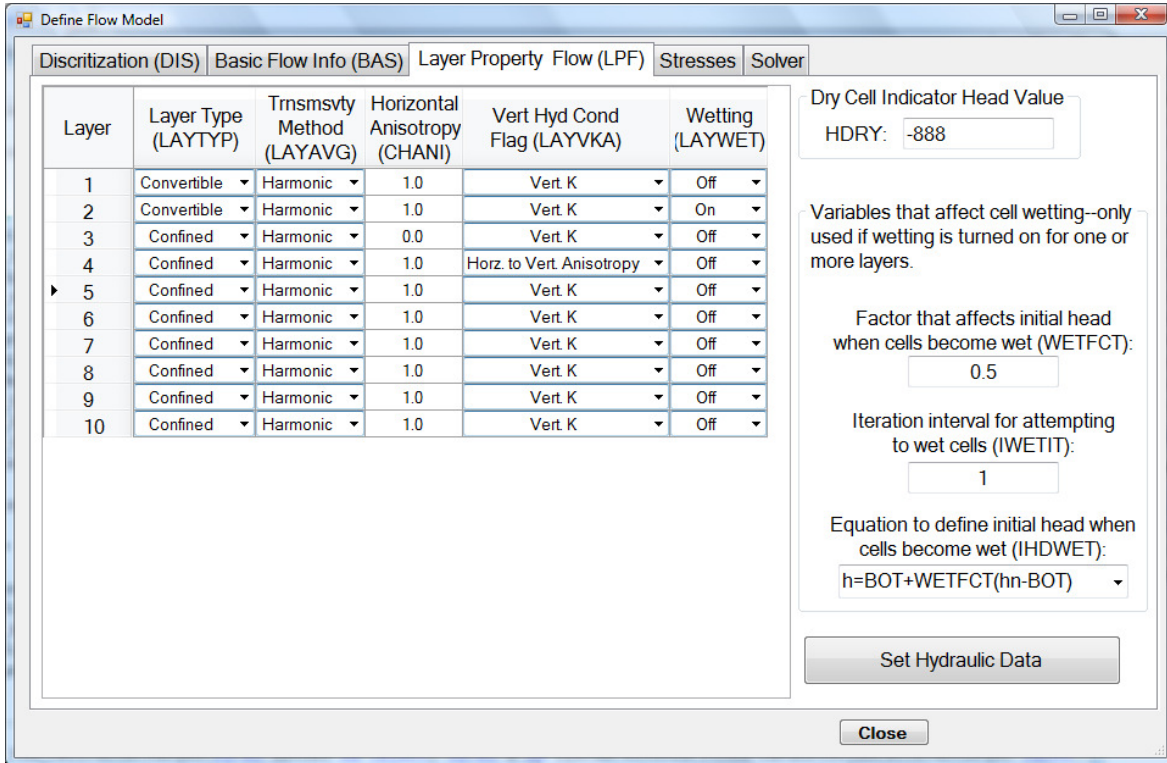
Figure 7.15: Flow Model Definition—LPF Tab (LAYWET Turned On)

Factor That Affects Initial Head When Cells Become Wet (WETFCT) is a variable that is included in the equation for the head to be established at a cell when the cell is converted from dry to wet (the equation is chosen by setting IHDWET).

Iteration Interval for Attempting to Wet Cells (IWETIT) determines the iterations at which wetting is attempted at wettable cells. Wetting is attempted every IWETIT iteration. If using the PCG solver, this value applies to outer iterations, not inner iterations.

Equation to Define Initial Head When Cells Become Wet (IHDWET) is an option that determines which equation to use in determining the initial head at cells that convert from dry to wet:

- BOT + WETFCT (hn - BOT)
- BOT + WETFCT (WETDRY)

Clicking the "Set Hydraulic Data" button on the LPF Tab opens the Hydraulic Data screen shown in Figure 7.16.
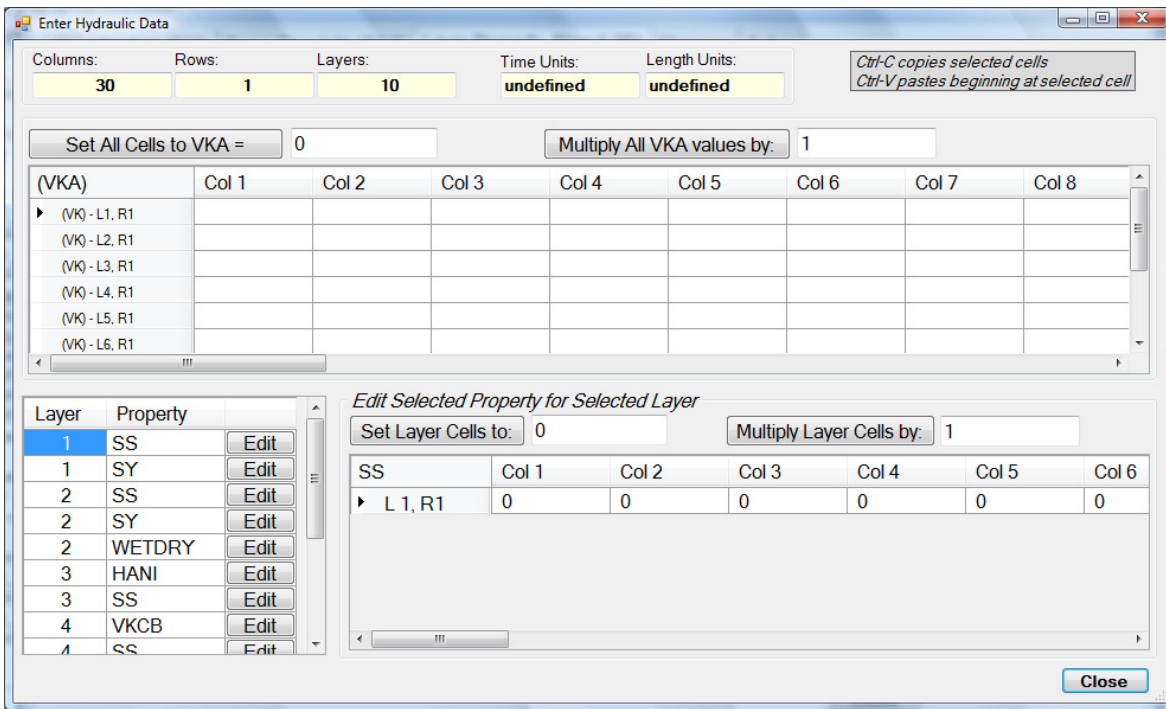
Figure 7.16: Flow Model Definition—Set Hydraulic Data Screen

VKA is entered for every model cell. It is either the vertical hydraulic conductivity or the ratio of horizontal hydraulic conductivity (HY) to vertical hydraulic conductivity, depending on the value of LAYVKA for each layer.

This screen also allows other hydraulic data (SS, SY, WETDRY, HANI, and VKCB) to be entered for each layer as required according to the options set on the LPF Tab such as steady state versus transient, wetting on or off, and layer type. Applicable properties that need to be entered appear in the table at the bottom-left of the screen. Clicking on "Edit" next to a property will open a data entry grid in the bottom-right corner. Clicking "Edit" for a different property will change the data entry grid accordingly.

SS is the specific storage. This array is required for every layer when there is at least one transient stress period.

SY is the specific yield. This array is only required for layers that are convertible, when there is at least one transient stress period.

WETDRY is a combination of the wetting threshold and a flag to indicate which neighboring cells can cause a cell to become wet. If WETDRY < 0, only the cell below a dry cell can cause the cell to become wet. If WETDRY > 0, the cell below a dry cell or the four horizontally adjacent cells can cause a cell to become wet. If WETDRY is 0, the cell cannot be wetted. The absolute value of WETDRY is the wetting threshold. When the sum of BOT (the cell bottom elevation) and the absolute value of WETDRY at a dry cell is equaled or exceeded by the head at an adjacent cell, the cell is wetted. This array is required only for layers that are wettable.

HANI is the ratio of hydraulic conductivity along columns (Y direction) to the hydraulic conductivity along rows (X direction). This array is only required for layers in which CHANI is 0.0.

VKCB is the vertical hydraulic conductivity of a Quasi-3D confining bed. This array is only required for layers that are underlain by a Quasi-3D confining bed.

Figure 7.17 shows the Stresses Tab, with sub-tabs for the seven available stress processes. Recharge and Evapotranspiration are areal stresses defined for entire layers, while the other five are point stresses applied at selected model cells.
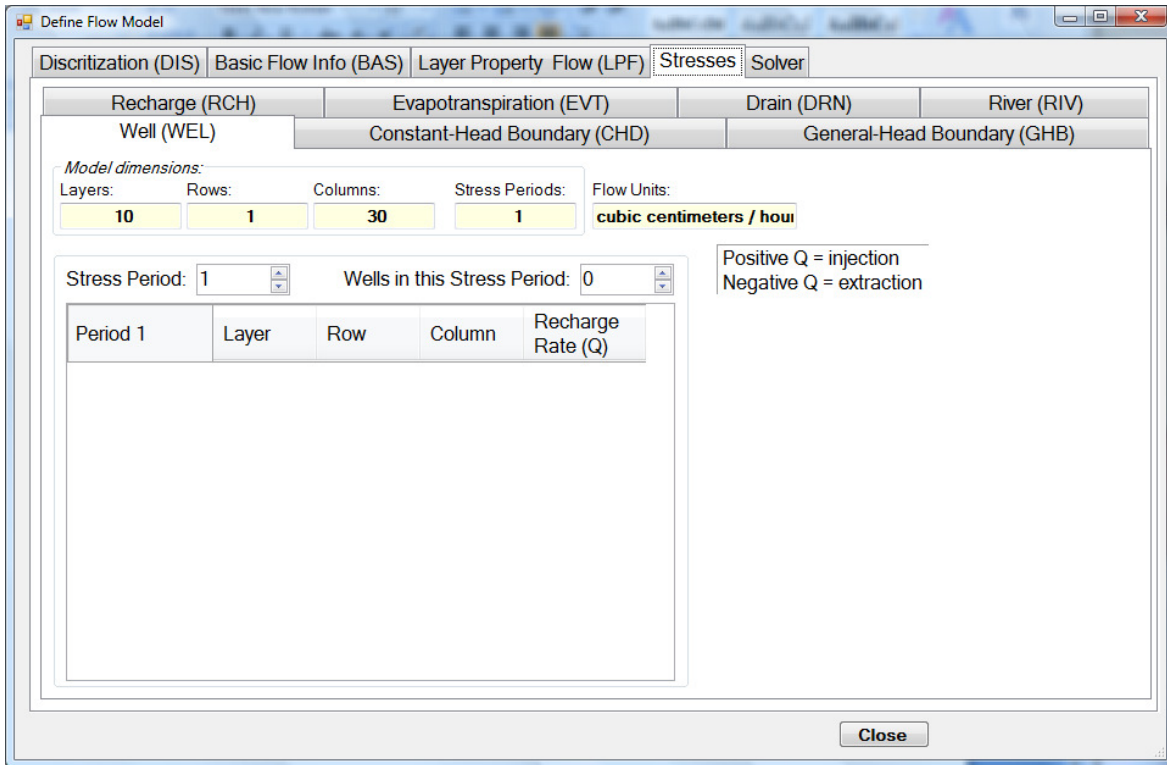
Figure 7.17: Flow Model Definition—Stresses (WEL Package) Tab

Begin by selecting the Stress Period that you want to set or edit well data for. Next, set the number of wells to be simulated in the selected Stress Period. Finally, the following fields must be defined for each well:

Layer—the layer number of the cell containing the well.

Row—the row number of the cell containing the well.

Column—the column number of the cell containing the well.

Well Recharge Rate (Q)—negative values indicate pumping.
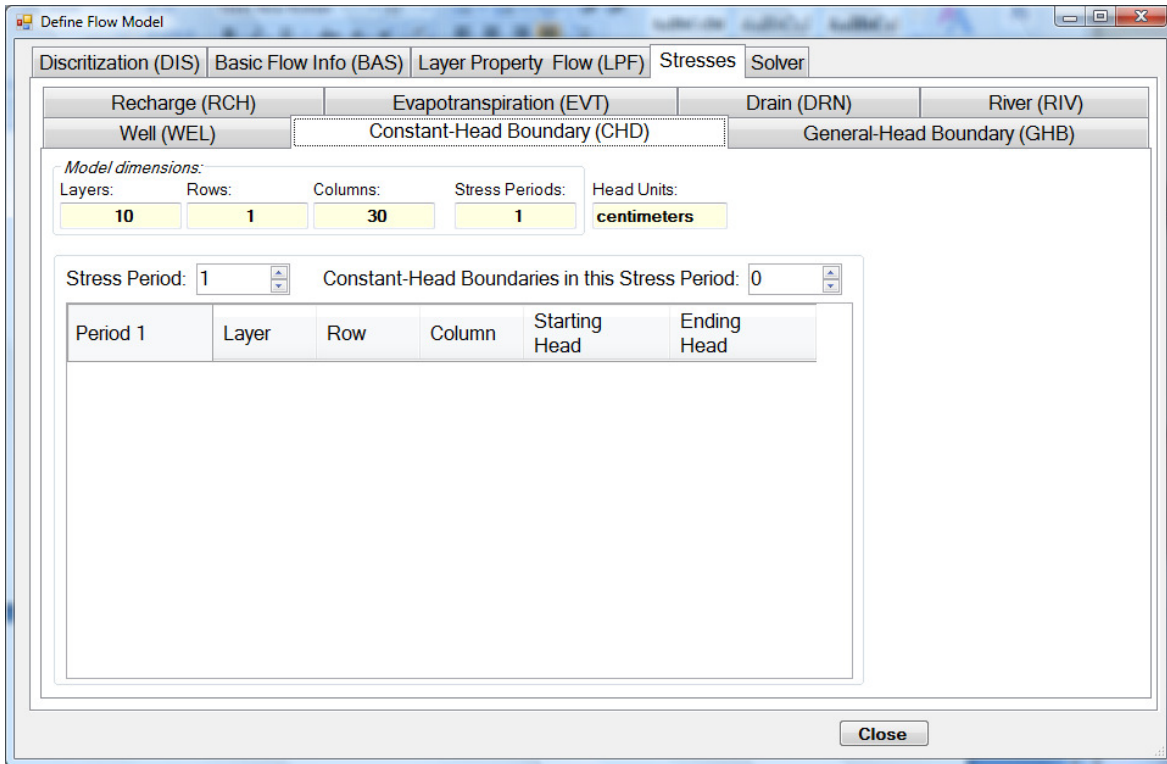
Figure 7.18: Flow Model Definition—Stresses (CHD Package) Tab

Begin by selecting the Stress Period that you want to set or edit constant head boundary data for. Next, set the number of constant head boundaries to be simulated in the selected Stress Period. Finally, the following fields must be defined for each constant head boundary:

Layer—the layer number of the cell containing the constant head boundary.

Row—the row number of the cell containing the constant head boundary.

Column—the column number of the cell containing the constant head boundary.

Starting Head—the head at the boundary at the start of the stress period.

Ending Head—the head at the boundary at the end of the stress period.

Figure 7.19: Flow Model Definition—Stresses (GHB Package) Tab

Begin by selecting the Stress Period that you want to set or edit general head boundary data for. Next, set the number of general head boundaries to be simulated in the selected Stress Period. Finally, the following fields must be defined for each general head boundary:

Layer—the layer number of the cell containing the general head boundary.

Row—the row number of the cell containing the general head boundary.

Column—the column number of the cell containing the general head boundary.

Boundary Head—the head on the boundary.

Boundary Conductance—the hydraulic conductance of the interface between the aquifer cell and the boundary.
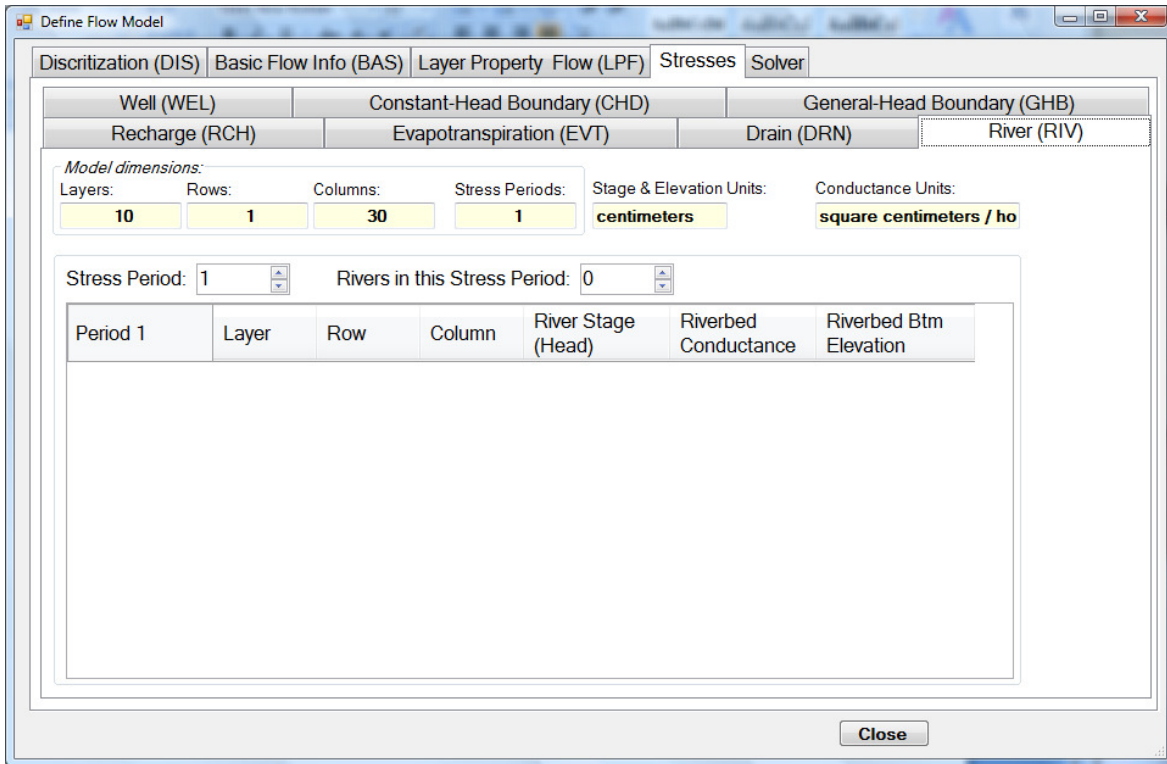
Figure 7.20: Flow Model Definition—Stresses (RIV Package) Tab

Begin by selecting the Stress Period that you want to set or edit river reach data for. Next, set the number of river reaches to be simulated in the selected Stress Period. Finally, the following fields must be defined for each river reach:

Layer—the layer number of the cell containing the river reach.

Row—the row number of the cell containing the river reach.

Column—the column number of the cell containing the river reach.

Stage—the head in the river.

Cond—the riverbed hydraulic conductance.

Rbot—the elevation of the bottom of the riverbed.
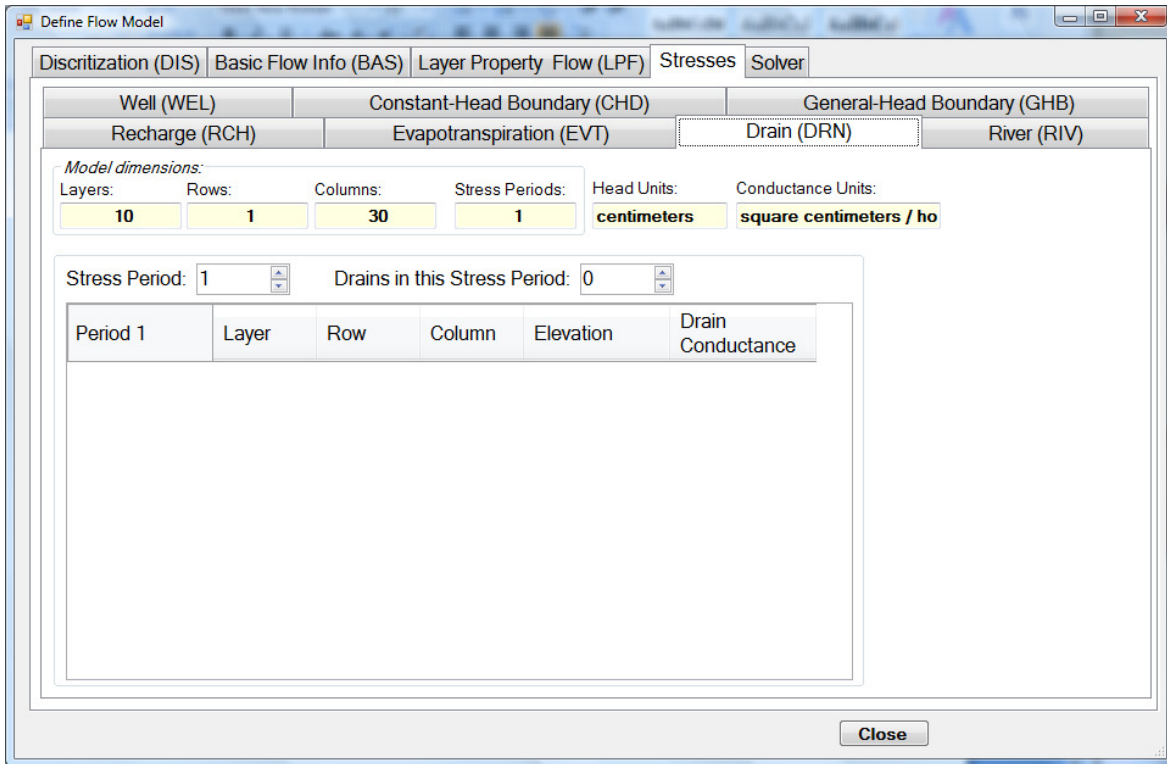
Figure 7.21: Flow Model Definition—Stresses (DRN Package) Tab

Begin by selecting the Stress Period that you want to set or edit drain data for. Next, set the number of drains to be simulated in the selected Stress Period. Finally, the following fields must be defined for each drain:

Layer—the layer number of the cell containing the drain.

Row—the row number of the cell containing the drain.

Column—the column number of the cell containing the drain.

Elevation—the elevation of the drain.

Cond—the hydraulic conductance of the interface between the aquifer and drain.
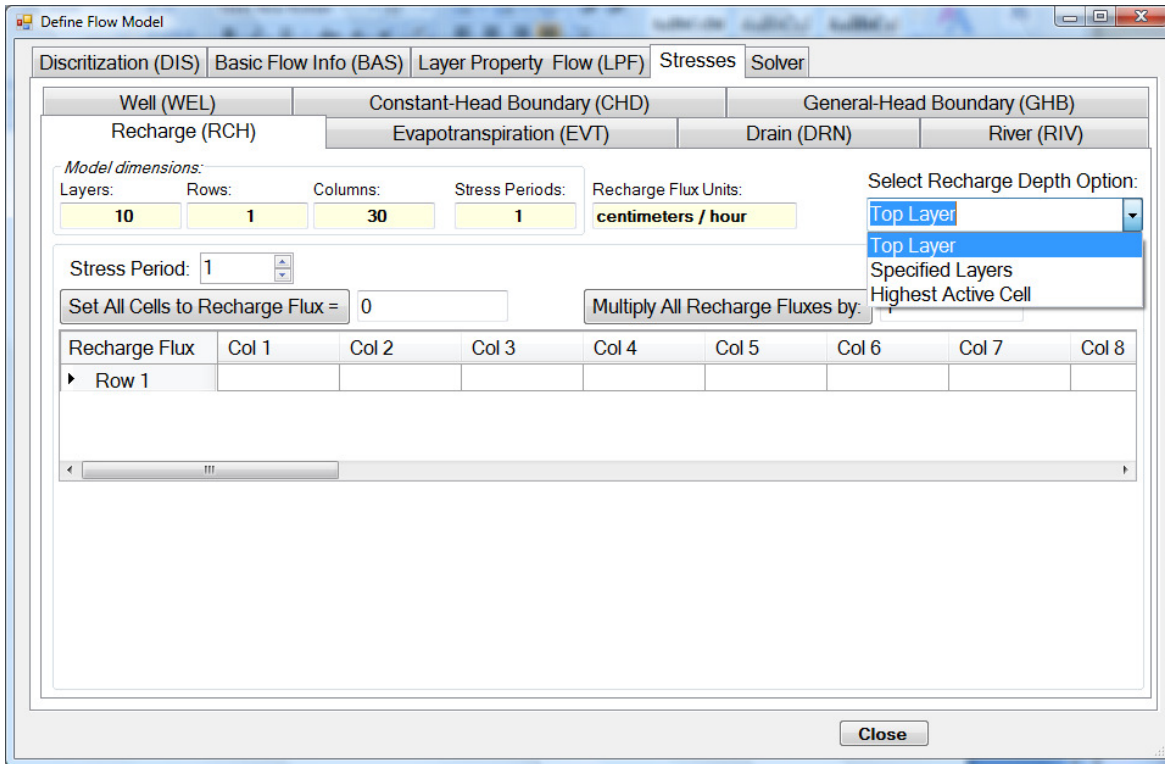
Figure 7.22: Flow Model Definition—Stresses (RCH Package) Tab

Begin by selecting the Stress Period that you want to set or edit recharge data for. Next, select a "Depth Option," to specify the vertical location to apply recharge:

- Top Layer—recharge is applied to layer 1.
- Specified Layers—recharge is applied to the layer specified in the IRCH data grid that appears (as shown in Figure 7.23) when this choice is selected.
- Automatic Selection—recharge passes vertically through no-flow cells until it reaches a variable-head cell or a constant-head cell. A constant-head cell intercepts the recharge and prevents deeper infiltration.

Recharge Flux (RECH)—enter recharge flux for every cell of the recharge layer

Recharge Layer (IRCH)—(visible and required only if Depth Option is set to Specified Layers) enter the layer number defining the layer in each vertical column where recharge is to be applied.
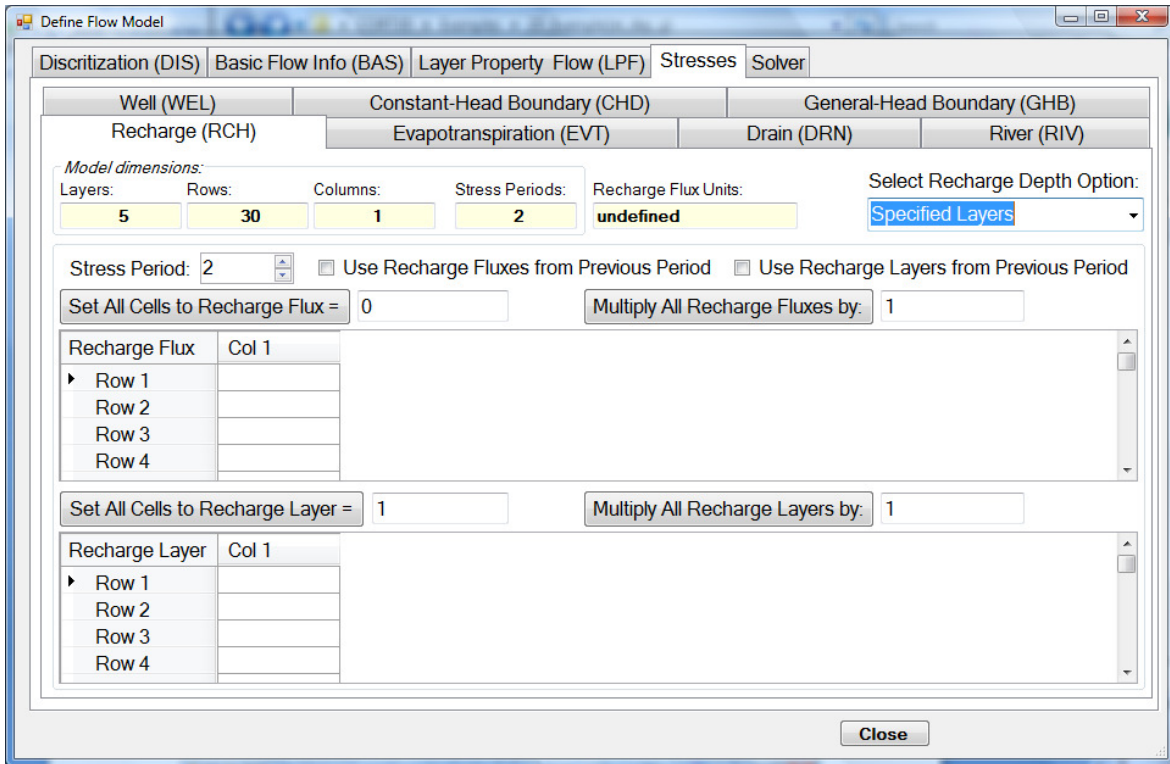
Figure 7.23: Flow Model Definition—RCH Package (Specify Recharge Layers and Stress Period > 1)

In simulations with multiple stress periods for each iteration, a check box will appear for each active recharge data entry grid when the second or higher stress period is selected (as shown in Figure 7.23). Checking a box will cause the data from the previous stress period for the respective variable to be used for the current stress period.
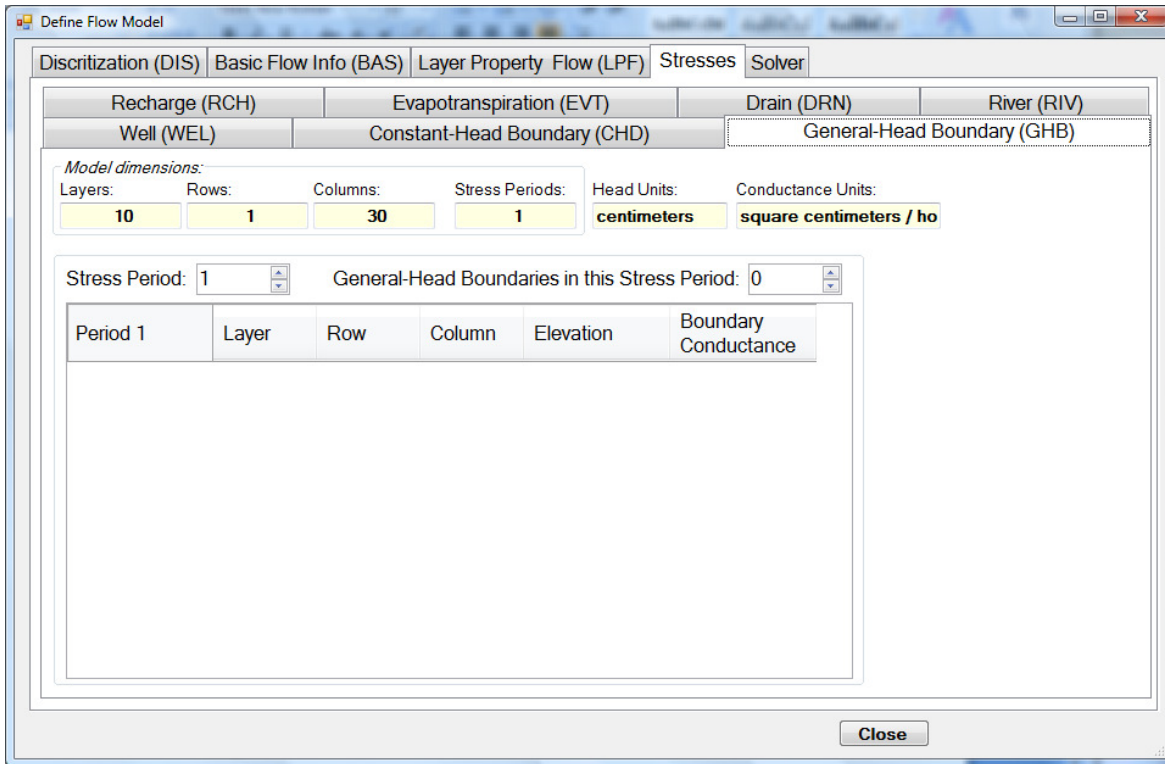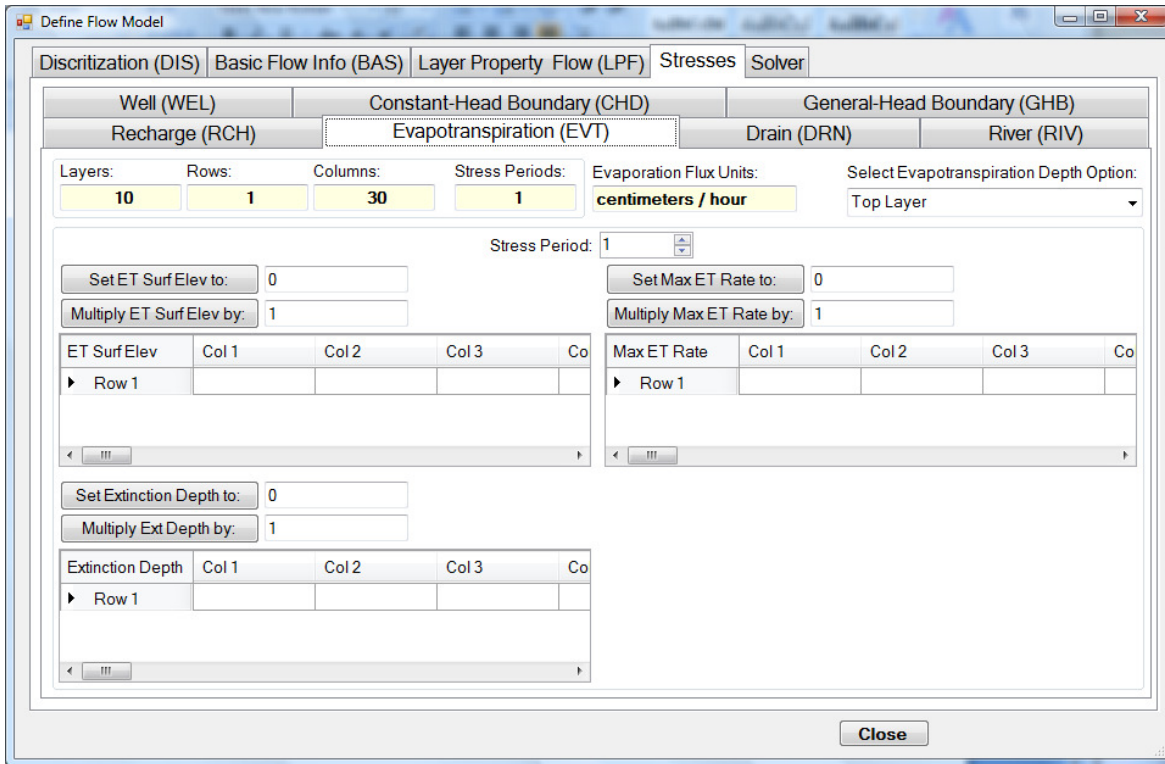
Figure 7.24: Flow Model Definition—Stresses (EVT Package) Tab

Begin by selecting the Stress Period that you want to set or edit evapotranspiration data for. Next, select a "Depth Option," to specify the vertical location to apply evapotranspiration:

- Top Layer—evapotranspiration is applied to layer 1.
- Specified Layers—evapotranspiration is applied to the layer specified in the IEVT data grid that appears (as shown in Figure 7.25) when this choice is selected.

Evapotranspiration Surface (SURF)—enter the elevation of the evapotranspiration surface.

Evapotranspiration Rate (EVTR)—enter the maximum evapotranspiration rate (volumetric flow rate per unit area) for every cell of the evapotranspiration layer in the data entry grid.

Evapotranspiration Extinction Depth (EXDP)—enter the evapotranspiration extinction depth for each vertical column.

Evapotranspiration Layer (IEVT)—(visible and required only if Depth Option is set to Specified Layers) enter the layer number defining the layer in each vertical column from which evapotranspiration is removed.
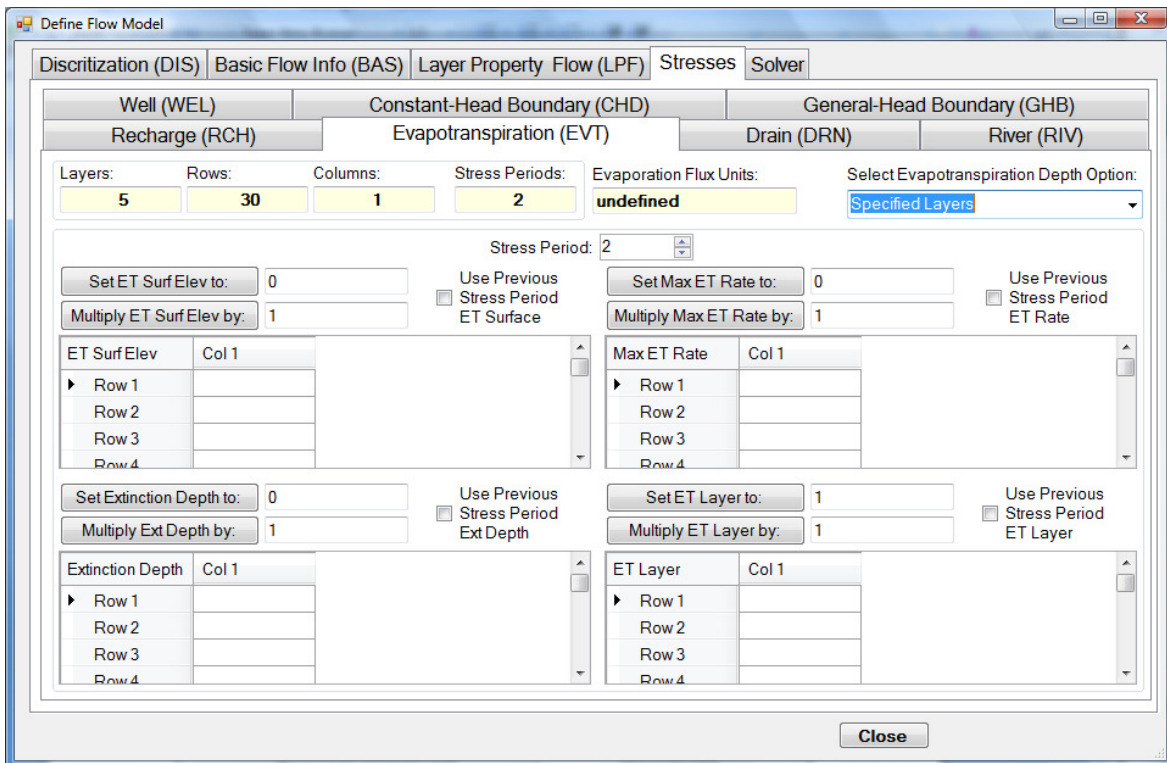
Figure 7.25: Flow Model Definition—EVT Package (Specify Recharge Layers and Stress Period > 1)

Just as with the Recharge stress input, in simulations with multiple stress periods for each iteration, a check box will appear for each active evapotranspiration data entry grid when the second or higher stress period is selected (as shown in Figure 7.25). Checking a box will cause the data from the previous stress period for the respective variable to be used for the current stress period.

Figure 7.26 shows the Solver tab, with sub-tabs for the four available solver packages. Recall that the most recent solver that you access is the one that will be activated for the simulation you are defining.
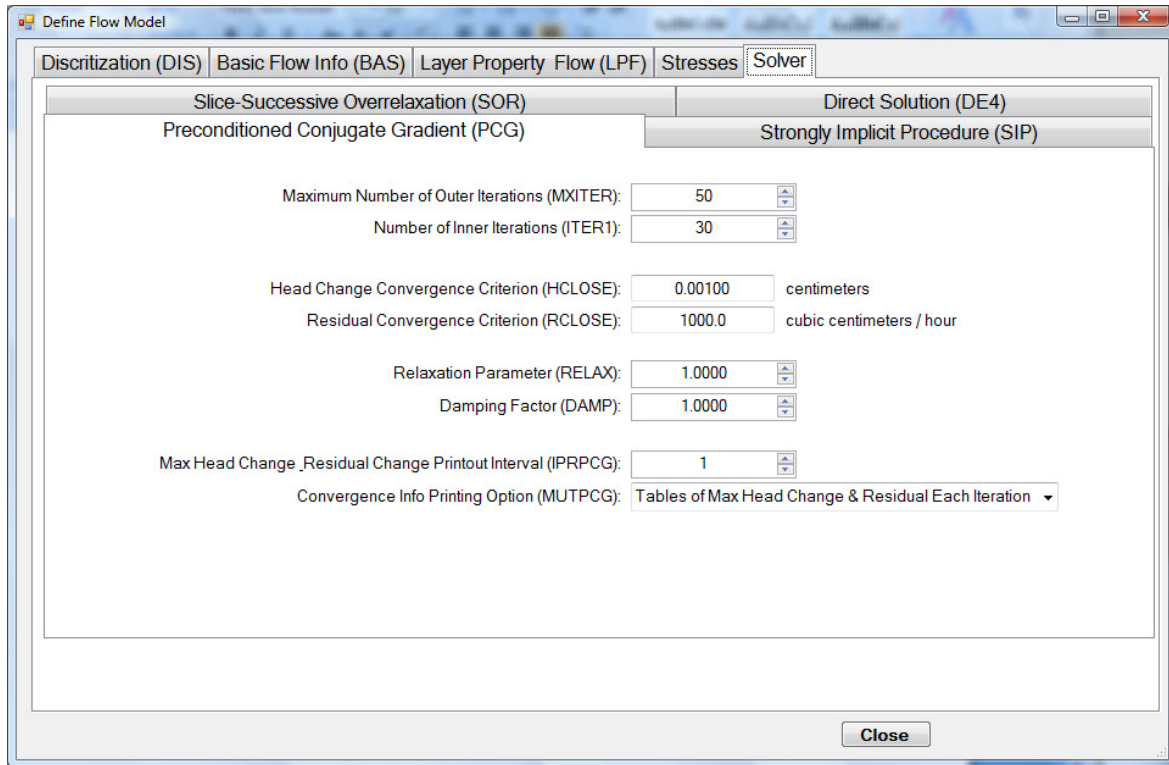
Figure 7.26: Flow Model Definition—Solver (PCG Package) Tab

MXITER is the maximum number of outer iterations (i.e., calls to the solution routine). For a linear problem MXITER should be 1, unless more than 50 inner iterations are required, when MXITER could be as large as 10. A larger number (generally less than 100) is required for a nonlinear problem.

ITER1 is the number of inner iterations. For nonlinear problems, ITER1 usually ranges from 10 to 30; a value of 30 will be sufficient for most linear problems. Note that for nonlinear problems, convergence is achieved when the convergence criteria are satisfied for the first inner iteration.

HCLOSE is the head change criterion for convergence, in units of length. When the maximum absolute value of head change from all nodes during an iteration is less than or equal to HCLOSE, and the criterion for RCLOSE is also satisfied (see below), iteration stops.

RCLOSE is the residual criterion for convergence, in units of cubic length per time. When the maximum absolute value of the residual at all nodes during an iteration is less than or equal to RCLOSE, and the criterion for HCLOSE is also satisfied (see above), iteration stops.

RELAX is the relaxation parameter. Usually, RELAX = 1.0, but for some problems a value of 0.99, 0.98, or 0.97 will reduce the number of iterations required for convergence.

DAMP is the damping factor. The damping factor typically is set equal to 1.0, which indicates no damping. A value less than 1.0 and greater than 0.0 causes damping.

IPRPCG is the printout interval for PCG. If IPRPCG is equal to 0, the variable is changed to 999. The maximum head change (positive or negative) and residual change are printed for each iteration of a time step whenever the time step is an even multiple of IPRPCG. This printout also occurs at the end of each stress period regardless of the value of IPRPCG.

MUTPCG is a flag that controls printing of solver convergence information:
- Print tables of maximum head change and residual every iteration.
- Print only the total number of iterations.
- No printing.
- Print only if convergence fails.
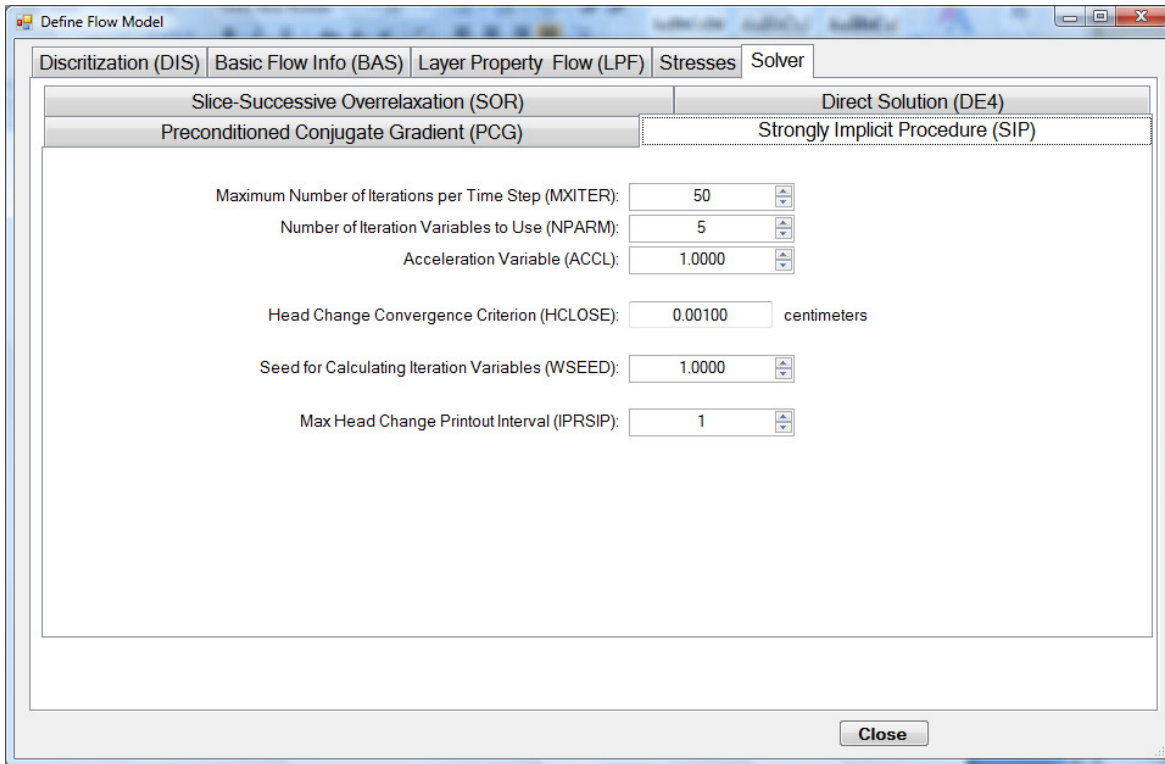
Figure 7.27: Flow Model Definition—Solver (SIP Package) Tab

MXITER is the maximum number of times through the iteration loop in one time
step in an attempt to solve the system of finite-difference equations.

NPARM is the number of iteration variables to be used. Five variables are
generally sufficient.

ACCL is the acceleration variable. The acceleration variable must be greater than
0.0 and is generally equal to 1.0.

HCLOSE is the head change criterion for convergence. When the maximum
absolute value of head change from all nodes during an iteration is less than
or equal to HCLOSE, iteration stops.

WSEED is the seed for calculating iteration variables.

IPRSIP—is the printout interval for SIP. The maximum head change (positive or negative) is printed for each iteration of a time step whenever the time step is an even multiple of IPRSIP. This printout also occurs at the end of each stress period regardless of the value of IPRSIP.
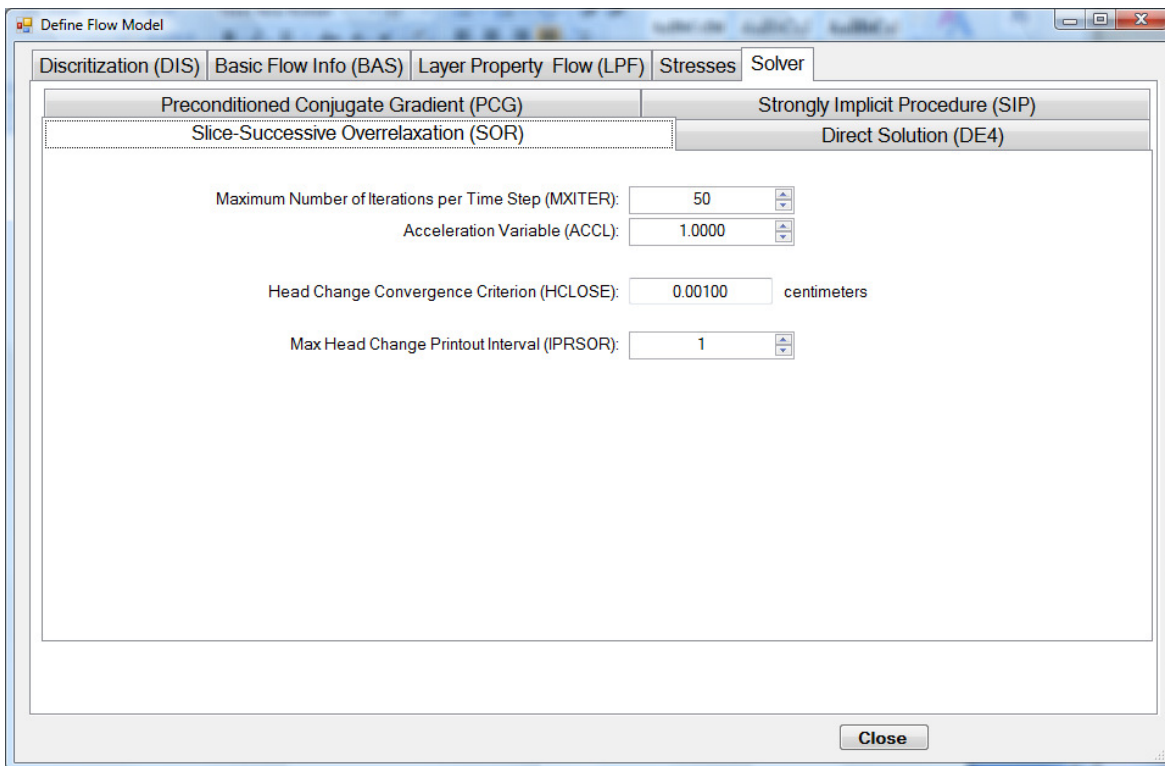
Figure 7.28: Flow Model Definition—Solver (SOR Package) Tab

MXITER is the maximum number of iterations allowed in a time step.

ACCL is the acceleration variable, usually between 1.0 and 2.0.

HCLOSE is the head change criterion for convergence. When the maximum absolute value of head change from all nodes during an iteration is less than or equal to HCLOSE, iteration stops.

IPRSOR is the printout interval for SOR. The maximum head change (positive or negative) is printed for each iteration of a time step whenever the time step is an even multiple of IPRSOR. This printout also occurs at the end of each stress period regardless of the value of IPRSOR.
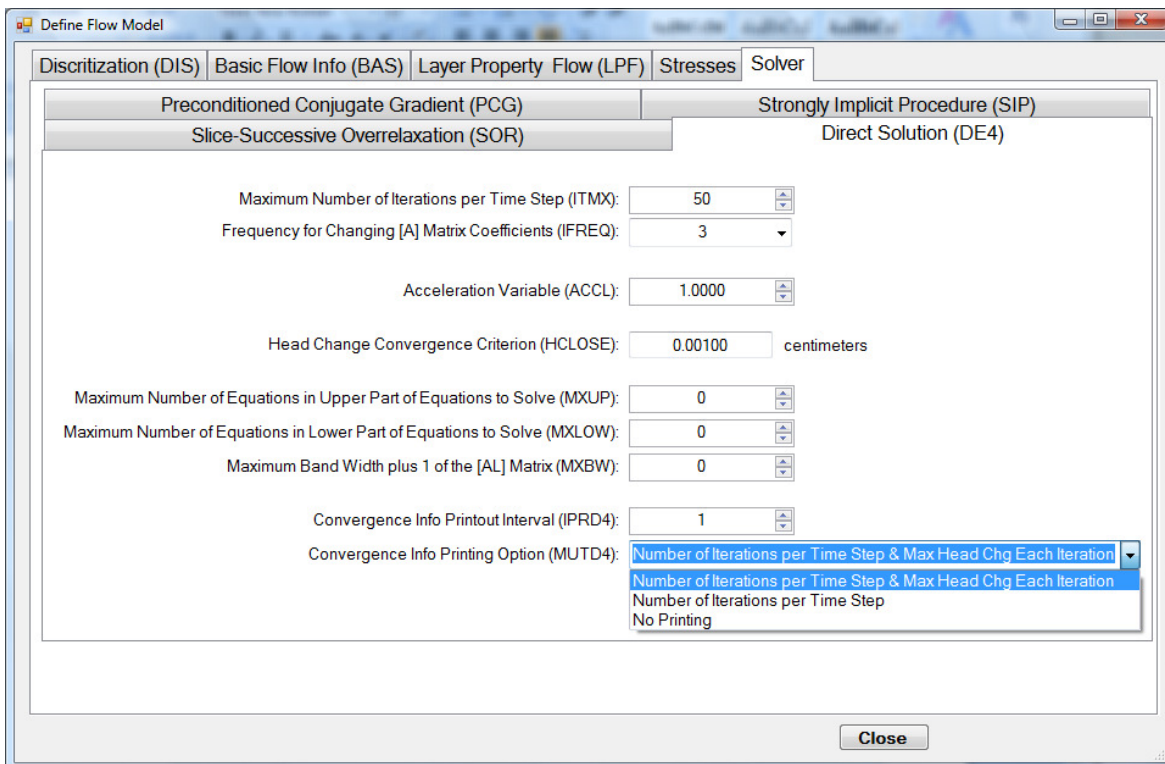
Figure 7.29: Flow Model Definition—Solver (DE4 Package) Tab

ITMX—is the maximum number of iterations for each time step. Specify ITMX = 1 if iteration is not desired. Ideally, iteration would not be required for direct solution; however, the iteration is necessary if the flow equation is nonlinear (see explanation for IFREQ = 3) or if computer precision limitations result in inaccurate calculations as indicated by a large water budget error (>1% for a 10,000-cell grid). For a nonlinear flow equation, each iteration is equally time consuming because [A] is changed at the start of each iteration and Gaussian elimination is required after each change.

Performing Gaussian elimination every iteration is called external iteration. For a linear equation, iteration is appreciably faster because [A] is changed, at most, once per time step; thus, Gaussian elimination is required, at most, once per time step. Iteration without performing Gaussian elimination every iteration is called internal iteration.

IFREQ is a flag indicating the frequency at which coefficients in [A] change. This affects the efficiency of solution; appreciable work can be avoided if [A] is known to remain constant all or part of the time.

- IFREQ = 1 indicates the flow equations are linear and that coefficients of simulated head for all stress terms are constant for all stress periods. To meet the linearity requirement, all model layers must be confined (LAYTYP in the LPF package equal to 0 for all layers), and formulations must not change based on head (such as seepage from a river changing from head dependent flow to a constant flow when head drops below the bottom of the riverbed). Examples of coefficients of simulated head for stress terms are riverbed conductance, drain conductance, maximum evapotranspiration rate, evapotranspiration extinction depth, and general-head boundary conductance.

- IFREQ = 2 indicates the flow equations are linear, but coefficients of simulated head for some stress terms may change at the start of each stress period. (See IFREQ = 1 for information about linear equations.) Examples of coefficients of simulated head for stress terms are riverbed conductance, drain conductance, maximum evapotranspiration rate, evapotranspiration extinction depth, and general-head boundary conductance. For simulations consisting of only one stress period, IFREQ = 2 has the same meaning as IFREQ = 1.

- IFREQ = 3 indicates that a nonlinear flow equation is being solved, which means that some terms in [A] depend on simulated head. Examples of head-dependent terms in [A] are transmissivity for water-table layers, where transmissivity is based on saturated thickness; flow

terms for rivers, drains, and evapotranspiration if they convert between head dependent flow and constant flow; and the change in storage coefficient when a cell converts between confined and unconfined. When a nonlinear flow equation is being solved, external iteration (ITMX > 1) normally is required to accurately approximate the nonlinearities. Note that when nonlinearities caused by water-table calculations are part of a simulation, obvious signs are not necessarily produced in the output from a simulation that does not use external iteration to indicate that iteration is needed. In particular, the budget error may be acceptably small without iteration even though appreciable error exists in head because of nonlinearity. To understand this, consider the water-table correction for transmissivity. Each iteration a new transmissivity is calculated based on the previous head. Then the flow equations are solved, and a budget is computed using the new head with the same transmissivities. No appreciable budget discrepancy results because heads are correct for the transmissivity being used at this point; however, the new heads may mean that an appreciable change in transmissivity has occurred. The new transmissivity will not be calculated unless there is another iteration. Therefore, when one or more layers are under water-table conditions, iteration always should be tried. The maximum change in head in each iteration (printed by DE4 when IPRD4 = 1 and MUTD4 = 0) provides an indication of the effect of all nonlinearities.

ACCL is a multiplier for the computed head change for each iteration. Normally, this value is 1, and should always be one for linear problems. A value greater than 1 may be useful for improving the rate of convergence when using external iteration to solve nonlinear problems (IFREQ = 3). When ITMX = 1, ACCL is changed to 1 regardless of the input value.

HCLOSE is the head change closure criterion. If iterating (ITMX > 1), iteration stops when the absolute value of head change at every node is less than or equal to HCLOSE. Though HCLOSE must be specified, it is not used if not iterating.

MXUP is the maximum number of equations in the upper part of the equations to be solved. This value affects the amount of memory used by the DE4 Package. If specified as 0, the program will calculate MXUP as half the number of cells in the model, which is an upper limit. The actual number of equations in the upper part will be less than half the number of cells whenever no-flow and constant-head cells exist because flow equations are not formulated for these cells. The actual number of equations in the upper part is printed when the DE4 Package runs. The printed value can be used for MXUP in future runs to minimize memory usage.

MXLOW is the maximum number of equations in the lower part of equations to be solved. This value affects the amount of memory used by the DE4 Package. If specified as 0, the program will calculate MXLOW as half the number of cells in the model, which is an upper limit. The actual number of equations in the lower part will be less than half the number of cells whenever no-flow and constant-head cells exist because flow equations are not formulated for these cells. The actual number of equations in the lower part is printed when the DE4 Package runs. The printed value can be used for MXLOW in future runs to minimize memory usage.

MXBW is the maximum band width plus 1 of the [AL] matrix. This value affects the amount of memory used by the DE4 Package. If specified as 0, the program will calculate MXBW as the product of the two smallest grid dimensions plus 1, which is an upper limit. The actual band width plus 1 is printed when the DE4 Package runs. The printed value can be used for MXBW in future runs to minimize memory usage.

IPRD4 is the time-step interval for printing out convergence information when iterating (ITMX > 1). For example, if IPRD4 is 2, convergence information is printed every other time step. A value is required, even if not iterating.

MUTD4 is a flag that indicates the quantity of information that is printed when convergence information is printed for a time step.
- Number of iterations in the time step and the maximum head change are printed after each iteration.
- Number of iterations in the time step is printed.
- No information is printed.

7.2.5 Defining Transport Model

From the Main screen, clicking on the "Define Transport Model" button will bring up the Transport Model screen shown in Figure 7.30. Just as with the Flow Model screen, there are a number of tabs where data for the transport model input files are entered. The first tab is the Basic Transport tab (corresponding to the Transport Model BTN package).
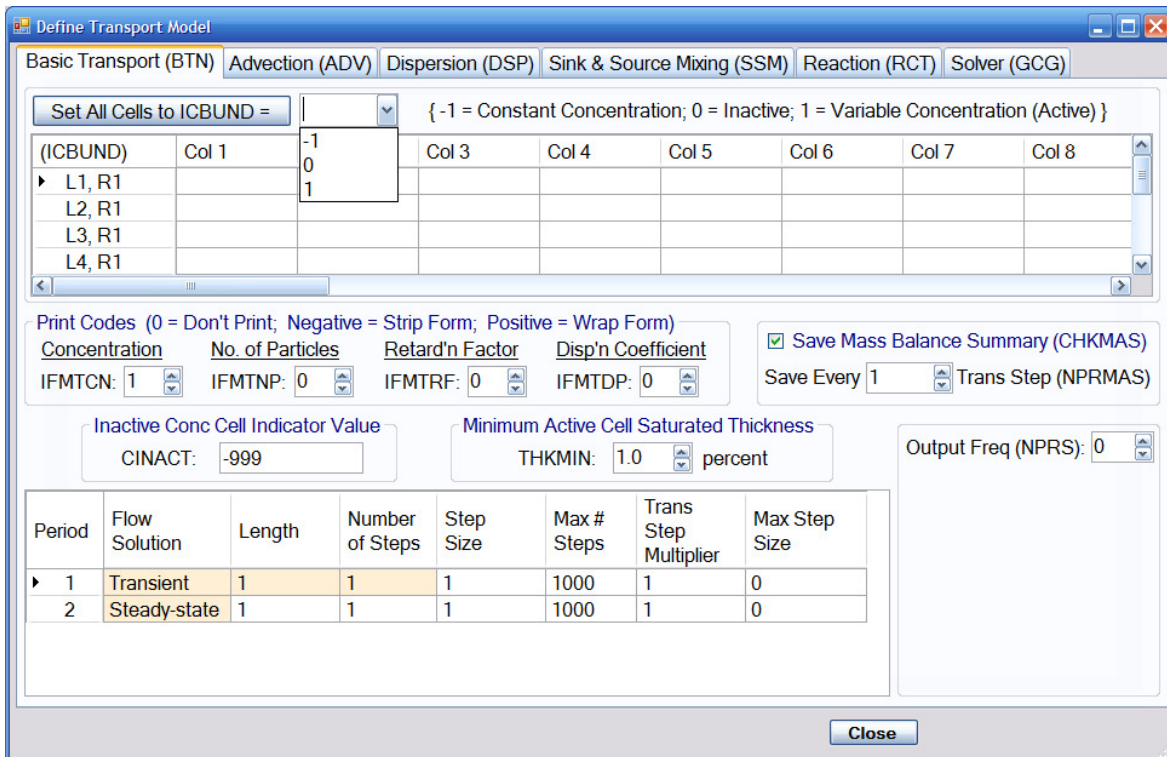
Figure 7.30: Transport Model Definition—Basic Transport (BTN Package) Tab

ICBUND is the boundary condition type. One value is read for every model cell. An ICBUND value of -1 means the cell has a constant concentration. A value of 0 means the cell is inactive. A value of 1 means the cell is active (the concentration can change). For multispecies simulation, ICBUND defines the boundary condition type shared by all species. Note that different species are allowed to have different constant-concentration conditions through an option in the Source and Sink Mixing Package.

IFMTCN is a flag indicating whether the calculated concentration should be printed to the standard output text file and also serves as a printing-format code if it is printed. The codes for print-formats are listed in Table 7.2.

- > 0, concentration is printed in the wrap form
- < 0, concentration is printed in the strip form
- = 0, concentration is not printed.

IFMTNP is a flag indicating whether the number of particles in each cell (integers) should be printed and also serves as a printing-format code if they are printed. The convention is the same as that used for IFMTCN.

IFMTRF is a flag indicating whether the model-calculated retardation factor should be printed and also serves as a printing-format code if it is printed. The convention is the same as that used for IFMTCN.

IFMTDP is a flag indicating whether the model-calculated, distance-weighted dispersion coefficient should be printed and also serves as a printing-format code if it is printed. The convention is the same as that used for IFMTCN.

Table 7.2: Printing Formats

Format Number	Real Numbers	Integers
1	11 G10.3	60 I1
2	9G 13.6	40 I2
3	15 F7.1	30 I3
4	15 F7.2	25 I4
5	15 F7.3	20 I5
6	15 F7.4	
7	20 F5.0	
8	20 F5.1	
9	20 F5.2	
10	20 F5.3	
11	20 F5.4	
12	10 G11.4	

NPRS is a flag indicating the frequency of output and also indicating whether the output frequency is specified in terms of total elapsed simulation time or the transport step number. Note: what is actually printed or saved is controlled by the values entered for IFMTCN, IFMTNP, IFMTRF, and IFMTDP.

- < 0, simulation results will be printed or saved whenever the number of transport steps is an even multiple of NPRS.
- = 0, simulation results will not be printed or saved except at the end of simulation.
- > 0, simulation results will be printed to the standard output text file or saved to the unformatted concentration file at times as specified in TIMPRS.

TIMPRS contains the total elapsed time(s) at which the simulation results are printed to the standard output text file or saved in the default unformatted (binary) concentration file. The number of TIMPRS entries is determined by the NPRS entry as shown in Figure 7.31.

CHKMAS is a logical flag indicating whether a one-line summary of mass balance information should be printed, for checking and post-processing purposes, in the file SIMNAMEnnn.MAS where SIMNAME is the name you gave the simulation and nnn is the species index number. If checked, mass balance information will be saved according to the frequency specified in NPRMAS. Otherwise, the mass balance summary file will not be saved (and the NPRMAS entry will not be visible as seen in Figure 7.31).

NPRMAS specifies how frequently the mass balance information should be saved in the mass balance summary file (if Mass Balance Summary is enabled). Mass balance information is saved every NPRMAS step.
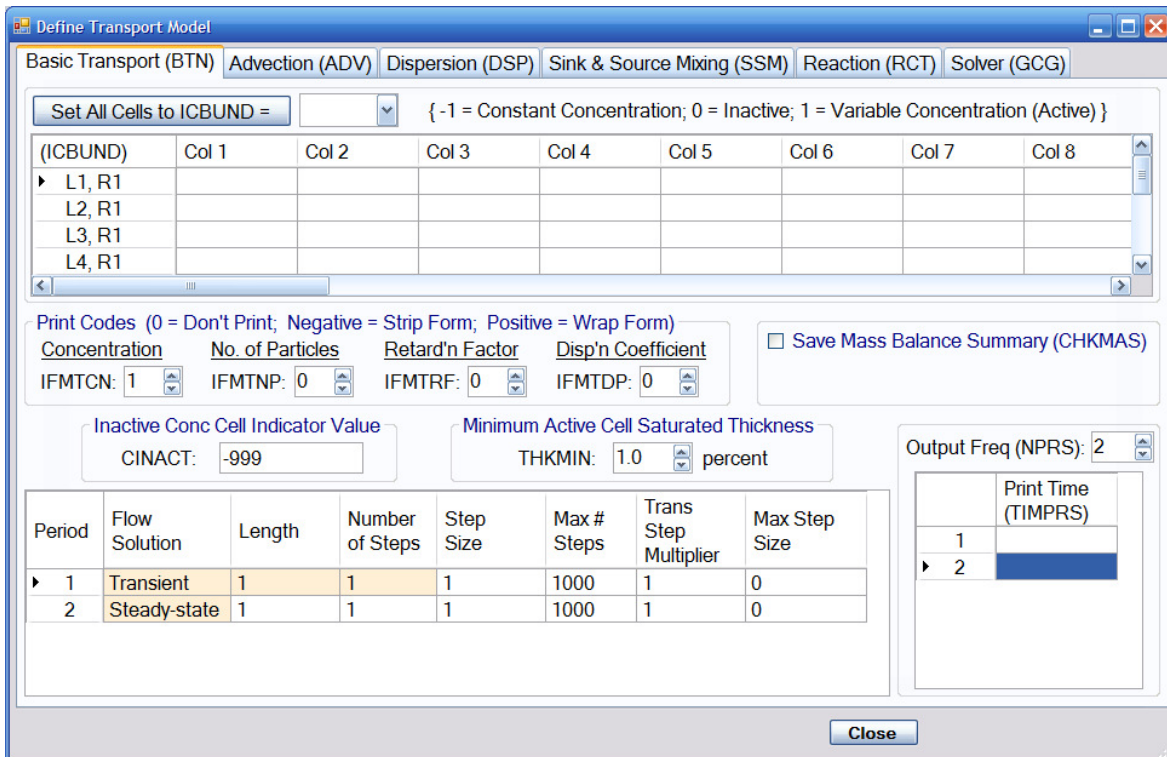
Figure 7.31: Transport Model Definition—BTN Package (CHKMAS & NPRS Details)

CINACT is the value for indicating an inactive concentration cell (ICBUND = 0). Even if inactive cells are not anticipated in the model, a value for CINACT is required.

THKMIN is the minimum saturated thickness in a cell, expressed as the percentage of the model layer thickness (DZ) below which the cell is considered inactive.

Stress Periods:

If flow model Stress Period information has not been defined (on the DIS tab of the Flow Model screen), the following parameters will not be available for entry on this screen. The flow model Stress Period information must be defined before the transport model-specific Stress Period information can be entered.

Flow Solution identifies the type of solution (transient or steady-state) assigned to the stress period in the flow model. This value is for reference only and is read-only. To change the stress period between transient or steady-state, return to the Flow Model Screen and update the Stress Period information on the DIS tab accordingly.

Length (PERLEN) is the length of the stress period. If the flow solution is transient, PERLEN will be equal to the length specified in the flow model, will be shaded orange and be read-only so it cannot be changed. If the flow solution is steady-state, PERLEN can be set to any desired length.

Number of Steps (NSTP) is the number of time-steps. If the flow solution is transient, NSTP will be equal to the number of steps specified in the flow model, will be shaded orange and be read-only so it cannot be changed. If the flow solution is steady-state, NSTP can be set to any value.

Step Size (DT0) is the user-specified transport step size within each time-step of the flow solution. DT0 is interpreted differently depending on whether the solution option chosen is explicit or implicit:

- For explicit solutions (i.e., the GCG solver is not used), the program calculates a maximum transport step size which meets the various stability criteria. Setting DT0 to zero causes the model-calculated transport step size to be used in the simulation. However, the model-calculated DT0 may not always be optimal. In this situation, DT0 should be adjusted to find a value that leads to the best results. If DT0 is greater than the model-calculated step size, the model-calculated step size will be used in the simulation.

- For implicit solutions (i.e., the GCG solver is used), DT0 is the initial transport step size. If it is set to zero, the model-calculated value of DT0, based on the user-specified Courant number in the Advection Package, will be used. The subsequent transport step size may increase

or remain constant depending on the user-specified transport step size multiplier TTSMULT and the solution scheme for the advection term.

Max # Steps (MXSTRN) is the maximum number of transport steps allowed within one time step of the flow solution. If the number of transport steps within a flow time-step exceeds MXSTRN, the simulation is terminated.

Trans Step Multiplier (TTSMULT) is the multiplier for successive transport steps within a flow time-step if the GCG solver is used and the solution option for the advection term is the standard finite-difference method. A value between 1.0 and 2.0 is generally adequate. If the GCG package is not used, the transport solution is solved explicitly as in the original MT3D code, and TTSMULT is set to 1.0 regardless of the user-specified input. Note that for the particle-tracking-based solution options (MOC, MMOC, and HMOC) and the third-order TVD scheme, TTSMULT does not apply.

Max Step Size (TTSMAX) is the maximum transport step size allowed when transport step size multiplier TTSMULT > 1.0. Setting TTSMAX=0 imposes no maximum limit.

Figure 7.32 displays the Advection tab (corresponding to the Transport Model ADV package).
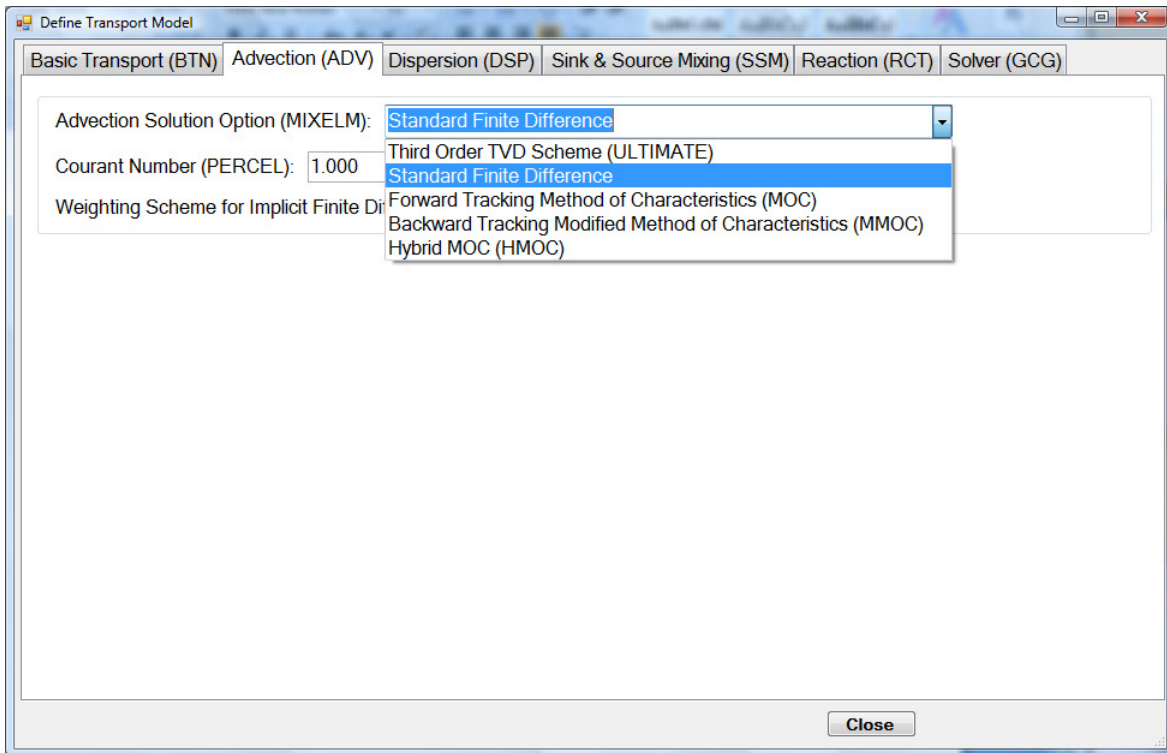
Figure 7.32: Transport Model Definition—Advection (ADV Package) Tab

The first step, here, is to select the desired solution option (MIXELM) from the five choices. Depending upon your choice of solver, different parameters will be displayed for entry/edit. Depending upon which solver is selected for MIXELM, refer to the appropriate Figure and corresponding description from the following list:

- Standard Finite Difference solver - Figure 7.33
- Forward Tracking Method of Characteristics (MOC) - Figure 7.34
- Backward Tracking Modified Method of Characteristics (MMOC) - Figure 7.35
- Hybrid Method of Characteristics (HMOC) - Figure 7.36
- Third-Order TVD Scheme (ULTIMATE) - Figure 7.37
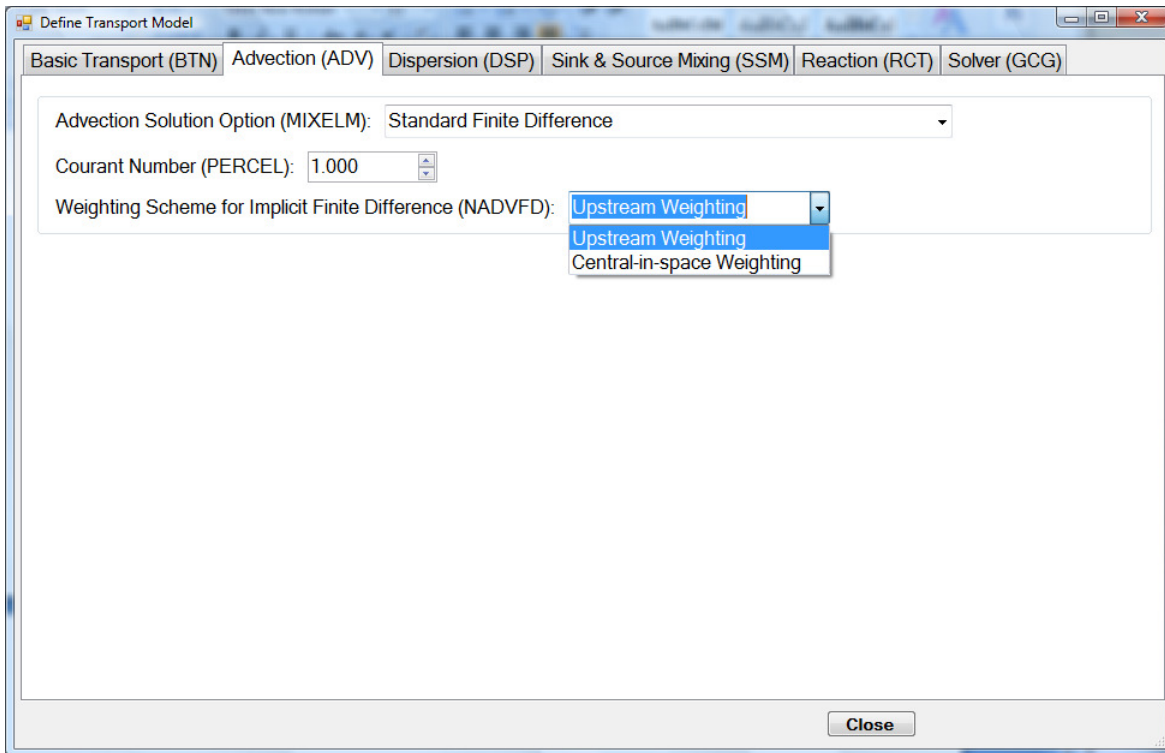
Figure 7.33: Transport Model Definition—ADV Package (Standard Finite Difference Solver)

PERCEL is the Courant number (i.e., the number of cells, or a fraction of a cell) advection will be allowed in any direction in one transport step. For implicit finite-difference or particle-tracking-based schemes, there is no limit on PERCEL, but for accuracy reasons, it is generally not set much greater than one. Note, however, that the PERCEL limit is checked over the entire model grid. Thus, even if PERCEL > 1, advection may not be more than one cell's length at most model locations. For the explicit finite-difference or the third-order TVD scheme, PERCEL is also a stability constraint which must not exceed one and will be automatically reset to one if a value greater than one is specified.

NADVFD is a flag indicating type of weighting to use for implicit solution scheme.

- Upstream weighting
- Central-in-space weighting

Figure 7.34: Transport Model Definition—ADV Package (Forward Tracking Method of Characteristics {MOC} Solver)

PERCEL is the Courant number (i.e., the number of cells, or a fraction of a cell) advection will be allowed in any direction in one transport step. For implicit finite-difference or particle-tracking-based schemes, there is no limit on PERCEL, but for accuracy reasons, it is generally not set much greater than one. Note, however, that the PERCEL limit is checked over the entire model grid. Thus, even if PERCEL > 1, advection may not be more than one cell's length at most model locations. For the explicit finite-difference or the third-order TVD scheme, PERCEL is also a stability constraint which must not exceed one and will be automatically reset to one if a value greater than one is specified.

MXPART is the maximum total number of moving particles allowed.

ITRACK is a flag indicating which particle-tracking algorithm to use for the Eulerian-Lagrangian methods.

- First-order Euler algorithm.
- Fourth-order Runge-Kutta algorithm; this option is computationally demanding and may be needed only when PERCEL is set >1.
- Hybrid first- and fourth-order algorithm is used; the Runge-Kutta algorithm is used in sink/source cells and the cells next to sinks/sources while the Euler algorithm is used elsewhere.

WD is a concentration weighting factor between 0.5 and 1. It is used for operator splitting in the particle-tracking-based methods. The value of 0.5 is generally adequate. The value of WD may be adjusted to achieve better mass balance. Generally, it can be increased toward 1.0 as advection becomes more dominant.

DCEPS is a small Relative Cell Concentration Gradient below which advective transport is considered negligible. A value around 10^{-5} is generally adequate.

NPLANE is a flag indicating whether the random or fixed pattern is selected for initial placement of moving particles.

- = 0, the random pattern is selected for initial placement. Particles are distributed randomly in both the horizontal and vertical directions by calling a random number generator (Refer to MT3DMS Manual for figure). This option is usually preferred and leads to smaller mass balance discrepancy in non-uniform or diverging/converging flow fields.
- > 0, the fixed pattern is selected for initial placement. The value of NPLANE serves as the number of vertical "planes" on which initial particles are placed within each cell block (Refer to MT3DMS Manual for figure). The fixed pattern may work better than the random pattern

only in relatively uniform flow fields. For 2-D simulations in plan view, set NPLANE = 1. For cross sectional or 3-D simulations, NPLANE = 2 is normally adequate. Increase NPLANE if more resolution in the vertical direction is desired.

NPL is the number of initial particles per cell to be placed at cells where the relative Cell Concentration Gradient is less than or equal to DCEPS. Generally, NPL can be set to zero since advection is considered insignificant when the Relative Cell Concentration Gradient is less than or equal to DCEPS. Setting NPL equal to NPH causes a uniform number of particles to be placed in every cell over the entire grid (i.e., the uniform approach).

NPH is the number of initial particles per cell to be placed at cells where the Relative Cell Concentration Gradient is greater than DCEPS. The selection of NPH depends on the nature of the flow field and also the computer memory limitation. Generally, a smaller number should be used in relatively uniform flow fields and a larger number should be used in relatively non-uniform flow fields. However, values exceeding 16 in 2-D simulation or 32 in 3-D simulation are rarely necessary. If the random pattern is chosen, NPH particles are randomly distributed within the cell block. If the fixed pattern is chosen, NPH is divided by NPLANE and then rounded to 1, 4, 5, 8, 9, or 16 to yield the number of particles to be placed per vertical plane.

NPMIN is the minimum number of particles allowed per cell. If the number of particles in a cell at the end of a transport step is fewer than NPMIN, new particles are inserted into that cell to maintain a sufficient number of particles. NPMIN can be set to zero in relatively uniform flow fields and to a number greater than zero in diverging/converging flow fields. Generally, a value between 0 and 4 is adequate.

NPMAX is the maximum number of particles allowed per cell. If the number of particles in a cell exceeds NPMAX, all particles are removed from that cell and replaced by a new set of particles equal to NPH to maintain mass balance. Generally, NPMAX can be set to approximately two times the value of NPH.
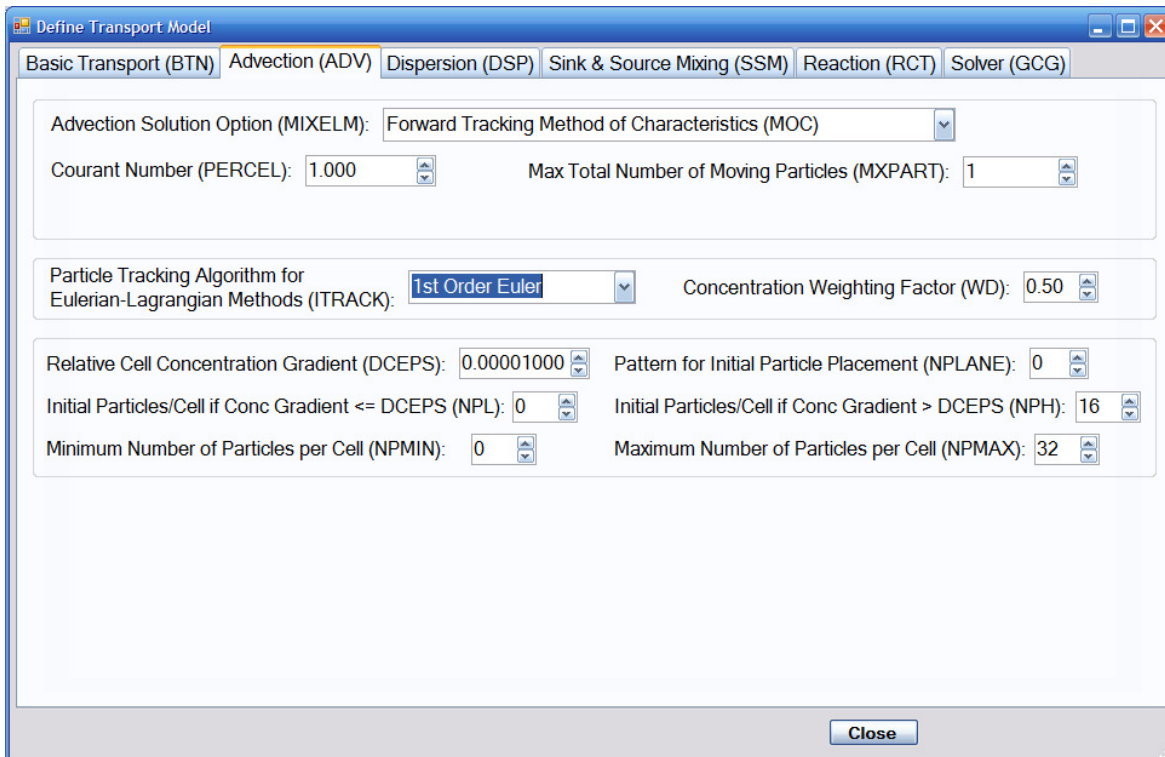

Figure 7.35: Transport Model Definition—ADV Package (Backward Tracking Modified Method of Characteristics {MMOC} Solver)

PERCEL is the Courant number (i.e., the number of cells, or a fraction of a cell) advection will be allowed in any direction in one transport step. For implicit finite-difference or particle-tracking-based schemes, there is no limit on PERCEL, but for accuracy reasons, it is generally not set much greater than one. Note, however, that the PERCEL limit is checked over the entire model grid. Thus, even if PERCEL > 1, advection may not be more than one cell's length at most model locations. For the explicit finite-difference or the third-order TVD scheme, PERCEL is also a stability constraint which

must not exceed one and will be automatically reset to one if a value greater than one is specified.

ITRACK is a flag indicating which particle-tracking algorithm to use for the Eulerian-Lagrangian methods.
- First-order Euler algorithm.
- Fourth-order Runge-Kutta algorithm; this option is computationally demanding and may be needed only when PERCEL is set >1.
- Hybrid first- and fourth-order algorithm is used; the Runge-Kutta algorithm is used in sink/source cells and the cells next to sinks/sources while the Euler algorithm is used elsewhere.

WD is a concentration weighting factor between 0.5 and 1. It is used for operator splitting in the particle-tracking-based methods. The value of 0.5 is generally adequate. The value of WD may be adjusted to achieve better mass balance. Generally, it can be increased toward 1.0 as advection becomes more dominant.

NLSINK is a flag indicating whether the random or fixed pattern is selected for initial placement of particles to approximate sink cells in the MMOC scheme.
- = 0, the random pattern is selected for initial placement. Particles are distributed randomly in both the horizontal and vertical directions by calling a random number generator (Refer to MT3DMS Manual for figure). This option is usually preferred and leads to smaller mass balance discrepancy in non-uniform or diverging/converging flow fields.
- > 0, the fixed pattern is selected for initial placement. The value of NLSINK serves as the number of vertical "planes" on which initial particles are placed within each cell block (Refer to MT3DMS Manual for figure). The fixed pattern may work better than the random pattern

only in relatively uniform flow fields. For 2-D simulations in plan view, set NLSINK = 1. For cross sectional or 3-D simulations, NLSINK = 2 is normally adequate. Increase NLSINK if more resolution in the vertical direction is desired.

NPSINK is the number of particles used to approximate sink cells in the MMOC scheme. The selection of NPSINK depends on the nature of the flow field and also the computer memory limitation. Generally, a smaller number should be used in relatively uniform flow fields and a larger number should be used in relatively non-uniform flow fields. However, values exceeding 16 in 2-D simulation or 32 in 3-D simulation are rarely necessary. If the random pattern is chosen, NPSINK particles are randomly distributed within the cell block. If the fixed pattern is chosen, NPSINK is divided by NLSINK and then rounded to 1, 4, 5, 8, 9, or 16 to yield the number of particles to be placed per vertical plane.
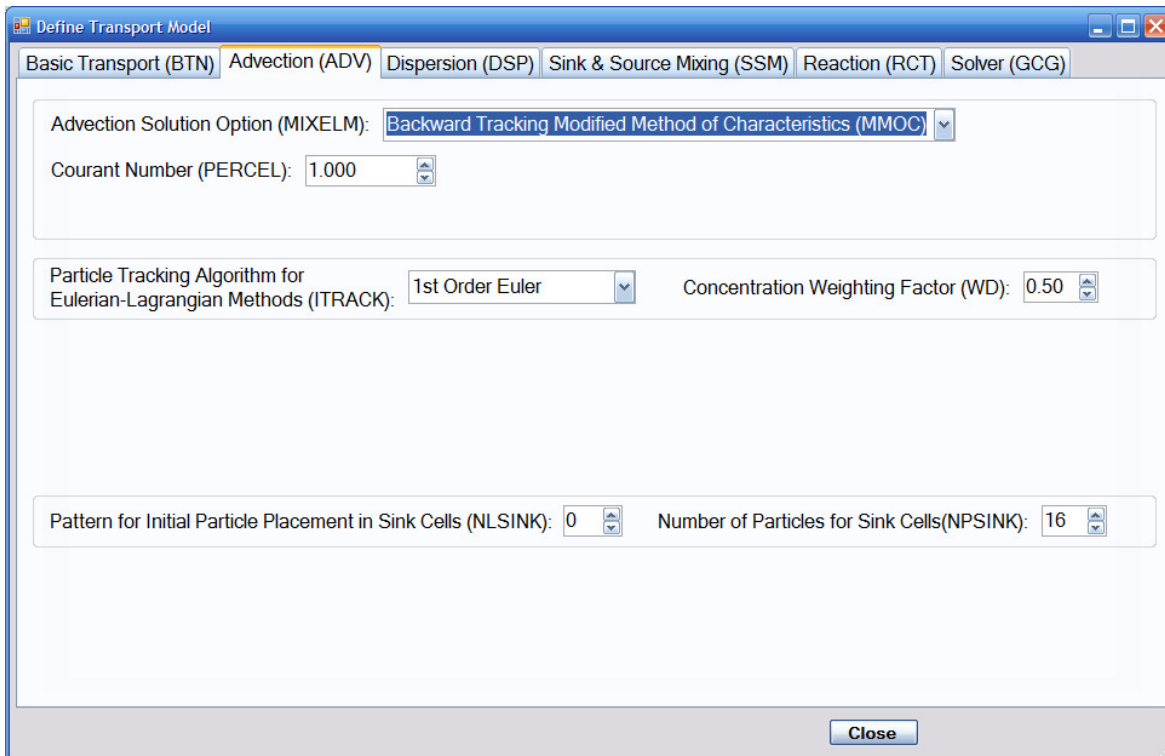
Figure 7.36: Transport Model Definition—ADV Package (Hybrid Method of Characteristics {HMOC} Solver)

PERCEL is the Courant number (i.e., the number of cells, or a fraction of a cell) advection will be allowed in any direction in one transport step. For implicit finite-difference or particle-tracking-based schemes, there is no limit on PERCEL, but for accuracy reasons, it is generally not set much greater than one. Note, however, that the PERCEL limit is checked over the entire model grid. Thus, even if PERCEL > 1, advection may not be more than one cell's length at most model locations. For the explicit finite-difference or the third-order TVD scheme, PERCEL is also a stability constraint which must not exceed one and will be automatically reset to one if a value greater than one is specified.

MXPART is the maximum total number of moving particles allowed.

ITRACK is a flag indicating which particle-tracking algorithm to use for the Eulerian-Lagrangian methods.

- First-order Euler algorithm.
- Fourth-order Runge-Kutta algorithm; this option is computationally demanding and may be needed only when PERCEL is set >1.
- Hybrid first- and fourth-order algorithm is used; the Runge-Kutta algorithm is used in sink/source cells and the cells next to sinks/sources while the Euler algorithm is used elsewhere.

WD is a concentration weighting factor between 0.5 and 1. It is used for operator splitting in the particle-tracking-based methods. The value of 0.5 is generally adequate. The value of WD may be adjusted to achieve better mass balance. Generally, it can be increased toward 1.0 as advection becomes more dominant.

DCEPS is a small Relative Cell Concentration Gradient below which advective transport is considered negligible. A value around 10^{-5} is generally adequate.

NPLANE is a flag indicating whether the random or fixed pattern is selected for initial placement of moving particles.

- = 0, the random pattern is selected for initial placement. Particles are distributed randomly in both the horizontal and vertical directions by calling a random number generator (Refer to MT3DMS Manual for figure). This option is usually preferred and leads to smaller mass balance discrepancy in non-uniform or diverging/converging flow fields.
- > 0, the fixed pattern is selected for initial placement. The value of NPLANE serves as the number of vertical "planes" on which initial particles are placed within each cell block (Refer to MT3DMS Manual for figure). The fixed pattern may work better than the random pattern

only in relatively uniform flow fields. For 2-D simulations in plan view, set NPLANE = 1. For cross sectional or 3-D simulations, NPLANE = 2 is normally adequate. Increase NPLANE if more resolution in the vertical direction is desired.

NPL is the number of initial particles per cell to be placed at cells where the relative Cell Concentration Gradient is less than or equal to DCEPS. Generally, NPL can be set to zero since advection is considered insignificant when the Relative Cell Concentration Gradient is less than or equal to DCEPS. Setting NPL equal to NPH causes a uniform number of particles to be placed in every cell over the entire grid (i.e., the uniform approach).

NPH is the number of initial particles per cell to be placed at cells where the Relative Cell Concentration Gradient is greater than DCEPS. The selection of NPH depends on the nature of the flow field and also the computer memory limitation. Generally, a smaller number should be used in relatively uniform flow fields and a larger number should be used in relatively non-uniform flow fields. However, values exceeding 16 in 2-D simulation or 32 in 3-D simulation are rarely necessary. If the random pattern is chosen, NPH particles are randomly distributed within the cell block. If the fixed pattern is chosen, NPH is divided by NPLANE and then rounded to 1, 4, 5, 8, 9, or 16 to yield the number of particles to be placed per vertical plane.
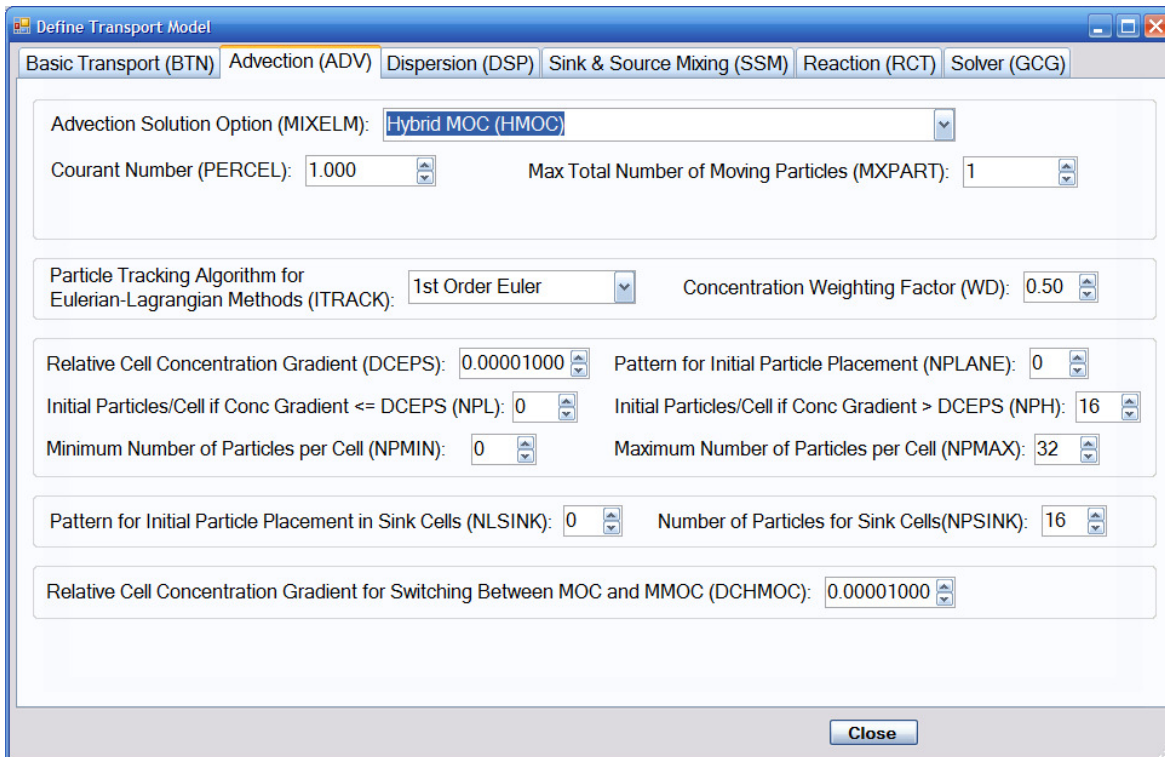
NPMIN is the minimum number of particles allowed per cell. If the number of particles in a cell at the end of a transport step is fewer than NPMIN, new particles are inserted into that cell to maintain a sufficient number of particles. NPMIN can be set to zero in relatively uniform flow fields and to a number greater than zero in diverging/converging flow fields. Generally, a value between 0 and 4 is adequate.

NPMAX is the maximum number of particles allowed per cell. If the number of particles in a cell exceeds NPMAX, all particles are removed from that cell and replaced by a new set of particles equal to NPH to maintain mass balance. Generally, NPMAX can be set to approximately two times the value of NPH.

NLSINK is a flag indicating whether the random or fixed pattern is selected for initial placement of particles to approximate sink cells in the MMOC scheme.
- = 0, the random pattern is selected for initial placement. Particles are distributed randomly in both the horizontal and vertical directions by calling a random number generator (Refer to MT3DMS Manual for figure). This option is usually preferred and leads to smaller mass balance discrepancy in non-uniform or diverging/converging flow fields.
- > 0, the fixed pattern is selected for initial placement. The value of NLSINK serves as the number of vertical "planes" on which initial particles are placed within each cell block (Refer to MT3DMS Manual for figure). The fixed pattern may work better than the random pattern only in relatively uniform flow fields. For 2-D simulations in plan view, set NLSINK = 1. For cross sectional or 3-D simulations, NLSINK = 2 is normally adequate. Increase NLSINK if more resolution in the vertical direction is desired.

NPSINK is the number of particles used to approximate sink cells in the MMOC scheme. The selection of NPSINK depends on the nature of the flow field and also the computer memory limitation. Generally, a smaller number should be used in relatively uniform flow fields and a larger number should be used in relatively non-uniform flow fields. However, values exceeding 16 in 2-D simulation or 32 in 3-D simulation are rarely necessary. If the random pattern is chosen, NPSINK particles are randomly distributed

within the cell block. If the fixed pattern is chosen, NPSINK is divided by NLSINK and then rounded to 1, 4, 5, 8, 9, or 16 to yield the number of particles to be placed per vertical plane.

DCHMOC is the critical Relative Concentration Gradient for controlling the selective use of either MOC or MMOC in the HMOC solution scheme. The MOC solution is selected at cells where the Relative Concentration Gradient is greater than DCHMOC. The MMOC solution is selected at cells where the Relative Concentration Gradient is less than or equal to DCHMOC.
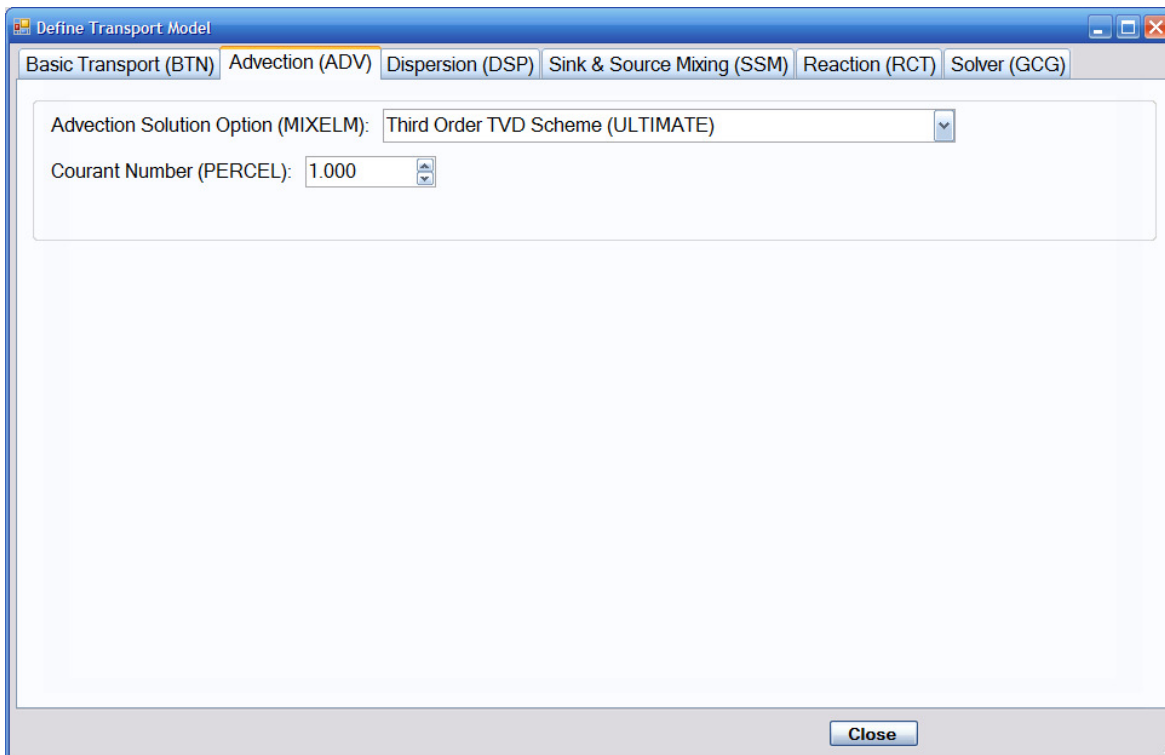
Figure 7.37: Transport Model Definition—ADV Package (Third-Order TVD Scheme {ULTIMATE} Solver)

PERCEL is the Courant number (i.e., the number of cells, or a fraction of a cell) advection will be allowed in any direction in one transport step. For implicit finite-difference or particle-tracking-based schemes, there is no limit on

PERCEL, but for accuracy reasons, it is generally not set much greater than one. Note, however, that the PERCEL limit is checked over the entire model grid. Thus, even if PERCEL > 1, advection may not be more than one cell's length at most model locations. For the explicit finite-difference or the third-order TVD scheme, PERCEL is also a stability constraint which must not exceed one and will be automatically reset to one if a value greater than one is specified.

Figure 7.38 displays the Dispersion tab (corresponding to the Transport Model DSP package).
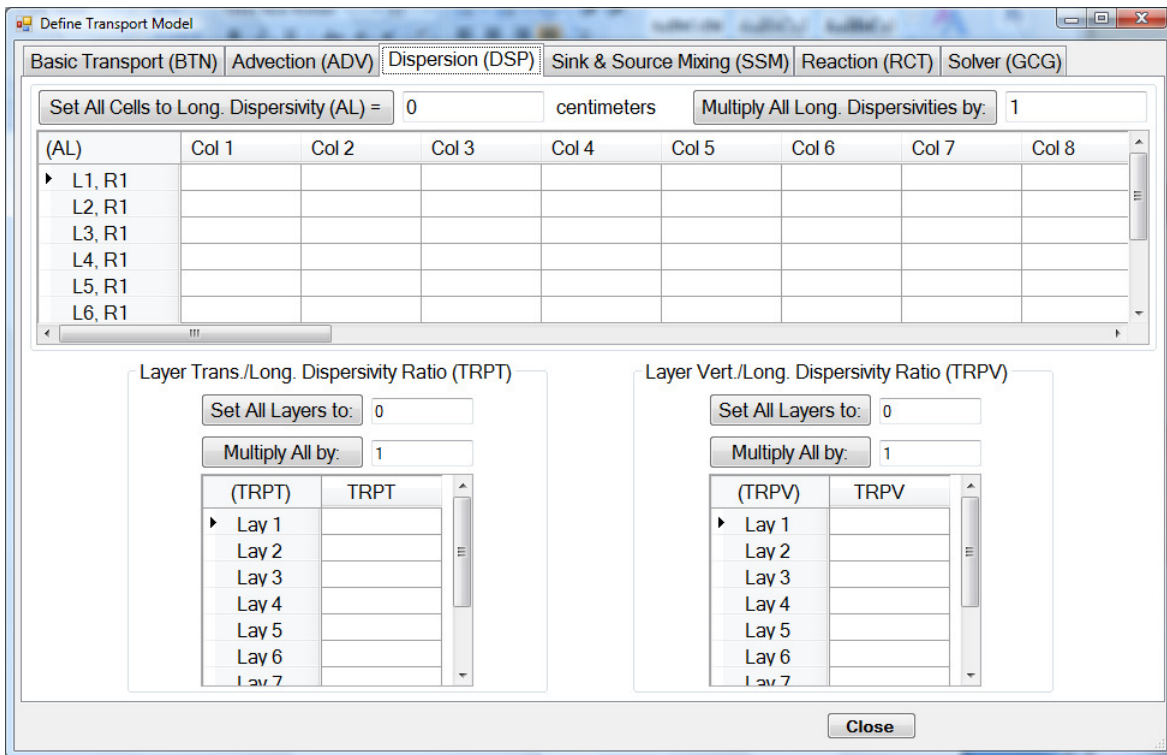
Figure 7.38: Transport Model Definition—Dispersion (DSP Package) Tab

AL is the longitudinal dispersivity, α_L, for every cell of the model grid (unit, L).

TRPT is the ratio of the horizontal transverse dispersivity, α_{TH}, to the longitudinal dispersivity, α_L. Each value corresponds to one model layer. Some field studies suggest that TRPT is generally not greater than 0.1.

TRPV is the ratio of the vertical transverse dispersivity, α_{TV}, to the longitudinal dispersivity, α_L. Each value corresponds to one model layer. Some field studies suggest that TRPT is generally not greater than 0.01.

Figure 7.39 displays the Sink and Source Mixing tab (corresponding to the Transport Model SSM package). The top-right corner of the screen displays the possible Flow Model point and areal stresses (except for Constant Head). If any of these stresses are active in the flow model, the box(es) will be checked and the sources will be displayed in the Point and/or Areal Source data grids. If the flow model does not include any sinks or sources, the data grid area will initially be blank as shown.
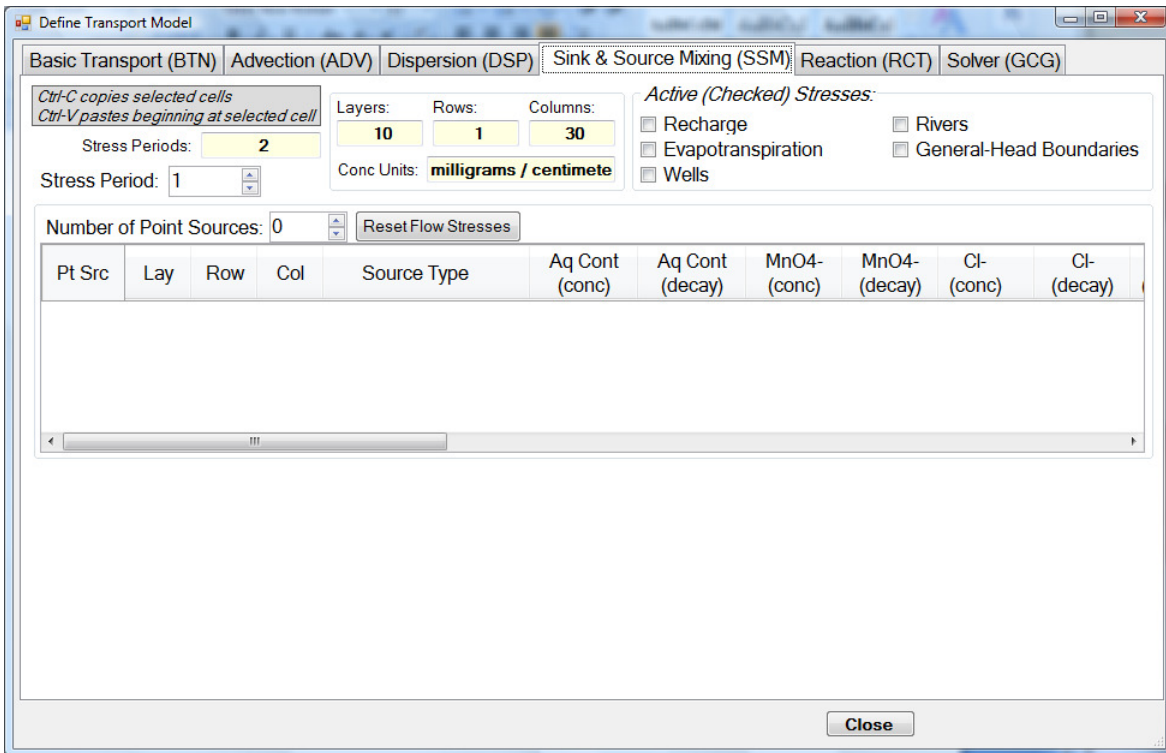
Figure 7.39: Transport Model Definition—Sink & Source Mixing (SSM Package) Tab

However, if there are sinks or sources defined in the flow model (including Constant Head cells and Constant Head Dependent Boundaries), the Point Source data grid will contain entries for each flow model point source (e.g., point sources 1 and 2 in Figure 7.40). These point sources cannot be deleted and the cells shaded orange cannot be changed; however, by leaving all component concentrations set to zero they are effectively shut off for the transport simulation. Just as with the Stress tabs on the Flow Model Screen, you can select the Stress Period that you want to view or edit source and sink data for.
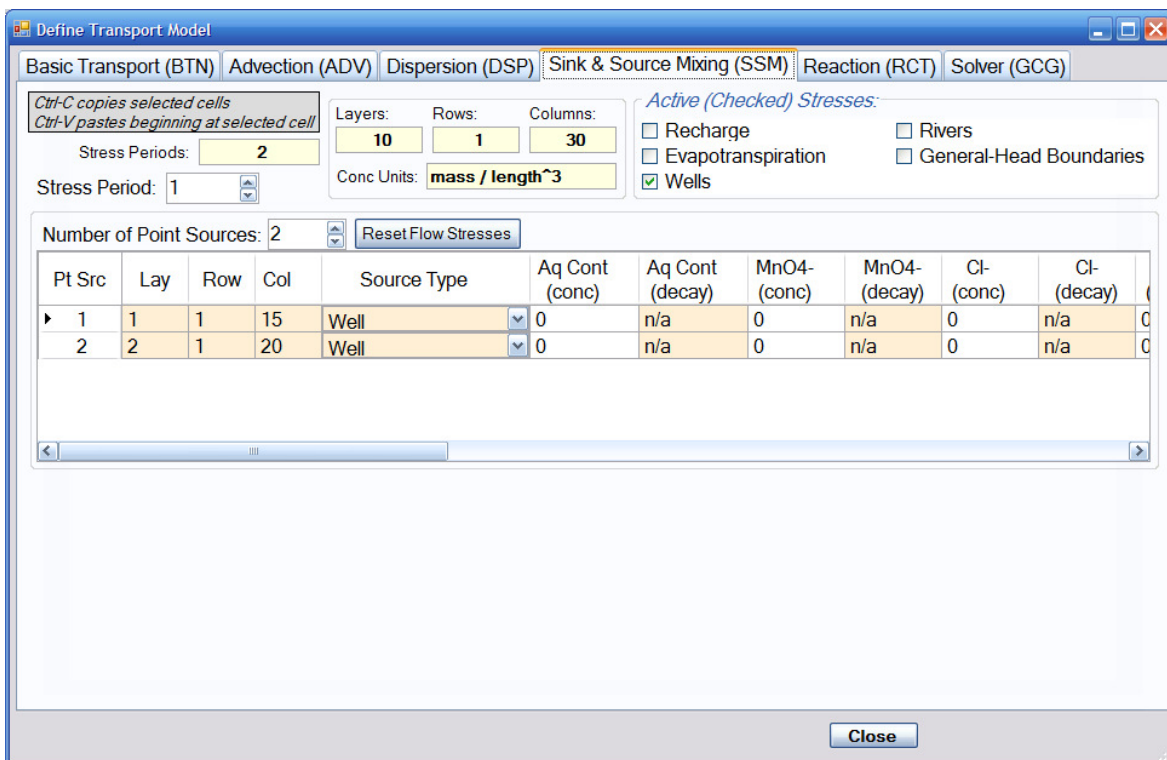
Figure 7.40: Transport Model Definition—SSM Package (Flow Model Point Sources)

Additional, user-specified point sources (typically either Constant Concentration or Decaying Source) can be added to the model by increasing the value for "Number of Point Sources." This adds additional point sources to the end of the data grid, which can then be modified as necessary. Conversely, point sources can be removed from the model by

decreasing the value for "Number of Point Sources." This will prompt you to confirm to removal of the indicated number of point sources from the bottom of the data grid.
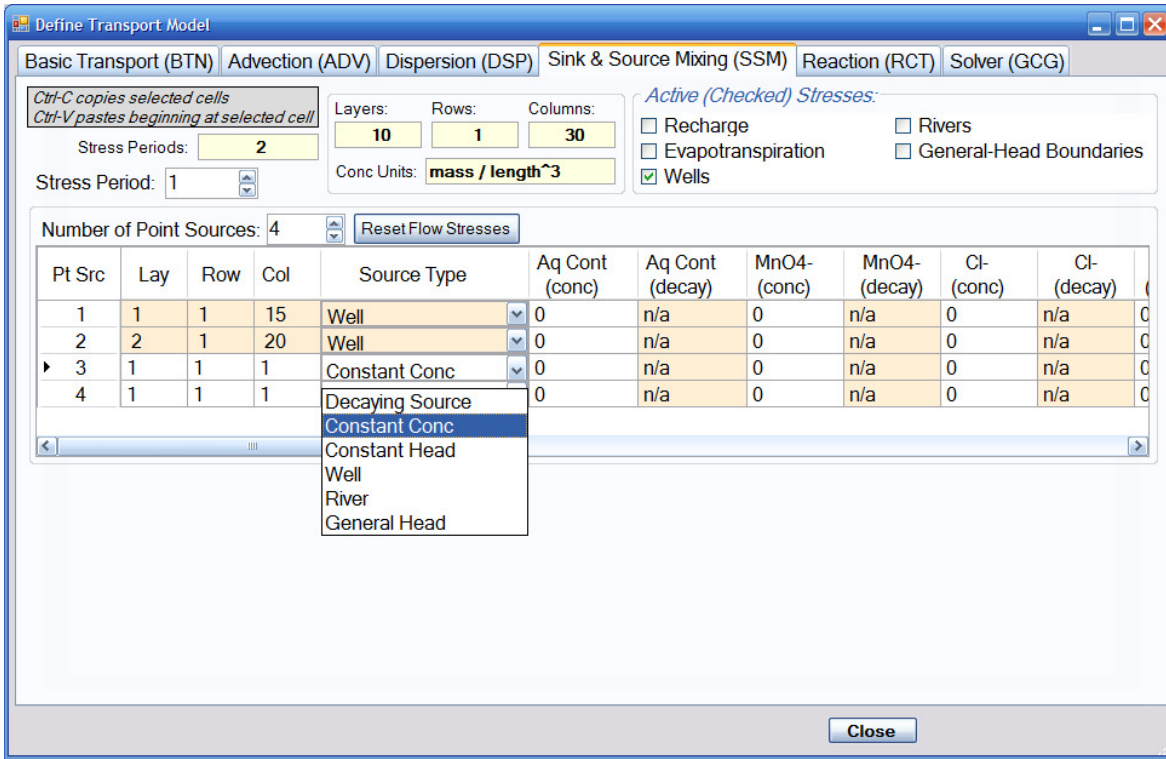
Figure 7.41: Transport Model Definition—SSM Package (User-Specified Point Sources)

When a user-specified point source is added, the following parameters need to be defined:

Layer—the layer number of the cell containing the point stress.

Row—the row number of the cell containing the point stress.

Column—the column number of the cell containing the point stress.

Source Type—select the type of point source from six available options. Constant Head, Well, River, and General Head Boundary point sources are not usually added as

user-specified point sources; they should normally match the stresses defined in the flow model.

- Constant Head
- Well
- River
- General Head Boundary
- Decaying Source. Simulates a decaying source, starts at a given initial concentration and decaying at a first-order rate according to Equation 7-1.

$$C_i = C_{i,0} \cdot \exp(-\lambda_i \cdot t) \tag{7-1}$$

where C_i is the concentration of species i at time t, $C_{i,0}$ is the initial concentration of species i in the source, and λ_i is the source decay constant for species i. For example, the decaying source feature can be used to model a waste pit with a depleting DNAPL source.

- Constant Concentration. This is similar to setting a constant-concentration boundary condition (i.e., setting ICBUND = -1 in the BTN package), with two major differences: 1) the concentration may be different in each stress period and 2) concentrations need not be held constant for all species.

Concentration (Aqueous Contaminant, $MnO4^-$, Cl^-)—Enter the point source concentration of the respective mobile component. When the point source type is either Constant Concentration or Decaying Source, positive Concentration values are used as constant/decaying source concentrations and negative values are indicators that those components should not have their concentrations held constant.

Decay Rate (each component)—Enter the first-order decay constant for the respective component, as applicable. The value should be positive if the source is decreasing with time and negative if it is increasing with time. Specify decay value as zero for the species that were assigned negative

concentration values. Also, zero can be used for non-decaying species. Note that decay rate values can only be entered for point sources of the Decaying Source type.

Mass Fraction (MnO$_2$, DNAPL, Sorbed Contaminant, Fast NOD, Slow NOD)— Enter the point source mass fraction of the respective immobile component. Note that source/sink mass fractions of immobile species are used (and can be defined) only when the point source type is either Constant Concentration or Decaying Source.

Once any parameter is manually changed for any Point Source, the "Reset Flow Stresses" button turns red as shown in Figure 7.42. This is a visual notification that any subsequent changes to flow model stresses defined on the Flow Model Screen will not be automatically reflected in the transport model Point Stresses. If you make add, remove, or change any flow model stresses on the Flow Model Screen, return to this screen and click on the "Reset Flow Stresses" button. This will re-establish the link between the flow model and transport model stresses, and the button color will return to gray.
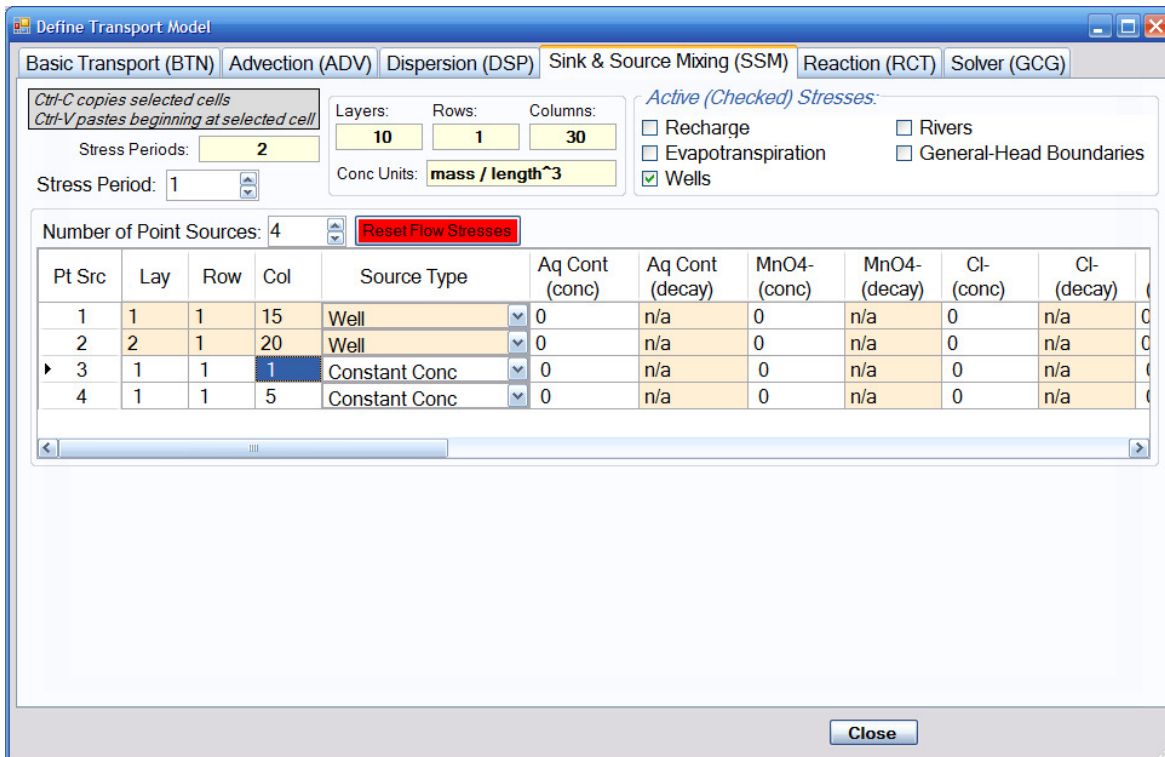
Figure 7.42: Transport Model Definition—SSM Package (Resetting Flow Model Point Sources)

If Recharge, Evapotranspiration, or both areal stresses are active in the flow model, the lower Areal Source data grid will be visible as shown in Figure 7.43. If an areal stress is active, concentration values must be entered for every cell in the stress layer. Further, values must be entered for every mobile component, for every stress period. Select the desired mobile species for entry/editing from the pull-down menu as shown in figure 7.43.

For Recharge, enter the concentration of recharge flux for the selected species. If the recharge flux is positive, it acts as a source whose concentration can be specified as desired. If the recharge flux is negative, it acts as a sink (discharge) whose concentration is always set equal to the concentration of groundwater at the cell where discharge occurs.

For Evapotranspiration, enter the concentration of evapotranspiration flux for the selected species. Evapotranspiration is the only type of sink whose concentration may be specified externally. Note that the concentration of a sink cannot be greater than that of the

aquifer at the sink cell. Thus, if the sink concentration is specified greater than that of the aquifer, it is automatically set equal to the concentration of the aquifer.
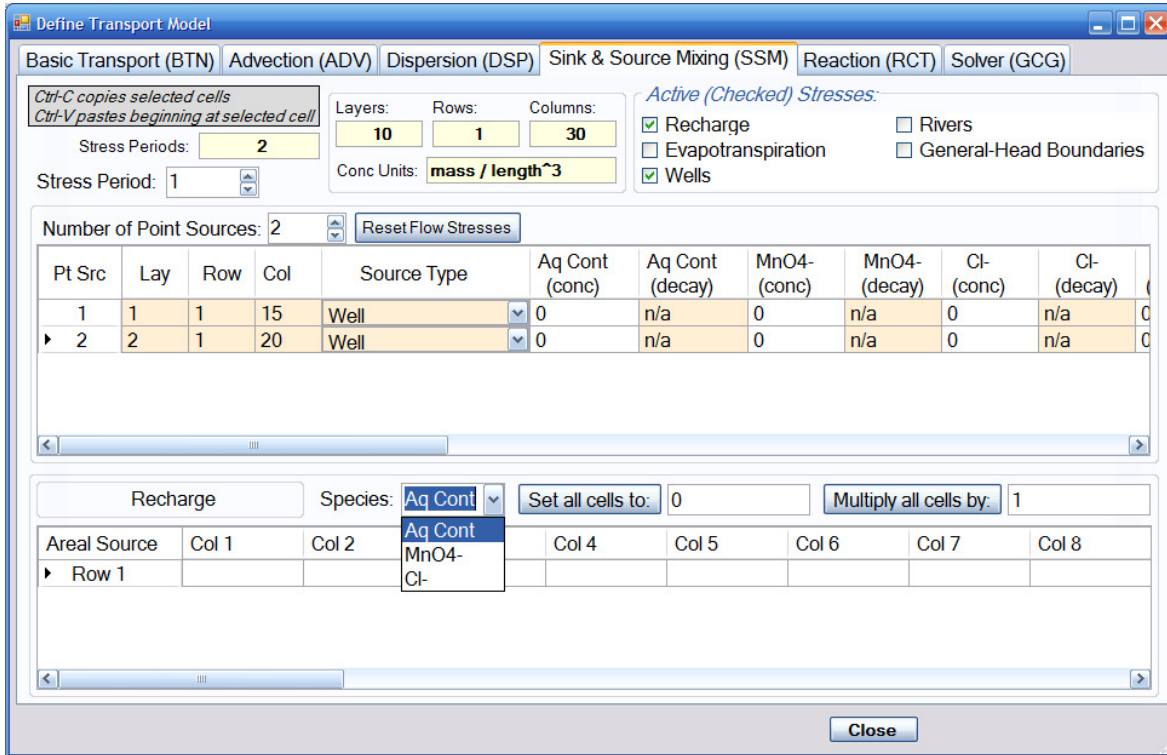
Figure 7.43: Transport Model Definition—SSM Package (Single Areal Source)

The upper-left corner of the data grid displays what type of areal source (Recharge or Evapotranspiration) is being displayed. If both Recharge and Evapotranspiration are active and defined in the flow model, there will be radio buttons in the upper-left corner of the data grid as shown in Figure 7.44. Simply click the radio button for the one you want to view/edit.
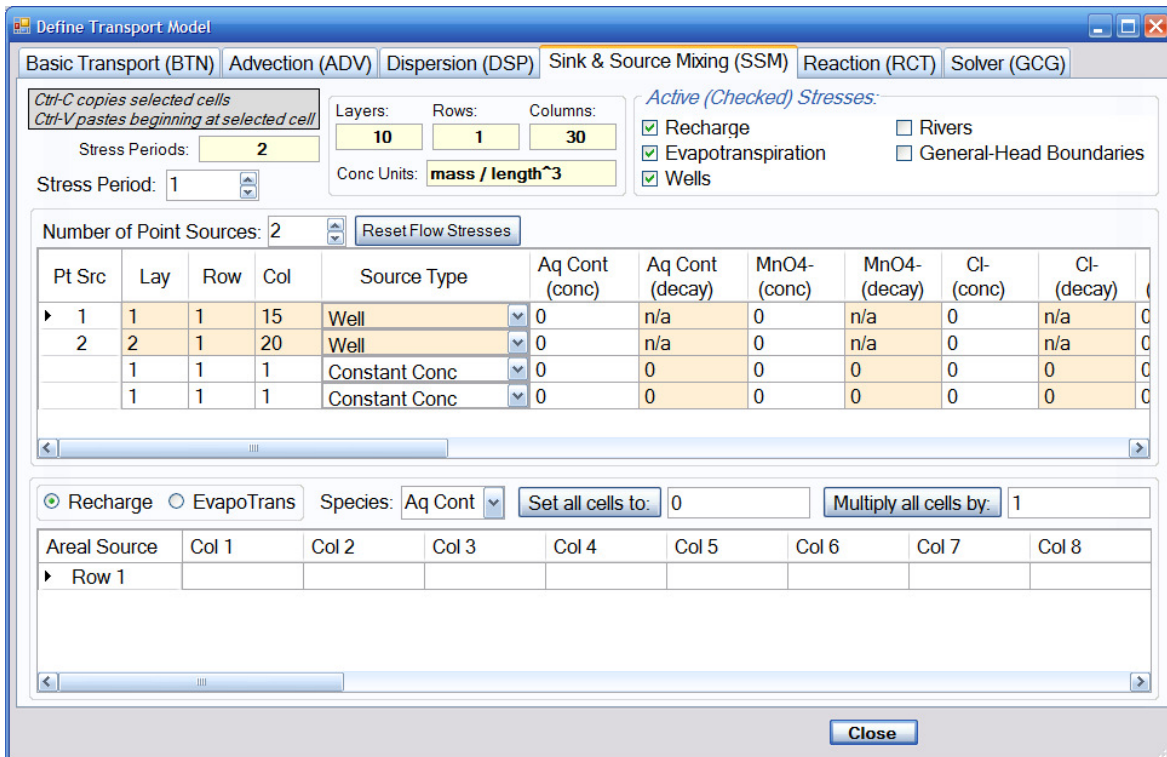
Figure 7.44: Transport Model Definition—SSM Package (Both Areal Sources)

Figure 7.45 displays the Reaction tab (corresponding to the Transport Model RCT package).
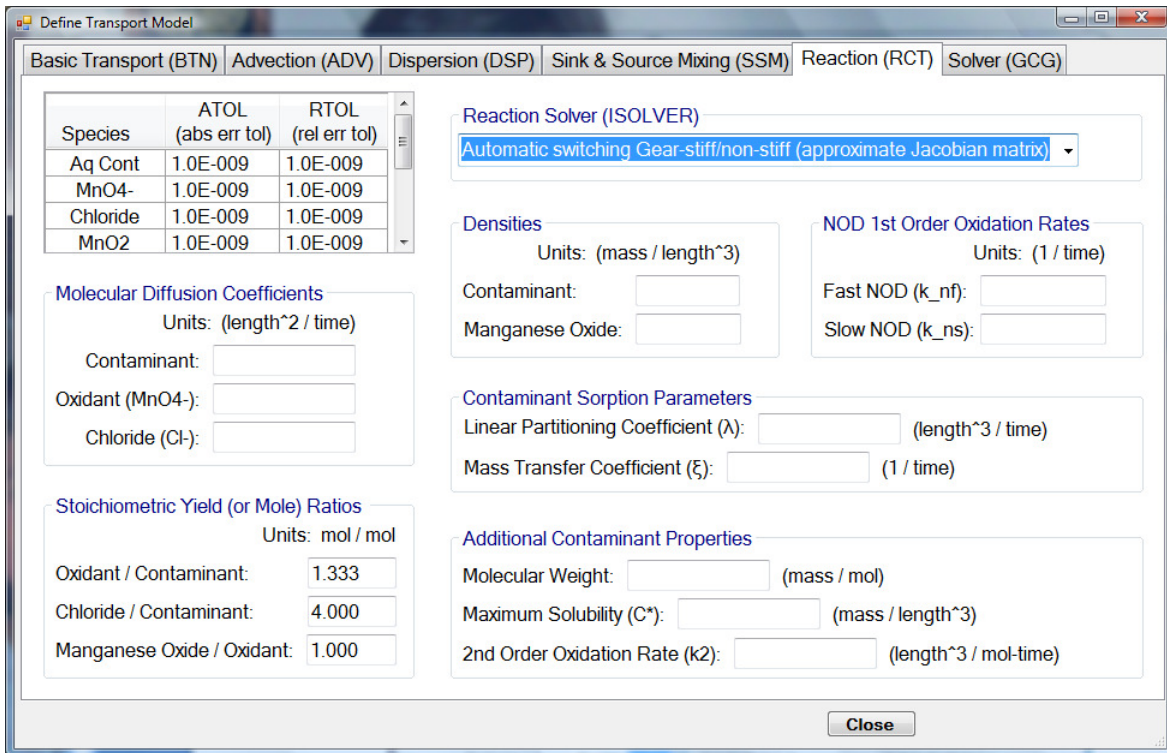
Figure 7.45: Transport Model Definition—Reaction (RCT Package) Tab

Reaction Solver (ISOLVER)—Select the desired solution option from the three choices.

- Automatic Switching Gear-Stiff/Non-Stiff Solver (Approximate Jacobian Matrix)—For stiff systems, this option will automatically compute the Jacobian matrix using finite-difference approximations.
- Automatic Switching Gear-Stiff/Non-Stiff Solver (External Jacobian Matrix)—For stiff systems, this option will utilize an external routine to compute analytical Jacobian.
- Fehlberg Fourth-Fifth Order Runge-Kutta Method

Absolute and Relative Error Tolerance (ATOL and RTOL)—are used by the solver to determine how accurate the solution for each component concentration must be.

If either Automatic Switching Gear-Stiff/Non-Stiff Solver is selected, then the ATOL and RTOL values specified for each species are used by the solvers.

If the Fehlberg Fourth-Fifth Order Runge-Kutta Solver is selected, then only the first pair of values, ATOL (Aq Cont) and RTOL (Aq Cont), is used by the solver. However, remaining ATOL and RTOL inputs must still have dummy values specified.

The differential equation solver will attempt to control the component's concentration local error, $e(i)$, such that, for each component, the local error has (approximately) a smaller magnitude than the error weight, $ewt(i)$:

$$|e(i)| \leq ewt(i) \qquad (7\text{-}2)$$

where,

$$ewt(i) = RTOL(i) \cdot |y(i)| + ATOL(i) \qquad (7\text{-}3)$$

Here $ewt(i)$ is a vector of weights which must always be positive, and the values of RTOL and ATOL should all be non-negative. Setting $ATOL(i) = 0.0$ results in a pure relative error test on that component. Setting $RTOL(i) = 0.0$ results in a pure absolute error test on that component. A mixed test with non-zero $RTOL(i)$ and $ATOL(i)$ corresponds roughly to a relative error test when the solution component, $y(i)$, is much bigger than ATOL and to an absolute error test when the solution component is smaller than the threshold ATOL.

For practical problems, the following rules of thumb may be used to set ATOL and RTOL values. $ATOL(i)$ should be set to a tolerable absolute error level (usually around 10^{-6} to 10^{-9}). Defining m as the number of significant digits required in the solution for species $y(i)$, set $RTOL(i) = 10^{-(m+1)}$. **Caution: Actual (global) errors may exceed the local tolerances, so choose ATOL(i) and RTOL(i) conservatively.**

Contaminant Molecular Diffusion Coefficient (Dm_cont)—Enter the molecular diffusion coefficient of the aqueous contaminant (L^2T^{-1}).

Oxidant Molecular Diffusion Coefficient (Dm_mno4)—Enter the molecular diffusion coefficient for permanganate (L^2T^{-1}).

Chloride Molecular Diffusion Coefficient (Dm_cl)—Enter the molecular diffusion coefficient for chloride (L^2T^{-1}). If oxidation of a non-chlorinated contaminant is being simulated, enter the molecular diffusion coefficient of an appropriate aqueous by-product of oxidation.

Oxidant/Contaminant Stoichiometric Mole Ratio (Y_mno4_cont)—Enter the number of moles of oxidant consumed in destroying one mole of contaminant ($MolMol^{-1}$).

Chloride/Contaminant Stoichiometric Mole Ratio (Y_cl_cont)—Enter the number of moles of chloride created by destroying one mole of contaminant ($MolMol^{-1}$). If oxidation of a non-chlorinated contaminant is being simulated, select an appropriate aqueous by-product of oxidation and enter the number of moles of by-product created in destroying one mole of contaminant.

Manganese Oxide/Oxidant Stoichiometric Mole Ratio (Y_mno2_mno4)—Enter the number of moles of manganese oxide created from consumption of one mole of permanganate ($MolMol^{-1}$). This parameter can be set to zero, if using CORT3D to simulate a different oxidant that does not generate a by-product with potential to plug soil pore space.

Contaminant Density (rho_cont)—Enter density of contaminant (ML^{-3}).

Manganese Oxide Density (rho_mno2)—Enter the effective density of manganese oxide solids (ML^{-3}). The manganese oxide solids formed during in situ oxidation tend to be amorphous in nature, so the value entered here is typically far lower than the density of crystalline manganese oxide.

Fast NOD Oxidation Rate (k_nf)—Enter the first-order kinetic rate constant for oxidation of the fraction of NOD with a faster rate (T^{-1}).

Slow NOD Oxidation Rate (k_ns)—First-order kinetic rate constant for oxidation of the fraction of NOD with a slower rate (T^{-1}).

Sorption Linear Partitioning Coefficient (lambda_c)—Enter the linear sorption coefficient $(L^{3}M^{-1})$.

Sorption Mass Transfer Coefficient (xi)—Enter the rate-limited sorption mass transfer coefficient (T^{-1}).

Contaminant Molecular Weight (MW_cont)—Enter the molecular weight of the contaminant $(MMol^{-1})$.

Contaminant Maximum Solubility (C_c_star)—Enter the maximum aqueous solubility for the contaminant (ML^{-3}).

Contaminant Oxidation Rate (k2_cont)—Enter the second-order kinetic rate constant for oxidation of the contaminant $(L^{3}Mol^{-1}T^{-1})$.

Figure 7.46 shows the Solver tab (corresponding to the Transport Model GCG Package)
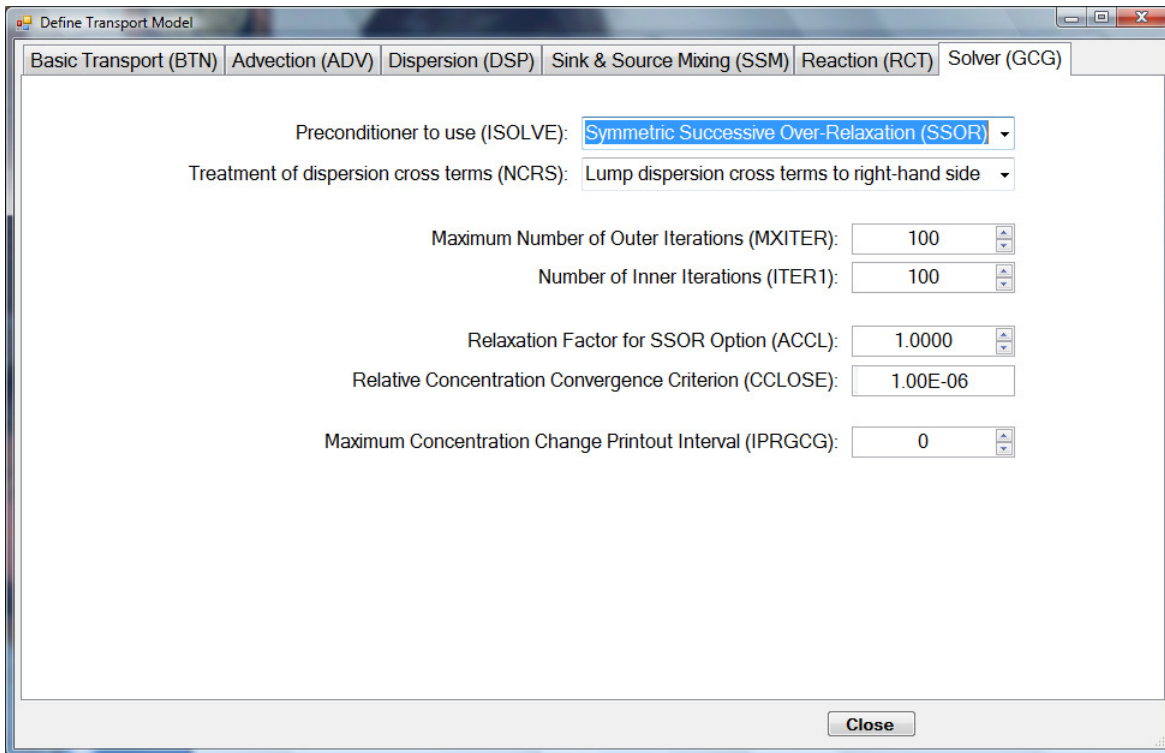
Figure 7.46: Transport Model Definition—Solver (GCG Package) Tab

MXITER is the maximum number of outer iterations.

ITER1 is the maximum number of inner iterations.

ISOLVE is the type of preconditioner to be used with the Lanczos/ORTHOMIN
acceleration scheme:

- Jacobi

- Symmetric Successive Over-Relaxation (SSOR)

- Modified Incomplete Cholesky (MIC). This usually converges faster,
but it needs significantly more memory.

-

NCRS is an integer flag for treatment of dispersion tensor cross terms:

- Lump Dispersion Cross Terms to the Right-hand Side. This is
approximate but highly efficient.

- Include Full Dispersion Tensor. This is memory intensive.
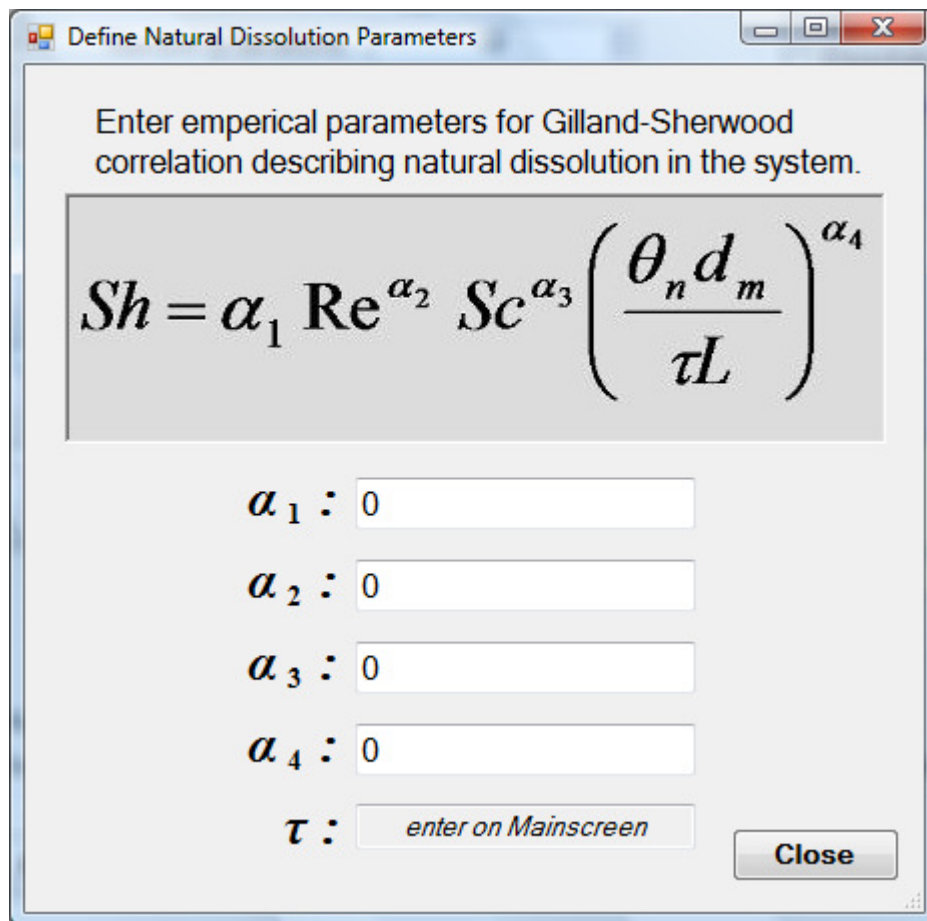
ACCL is the relaxation factor for the SSOR option; a value of 1.0 is generally adequate. Note that a value is needed even if a different acceleration scheme is selected for ISOLVE.

CCLOSE is the convergence criterion in terms of relative concentration; a real value between 10-4 and 10-6 is generally adequate.

IPRGCG is the interval for printing the maximum concentration changes of each solver iteration. Set IPRGCG to zero for printing at the end of each stress period.

7.2.6 *Defining DNAPL Natural Dissolution*

From the Main screen, clicking on the "Define Natural Dissolution" button will bring up the Natural Dissolution screen shown in Figure 7.47. Unlike the Flow Model and Transport Model screens, there are no tabs to be filled out. Just enter the four empirical "alpha" parameters describing the DNAPL natural dissolution process for the system being simulated.

Figure 7.47: Natural Dissolution Definition

α_1—Pre-multiplier in Gilland-Sherwood relationship for natural dissolution.

α_2—Exponent of Reynolds number in Gilland-Sherwood relationship.

α_3—Exponent of Schmidt number in Gilland-Sherwood relationship.

α_4—Exponent of $\left(\dfrac{\theta_n d_{50}}{\tau L} \right)$ term in Gilland-Sherwood relationship.

Soil tortuosity factor (τ)—used in Gilland-Sherwood. Note that this parameter is entered on the Main screen, and displayed here for reference.

7.2.7 Defining Oxidation Initial Aquifer Properties

From the Main screen, clicking on the "Define Oxidation Initial Aquifer Properties" button will bring up the Initial Aquifer Properties screen shown in Figure 7.48. Like the Flow Model and Transport Model screens, there are a number of tabs where data are entered. The first tab is the Initial Porosity (Phi0).
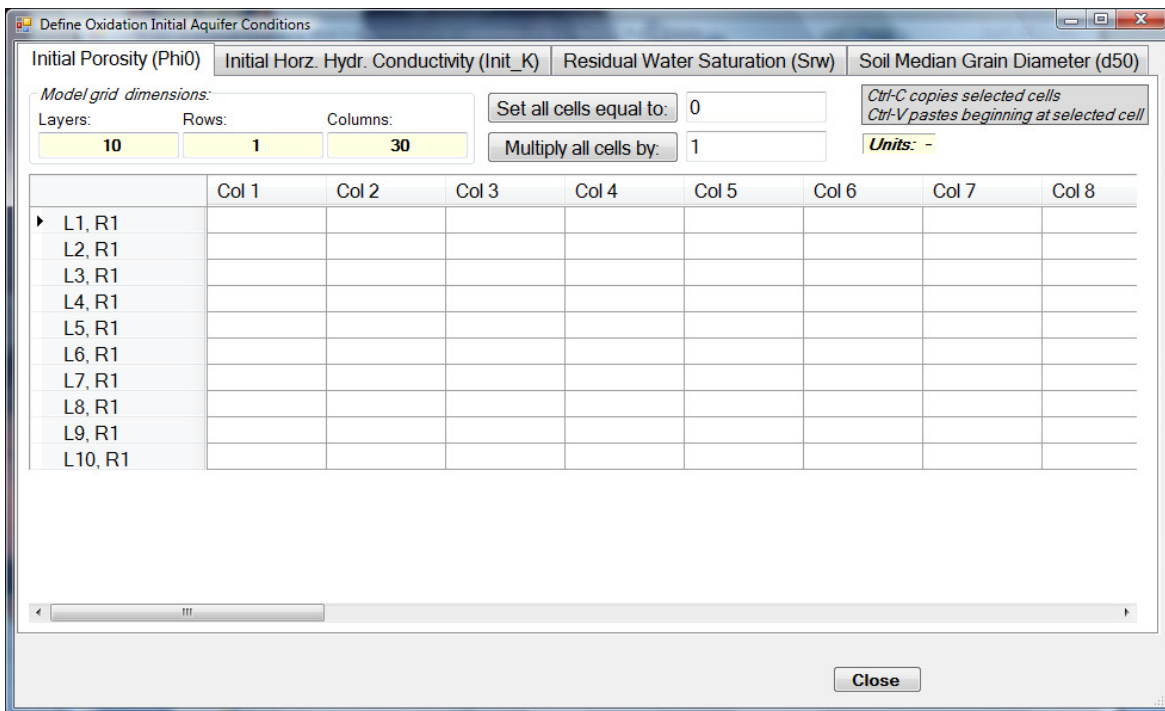
Figure 7.48: Oxidation Initial Oxidation Aquifer Properties Definition (Initial Porosity Tab)

Phi0—enter the initial total porosity (available to contain water, DNAPL, and/or $MnO_{2\,(s)}$) of each cell within the system.

Figure 7.49 shows the Initial Horizontal Hydraulic Conductivity Tab.
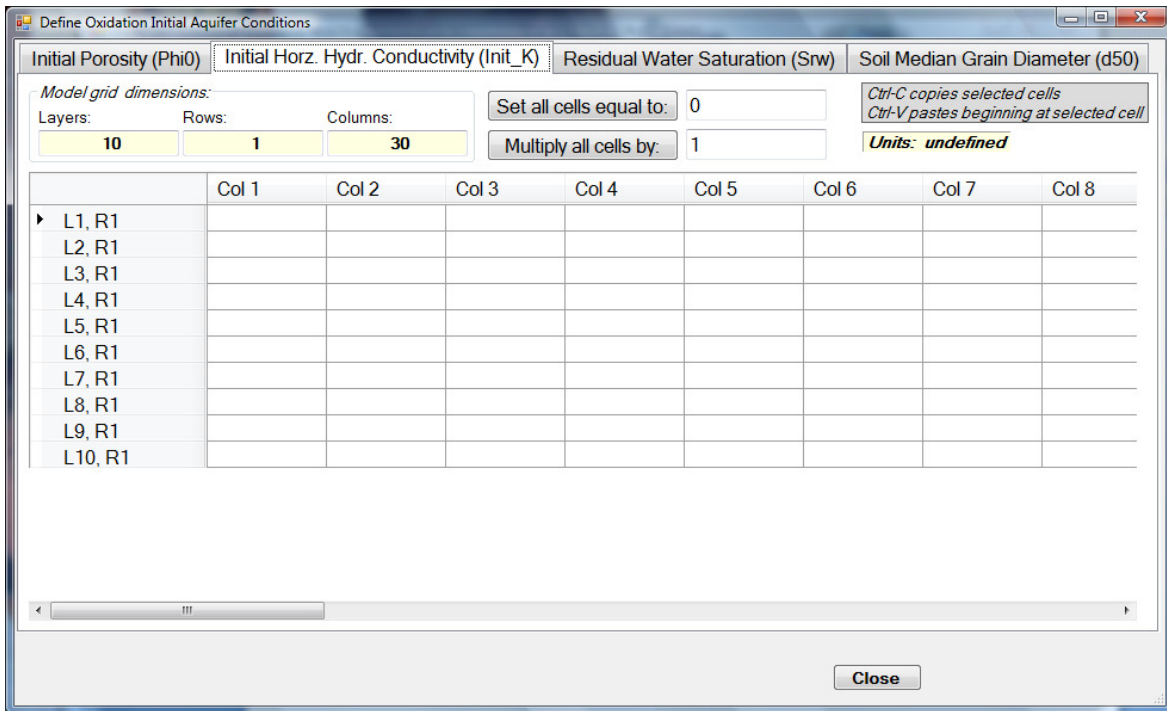
Figure 7.49: Oxidation Initial Oxidation Aquifer Properties Definition (Initial Horizontal Hydraulic Conductivity Tab)

Init_K—enter the initial (fully water-saturated), horizontal hydraulic conductivity of each cell (i.e., the hydraulic conductivity when none of the pore space is containing DNAPL or $MnO_{2\ (s)}$). This value is multiplied by HANI or CHANI (entered on the LPF tab of the Flow Model screen) to obtain hydraulic conductivity along columns.

Figure 7.50 shows the Residual Water Saturation Tab.
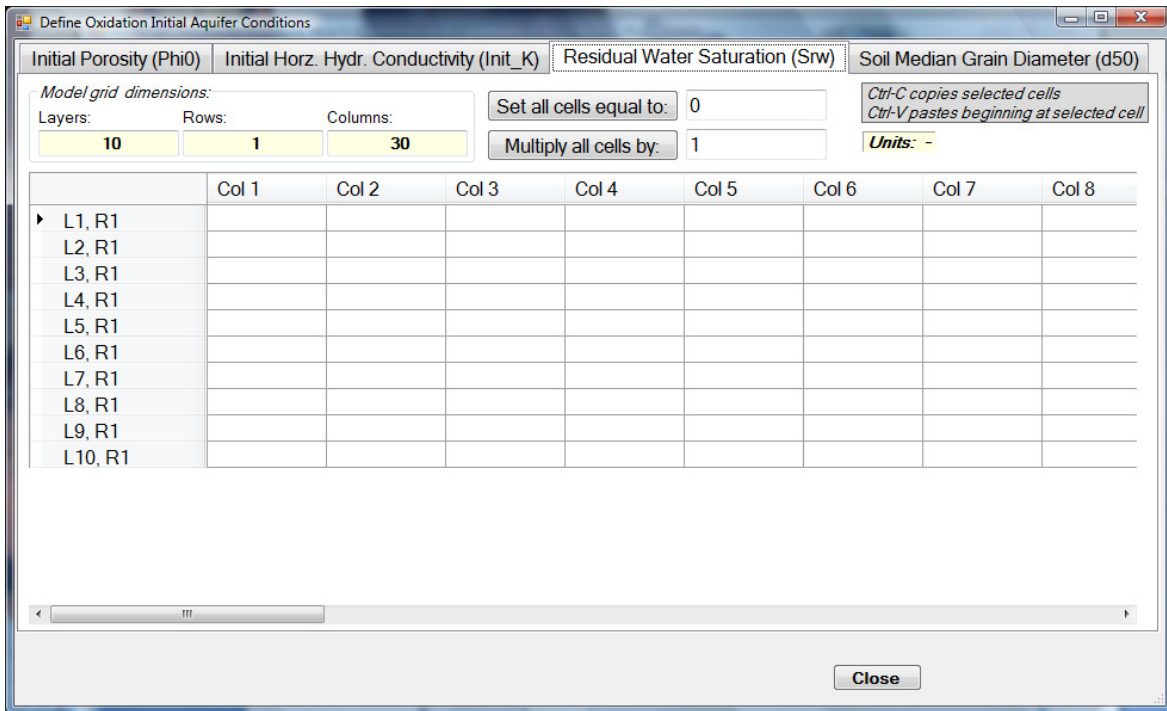
Figure 7.50: Oxidation Initial Oxidation Aquifer Properties Definition (Residual Water Saturation Tab)

Srw—enter the residual water saturation of each cell within the system.

Figure 7.51 shows the Soil Median Grain Diameter Tab.
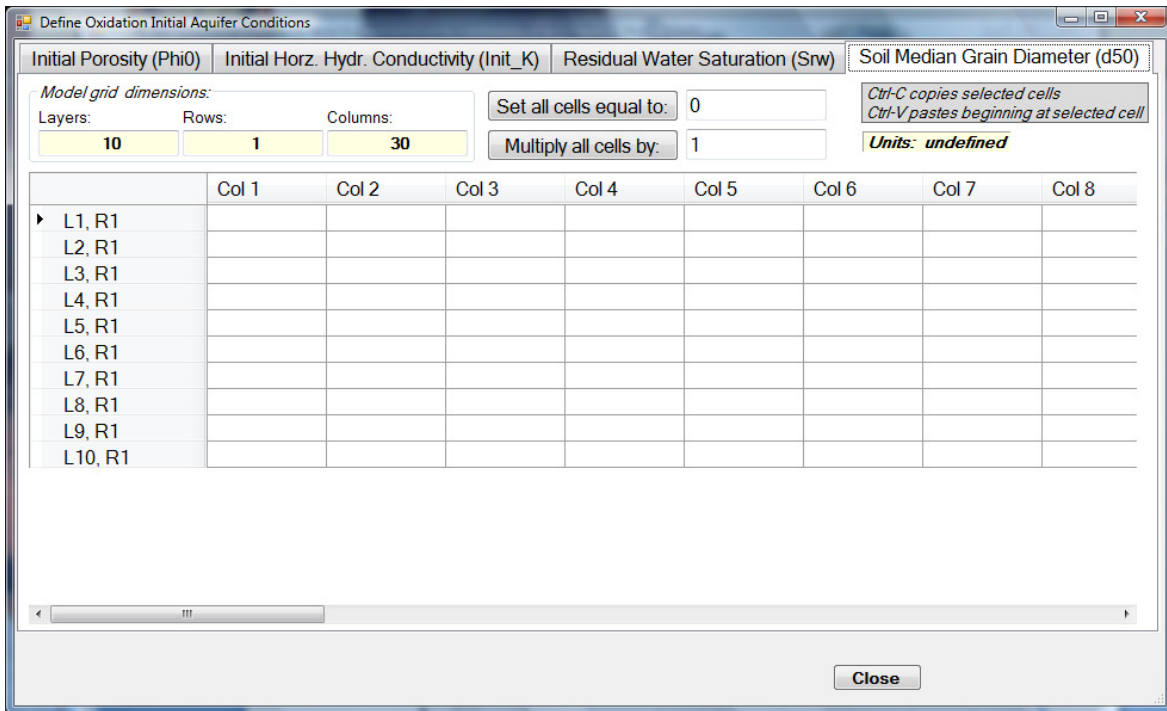
Figure 7.51: Oxidation Initial Oxidation Aquifer Properties Definition (Soil Median Grain Diameter Tab)

d50—enter the soil particle size (specifically, the median soil grain size diameter) for each cell in the system.

7.2.8   *Defining Initial Concentrations, Mass Fractions, and DNAPL Saturation*

From the Main screen, clicking on the "Define Initial Concentrations/Mass Fractions" button will bring up the Initial Concentrations, Mass Fractions, and DNAPL Saturation screen shown in Figure 7.52. Again, there are a number of tabs where data are entered. The first tab is for entering the Initial DNAPL saturation.
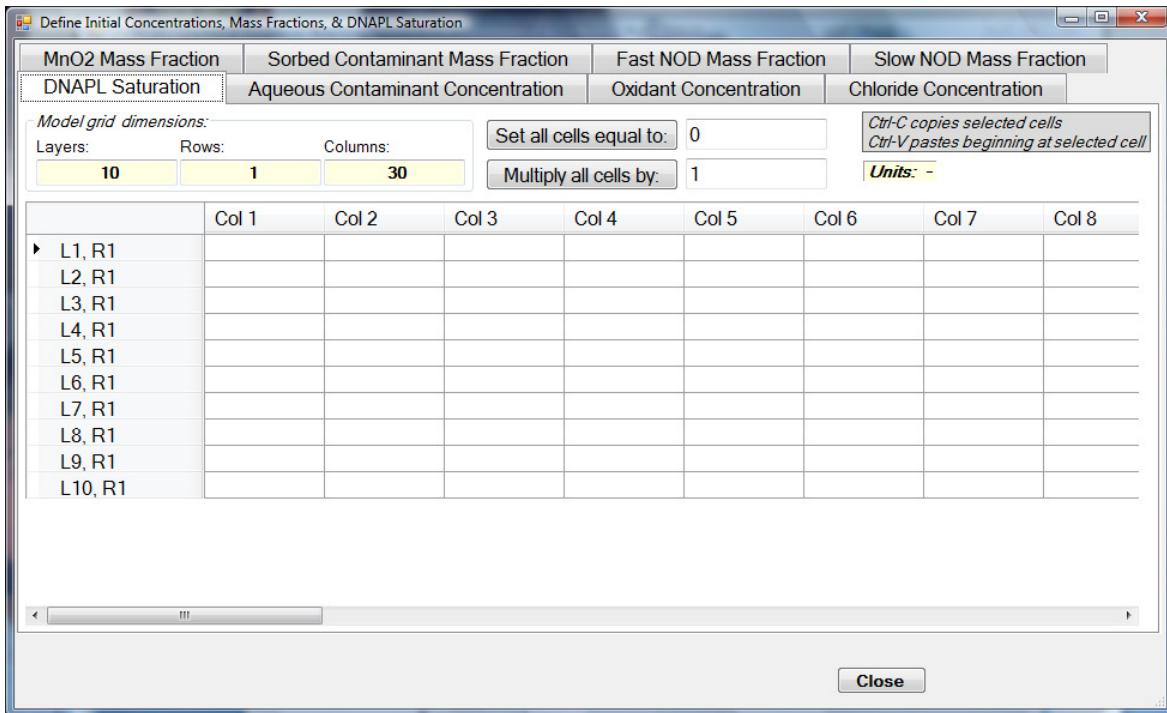
Figure 7.52: Setting Initial Concentrations/Mass Fractions (DNAPL Saturation Tab)

DNAPL Saturation (S_n)—enter the initial DNAPL saturation value for each cell in the model.

Figure 7.53 shows the Initial Aqueous Contaminant Concentration Tab.
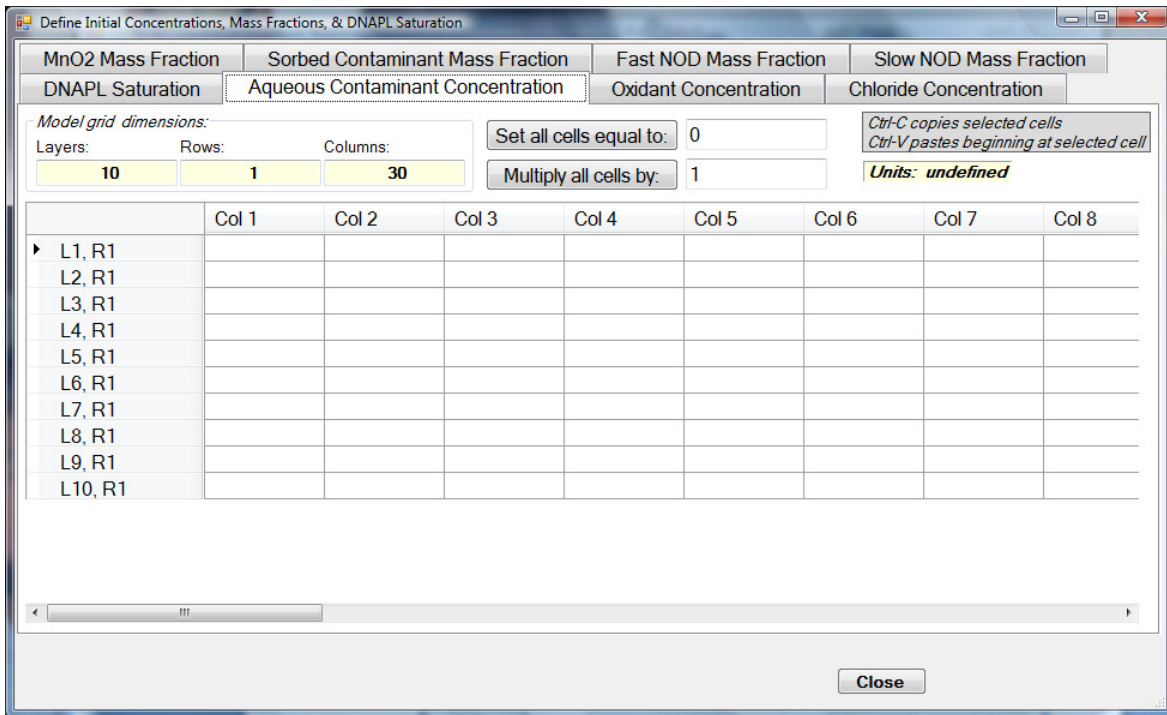
Figure 7.53: Setting Initial Concentrations/Mass Fractions (Aqueous Contaminant Concentration Tab)

Aqueous Contaminant Concentration (C_{cont})—enter the initial aqueous or dissolved contaminant concentration present in each cell in the model.

Figure 7.54 shows the Initial Oxidant Concentration Tab.
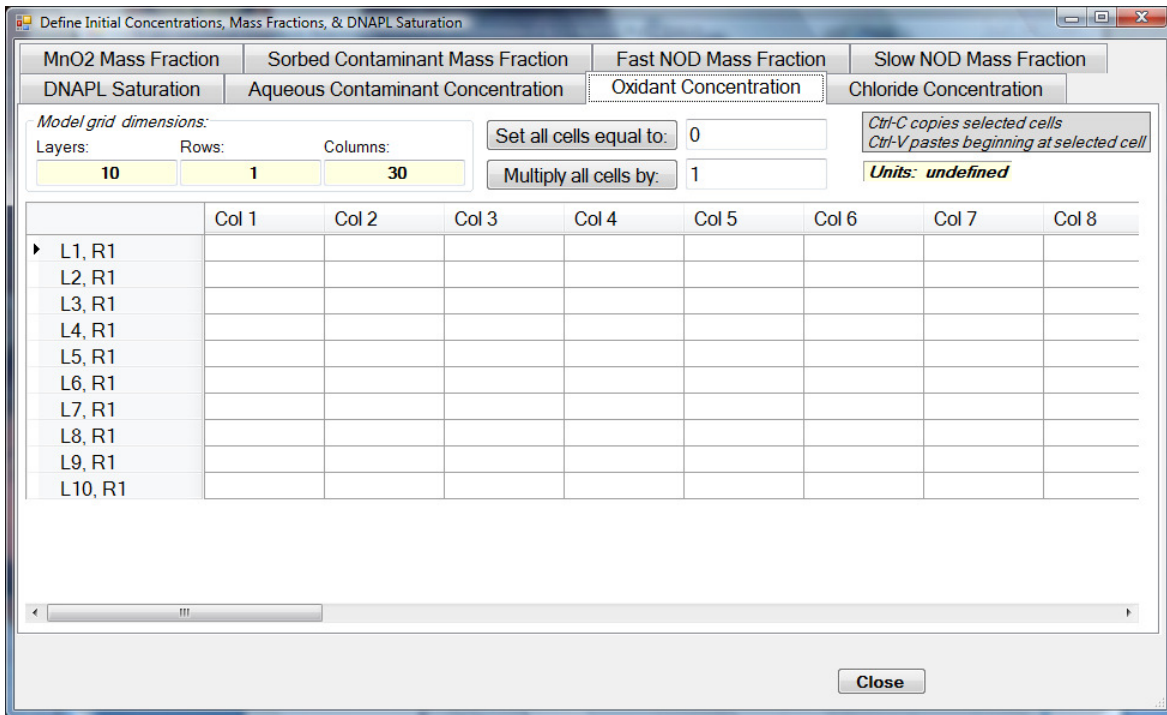
Figure 7.54: Setting Initial Concentrations/Mass Fractions (Oxidant Concentration Tab)

Oxidant Concentration ($C_{oxidant}$)—enter the initial oxidant concentration present in each cell in the model.

Figure 7.55 shows the Initial Chloride Concentration Tab.
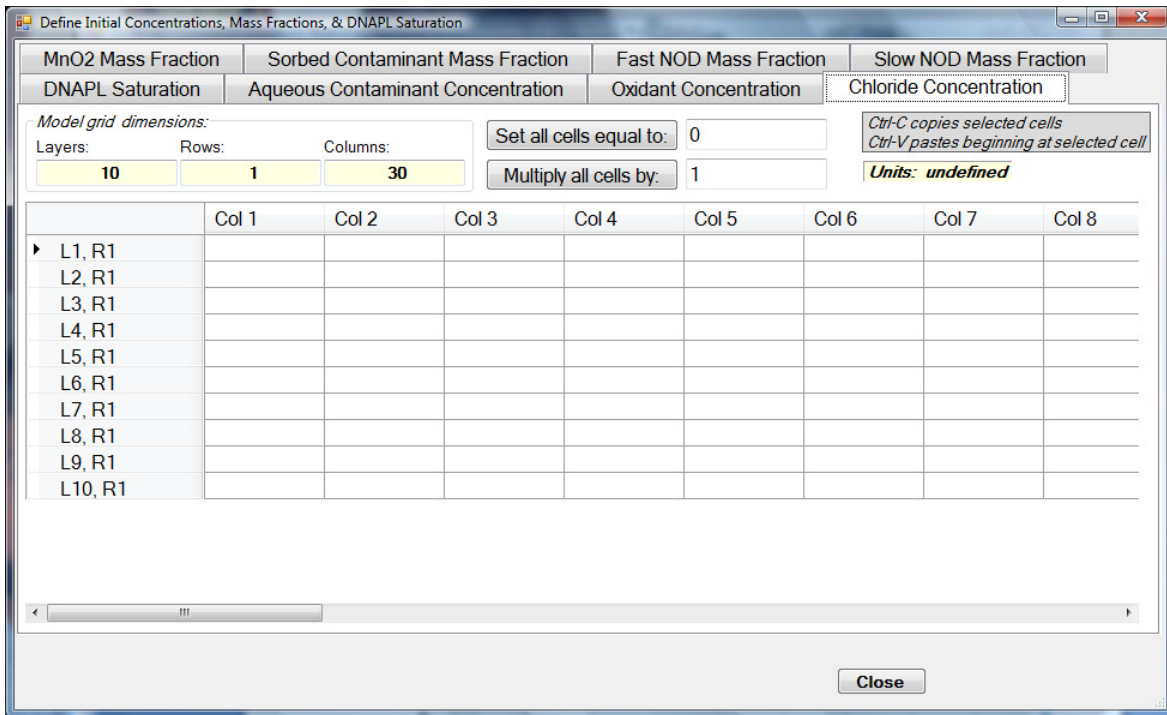
Figure 7.55: Setting Initial Concentrations/Mass Fractions (Chloride Concentration Tab)

Chloride Concentration (C_{cl})—enter the initial chloride concentration present in each cell in the model. If a non-chlorinated contaminant is being simulated, the concentration an appropriate aqueous by-product of oxidation can be entered here.

Figure 7.56 shows the Initial Manganese Oxide Mass Fraction Tab.
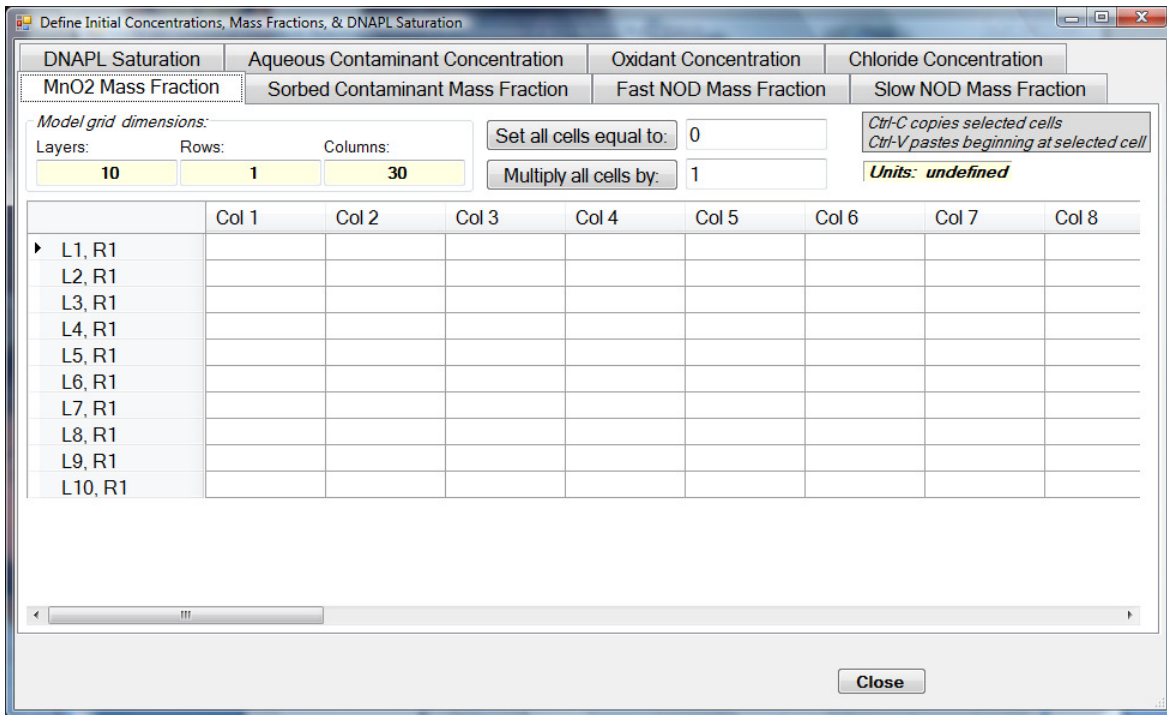
Figure 7.56: Setting Initial Concentrations/Mass Fractions (Mangenese Oxide Mass Fraction Tab)

Manganese Oxide Mass Fraction (X_{mno2})—enter the initial mass fraction of manganese oxide present in each cell in the model.

Figure 7.57 shows the Initial Sorbed Contaminant Mass Fraction Tab.
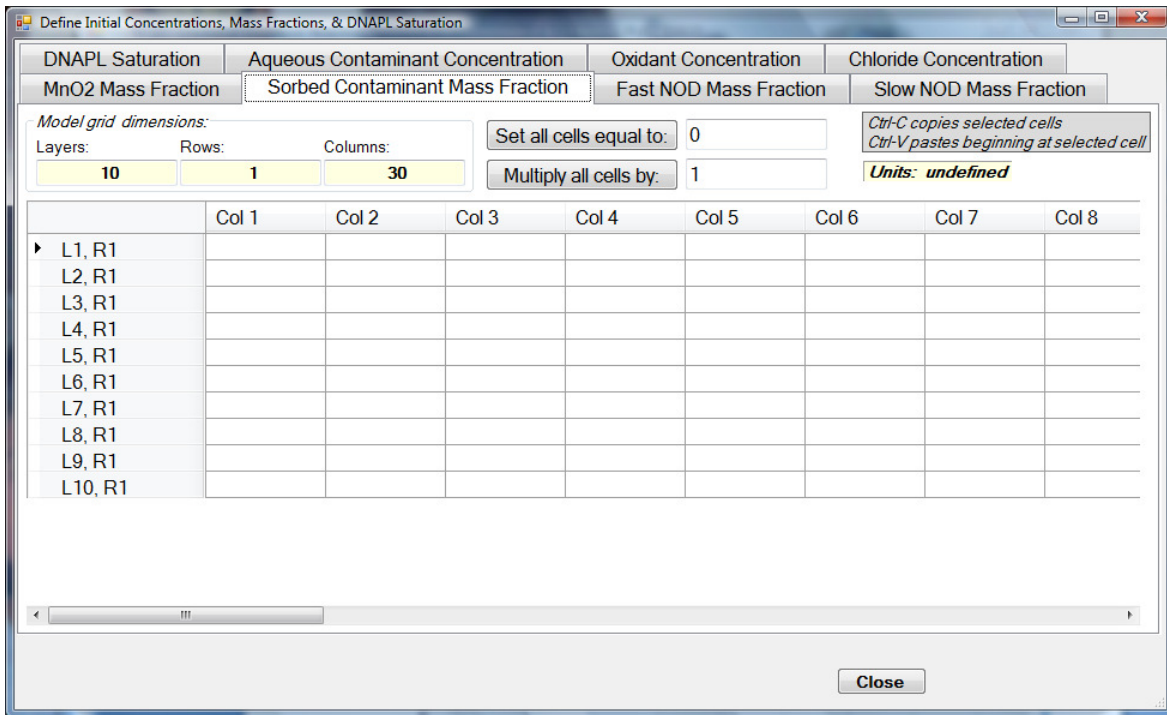
Figure 7.57: Setting Initial Concentrations/Mass Fractions (Sorbed Contaminant Mass Fraction Tab)

Sorbed Contaminant Mass Fraction (X_{sorb})—enter the initial mass fraction of sorbed contaminant present in each cell in the model.

Figure 7.58 shows the Initial Fast NOD Mass Fraction Tab.
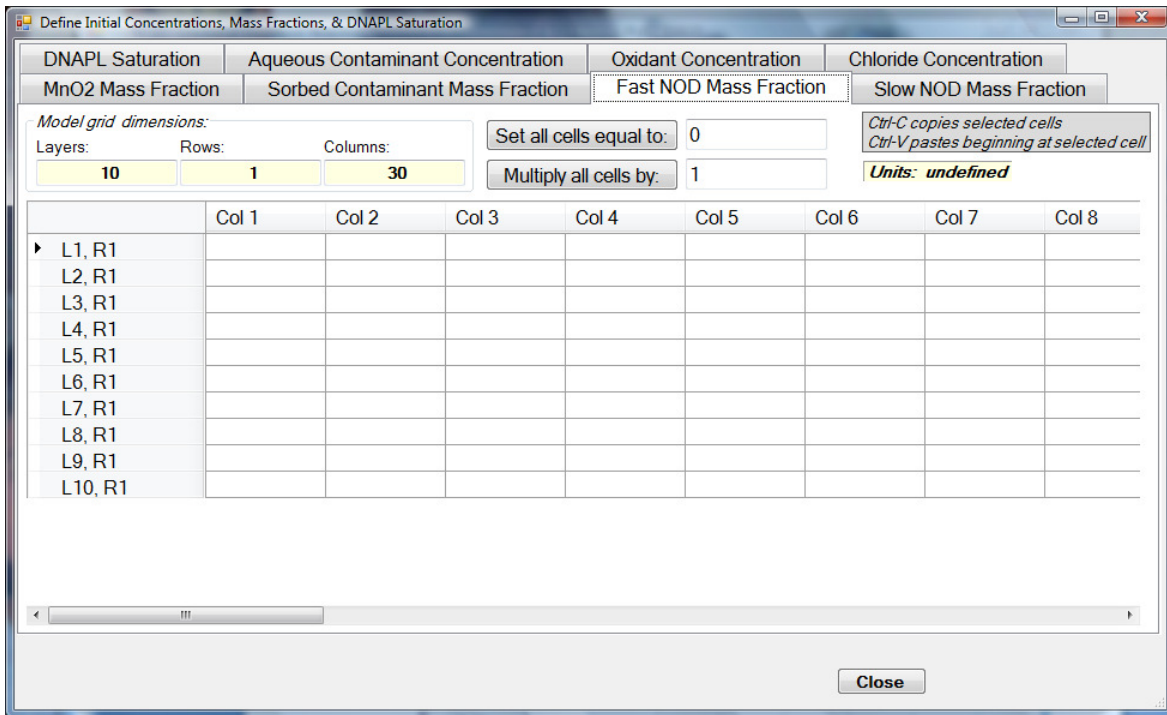
Figure 7.58: Setting Initial Concentrations/Mass Fractions (Fast NOD Mass Fraction Tab)

Fast NOD Mass Fraction (X_{f_nod})—enter the initial mass fraction of fast NOD present in each cell in the model.

Figure 7.59 shows the Initial Slow NOD Mass Fraction Tab.
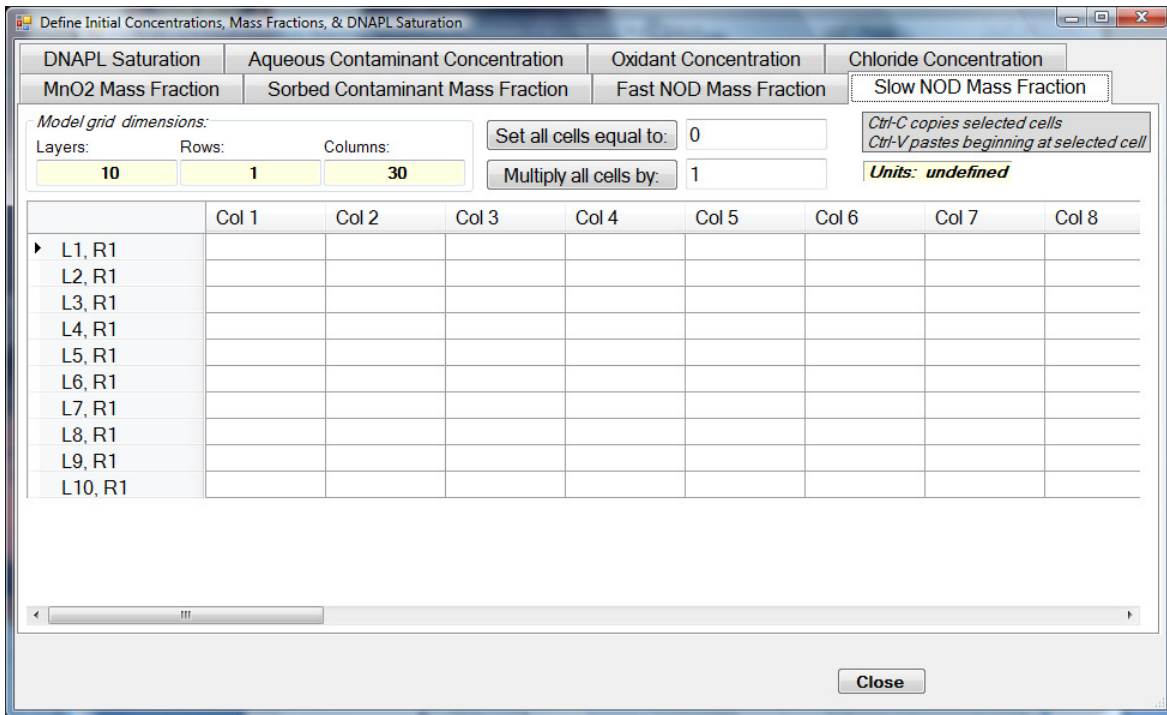
Figure 7.59: Setting Initial Concentrations/Mass Fractions (Slow NOD Mass Fraction Tab)

Slow NOD Mass Fraction (X_{s_nod})—enter the initial mass fraction of slow NOD present in each cell in the model.

7.2.9   *Defining Observation Locations*

From the Main screen, clicking on the "Define Observation Locations" button will bring up the Observation Locations screen shown in Figure 7.60. Just like the Natural Dissolution screen, there are no tabs to be filled out. The observation locations specified will be used in creating several useful output text files.

The concentration of each mobile component at designated observation points and effluent column, along with total aqueous flow rate at effluent, at end of each iteration, will be recorded in the "obs_c.out" file.

The mass fraction of each immobile component at designated observation points, at end of each iteration, will be recorded in the "obs_m.out" file.

The hydraulic head at each observation point, at end of each iteration, will be recorded in the "obs_h.out" file.
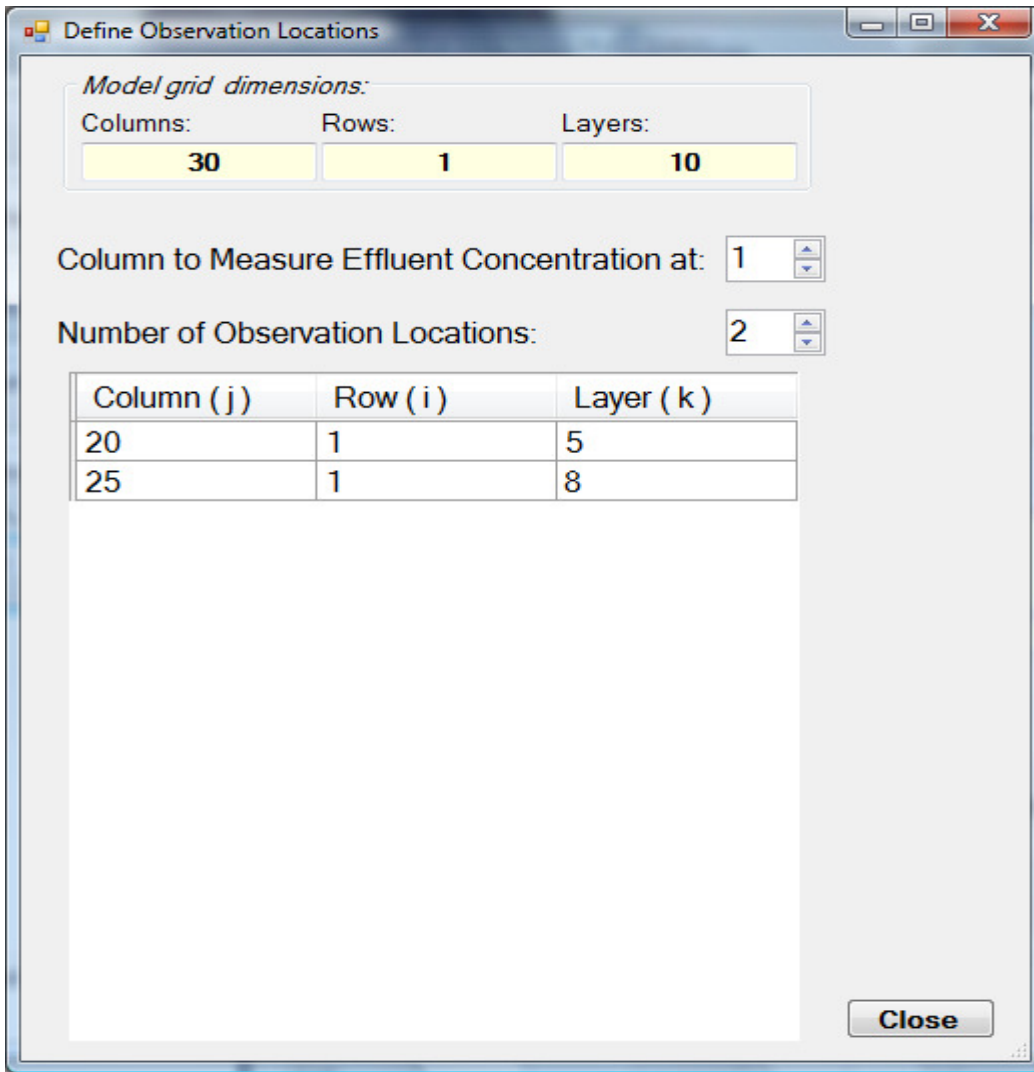
Figure 7.60: Observation Location Definition

Column to Measure Effluent—enter column number to use for calculating and recording effluent concentrations and flow rate

Number of Observation Locations—enter number of observations points at which to record concentration, mass fraction, and hydraulic head for each iteration.

Column, Row, Layer (j,i,k) of each observation point—enter the model cell coordinates of each observation location.

8. Example Simulations

Example simulation inputs are shown here for both a 2-D and a 1-D example. Complete sets of data files for these and additional examples (including 3-D, without NOD, and using different units) are included with the software distribution.

8.1. *ISCO (Using Permanganate) of Entrapped DNAPL PCE in 2-D Aquifer Containing Uniformly Distributed Fast and Slow NOD*

This simulation includes transient dissolution and chemical oxidation of stably entrapped dense non-aqueous phase liquid (DNAPL) PCE in a *confined* hypothetical 2-D aquifer. The aquifer has a dimension of 25 m long, 5 m high, and 0.05 m wide. The aquifer material exerts a uniformly distributed fast natural oxidant demand (fast NOD) of 0.0007 kg MnO_4^-/kg soil and a slow NOD of 0.0014 kg MnO_4^-/kg soil. The aquifer material has zero sorption potential, and there is no aqueous chloride or manganese oxide originally present. The saturation distribution of a DNAPL source zone is shown in Figure 8.1. In order to simulate transient dissolution of PCE and the transport of the dissolved constituent, groundwater velocity must be calculated using MODFLOW. Then, the *reactive* contaminant transport program RT3D takes over to simulate mass transfer. Additional software modules are executed before and after MODFLOW and RT3D, as appropriate, to generate or format input parameters and conditions.

In the example simulation, the aquifer is discretized into 25 columns, 10 layers, and 1 row. The simulation covers five days, broken down into 40 three-hour intervals. The injection well array is located upstream of the source zone to drive groundwater containing oxidant through aquifer. A total injection rate of 0.25 m^3/day (0.025 m^3/day into each of the 10 cells of the injection well), corresponding to a Darcy velocity of 1.0 m/day, is used in this simulation. The oxidant is permanganate (MnO_4^-) at a concentration of 10,000 mg/L (entered as 10.0 g/L which is equal to 10 kg/m^3 utilizing consistent units) or 1.0% by weight. The hydraulic head at the end of the test aquifer is kept constant at 5m. The LPF, BTN, RCT, and CORT3D.INP input files for this example are shown in Figures 8.2, 8.3-8.5, 8.6, and 8.7, respectively.
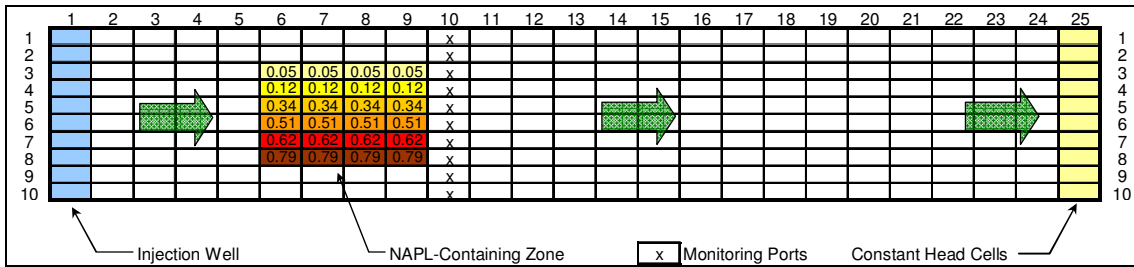
Figure 8.1: Test Aquifer for Example Problem 1.


```
        62   -888.00         0  ILPFCB,HDRY,NPLPF
 0 0 0 0 0 0 0 0 0 0
 0 0 0 0 0 0 0 0 0 0
 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1
 0 0 0 0 0 0 0 0 0 0
OPEN/CLOSE  fort.6001  1.0  (free) 0  HK layer  1
CONSTANT    1.000000E+00                VKA layer  1
OPEN/CLOSE  fort.6002  1.0  (free) 0  HK layer  2
CONSTANT    1.000000E+00                VKA layer  2
OPEN/CLOSE  fort.6003  1.0  (free) 0  HK layer  3
CONSTANT    1.000000E+00                VKA layer  3
OPEN/CLOSE  fort.6004  1.0  (free) 0  HK layer  4
CONSTANT    1.000000E+00                VKA layer  4
OPEN/CLOSE  fort.6005  1.0  (free) 0  HK layer  5
CONSTANT    1.000000E+00                VKA layer  5
OPEN/CLOSE  fort.6006  1.0  (free) 0  HK layer  6
CONSTANT    1.000000E+00                VKA layer  6
OPEN/CLOSE  fort.6007  1.0  (free) 0  HK layer  7
CONSTANT    1.000000E+00                VKA layer  7
OPEN/CLOSE  fort.6008  1.0  (free) 0  HK layer  8
CONSTANT    1.000000E+00                VKA layer  8
OPEN/CLOSE  fort.6009  1.0  (free) 0  HK layer  9
CONSTANT    1.000000E+00                VKA layer  9
OPEN/CLOSE  fort.6010  1.0  (free) 0  HK layer 10
CONSTANT    1.000000E+00                VKA layer 10
```

Figure 8.2: LPF Input File for 2D Example

```
DISSOLUTION OF PCE: 2D TEST PROBLEM                            COMMENT1
DISSOLUTION & CHEMOX MODELING                                  COMMENT2
        10         1         25        1         8         3 NLAY,NROW,NCOL,NPER,NCOMP,MCOMP
 day   m  kg                                                  TUNIT,LUNIT,MUNIT
 T T T T T F F F F F                                          TRNOP(ADV,DSP,SSM,RCT,GCG,5@N/A)
 0 0 0 0 0 0 0 0 0 0                                          LAYCON
         0       1.0                                          DELR
         0       0.05                                         DELC
         0       5.0                                          HTOP
      1001       1.0                              0           DZ(K)
      1002       1.0                              0
      1003       1.0                              0
      1004       1.0                              0
      1005       1.0                              0
      1006       1.0                              0
      1007       1.0                              0
      1008       1.0                              0
      1009       1.0                              0
      1010       1.0                              0
      4001       1.0                              0           PRSTY_EFF
      4002       1.0                              0
      4003       1.0                              0
      4004       1.0                              0
      4005       1.0                              0
      4006       1.0                              0
      4007       1.0                              0
      4008       1.0                              0
      4009       1.0                              0
      4010       1.0                              0
```

Figure 8.3: BTN Input File for 2D Example (part 1)

```
       0      1                                           ICBUND
       0      1
       0      1
       0      1
       0      1
       0      1
       0      1
       0      1
       0      1
       0      1
    7001    1.0                             0             CONC FOR CONT (M/L3)
    7002    1.0                             0
    7003    1.0                             0
    7004    1.0                             0
    7005    1.0                             0
    7006    1.0                             0
    7007    1.0                             0
    7008    1.0                             0
    7009    1.0                             0
    7010    1.0                             0
    8001    1.0                             0             CONC FOR MNO4 (M/L3)
    8002    1.0                             0
    8003    1.0                             0
    8004    1.0                             0
    8005    1.0                             0
    8006    1.0                             0
    8007    1.0                             0
    8008    1.0                             0
    8009    1.0                             0
    8010    1.0                             0
    9001    1.0                             0             CONC FOR CL (M/L3)
    9002    1.0                             0
    9003    1.0                             0
    9004    1.0                             0
    9005    1.0                             0
    9006    1.0                             0
    9007    1.0                             0
    9008    1.0                             0
    9009    1.0                             0
    9010    1.0                             0
   10001    1.0                             0             MASSFRAC FOR MNO2 (M/M)
   10002    1.0                             0
   10003    1.0                             0
   10004    1.0                             0
   10005    1.0                             0
   10006    1.0                             0
   10007    1.0                             0
   10008    1.0                             0
   10009    1.0                             0
   10010    1.0                             0
   11001    1.0                             0             MASSFRAC FOR DNAPL CONT (M/M)
   11002    1.0                             0
   11003    1.0                             0
   11004    1.0                             0
   11005    1.0                             0
   11006    1.0                             0
   11007    1.0                             0
   11008    1.0                             0
   11009    1.0                             0
   11010    1.0                             0
```

Figure 8.4: BTN Input File for 2D Example (part 2)

```
12001        1.0                             0        MASSFRAC FOR SORBED CONT (M/M)
12002        1.0                             0
12003        1.0                             0
12004        1.0                             0
12005        1.0                             0
12006        1.0                             0
12007        1.0                             0
12008        1.0                             0
12009        1.0                             0
12010        1.0                             0
13001        1.0                             0        MASSFRAC FOR FAST NOD (M/M)
13002        1.0                             0
13003        1.0                             0
13004        1.0                             0
13005        1.0                             0
13006        1.0                             0
13007        1.0                             0
13008        1.0                             0
13009        1.0                             0
13010        1.0                             0
14001        1.0                             0        MASSFRAC FOR SLOW NOD (M/M)
14002        1.0                             0
14003        1.0                             0
14004        1.0                             0
14005        1.0                             0
14006        1.0                             0
14007        1.0                             0
14008        1.0                             0
14009        1.0                             0
14010        1.0                             0
 -999.0      0.01                                     CINACT, THKMIN
     1         0         0         0        T         IFMTCN,IFMTNP,IFMTRF,IFMTDP,SAVUCN
     0                                                NPRS {save results at end}
     0         1                                      NOBS, NPROBS
     T         1                                      CHKMAS, NPRMAS
 0.125         6       1.0                             PERLEN,NSTP,TSMULT
   0.0    100000       1.0       0.0                   DT0,MXSTRN,TTSMULT,TTSMAX
```

Figure 8.5: BTN Input File for 2D Example (part 3)

```
        0          10         15         2          1          2
    2001      1.0                                    2                   RHOB (M/L3)
    2002      1.0                                    2
    2003      1.0                                    2
    2004      1.0                                    2
    2005      1.0                                    2
    2006      1.0                                    2
    2007      1.0                                    2
    2008      1.0                                    2
    2009      1.0                                    2
    2010      1.0                                    2
1.0e-010 1.0e-009                                                        ATOL,RTOL
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
0.000075168                                                     rc(1):Dm_cont   (L2/T)
0.00014112                                                      rc(2):Dm_mno4   (L2/T)
0.000175392                                                     rc(3):Dm_cl     (L2/T)
1.3333                                                          rc(4):Y_mno4_cont (mol/mol)
4.0                                                             rc(5):Y_cl_cont   (mol/mol)
1.0                                                             rc(6):Y_mno2_mno4 (mol/mol)
1000.0                                                          rc(7):rho_mno2  (M/L3)
0.165875                                                        rc(8):MW_cont   (M/mol)
1630.0                                                          rc(9):rho_cont  (M/L3)
3.888                                                           rc(10):k2_cont  (L3/mol-T)
0.200                                                           rc(11):C_c_star (M/L3)
0.0                                                             rc(12):xi       (1/T)
0.15                                                            rc(13):lambda_c (L3/M)
4.8                                                             rc(14):k_nod_f  (1/T)
0.48                                                            rc(15):k_nod_s  (1/T)
    3001      1.0                                    2          vrc(1):k_La     (1/T)
    3002      1.0                                    2
    3003      1.0                                    2
    3004      1.0                                    2
    3005      1.0                                    2
    3006      1.0                                    2
    3007      1.0                                    2
    3008      1.0                                    2
    3009      1.0                                    2
    3010      1.0                                    2
    5001      1.0                                    2          vrc(2):initial porosity
    5002      1.0                                    2
    5003      1.0                                    2
    5004      1.0                                    2
    5005      1.0                                    2
    5006      1.0                                    2
    5007      1.0                                    2
    5008      1.0                                    2
    5009      1.0                                    2
    5010      1.0                                    2
```

Figure 8.6: RCT Input File for 2D Example

```
EX1.nam             / MODFLOW name (NAM or MFN) file
EX1.rts             / MODFLOW RT3D super (RTS) file
40                  / number of iterations to perform
N                   / is this a continuation of another run (Y/N)?
init_K.inp          / input file containing hydraulic conductivity for all layers
phi0.inp            / input file containing porosity for all layers (w/ no napl)
d50.inp             / input file containing d50 for all layers
srw.inp             / input file containing residual water saturation for all layers
sn.inp              / input file containing DNAPL saturation for all layers
smn.inp             / input file containing MnO2 pseudo-saturation for all layers
conc7.out           / output file containing contaminant concentration
conc8.out           / output file containing permanganate concentration
conc9.out           / output file containing chloride concentration
mfrac10.out         / output file containing MnO2 mass fraction
mfrac11.out         / output file containing NAPL mass fraction
mfrac12.out         / output file containing Sorbed contaminant mass fraction
mfrac13.out         / output file containing Fast NOD mass fraction
mfrac14.out         / output file containing Slow NOD mass fraction
mass.out            / output file containing mass of immobile species within model
obs_c.out           / output file containing mobile species conc. at obs. points
obs_m.out           / output file containing immobile species mass frac. at obs. points
obs_h.out           / output file containing heads at observation points
2710.0              / density of the solid phase (M/L3)
2.0                 / tortuosity factor (tau)
9.170               / alpha_1 - empirical parameter for natural dissolution
0.216               / alpha_2 - empirical parameter for natural dissolution
0.5                 / alpha_3 - empirical parameter for natural dissolution
1.071               / alpha_4 - empirical parameter for natural dissolution
10                  / number of obs pts.
8  1   1            / col row lay (j,i,k) for obs. pts.
8  1   2
8  1   3
8  1   4
8  1   5
8  1   6
8  1   7
8  1   8
8  1   9
8  1  10
24                  / effluent concentration measured at column #
```

Figure 8.7: <u>CORT3D.INP</u> Input File for 2D Example

Next, the initial concentrations and mass fractions must be defined. For this simulation, the initial concentration of PCE, oxidant, and chloride are all zero throughout the aquifer. The initial mass fractions of $MnO_{2\,(s)}$ and sorbed contaminant are also zero. Consequently, the 'file_gen.y000' files for these components are configured to set the value for each respective component to zero in all cells as demonstrated for PCE using the 'file_gen.7000' file shown in Figure 8.8. **Note that the C3DI front-end program does not read in values generated from a 'file_gen.y000' file. C3DI will only read in initial concentrations and mass fractions defined in 'fort.xxyyy.ini' files.**

```
7000            / starting file series number
0.0             / value to be written
```

Figure 8.8: FILE_GEN.Y000 Input File Structure (Example FILE_GEN.7000 to set Initial Contaminant Concentration throughout Model to Zero)

However, there is both fast and slow NOD present throughout the site. In order to demonstrate both methods of setting the initial concentration or mass fraction of a species, the 'fort.yxxx.ini' method is used for the slow NOD (where 'y' = 13) and the 'file_gen.yxxx' method is used for the fast NOD (where 'y' = 14, and 'xxx' is each layer in turn), as shown in Figures 8.9 and 8.10, respectively. For this example, the 'file_gen.yxxx' method could have been used for both NOD components, since the initial mass fraction of each is uniform throughout the site. If the initial mass fraction of slow NOD actually varied throughout the site, the 'fort.13xxx' files would be set up to contain varying values for each cell within the specified layer.

```
0.000700000000000E+000   0.000700000000000E+000   0.000700000000000E+000
0.000700000000000E+000   0.000700000000000E+000   0.000700000000000E+000
0.000700000000000E+000   0.000700000000000E+000   0.000700000000000E+000
0.000700000000000E+000   0.000700000000000E+000   0.000700000000000E+000
0.000700000000000E+000   0.000700000000000E+000   0.000700000000000E+000
0.000700000000000E+000   0.000700000000000E+000   0.000700000000000E+000
0.000700000000000E+000   0.000700000000000E+000   0.000700000000000E+000
0.000700000000000E+000   0.000700000000000E+000   0.000700000000000E+000
0.000700000000000E+000
```

Figure 8.9: FILE_GEN.YXXX.INI Input File Structure (Example FILE_GEN.13001.INI for Fast NOD in Layer 1)

```
14000           / starting file series number
0.0014          / value to be written
```

Figure 8.10: FILE_GEN.14000 Input File (Setting Uniform Initial Mass Fraction for Slow NOD throughout Model)

Finally, the D50.INP, INIT_K.INP, PHI0.INP, SRW.INP, and SN.INP.INI files need to be built. For this example, all cells have a median soil grain size diameter of

0.0025 m within the DNAPL source zone and 0.001 m elsewhere (entered in 'D50.INP' file), an initial fully water-saturated hydraulic conductivity of 25.0 m/day in the source zone and 7.5 m/day elsewhere, an initial total porosity of 0.45 in the source zone and 0.34 elsewhere, a uniform residual water saturation of 0.04, an initial DNAPL saturation distribution as shown in Figure 8.1, and an initial uniform MnO_2 (s) pseudo-saturation of zero. Figure 8.11 demonstrates using the multiplier method to setup the 'SRW.INP.INI' file since all cells have the same value (i.e., 10 rows by 25 columns by 1 layer equals 250 cells with a value of 0.04). If the residual saturations vary spatially, individual values must be entered for each cell. Figure 8.12 demonstrates building the initial DNAPL saturation distribution ('SN.INI.INP' file) entering a value for each cell since cell values are not uniform (**this method must also be used if the input file will be read into the C3DI.EXE front-end program**).

```
250*0.04
```

Figure 8.11: SRW.INP Input File Structure (Example of Using Multiplier to Enter Values)

```
0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.05   0.05   0.05   0.05   0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.12   0.12   0.12   0.12   0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.34   0.34   0.34   0.34   0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.51   0.51   0.51   0.51   0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.62   0.62   0.62   0.62   0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.79   0.79   0.79   0.79   0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
```

Figure 8.12: SN.INP.INI Input File (Columns 1-11 Only, Remaining Columns are Zero)

Once all files are created, execute the simulation. Upon simulation completion, results can be analyzed using the USGS Model Viewer, GMS, or a spreadsheet.

8.2. ***ISCO (Using Permanganate) of Entrapped DNAPL PCE in 1-D Column Containing Uniformly Distributed Fast and Slow NOD***

This simulation includes transient dissolution and chemical oxidation of stably entrapped, residual dense non-aqueous phase liquid (DNAPL) PCE in a hypothetical 1-D column. The column has a dimension of 40 cm long, 4.5 cm high, and 4.5 cm wide. The aquifer material exerts a uniformly distributed fast natural oxidant demand (fast NOD) of 0.0007 kg MnO_4^-/kg soil and a slow NOD of 0.0014 kg MnO_4^-/kg soil. The aquifer material has zero sorption potential, and there is no aqueous chloride or manganese oxide originally present. The residual PCE (1.0% saturation) is distributed in the column as shown in Figure 8.13. In this example simulation, the column is discretized into 40 columns, 1 layer, and 1 row. The simulation covers 14 days, broken down into 56 six-hour intervals. The injection is located upstream of the source zone to drive groundwater containing oxidant through column. An injection rate of 0.886 mL/min, corresponding to a Darcy velocity of 63.0 cm/day, is used in this simulation. The oxidant is permanganate (MnO_4^-) at a concentration of 7,500 mg/L (entered as 7.5 g/L which is equal to 7.5 kg/m^3 utilizing consistent units) or 0.75% by weight. The hydraulic head at the end of the test column is kept constant at 4.5 cm. The BTN, RCT, and CORT3D.INP input files for this example are shown in Figures 8.14, 8.15, 8.16 and 8.17, respectively.
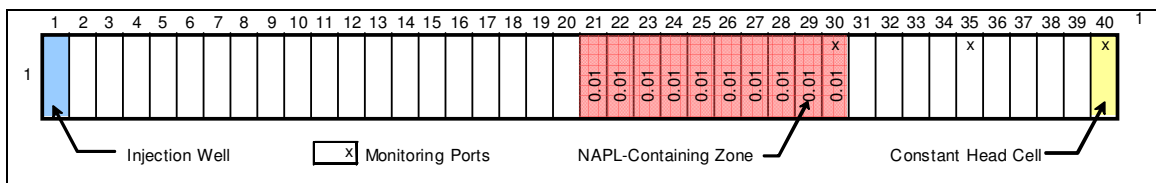

Figure 8.13: Test Column for Example Problem 2.

```
40   -888.0   0
1
0
-1.0
1
0
OPEN/CLOSE  fort.6001   1.0  (free) 0  HK layer  1
CONSTANT 1.0
CONSTANT 1.0
```

Figure 8.14: LPF Input File for 1D Example

```
GMS MT3D Simulation                               COMMENT1
08 November 2004                                  COMMENT2
         1         1        40        1        8        3
 hr  cm  mg                                       TUNIT,LUNIT,MUNIT
T T T T F F F F F                                 TRNOP(ADV,DSP,SSM,RCT,GCG,5@N/A)
1                                                 LAYCON
        0 1.0000000                               DELR
        0 4.5000000                               DELC
        0 4.5000000                               HTOP
     1001       1.0                        0      DZ(K)
     4001       1.0                        0      PRSTY_EFF
        0         1                               ICBUND
     7001       1.0                        0      CONC FOR CONT (M/L3)
     8001       1.0                        0      CONC FOR MNO4 (M/L3)
     9001       1.0                        0      CONC FOR CL (M/L3)
    10001       1.0                        0      MASSFRAC FOR MNO2 (M/M)
    11001       1.0                        0      MASSFRAC FOR DNAPL CONT (M/M)
    12001       1.0                        0      MASSFRAC FOR SORBED CONT (M/M)
    13001       1.0                        0      MASSFRAC FOR FAST NOD (M/M)
    14001       1.0                        0      MASSFRAC FOR SLOW NOD (M/M)
-999.0000                                         CINACT, THKMIN
        1         0         0         0        T  IFMTCN,IFMTNP,IFMTRF,IFMTDP,SAVUCN
        0                                         NPRS
        0         1                               NOBS, NPROBS
        T         1                               CHKMAS, NPRMAS
  6.00000        12 1.0000000                     PERLEN,NSTP,TSMULT
     0.0      1000 1.0000000              0.0     DT0,MXSTRN,TTSMULT,TTSMAX
```

Figure 8.15: BTN Input File for 1D Example

```
         0        10        15         2         1         2
      2001       1.0                              2          RHOB (M/L3)
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
1.0e-010 1.0e-009
0.03132                                          rc(1):Dm_cont   (L2/T)
0.0588                                           rc(2):Dm_mno4   (L2/T)
0.07308                                          rc(3):Dm_cl     (L2/T)
1.3333                                           rc(4):Y_mno4_cont (mol/mol)
4.0                                              rc(5):Y_cl_cont   (mol/mol)
1.0                                              rc(6):Y_mno2_mno4 (mol/mol)
3000.0                                           rc(7):rho_mno2 (M/L3)
165830.0                                         rc(8):MW_cont  (M/mol)
1630.0                                           rc(9):rho_cont (M/L3)
262000.0                                         rc(10):k2_cont  (L3/mol-T)
0.200                                            rc(11):C_c_star (M/L3)
0.0                                              rc(12):xi  (1/T)
150.0                                            rc(13):lambda_c (L3/M)
52152.35                                         rc(14):k_nod_f  (1/T)
3.36e-005                                        rc(15):k_nod_s  (1/T)
      3001       1.0                              2          vrc(1):k_La (1/T)
      5001       1.0                              2          vrc(2):initial porosity
```

Figure 8.16: RCT Input File for 1D Example

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```
ex2.mfn          / MODFLOW name (NAM or MFN) file
ex2.rts          / MODFLOW RT3D super (RTS) file
56               / number of iterations to perform
n                / is this a continuation of another run (Y/N)?
init_K.inp       / input file containing hydraulic conductivity for all layers
phi0.inp         / input file containing porosity for all layers (w/ no DNAPL)
d50.inp          / input file containing d50 for all layers
srw.inp          / input file containing residual water saturation for all layers
sn.inp           / input file containing DNAPL saturation for all layers
smn.inp          / input file containing MnO2 pseudo-saturation for all layers
conc7.out        / output file containing contaminant concentration
conc8.out        / output file containing permanganate concentration
conc9.out        / output file containing chloride concentration
mfrac10.out      / output file containing MnO2 mass fraction
mfrac11.out      / output file containing DNAPL mass fraction
mfrac12.out      / output file containing Sorbed contaminant mass fraction
mfrac13.out      / output file containing Fast NOD mass fraction
mfrac14.out      / output file containing Slow NOD mass fraction
mass.out         / output file containing mass of immobile species within model
obs_c.out        / output file containing mobile species conc. at obs. points
obs_m.out        / output file containing immobile species mass frac. at obs. points
obs_h.out        / output file containing heads at observation points
2700.0           / density of the solid phase (M/L3)
2.0              / tortuosity factor (tau)
9.170            / alpha_1 - empirical parameter for natural dissolution
0.216            / alpha_2 - empirical parameter for natural dissolution
0.5              / alpha_3 - empirical parameter for natural dissolution
1.071            / alpha_4 - empirical parameter for natural dissolution
3                / number of obs pts.
30  1   1        / col row lay (j,i,k) for obs. pts.
35  1   1
40  1   1
39               / effluent concentration measured at this column
```

Figure 8.17: <u>CORT3D.INP</u> Input File for 1D Example

Next, the initial concentrations and mass fractions must be defined. For this simulation, the initial concentration of PCE, oxidant, and chloride are all zero throughout the aquifer. The initial mass fractions of $MnO_{2\ (s)}$ and sorbed contaminant are also zero. Consequently, the 'file_gen.y000' files for these components are configured to set the value for each respective component to zero in all cells as demonstrated for PCE using the 'file_gen.7000' file shown in Figure 8.8.

However, there is both fast and slow NOD present throughout the site. In order to demonstrate both methods of setting the initial concentration or mass fraction of a species, the 'fort.yxxx.ini' method is used for the slow NOD (where 'y' = 13) and the 'file_gen.yxxx' method is used for the fast NOD (where 'y' = 14, and 'xxx' is each layer in turn). For this example, the 'file_gen.yxxx' method could have been used for both NOD components, since the initial mass fraction of each is uniform throughout the site. If the initial mass fraction of slow NOD actually varied throughout the site, 'fort.13xxx.ini' files would be set up to contain varying values for each cell within the specified layer. **Note**

that the C3DI front-end program does not read in values generated from a 'file_gen.y000' file. C3DI will only read in initial concentrations and mass fractions defined in 'fort.xxyyy.ini' files.

Finally, the D50.INP, INIT_K.INP, PHI0.INP, SRW.INP, and SN.INP.INI files need to be built. For this example, all cells have a uniform median soil grain size diameter of 0.13 cm (entered in 'D50.INP' file), a uniform initial fully water-saturated hydraulic conductivity of 87.5 cm/hr, a uniform initial total porosity of 0.41, a uniform residual water saturation of 0.04, and an initial DNAPL saturation distribution as shown in Figure 8.13.

Once all files are created, execute the simulation. Upon simulation completion, results can be analyzed using the USGS Model Viewer, GMS, or a spreadsheet.

9.   Post-processing

Upon completion of a simulation run, the CORT3D code creates text-based output files that can be imported into a spreadsheet program for analysis. Additionally, binary output files are created to facilitate post-processing using two readily available software packages: Model Viewer 1.2 from the USGS, and GMS 6.5 from US Army Corps of Engineers.

9.1.   Model Viewer 1.2

If Model Viewer software is installed, using it for post-processing is fairly straight-forward. After running the CORT3D simulation, double-click the Model Viewer file (i.e. 'MV_species.MV') for the desired species, where 'species' indicates the species as indicated in Table 9.1. This will open the desired data files in Model Viewer, and you will see something like what is shown in Figure 9.1. The next step is to update the display to show the entire model grid.

Table 9.1: Model Viewer Species Files

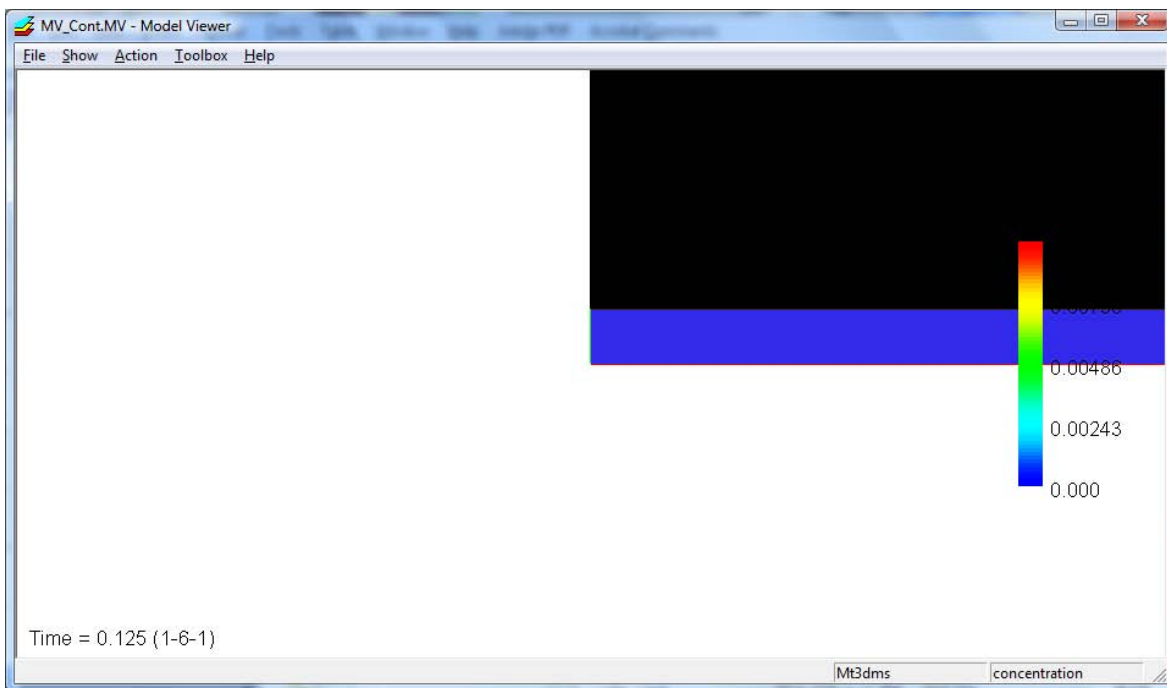| Species	Model Viewer File
Contaminant	MV_Cont.MV
Oxidant	MV_Oxid.MV
Chloride	MV_Cl.MV
Manganese Oxide	MV_MnO2.MV
DNAPL Contaminant	MV_NAPL.MV
Sorbed Contaminant	MV_Sorb.MV
Fast NOD	MV_FNOD.MV
Slow NOD	MV_SNOD.MV

Figure 9.1: Model Viewer Initial Display

Updating the display is accomplished by clicking on "Reset Viewport" under the "Action" pull-down menu as shown in Figure 9.2. This will resize the display so the entire model grid is displayed on the screen. Next, you need to choose what direction to view the model grid from. This is done by clicking "View From Direction" on the "Action" pull-down menu, and then clicking on the desired direction (e.g. +x, -x, +y, -y, +z, -z). The axes are defined as follows: the positive x axis is oriented along a row of cells and points in the direction of increasing column numbers (as defined in MODFLOW), the positive y

axis is oriented along a column of cells and points in the direction of decreasing row numbers (as defined in MODFLOW), and the positive z axis points vertically upward. Once you have the display configured, save the configuration by clicking "Save" from the "File" pull-down menu.
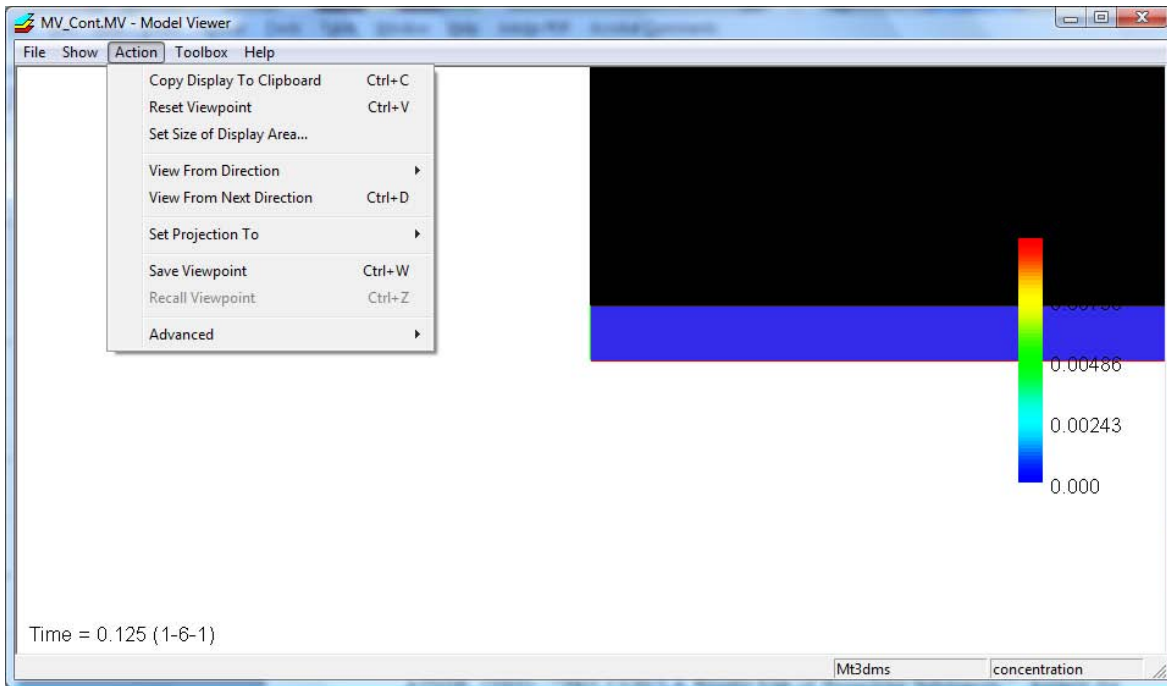
Figure 9.2: Model Viewer Action Pull-down Menu

In order to view the model at a specific point in time, or to create an animation of the simulation, choose "Animation" from the "Toolbox" pull-down menu. The Animation Toolbox will then be displayed as shown in Figure 9.3. To view a specific time point, click the arrow next to "Set to Time," select the desired time point, and then click "Set." If the display is set to any time point, other than the final one, you can click "Advance" to set the display to the next time point. Alternately, you can click "Run" to view an animation from the current time point through the final time point. The speed of the animation can be adjusted by clicking the "Options" tab of the Animation toolbox and adjusting the "Delay" value.
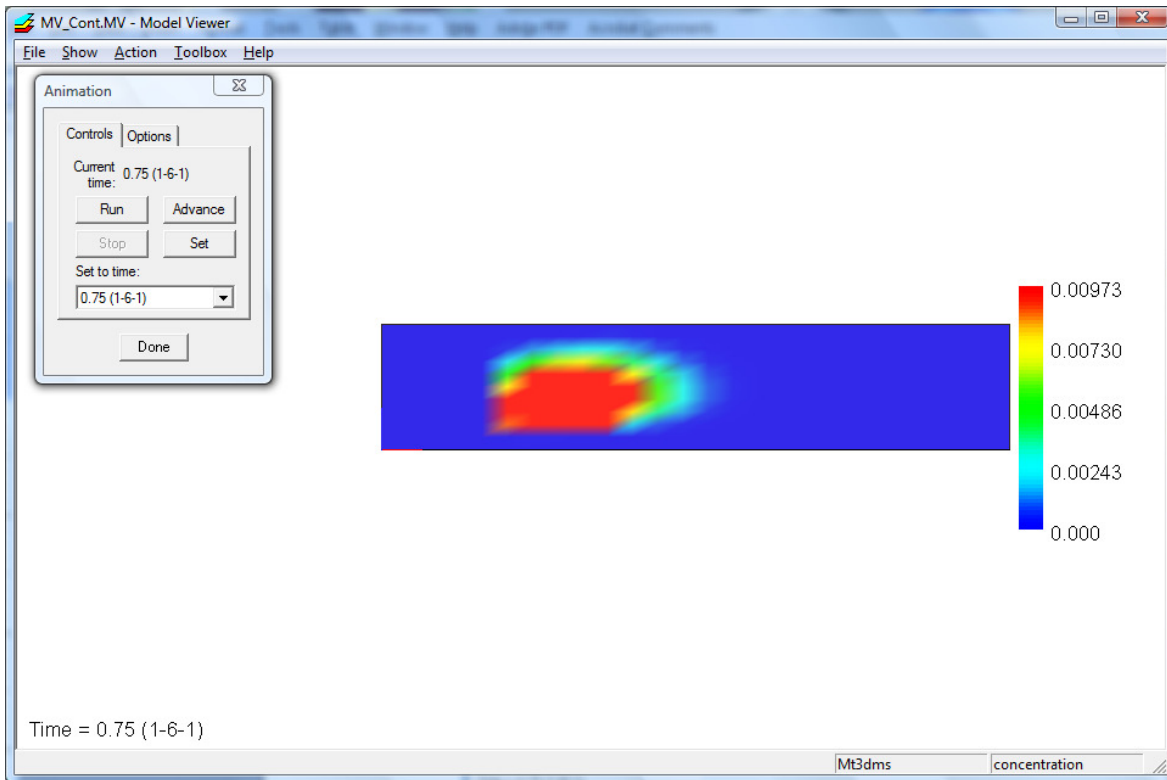
Figure 9.3: Model Viewer Animation Toolbar

Refer to Figure 9.4 for additional toolboxes you will find useful. The "Scalar" tab of the "Data" toolbox displays the maximum and minimum data values. These values are useful in configuring the limits to use for the contour coloring, on the "Limits" tab of the "Color Bar" toolbox. The "Size" tab of the "Color Bar" toolbox allows you to set the size of the color bar, as well as the distance from the right edge of the color bar in pixels to the right side of the display area. The "Scale" tab of the "Geometry" toolbox is used to set the scale factor for viewing the model grid. Finally, the "Controls" tab of the "Crop" toolbox is used to display interior regions of the model—this is especially useful for 3-D models. For more information on the capabilities of Model Viewer, and detailed instructions, refer to the Model Viewer User's Guide or Online Help.
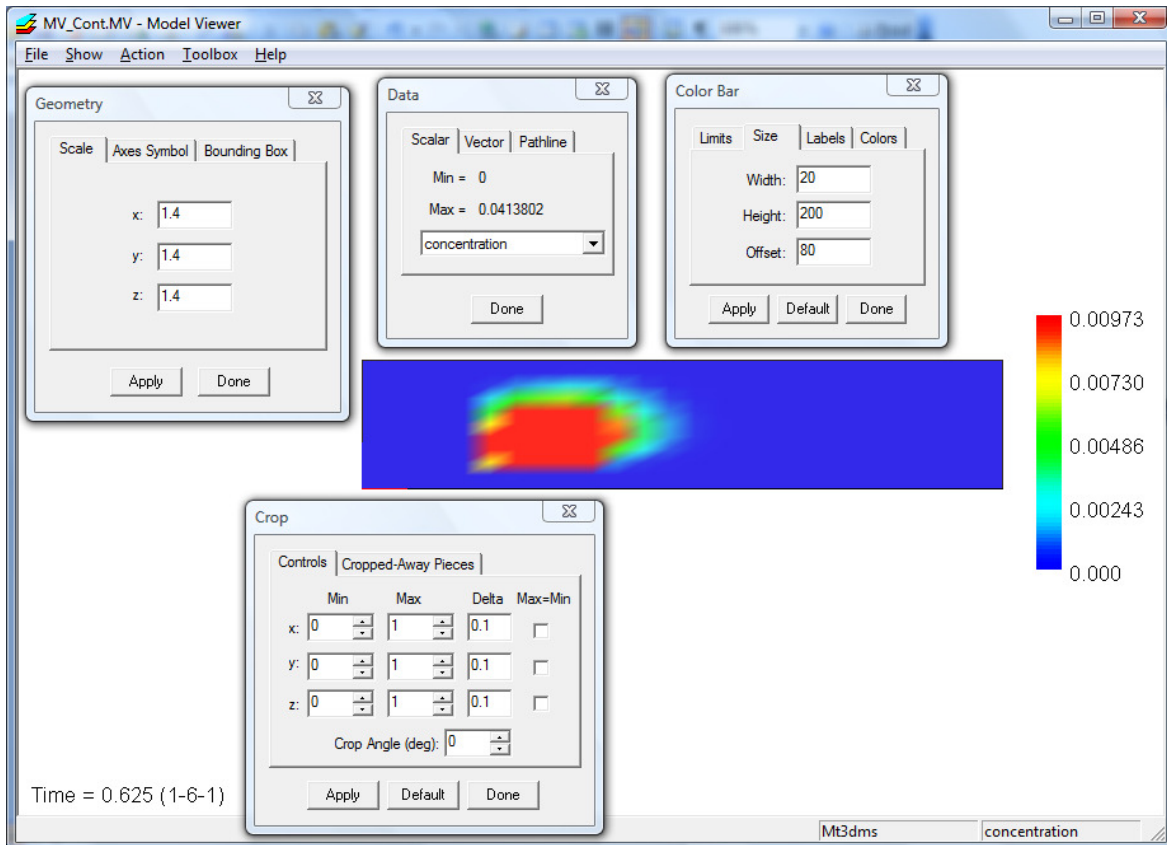
Figure 9.4: Model Viewer Other Useful Toolbars

9.2. Groundwater Modeling System (GMS) 6.5

If you have GMS, you can use it to view and analyze the results from CORT3D. The following instructions assume you already have a working copy of GMS version 6.5 installed. However, it is expected that any version of GMS from 5.0 and later will work as well.

After running the CORT3D simulation, open GMS which will look much like Figure 9.5. The first step is to open the MODFLOW Super file created by CORT3D. To do this, choose "Open" from the "File" pull-down menu. In the open file dialog box that appears (Figure 9.6), click the arrow next to the "Files of Type" field and select "Model Super Files." The open file dialog box now looks similar to Figure 9.7. Select the 'GMS.MFS' file and click "Open" to read the flow model setup.
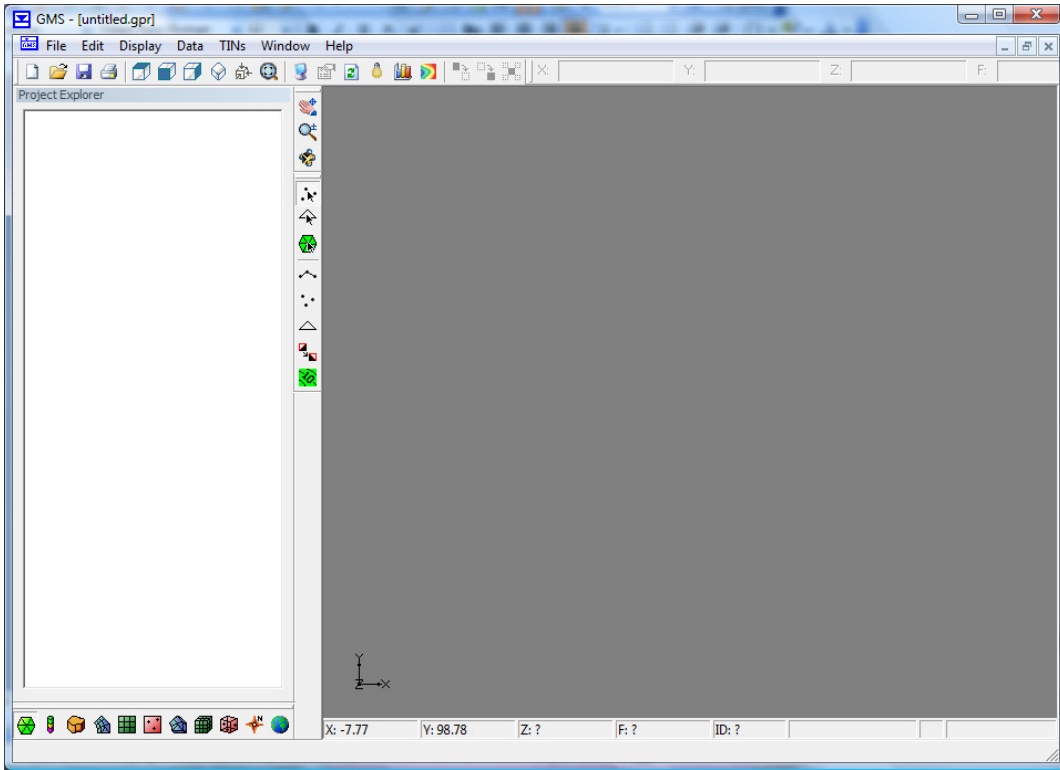
Figure 9.5: GMS Opening View
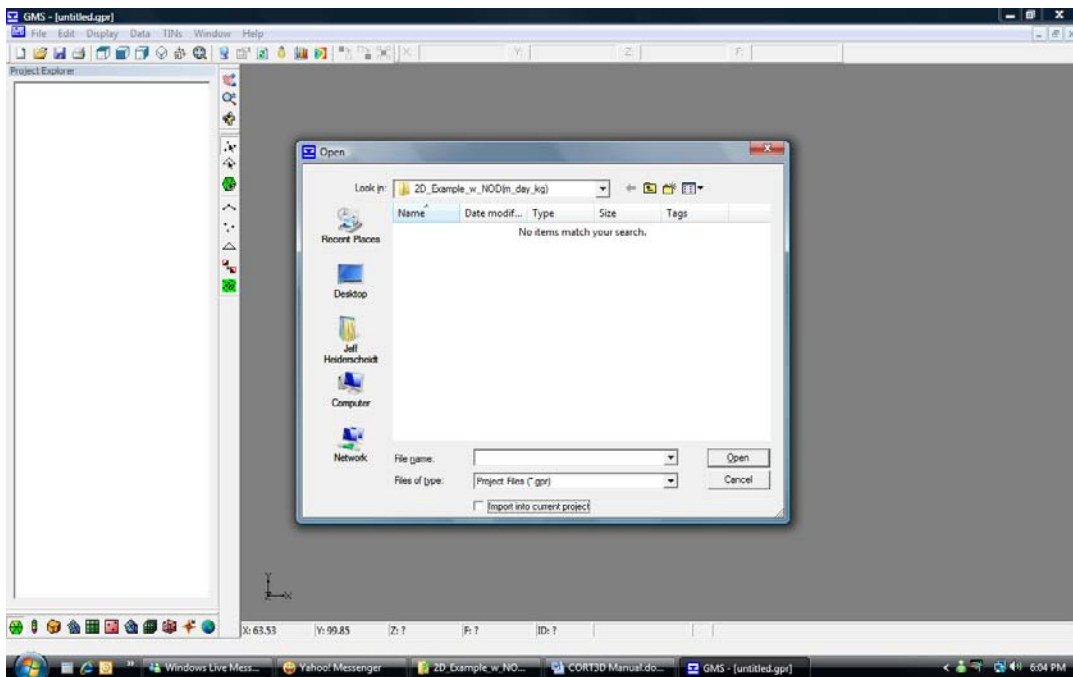
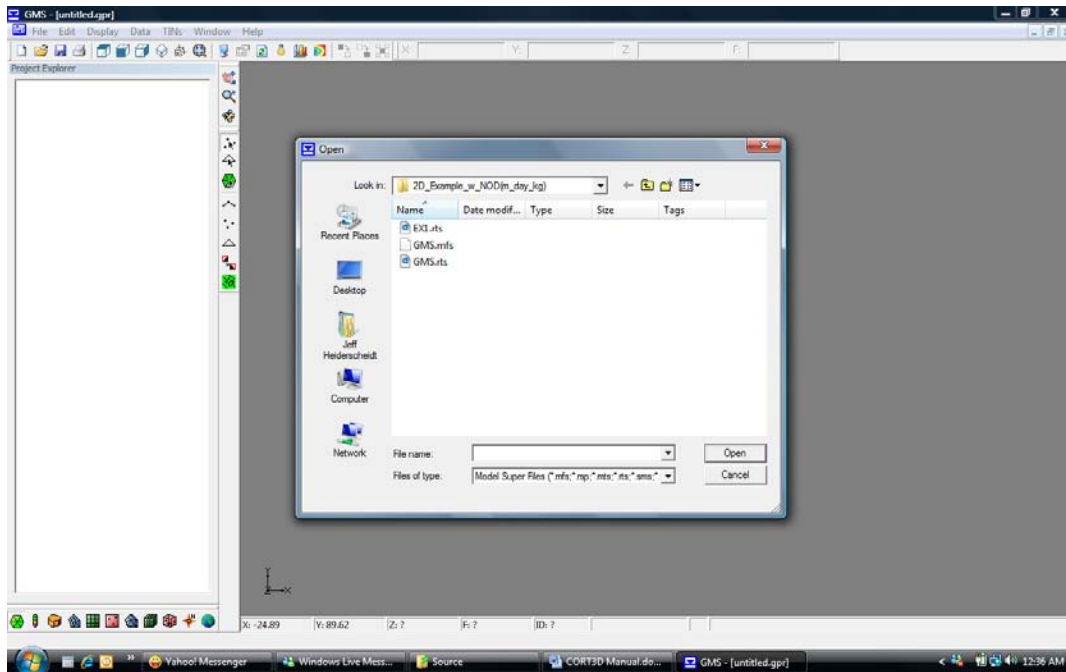**Figure 9.6: GMS Open File Dialog Box**

Figure 9.7: Opening MODFLOW Super File in GMS

After the flow solution is loaded, the model grid will be visible in the model window and the data tree will be visible on the left side of the display. Now, open the RT3D Super File by again choosing "Open" from the "File" pull-down menu. This time, it will default to "Files of Type" field already being set to "Model Super Files," similar to Figure 9.8. Select the 'GMS.RTS' file and click "Open" to read the transport solution. A dialog box will appear asking if you want to continue reading an old Advection Package file (Figure 9.9). Click "OK" to read the transport model setup.
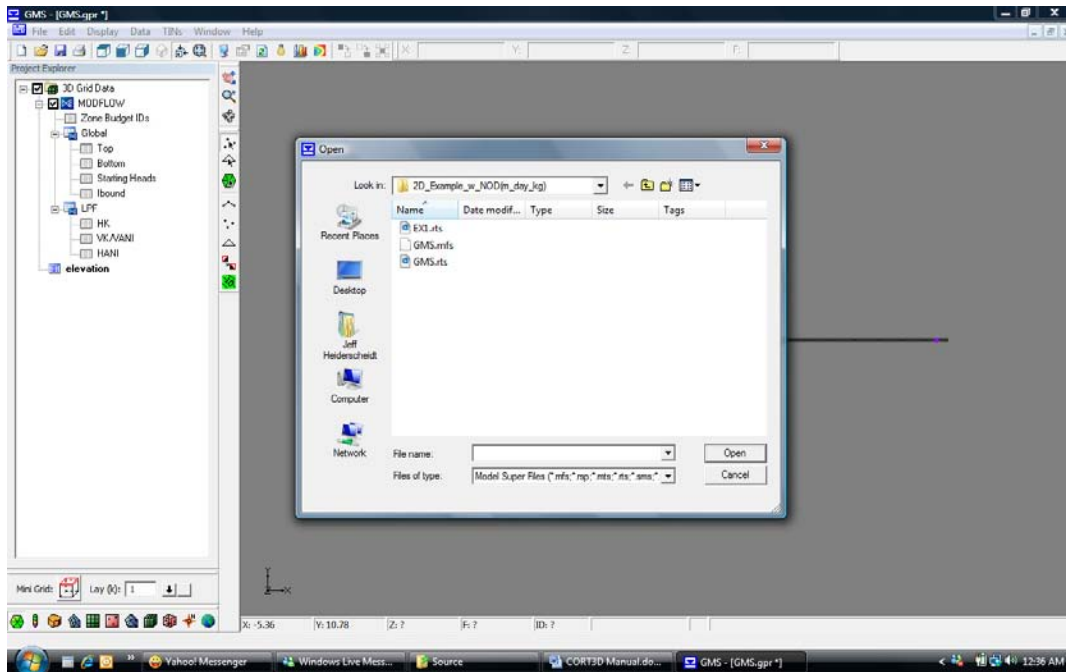
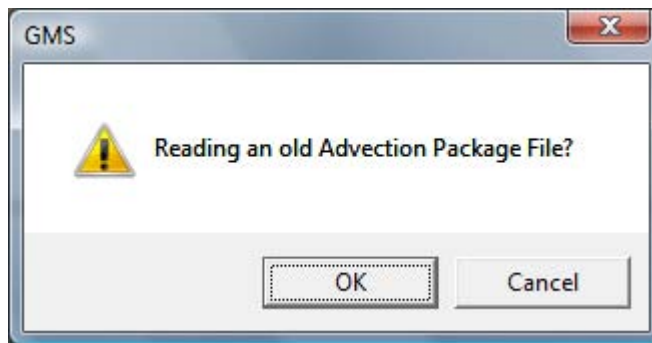**Figure 9.8: Opening RT3D Super File in GMS**

Figure 9.9: Read Old Advection Package File Dialog Box

Now that the flow and transport models have been loaded, click the "3-D Grid" button at the bottom, left of the display (Figure 9.10), and a new set of pull-down menus and toolbars will appear as shown in Figure 9.11. Select which type of view you want of the model grid by clicking on one of the view buttons (plan, front, or side, respectively) indicated in Figure 9.11. The next step is to read in the flow and transport solutions.
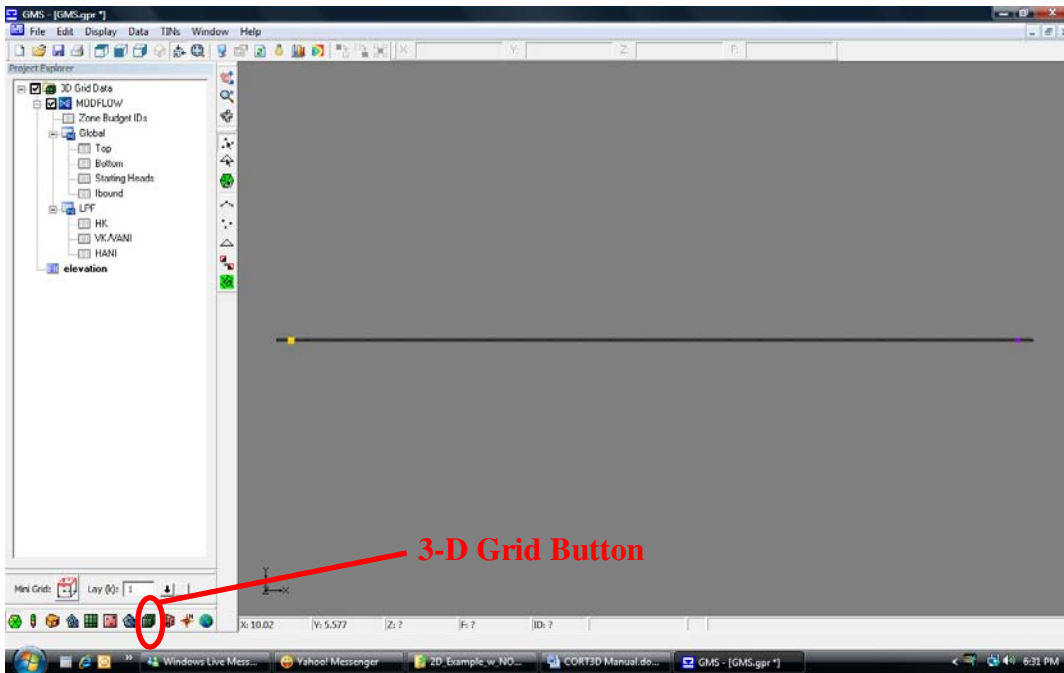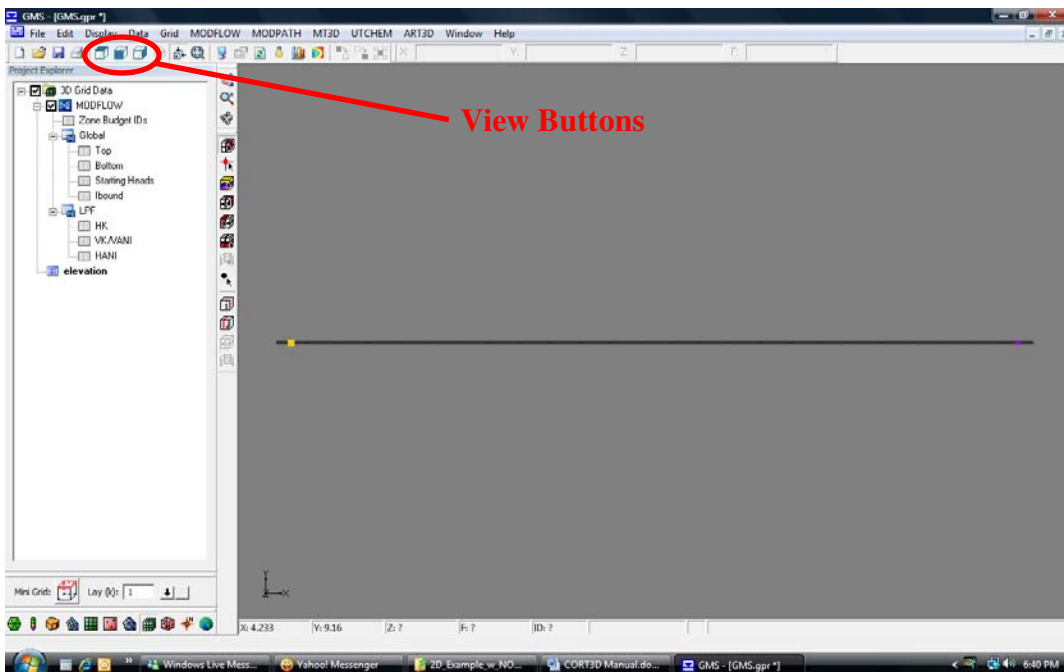
Figure 9.10: 3-D Grid Button

Figure 9.11: 3-D Grid Display with Flow and Transport Menus

To read in the flow solution, select "Read Solution…" from the "MODFLOW" pull-down menu and select the 'GMS.MFS' file as shown in Figure 9.12, then click "Open." Similarly, to read in the transport solution, select "Read Solution…" from the "MT3D" pull-down menu and select the 'GMS.RTSS' file as shown in Figure 9.13, then click "Open."
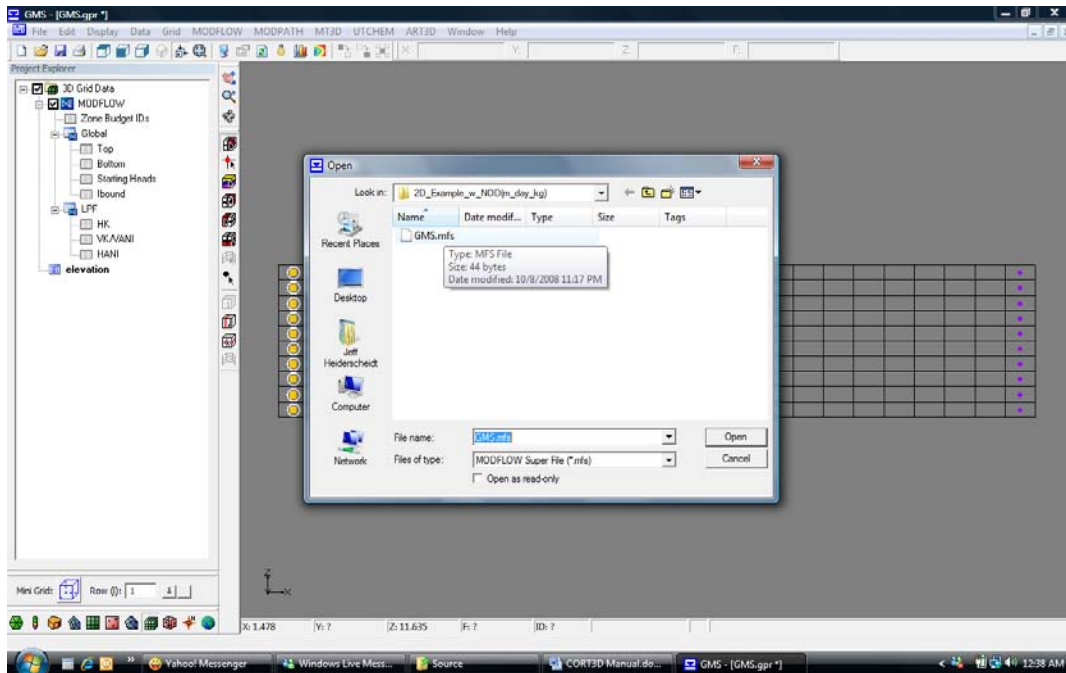

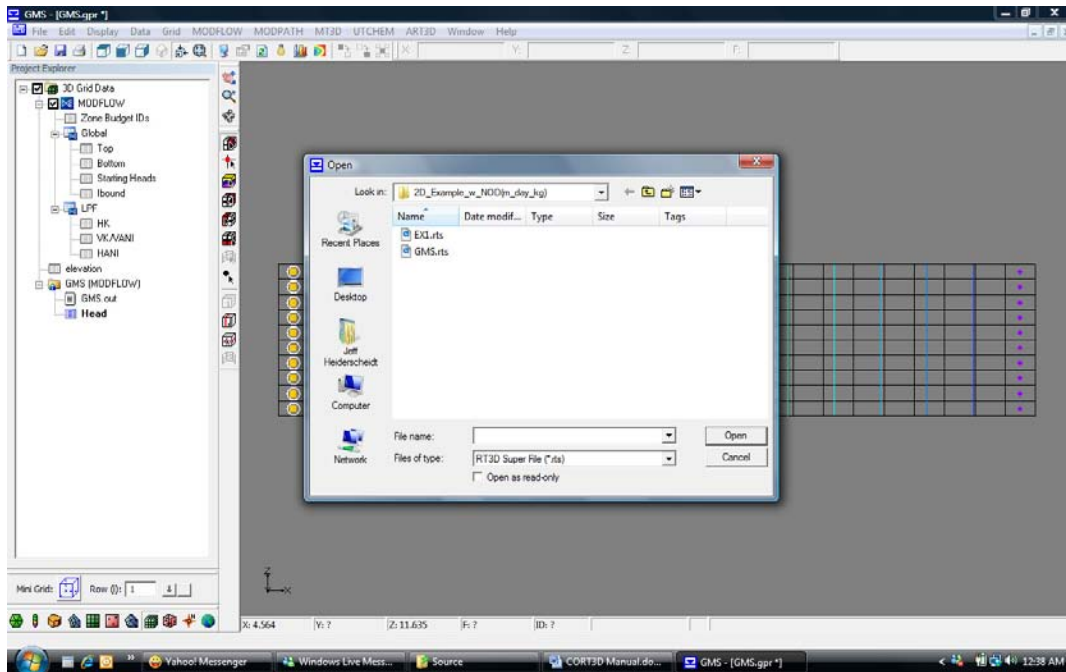**Figure 9.12: Opening Flow (MODFLOW) Solution File**

Figure 9.13: Opening Transport (RT3D) Solution File

After reading in the flow and transport solutions, ensure the simulation units are set to the correct values. This is accomplished by selecting "Units" from the "Edit" pull-down menu. The resulting dialog box will resemble the one in Figure 9.14. The "Length" and "Time" units should be correct as they are read from the MODFLOW DIS file. However, the "Mass" and "Concentration" values may need to be updated since default values ("mg" and "mg/L") are used instead of reading in values from BTN file. **It is critical that you select the same "Mass" unit you entered in the BTN file, and select a "Concentration" unit that is equivalent to the ("Mass" unit divided by the "Length" unit cubed).** Once all the units are set correctly, click "OK."

At this point, be sure to save the GMS project. To do this, select "Save" from the "File" pull-down menu. The resulting project file is 'GMS.GPR' and can be re-opened later by simply double-clicking it. Alternately, the project can be saved under a different name by selecting "Save As…" under the "File" menu.
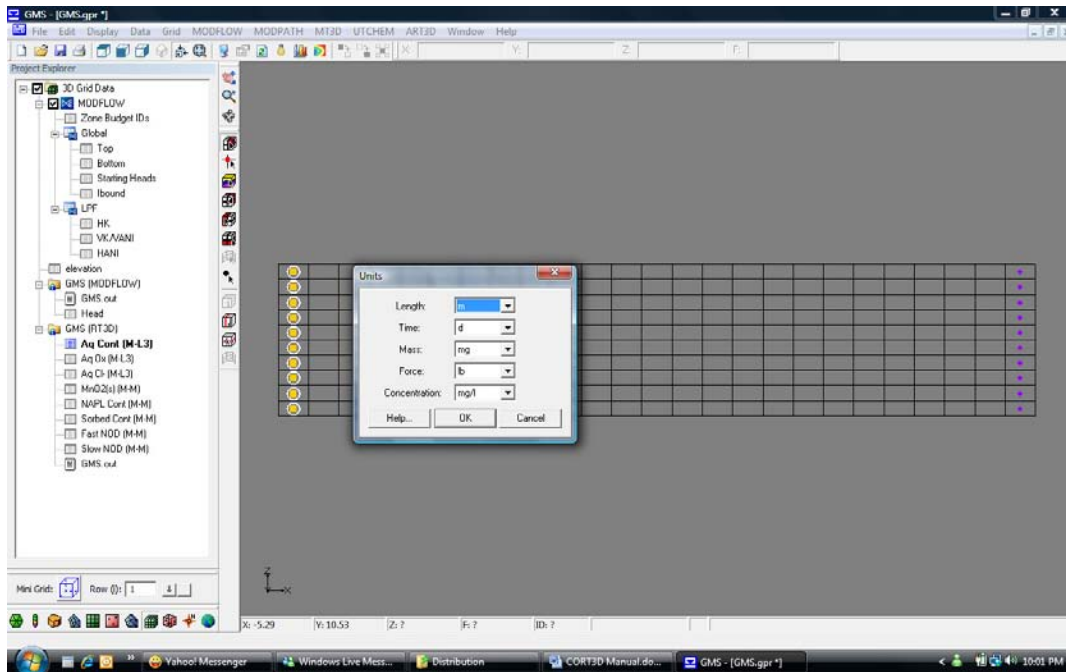
Figure 9.14: Verifying Correct Units

At this point, the display will show the first time step of the first species (aqueous contaminant) as seen in Figure 9.15. The active data set is shown in bold on the data tree on the left side of the display. Click on the bold data set ("Aq Cont M-L3") and the "Time Step Window" will appear in the bottom, left corner as shown in Figure 9.16.

From here, you can manipulate the display as needed to analyze results. Click on the desired time step in the "Time Step Window" to update the display to that time step. In the data tree on the left side, click on the desired species under the "GMS (RT3D)" branch to view the concentration or mass fraction distribution of that species. Similarly, you can click on "Head" under the "GMS (MODFLOW)" branch to see the head distribution. You can also click on the "View Buttons" (Figure 9.11), as described previously, to view the model grid from a different direction. Refer to GMS documentation and Online Help for more detailed instructions and capabilities.
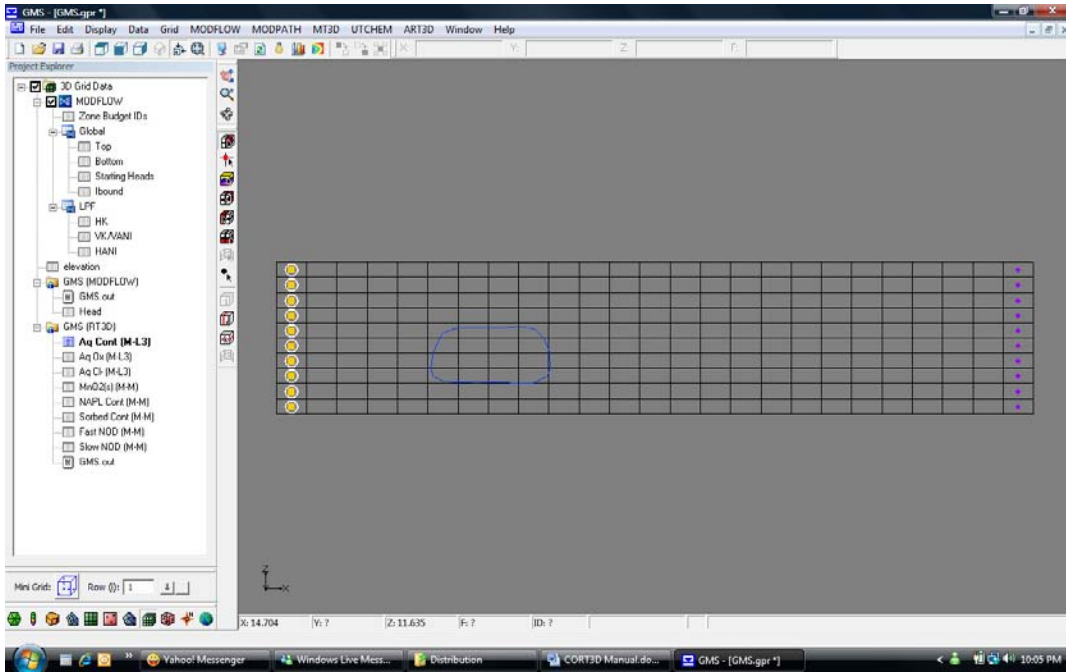
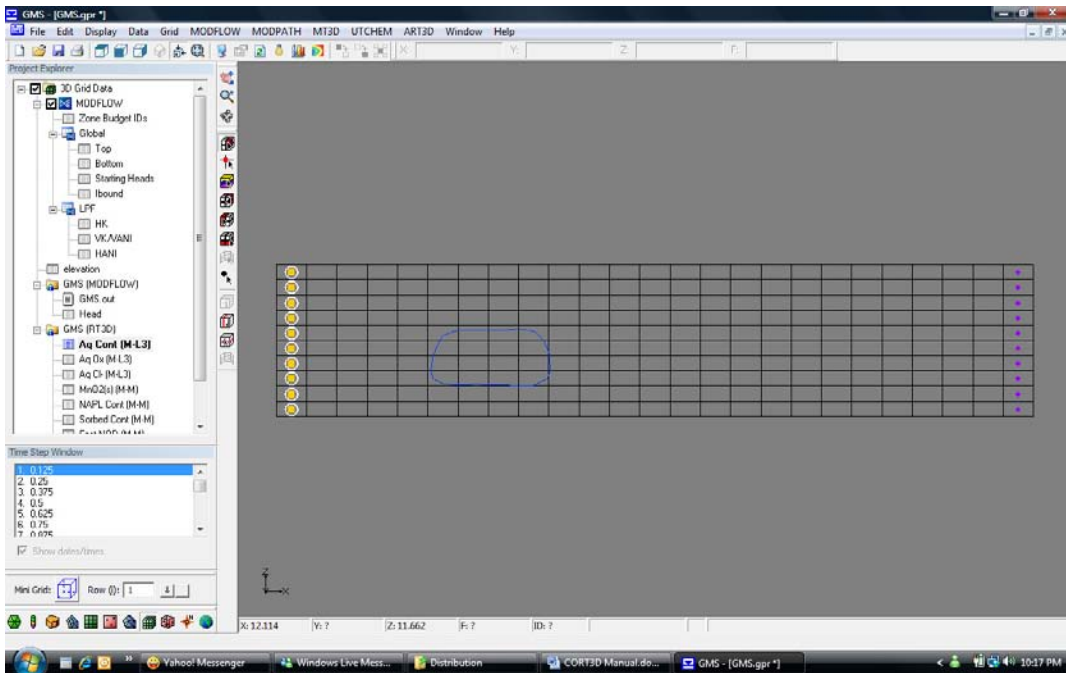**Figure 9.15: Selecting Data Set with Data Tree**

Figure 9.16: Selecting Time Step to View

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