GROWTOX - A Numerical Simulator for Shallow Groundwater Flow and Species Transport in the Subsurface

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Summary

This report contains a technical description of the GROWTOX computer program for simulating the shallow groundwater (confined/unconfined) flow and species transport in saturated porous media. The physical processes taken into account in GROWTOX are discussed, and the governing equations solved by the simulator are stated in full detail. A brief overview is given of the mathematical and numerical methods. The report provides description of GROWTOX input file. Code applications are illustrated by means of two sample problems.

Contents

1 Introduction

GROWTOX code is developed to simulate shallow confined-unconfined groundwater flow and transport of radionuclides, heavy metals, or other contaminants in saturated subsurface environment. The description of porous media contamination is founded on governing conservation equations and associated constitutive functions. Groundwater flow through the subsurface environment occurs in response to gradients in liquid pressures and gravitational body forces according to Darcy's flow law under assumption that the resistance to flow in the vertical direction may be neglected. Species transport through the saturated porous media occurs by molecular diffusion, hydrodynamic dispersion, and advection. Interphase species mass transfer between exchangeable sorbed solid aqueous phases is assumed being under thermodynamic and geochemical equilibrium conditions. These equilibrium condition assumptions require that time scales for thermodynamic and geochemical phenomena are small when compared with those for transport phenomena. Slow sorption/desorption processes between exchangeable sorbed solid and fixed solid phases are considered as non-equilibrium exchangeable processes which are described by first-order kinetic equations.

GROWTOX is designed to solve one-, or two-dimensional problems. A problem can be defined and solved using either Cartesian or cylindrical coordinates.

Governing equations are partial differential equations for the conservation of liquid mass and species mass. The governing partial differential equations are solved by discretizing governing equations to algebraic form with integrated finite-difference method. The resulting system of algebraic equations is non-linear. The non-linear algebraic forms of the conservation equations are converted to a linear form using residual-based, global Newton's iteration technique. The technique generally yields quadratic convergence of the residuals with iterations, given initial estimates of the unknowns that are sufficiently close to the solution. Conjugate gradient scheme is used for the solution of the linearized algebraic form of the conservation equations.

2 Governing Equations

2.1 *Shallow Groundwater Flow Equations*

Assume that the Dupuit-Forchheimer assumption [1-2] is applicable. This assumption is identified with the assumption that the vertical component of the specific discharge vector is neglected or the resistance to flow in the vertical direction is negligible [3]. Then shallow groundwater flow is described by the equation:

$$\frac{\partial}{\partial x}\left(T_x \frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T_y \frac{\partial h}{\partial y}\right)-\frac{h-h^*}{c}+N=\frac{\partial}{\partial t}(Sh)\,, \tag{1}$$

where t is the time (s); x, y are the Cartesian spatial coordinates (m); h is the hydraulic head (m); T is the transmissivity (m^2 s^{-1}); N is the infiltration rate (m s^{-1}); S is the storage coefficient (dimensionless); c is the resistance of a semipermeable layer, equal to its thickness divided by its hydraulic conductivity (s); h^* is the hydraulic head at a point separated from the aquifer by a semipermeable layer (m).

The third term on the left-hand side of the equation (1) is added to cover cases of flow in leaky aquifers. For shallow confined flow T equals $k(\eta$-$\xi)$, for shallow unconfined flow T equals $k(h$-$\xi)$, where k is the hydraulic conductivity tensor (m s^{-1}); η and ξ are the upper surface and bottom surface elevation of the aquifer, respectively (m).

For shallow unconfined flow S is the coefficient of phreatic storage, representing the fraction of a unit volume available for storage due to vertical movement of a phreatic surface. For shallow confined flow S is defined by expression:

$$S=(\eta-\xi)S_s=(\eta-\xi)\rho g(m_v+\phi\beta)\,,$$

where S_s is the coefficient of specific storage (m^{-1}); ϕ is the porosity (dimensionless); g is the acceleration due to gravity (m s^{-2}); ρ is the density of water (kg m^{-3}); β is the compressibility of water (m^2 N^{-1}); m_v is the coefficient soil volume compressibility (m^2 N^{-1}).

There are many sources of infiltration into groundwater, rainfall being the most common one. Rivers and lakes also may be sources of infiltration. Rivers and lakes usually have deposits along their bottoms, which often are less permeable than the aquifer underneath. If the river bottom is above the groundwater table, the leakage through the bottom is downward and independent of the flow in the aquifer, assuming that the pressure below the river bottom is atmospheric. The rate of infiltration N than may be expressed as follows:

$$N=\frac{h^*-h_b}{c}\,,$$

where h^* is the head in the river (m); c is the resistance of the river bottom (s); and h_b is the elevation of points in the aquifer just below the river bottom (s). Note that in this case, the infiltration rate is indeed independent of the head h in the aquifer. If h is greater than h_b, the leakage depends upon the head in aquifer, and

$$N = \frac{h^* - h}{c}.$$

The initial conditions for equation (1) consist of initial values of hydraulic head, specified by:

$$h(0, x, y) = \varphi(x, y),$$

where x, y are the spatial coordinates and φ is a prescribed function.

Boundary conditions may be Dirichlet (type 1):

$$h(t, x, y) = g_1(t, x, y) \qquad \text{on } \Gamma_1,$$

or Neumann (type 2):

$$-T\frac{\partial h}{\partial n} = g_2(t, x, y) \qquad \text{on } \Gamma_2,$$

where g_1 is the prescribed hydraulic head on the boundary Γ_1; $\partial/\partial n$ represents differentiation in the direction of the outward normal to the boundary Γ_2; and g_2 is the prescribed outward water flux normal to Γ_2. Γ_1 and Γ_2 comprise the entire boundary of the domain. Usually Γ_1 is the part of boundary at which surface-water bodies are intercepted by aquifers; Γ_2 are the boundaries across which fluid passes at a specific rate (impervious boundaries, areas of infiltration or evapotranspiration, points of injection and withdrawal, etc.).

2.2 *Species Transport Equations*

Let c_l represent the volumetric radionuclide activity in the aqueous phase (Bq m^{-3}); c_s the volumetric exchangeable sorbed activity in solid phase (Bq m^{-3}); and c_f the volumetric activity which is fixed in the mineral lattice (Bq m^{-3}). Assuming that the ion-exchange reaction transferring activity between aqueous and solid exchangeable phases has a sufficiently short timescale, we will consider this reaction as instantaneous which is described by a linear equilibrium isotherm. Transfers of activity to and from the fixed phase are modelled by first-order rate constants α_{sf} and α_{fs}, respectively, as shown in Figure 1 [4].

The leaching of radionuclides from the fuel particles is modelled by a first-order equation

$$\frac{\partial c_p}{\partial t} = -(\alpha_p + \lambda)c_p, \qquad (2)$$

$$c_p(0,x) = c_p^0(x),$$

where x is the spatial coordinate vector (m); c_p is the radionuclide activity in the fuel particles per soil solid volume (Bq m^{-3}); α_p is the first-order constant of radionuclide leaching from fuel particles (s^{-1}); λ is the radionuclide decay constant (s^{-1}); $c_p^{\,0}$ is the initial radionuclide activity in the fuel particles (Bq m^{-3}).

Ignoring chemical diffusion in the solid phase, the equation for advective-dispersive transport of radionuclide activity in the exchangeable phase for shallow groundwater flow may be written in the form

$$\frac{\partial}{\partial t}(Hc) = \frac{\partial}{\partial x_i}\left(H\phi D_{ij}\frac{\partial c_l}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(Q_i c_l) - \lambda Hc +$$

$$(1-\phi_T)H(\alpha_p c_p + \alpha_{fs} c_f - \alpha_{sf} c_s) + f \qquad (3)$$

where x_i are the Cartesian spatial coordinates (m); c is the radionuclide activity per total volume (Bq m^{-3}); f is the species source-sink (Bq m^{-3} s^{-1}).

For shallow confined groundwater flow H equals (η-ξ), for shallow unconfined flow H equals (h-ξ). The discharge vector Q is defined as

$$Q_i = -T_i \frac{\partial h}{\partial x_i}.$$

D_{ij} is the dispersion tensor, defined by:

$$\phi D_{ij} = \alpha_T |v| \delta_{ij} + (\alpha_L - \alpha_T)\frac{v_i v_j}{|v|} + \phi\tau D_0 \delta_{ij}$$

where α_L and α_T are the longitudinal and transverse dispersivities (m), respectively; δ_{ij} is the Kronecker delta; $|v|$ is the magnitude of the Darcy velocity; D_0 is the molecular

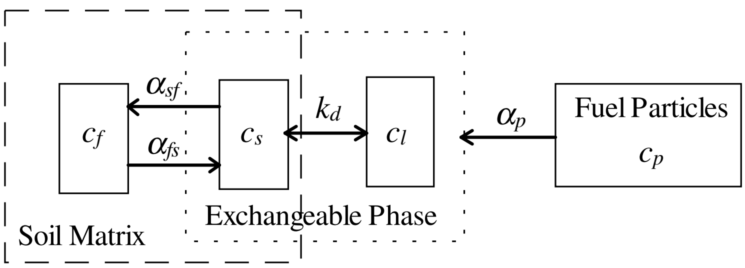

Figure 1. Schematic representation of the kinetic sorption model.

diffusion coefficient ($m^2\ s^{-1}$); τ is the tortuosity.

The total radionuclide activity is defined by:

$$c = \phi c_l + (1 - \phi_T) c_s$$

where ϕ_T is the total porosity of the medium; and volumetric phase activities are interrelated through solid-aqueous partition coefficient k_d, according to relationship

$$k_d = \frac{c_s \rho}{c_l \rho_s}$$

where ρ_s is the soil solid density (kg m^{-3}).

Initial conditions for equation (3) consist of specification of initial radionuclide activity in the aqueous phase:

$$c_l(t, x) = c_0(x)$$

Boundary conditions for inflow boundaries are Dirichlet (type 1):

$$c_l = c_1 \qquad \text{on } \Gamma_3$$

or Cauchy (type 3):

$$\left(-H\phi D_{ij} \frac{\partial c_l}{\partial x_j} + Q_i c_l \right) n_i = Q_b c_b \qquad \text{on } \Gamma_4$$

where c_1 is prescribed radionuclide activity on the boundaries Γ_3; n_i is the unit vector normal to boundaries, direction inwards; Q_b is the prescribed fluid flux over the thickness of the aquifer normal to the boundaries Γ_4; and c_b is the prescribed radionuclide activity associated with the prescribed fluid flux.

At outflow boundaries the assumption is often made that transport across the boundaries, according to Frind[5], occurs by advection only and a Neumann (type 2) boundary condition is specified by:

$$\frac{\partial c_l}{\partial x_j} = 0 \qquad \text{on } \Gamma_5$$

where $\Gamma_3 + \Gamma_4 + \Gamma_5 = \Gamma$ is the boundary of the domain.

The transport of activity in the fixed phase is described by

$$\frac{\partial c_f}{\partial t} = \alpha_{sf} c_s - \alpha_{fs} c_f - \lambda c_f, \tag{4}$$

$$c_f(0,x) = c_f^0(x),$$

where c_f^0 is the initial activity in the fixed phase.

3 Numerical Approximation

The flow domain is spatially discretized into a computational domain composed of a number of non-overlapping control volumes. Each control volume surrounds a single grid point, which defines the position of intrinsic property variables. Surfaces between nodes are located at the midpoint between two adjacent nodes. Control volumes are defined by their bounding surfaces.

3.1 *Shallow Groundwater Flow Equations*

The shallow groundwater flow equation is discretized by integration the equation (1) over a control volume V and a short time interval τ.

$$\int_t^{t+\tau}\int_V\left[\frac{\partial}{\partial t}(Sh)-\frac{\partial}{\partial x_i}\left[T_i\frac{\partial h}{\partial x_i}\right]+\frac{h-h^*}{c}-N\right]dVdt= \tag{5}$$

$$=\int_V (Sh)\Big|_t^{t+\tau}dV-\int_t^{t+\tau}\int_\Gamma\left[T_i\frac{\partial h}{\partial x_i}\right]\cdot n\, d\Gamma dt+\int_t^{t+\tau}\int_V\left(\frac{h-h^*}{c}-N\right)dVdt=0$$

where Γ is the boundary surface of the control volume V; n is the unit vector normal to the boundary Γ.

Using fully implicit temporal discretization and approximating the surface integrals as summations over the bounding control volume surfaces, the equation (5) can be rewritten in form

$$V\frac{(Sh)^{t+\tau}-(Sh)^t}{\tau}-\sum_\gamma Q_\gamma^{t+\tau}A_\gamma+V\left(\frac{h-h^*}{c}-N\right)^{t+\tau}=0 \tag{6}$$

$$Q_\gamma=-T_i\frac{\partial h}{\partial x_i}$$

where A_γ is the area of control volume bounding surface γ; Q_γ is the discharge occurring over the thickness of the aquifer across the surface γ.

In order to define a value of Q_γ at the surface γ located between two adjacent nodes $x_{j,p}$ and $x_{j,p-1}$, we integrate $\frac{1}{T_j}Q_\gamma$ over the interval $[x_{j,p-1}, x_{j,p}]$

$$-\int_{x_{j,p-1}}^{x_{j,p}}\frac{Q_\gamma}{T_j}dx_j=\int_{x_{j,p-1}}^{x_{j,p}}\frac{\partial h}{\partial x_j}dx_j=h\Big|_{x_{j,p-1}}^{x_{j,p}}$$

Assuming constant Q_γ between two adjacent nodes $x_{j,p}$ and $x_{j,p-1}$ yields

$$Q_\gamma = -[a]_{j,p} h_{\bar{x}_{j,p}} \tag{7}$$

where

$$[a]_{j,p} = \left[\int_{x_{j,p-1}}^{x_{j,p}} \frac{1}{T_j}\, dx_j \right]^{-1} \tag{8}$$

$$y_{\bar{x}_{j,p}} = \frac{y(x_{j,p}) - y(x_{j,p-1})}{x_{j,p} - x_{j,p-1}}$$

The terms delimited with brackets indicate a suitable interface averaging (arithmetic, harmonic, geometric, or upwind) of the expression on the right-hand side of the equation (8).

Combining (6)-(7), the shallow groundwater flow equation (1) is approximated by fully implicit finite-difference scheme

$$(Sh)_{\bar{t}} - \left([a]_i \; h_{\bar{x}_i} \right)_{\hat{x}_i} + \frac{h - h^*}{c} - N = 0$$

where topped with bar subscript x_i represents the x_i-direction finite-difference left derivative and subscript x_i topped with circumflex represents the x_i-direction following finite-difference derivative

$$y_{\hat{x}_i} = \frac{y(x_{i,p+1}) - y(x_{i,p})}{0.5(x_{i,p+1} - x_{i,p-1})}$$

3.2 *Species Transport Equations*

Integration of the species transport equation (3) over a control volume V and a temporal interval $[t,t+\tau]$ and converting of the volumetric integrals into surface integrals yields

$$\int_t^{t+\tau} \int_V \left[\frac{\partial(Hc)}{\partial t} - \frac{\partial}{\partial x_i} \left(H\phi D_{ij} \frac{\partial c_l}{\partial x_j} \right) + \frac{\partial}{\partial x_i}(Q_i c_l) \right] dVdt +$$

$$\int_t^{t+\tau} \int_V \left[\lambda Hc - (1 - n_T) H (\alpha_p c_p + \alpha_{fs} c_f - \alpha_{sf} c_s) \right] dVdt =$$

$$= \int_V \left[H(x,t+\tau)c(x,t+\tau) - H(x,t)c(x,t) \right] dV - \int_t^{t+\tau} \int_\Gamma \left[H\phi D_{ij} \frac{\partial c_l}{\partial x_j} - Q_i c_l \right] \cdot n \, d\Gamma dt +$$

$$+ \int_t^{t+\tau} \int_V H\left[\lambda c - (1-n_T)(\alpha_p c_p + \alpha_{fs} c_f - \alpha_{sf} c_s) \right] dV dt = 0$$

Using fully implicit temporal discretization, applying the upstream-weighted approximation to advective flux term and approximating the surface integrals as summations over the control volume surface, we obtain the following monotone conservative implicit scheme

$$(Hc)_{\bar{t}} - ([b]_i \, c_{l\bar{x}_j})_{\hat{x}_i} + Q^{-}_{i+0.5} \, c_{lx_i} + Q^{+}_{i-0.5} \, c_{l\bar{x}_i} + Q_{i+0.5,\hat{x}_i} \, c_l -$$

$$-\lambda Hc + (1-n_T)H(\alpha_p c_p + \alpha_{fs} c_f - \alpha_{sf} c_s) = 0$$

where

$$[b]_{j,p} = \left[\int_{x_{j,p-1}}^{x_{j,p}} \frac{1}{H\phi D_{ij}} \, dx_j \right]^{-1}$$

$$y^{\pm} = 0.5(y \pm |y|)$$

$$y_{i\pm 0.5} = y(0.5(x_{i,p} + x_{i,p\pm 1}))$$

Integration the leaching equation (2) over a time interval leads to

$$c_p(t+\tau) = c_p(t) exp\left\{ -\left(\alpha_p + \lambda \right) \tau \right\}$$

Equation of radionuclide activity exchange between fixed and sorbed phases is discretized by integration the equation (4) over a small time interval

$$\int_t^{t+\tau} \left(\frac{\partial c_f}{\partial t} - \alpha_{sf} c_s + \alpha_{fs} c_f + \lambda c_f \right) dt =$$

$$c_f \Big|_t^{t+\tau} - \int_t^{t+\tau} \left(\alpha_{sf} c_s - \alpha_{fs} c_f - \lambda c_f \right) dt = 0 \qquad (9)$$

Using fully implicit temporal approximation, we rewrite (9) in form

$$c_{f\bar{t}} - \alpha_{sf} c_s + \alpha_{fs} c_f + \lambda c_f = 0$$

3.3 *Boundary Condition Approximation*

The discretization of the water flow and species transport equations described above were obtained for nodes positioned within the interior of the computational domain. For nodes located adjacent to the domain boundary, the discretization of the governing equations differs to account for conditions at the boundary. Boundary conditions are specified either with field variables or with surface fluxes on the boundary surfaces. Boundary conditions of the former type are referred to as Dirichlet, whereas the latter type are referred to as Neumann.

Implementation of Dirichlet boundary conditions requires relatively few modifications to the discretized governing conservation equations. These modifications are replacing the following field variables at the boundary nodes by their values on the boundary surfaces.

Neumann-type boundary conditions are accommodated by substituting the specified surface fluxes directly into the discretized form of the conservation equation. Default boundary conditions for GROWTOX are zero-flux Neumann-type boundaries.

4 Numerical Solution Method

The finite difference discretization of the water flow equations leads to a system of non-linear equations:

$$F(x) = 0 \qquad\qquad F\colon\ R^n \to R^n \tag{10}$$

The non-linear equations (10) are solved iteratively, using a multivariable, residual-based Newton technique

$$x^{s+1} = x^s + p_s \qquad\qquad s = 0,1,2,\ldots \tag{11}$$

$$p_s = -J(x^s)^{-1} F(x^s)$$

where s denotes an iteration number; and $J(x^s)$ is the Jacobian of $F(x)$.

Iteration continues until the criterion is satisfied

$$\max_{1 \le i \le n} \frac{\left| x_i^{s+1} - x_i^s \right|}{\left| x_i^s \right|} \le \varepsilon$$

where ε is a user-provided error tolerance.

The iteration routine starts, at a given time step, with an estimate of liquid pressures based on the previous time step. This estimate is used to update values of the governing equation residuals and to evaluate all of the partial derivatives that make up the Jacobian matrix. The resulting system of linear equations is then solved by using the conjugate gradient method with incomplete LU factorization. Solution of the system of equations yields changes to the liquid pressures. An iteration ends by updating the liquid pressures with the changes computed from the system of linear equations. If the criterion is satisfied, then the procedure is determined to have converged and a new time step begins. Otherwise, another iteration commences. If the criterion is not satisfied within a specified number of iterations, the system is considered non-convergent. Non-convergent systems are handled by reducing the simulation step, resetting the liquid pressures to their previous time-step values, and reinitiating the time-step procedures.

5 Comparisons with Existing Solutions

5.1 *One-Dimensional Groundwater Flow*

The purpose of this one-dimensional, time-dependent, unconfined shallow groundwater flow is to demonstrate that the GROWTOX code correctly solves the shallow groundwater equation for a spreading over an impervious base of flat groundwater hillock. The governing equation for this problem is the one-dimensional form of the Boussinesq's equation

$$\frac{\partial h}{\partial t} = \frac{k}{m}\frac{\partial}{\partial x}\left(h\frac{\partial h}{\partial x}\right) \qquad (12)$$

where t is the time; x is the spatial coordinate; k is the hydraulic permeability; h is the hydraulic head; m is the storage coefficient.

The analytic solution of the equation (12) reported by Barenblatt [6] is the solution with type of the instantaneous source and it can be written in the form

$$h(t,x) = -\frac{m}{6k}\frac{(x-x_0)^2}{(t+t_0)} + c(t+t_0)^{-1/3}$$

where t_0, x_0 and c are the arbitrary constants.

Consider the numerical solution of the equation (12) on the interval [0, 10 cm] for the following parameter values:

$m=0.03$

$k=0.05$ cm/h;

$t_0=1$ h;

$x_0=10$ cm;

$c=10$ cm $h^{1/3}$.

The initial conditions for the equation (12) are a hydraulic head equals $10\ [1 - (1-0.1\ x)^2]$ cm. The boundary conditions are Dirichlet type at the left boundary and zero flux for the right boundary, i.e.

$$h(t,0) = -\frac{0.1(x-10)^2}{(t+1)} + 10(t+1)^{-1/3}$$

$$kh\frac{\partial h}{\partial x}(t,10) = 0$$

The problem domain is discretized by a uniform mesh that contains 100 nodes. The time step used in calculations was *0.1* hour.

Comparison between the analytic and numerical solutions after *3.0* hours of simulation is given in Figure 2.

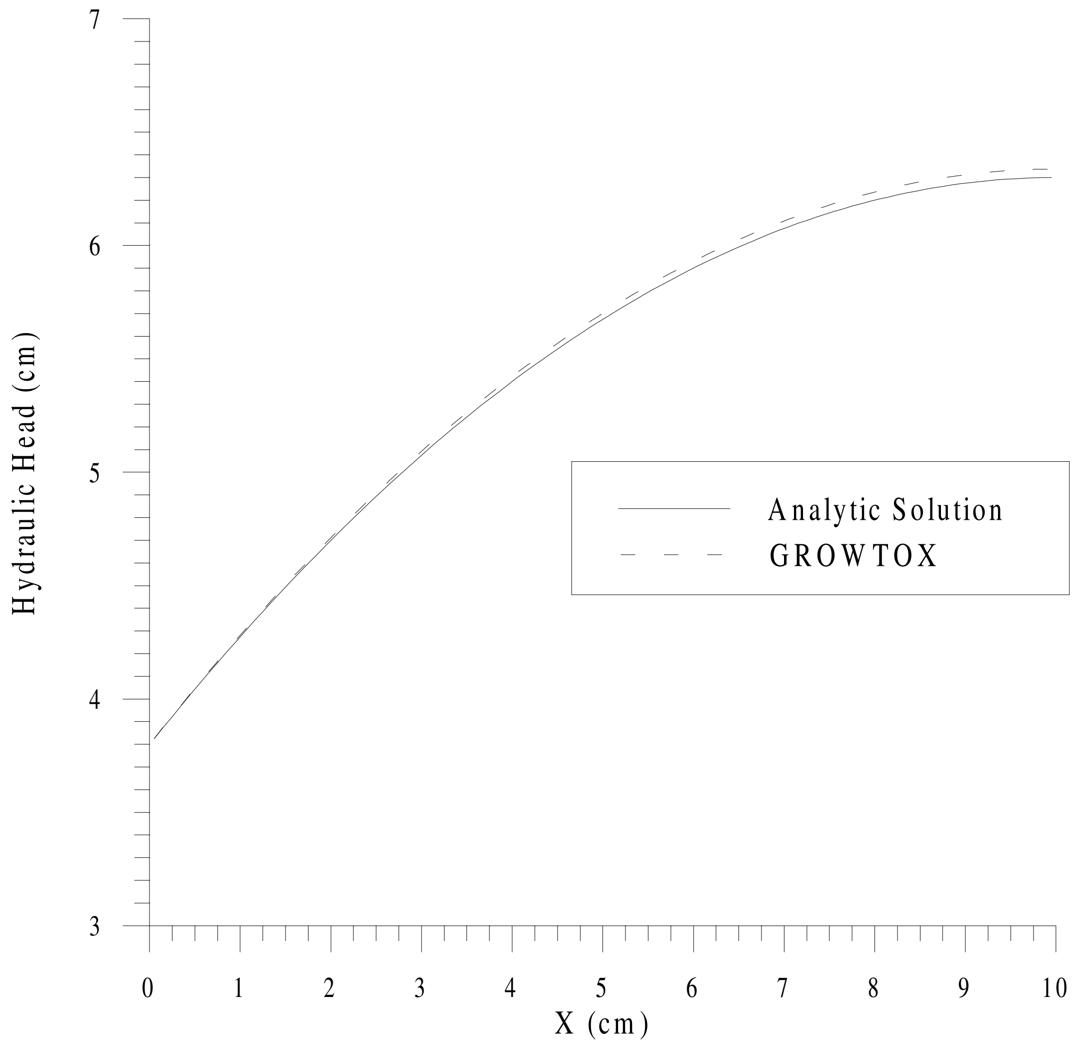

Figure 2. Comparison of GROWTOX Numerical Solution to the Analytical Solution After 3 Hours of Groundwater Hillock Spreading

The GROWTOX input file for one-dimensional groundwater flow is given in appendix A.

5.2 *Two-Dimensional Groundwater Flow*

Consider a two-dimensional groundwater hillock spreading over an impervious horizontal base in a two-dimensional rectangular (15 cm by 10 cm) domain. The purpose of the problem is to demonstrate how GROWTOX propagates the phreatic surface in two dimensions. The groundwater hillock spreading over an impervious bottom is described by the Boussinesq's equation

$$\frac{\partial h}{\partial t}=\frac{k}{m}\frac{\partial}{\partial x}\left(h\frac{\partial h}{\partial x}\right)+\frac{k}{m}\frac{\partial}{\partial y}\left(h\frac{\partial h}{\partial y}\right) \tag{13}$$

where t is the time; x and y are the spatial coordinates; k is the hydraulic permeability; h is the hydraulic head; m is the storage coefficient.

Sokolov [6] provided an analytical solution of the equation (13) which can be written in form

$$h(t,x,y)=-\frac{m}{8k}\frac{(x-x_0)^2+(y-y_0)^2}{t+t_0}+c\left|t+t_0\right|^{-1/2}$$

where x_0, y_0, t_0, and c are arbitrary constants.

Parameter values used in numerical simulations are

$m=0.02$

$k=0.05$ cm/h;

$t_0=1$ h;

$x_0=0$ cm;

$y_0=0$ cm;

$c=20$ cm $h^{1/2}$.

The whole right and upper boundaries are maintained at a prescribed head gradient of

$$\left.\frac{\partial h}{\partial x}\right|_{x=15\text{ cm}}=-\frac{3}{2}(1+t)^{-1}$$

$$\left.\frac{\partial h}{\partial y}\right|_{y=10\text{ cm}}=-(t+1)^{-1},$$

respectively. All other boundary surfaces are defined as zero-flux surfaces. Figure 3 provides a schematic of the problem and illustrates the discretization and boundary condition placement.

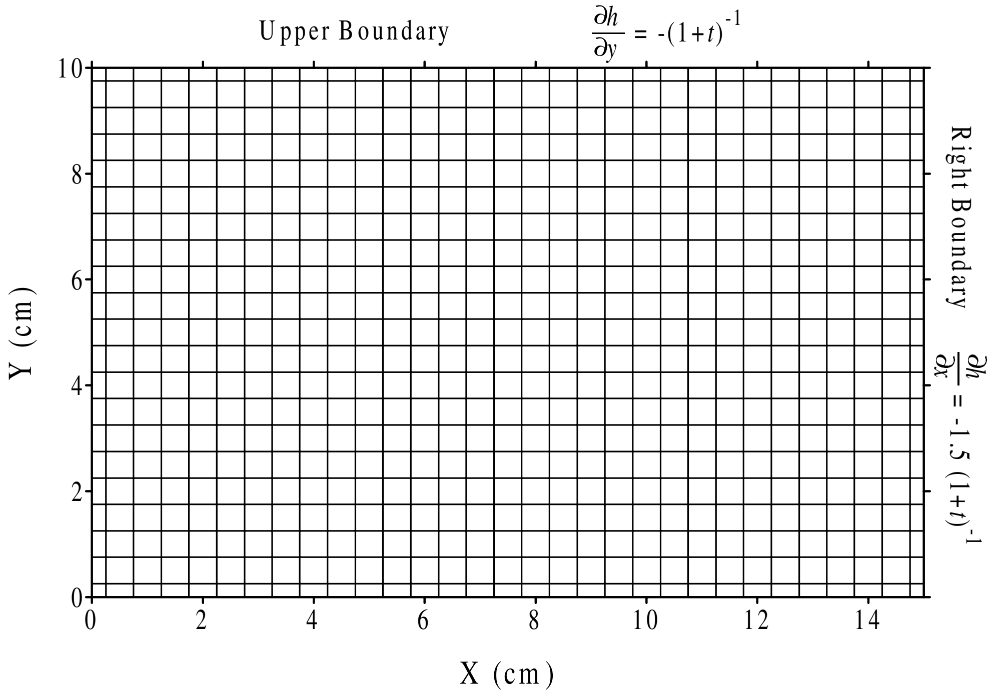

Figure 3. Two-Dimensional Groundwater-Flow Problem Geometry, Discretization, and Boundary Conditions.

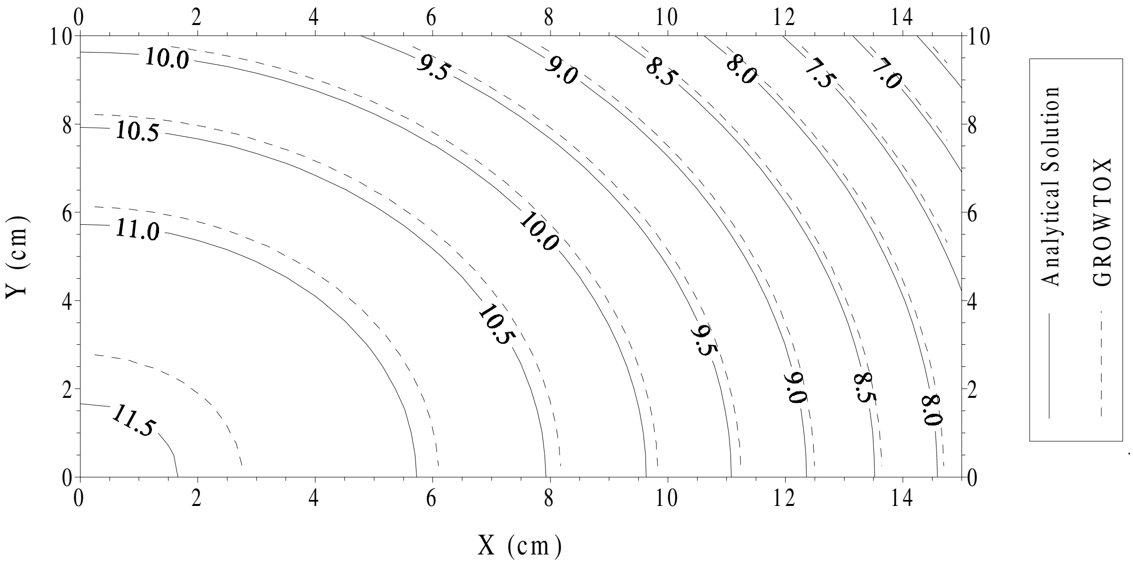

Figure 4. Comparison of Numerical Solution to the Analytical Solution After 2 Hours of Groundwater Hillock Spreading

Initial conditions for the equation (13) are

$$h(0,x,y) = -\frac{1}{20}(x^2 + y^2) + 20$$

The hydraulic head distribution predicted by GROWTOX after 2 hours is compared to the analytical solution in Figure 4.

The GROWTOX input file for two-dimensional groundwater flow is given in appendix B.

6 Modelling the Groundwater Flow on Right-Bank Floodplain of the Pripyat River

6.1 *Site Description*

Right bank floodplain of Pripyat River is located in 10-km zone of the Chernobyl NPP on the south-west by Yanovsky railroad bridge, on the north and north-west it is bounded by Pripyat River, on the west by Sakhan River, and on the east by the Cooling Pond. The Chernobyl NPP is located on the right bank of the Pripyat River. The NPP site is a flat river bench.

Most surface of the right bank floodplain is flat, with prevailing altitude at 106-108m, flooding which from separate lowering to a complete covering by water occurs over the range of discharge from 1200 up to 2600 cub.m per second. Flooding of the right bank floodplain occurs at water level of the Pripyat River more than at 106m.

There is wide distribution of alluvial sand in the upper part of geologic section in this region. Aquifers of this site are composed by fine, medium and sometimes coarse sands with interlayers of sand loam and loam. Medium sands prevail.

In the alluvial sands a fraction of 0.25-0.05mm prevails, constituting on the average from 42.5 up to 58.2%, contents of clay changes from 0.8 up to 3.5%. Porosity of the fine sands vary from 0.35 to 0.43, and medium sands from 0.31 to 0.4. The alluvial sands have hydraulic conductivity at saturation of 1.62-6.39 and 6.0-15.0 m/day according laboratory and field studies respectively.

The alluvial sands overlay marls of Kiev Eocene suite. These marls have very low permeability and act as an aquitard. The hydraulic conductivity at saturation of the marl changes from 10^{-2} to 10^{-4} m/day. Thickness of this layer is from 6 to 30 m.

Phreatic surface of the unconfined aquifer lays below 1 to 5 m of the land surface.

The riverbed for this site lays at from 98 to 102 m, slope of the free water surface is equal to 0.000087.

Amplitude of fluctuation of the level of water in Pripyat River during flooding reaches 3.5-5.0 m.

The unconfined aquifer of right bank floodplain is recharged by lateral groundwater flow, precipitation and floods infiltration, and partially by upward flow from lower confined aquifer of Eocene deposits. Natural discharge of unconfined aquifer is mainly into the river, floodplain water intake and also partially downward flow to low-lying confined aquifer of Eocene deposits.

The overall annual average sum of precipitation for this site is 550-600 mm, with extreme values of 762 mm in wet years and 301 mm in dry years. Average annual total evapotranspiration is equals 350-500 mm. The annual infiltration rate is equal 80-200 mm.

6.2 *Simulation Results*

Modelled aquifer is considered as a single unconfined aquifer with horizontal bed. The averaged hydraulic conductivity equals 10 m per day, the coefficient of phreatic storage equals 0.2.

For simulation of shallow groundwater flow on the right bank floodplain of Pripyat River the flow domain was discretized by a uniform rectangle mesh with 100-m distance between grid nodes. Time steps of 30 days were used.

The prescribed values of hydraulic head were specified on the whole boundary of the flow domain.

Seasonal fluctuations of the water level in Pripyat River varied between 103.8 m and 105.2 m; in Azbuchin Lake, between 104.3 m and 106.8 m; and in the Cooling Pond, between 109.8 m and 110.4 m [18]. These seasonal fluctuations of water level in surface water bodies and the variability over time of precipitation and evapotranspiration were taken into account in the simulations.

The contours obtained from numerical simulations are reproduced in Figure 5. The contour map prepared by interpolation of data of field observation in the vicinity of Chernobyl NPP is reproduced in Figure 6 and 7. Comparison of the obtained contours with measured contours shows that the model predictions are judged to be sufficiently realistic to conclude that the model could be used to predict the groundwater level distribution.

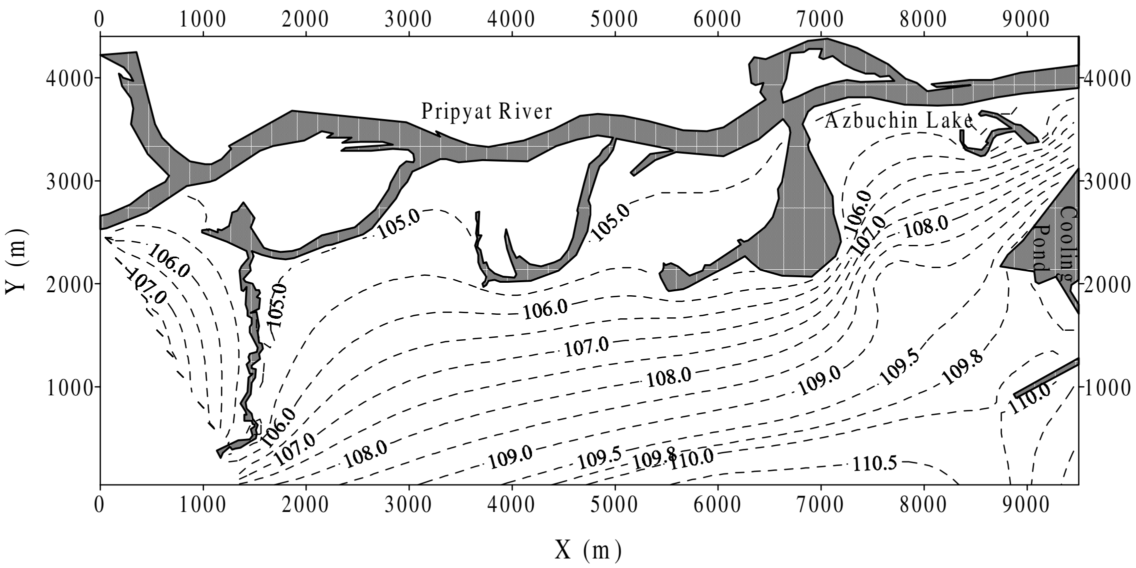

Figure 5. Contour levels predicted for the right bank floodplain of Pripyat River in September 1995 year.

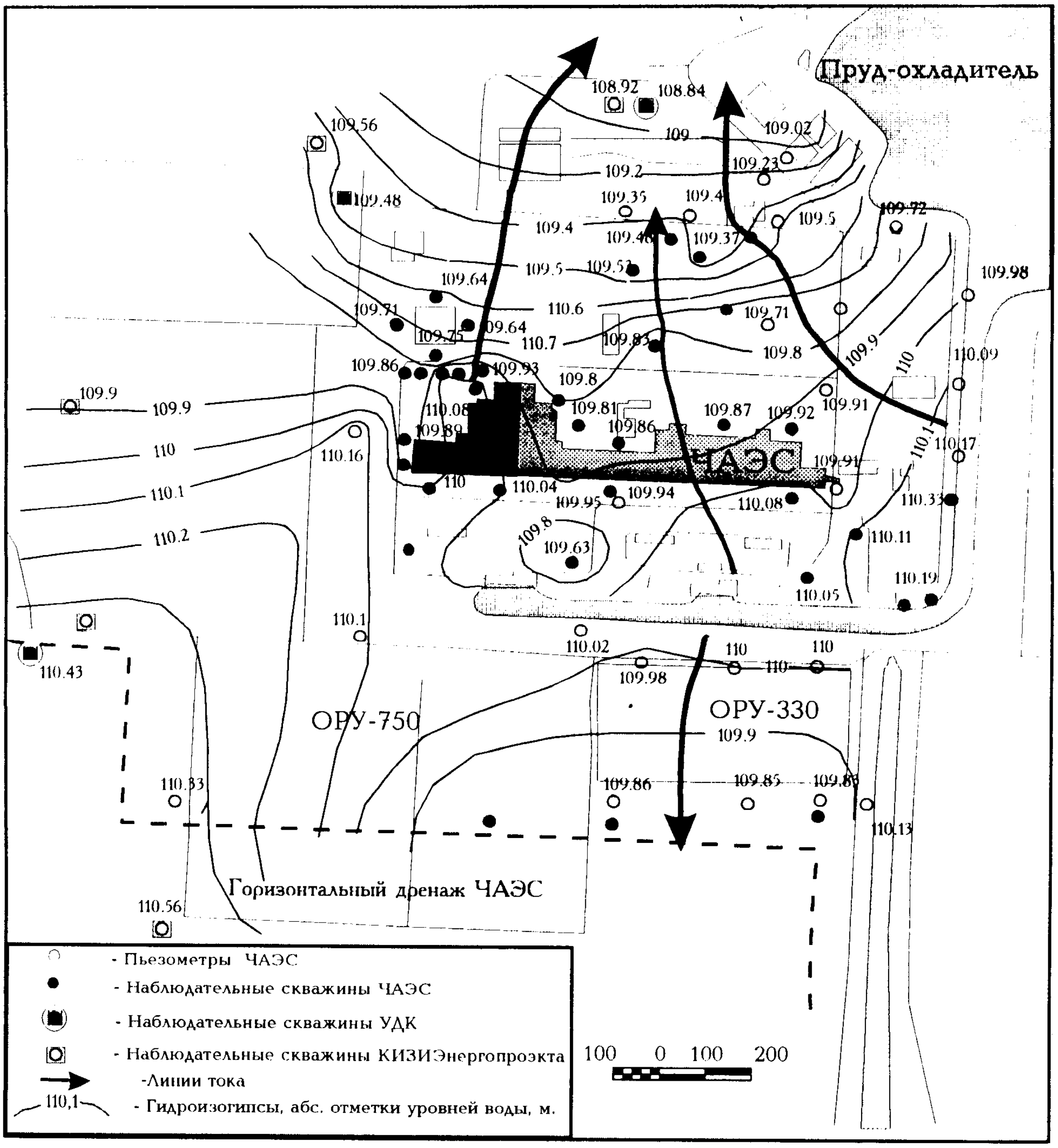

Figure 6. Streamlines and groundwater contour map in September 1995 year. Locations of observation wells are denoted by ○ and ●.

(prepared on the base of field observation by Institute of Geologic Sciences [10])

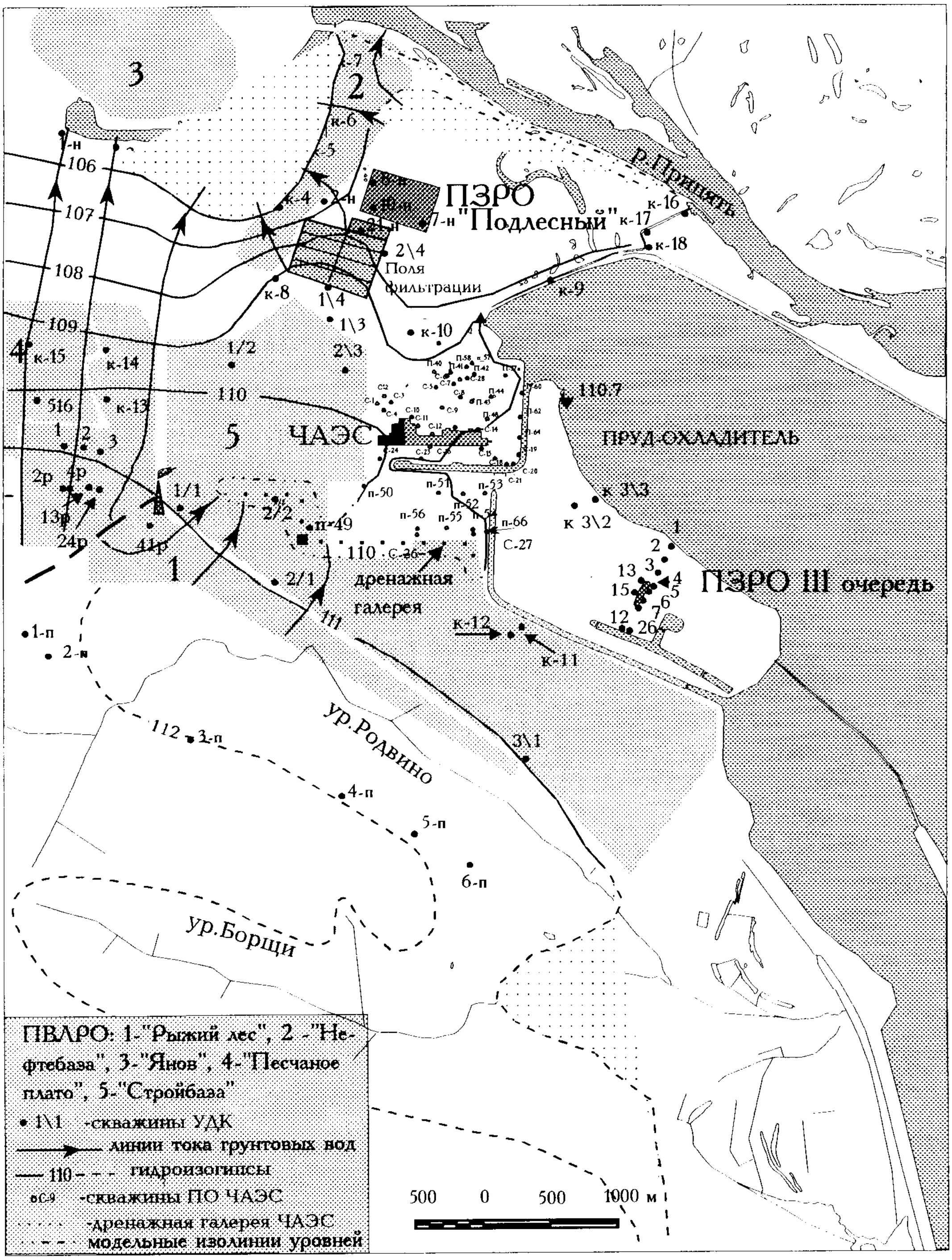

Figure 7. Streamlines and contour levels in the vicinity of Chernobyl NPP in November 1994.

(map prepared by interpolation of measured data by Institute of Geologic Sciences [11])

7 Input File Structure

Structure of GROWTOX Input file is similar to MSTS Input file structure [12-13].

7.1 *Simulation Title Card*

The Simulation Title card is used to specify information that identifies an Input file, including the title of the simulation, the user's name and affiliation, date and time of Input file creation, and any notes the user may enter.

Format:

Line 0	"~Simulation Title and Notes"
Line 1	Simulation Title {character*80}
Line 2	User Name {character*80}
Line 3	Company Name {character*40}
Line 4	Input File Creation Date {character*40}
Line 5	Input File Creation Time {character*40}
Line 6	N {integer} "line(s) of simulation title notes follows."
Line n	Simulation Title Notes {character*120}

7.2 *Solution Schemes Card*

The Solution Scheme card is used to restart options, control simulation time variables, and specify which governing equations to solve.

Format:

Line 0	"~Solution Schemes"
Line 1	Initial Conditions Only [true | false], Restart [true | false], Restart from Time Zero [true | false],
Line 2	Water Equation [true | false], Species Transport Equation [true | false],
Line 3	Simulation Time Limit, Units [s | min | h | day | wk | yr],
Line 4	Initial Time Step, Units [s | min | h | day | wk | yr],
Line 5	Time Step Acceleration Factor,
Line 6	Maximum Time Step, Units [s | min | h | day | wk | yr],
Line 7	Screen Echo [true | false],

7.3 *Numerical Control Card*

The Numerical Control card is used to control the iteration process, and specify the numerical convergence limits and averaging technique used for solution of each of the governing equations.

Format:

Line 0	"~Numerical Control"
Line 1	Number of Newton Iterations, Residuals Convergence [maximum residual | least squares]
Line 2	Criterion Error Tolerance of Water Equation Convergence,
Line 3	Water Equation Mean [harmonic | geometric | arithmetic | upwind],

7.4 *Grid Geometry Card*

The Grid Geometry card is used to select the problem coordinate system (Cartesian or cylindrical), specify the number of nodes in each cartesian direction, specify the physical length of the problem domain, and indicate the physical location of all nodes in the problem domain. The problem domain is discretized into a computational domain composed of non-overlapping node volumes. Node volumes are defined by their bounding surfaces. Surfaces between nodes are located at the midpoint between two adjacent nodes. Grid geometry should arrange a grid such that the lower and upper boundaries of problem domain are a bounding surfaces of node volumes, and the lower grid boundary in each dimension is at position zero. Node positions are referenced from the west, or south boundaries for the *x*-, and *y*-coordinate directions.

Format:

Line 0	"~Grid Geometry"
Line 1	Coordinate System [Cartesian | cylindrical],
Line 2	Number of Grid Nodes in the X- or R-direction, Number of Grid Nodes in the Y- or θ-direction,
Line 3	Physical Domain Length in X- or R-direction, Units [m | ft | cm], Physical Domain Length in Y- or θ-direction, Units [m | ft | cm],
Line 4	Inner Radius Length, Units [m | ft | cm],
Line 5	I {integer} "line(s) of grid geometry input follows."
Line i	"Node " i {integer}, X-direction Node Position, Units [m | ft | cm],
Next Line	J {integer} "line(s) of grid geometry input follows."
Line j	"Node " j {integer}, Y-direction Node Position, Units [m | ft | cm],

7.5 *Inactive Nodes Card*

The Inactive Nodes card is used to designate inactive, non-computational nodes in the problem domain. Often the rectangular grid required by the finite difference method does not provide the flexibility needed to describe complex geometry. The inactive node feature gives some flexibility in this regard.

Format:

Line 0 “~Inactive Nodes”
Line 1 N {integer} “line(s) of inactive nodes input follows.
Line n I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

7.6 *Aquifer Surfaces Card*

The Aquifer Surfaces card is used to specify elevation of confining boundaries for shallow confined flow, or soil surface and bed surface for shallow unconfined flow.

Format:

Line 0 “~Aquifer Surfaces”
Line 1 N {integer} “line(s) of aquifer top-surface input follows.”
Line n Surface Elevation {real},
Unit [m | ft | cm],
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},
Next Line N {integer} “line(s) of aquifer bottom-surface input follows.”
Line n Surface Elevation {real},
Unit [m | ft | cm],
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

7.7. *Rock or Soil Types Card*

The Rock or Soil Types card is used to group computational nodes with identical physical properties into unique rock or soil types.

Format:

Line 0 “~Rock or Soil Types”
Line 1 N {integer} “line(s) of rock or soil types notes follows.”
Line n Rock Notes {character*120}
Next Line N {integer} “line(s) of rock or soil types input follows.”
Line n Rock or Soil Type {character*80},
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

7.7 *Mechanical Properties Card*

The Mechanical Properties card is used to assign values of porosity, density, tortuosity, longitudinal and transverse dispersivities to rock or soil types identified with the Rock or Soil Types card.

Format:

Line 0 "~Mechanical Properties"
Line 1 N {integer} "line(s) of mechanical properties input follows."
Line n Rock or Soil Type {character*80},
Porosity {real},
Coefficient of Storage {real},
Tortuosity {real},
Rock or Soil Density {real},
Units [*M*/*L*^3],
Longitudinal Dispersivity {real},
Units [*L*],
Transverse Dispersivity {real},
Units [*L*],

where unit of *M* is [kg | gm | lbm]; and unit of *L* is [m | cm | mm | in | ft | yd].

7.8 *Hydraulic Properties Card*

The Hydraulic Properties card is used to assign values of intrinsic permeability or hydraulic conductivity (hc) to rock or soil types identified with the Rock or Soil Types card.

Format:

Line 0 "~Hydraulic Properties"
Line 1 N {integer} "line(s) of hydraulic properties input follows."
Line n Rock or Soil Type {character*80},
X-direction Intrinsic Permeability or Hydrailic Conductivity {real},
Y-direction Intrinsic Permeability or Hydrailic Conductivity {real},
Units [*L*^2 | hc:*L*/*T*],
Resistance of Leaky Layer {real},
Units [*T*],

where unit of *T* is [min | h | day | s | wk | yr]; and unit of *L* is [m | cm | mm | in | ft | yd].

7.9 *Species Properties Card*

The Species Properties card is used to assign a species name and associated molecular diffusion coefficient, partition coefficients, radioactive half-life, and slow sorption and desorption rate coefficients to each rock or soil types identified with the Rock or Soil Types card.

Format:

Line 0 "~Species Properties"
Line 1 N {integer} "line(s) of species properties input follows."
Line n Rock or Soil Type {character*80},
Species Name {character*80},
Molecular Diffusion Coefficient {real},
Units [*L*^2/*T*],
Solid-Liquid Partition Coefficient {real},
Units [*M* liq./*M* sol.],
Species Half-Life {real},
Units [s | min | h | day | wk | yr],
Slow Sorption Rate {real},
Units [1/s | 1/min | 1/h | 1/day | 1/wk | 1/yr],
Slow Desorption Rate {real},
Units [1/s | 1/min | 1/h | 1/day | 1/wk | 1/yr],

where unit of *M* is [kg | gm | lbm]; unit of *T* is [min | h | day | s | wk | yr]; and unit of *L* is [m | cm | mm | in | ft | yd].

7.10 *Liquid Boundary Conditions Card*

The Liquid Boundary Conditions card is used to specify the boundary conditions for hydraulic head, and liquid fluxes at the external boundaries of the problem domain and at the boundaries of inactive nodes.

Format:

Line 0 "~Liquid Boundary Conditions"
Line 1 N {integer} "line(s) of liquid boundary conditions input to follow."

Dirichlet Boundary

Line n Direction [X-Direction | Y-Direction]:
Surface [East | West | North | South] " Surface",
"Dirichlet @ Boundary",
Temporal Variation [constant | tabular],

Constant

Hydraulic Head {real},
Units [m | ft | cm],
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

Tabular

Table Name {character*20},
,
I Start {integer},
I End {integer},
J Start {integer},

J End {integer},

Neumann Boundary.

Line n Direction [X-Direction | Y-Direction]:
Surface [East | West | North | South] " Surface",
"Neumann @ Boundary",
Temporal Variation [constant | tabular],

Constant

Liquid Mass Flux {real},
Units [*M*/*L T*],
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

Tabular

Table Name {character*20},
,
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

where unit of *M* is [kg | gm | lbm]; unit of *T* is [min | h | day | s | wk | yr]; and unit of *L* is [m | cm | mm | in | ft | yd].

Tables for tabular data follow all functional input lines. Tables must be in ascending or descending order.

Line 1 N {integer} "line(s) of all boundary tables input follows."
Line n Time {real},
Units [s | min | h | day | wk | yr],
Boundary Value {real},
Boundary Value Units,

7.11 *Species Boundary Conditions Card*

The Species Boundary Conditions card is used to specify the boundary conditions for species concentrations and species boundary surface fluxes at the external boundaries of the problem domain and at the boundaries of inactive nodes.

Format:

Line 0 "~Species Boundary Conditions"
Line 1 N {integer} "line(s) of species boundary conditions input to follow."

Dirichlet Boundary

Line n Direction [X-Direction | Y-Direction]:
Surface [East | West | North | South] " Surface",

"Dirichlet @ Boundary",
Temporal Variation [constant | tabular],

Constant

Liquid-Phase Species Concentration {real},
Units [1/*L*^3],
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

where unit of *L* is [m | cm | mm | in | ft | yd].

Tabular

Table Name {character*20},
,
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

Neumann Boundary

Line n Direction [X-Direction | Y-Direction]:
Surface [East | West | North | South] " Surface",
"Neumann @ Boundary",
Temporal Variation [constant | tabular],

Constant

Liquid-Phase Species Flux {real},
Units [1/*L T*],
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

Tabular

Table Name {character*20},
,
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

where unit of *T* is [min | h | day | s | wk | yr]; and unit of *L* is [m | cm | mm | in | ft | yd].

Outflow Boundary

Line n Direction [X-Direction| Y-Direction]:
Surface [East|West|North|South] " Surface",

“Outflow @ Boundary”,
,
,
,
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

Tables for tabular data follow all functional input lines. Tables must be in ascending or descending order.

Line 1 N {integer} “line(s) of all boundary tables input follows.”
Line n Time {real},
Units [s | min | h | day | wk | yr],
Boundary Value {real},
Boundary Value Units,

7.12 *Fuel Particle Sources Card*

The Fuel Particle Sources card is used to specify initial contamination of problem domain by fuel particle, and portions of the exchangeable and fixed phases in this contamination.

Format:

Line 0 “~Fuel Particle Sources”
Line 1 N {integer} “line(s) of fuel particle sources input to follow.”
Line n Fuel Particle Concentration {real},
Unit [1/*L*^3],
Radionuclide Leaching Rate {real},
Unit [1/s | 1/min | 1/h | 1/day | 1/wk | 1/yr],
Exchangeable-phase portion in fuel contamination {real},
Fixed-phase portion in fuel contamination {real},
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

where unit of *L* is [m | cm | mm | in | ft | yd].

7.13 *Initial Conditions Card*

The Initial Conditions card is used to specify the values of field variables at the computational nodes at the start of a simulation. No field variable initial conditions are required for restart simulations.

Format:

Line 0 “~Initial Conditions”

Line 1 N {integer} "line(s) of initial conditions input to follow."
Line n Variable Name [Hydraulic Head | Leaky Hydraulic Head | Species Concentration | Species Liquid Concentration | X-Dir. Liquid Velocity | Y-Dir. Liquid Velocity],
Field Variable Value {real},
Units *Hydraulic Head*. [m | ft | cm],
Leaky Hydraulic Head. [m | ft | cm],
Velocity [*L/T*],
Concentration. [1/*L*^3 | 1/*V*],
X-Direction Gradient {real},
Units [1/m | 1/ft | 1/cm],
Y-Direction Gradient {real},
Units [1/m | 1/ft | 1/cm],
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

where unit of *V* is [liter | l | gal]; unit of *T* is [min | h | day | s | wk | yr]; and unit of *L* is [m | cm | mm | in | ft | yd].

7.14 *Sources and Sinks Card*

The Sources and Sinks card is used to identify the location and rate of sources and/or sinks of liquid mass and species mass. The source/sink rate either may be constant in time or may vary following tabular input.

Format:

Line 0 "~Sources & Sinks"
Line 1 N {integer} "line(s) of sources & sinks input to follow."
Line n Source Type [Liquid Mass | Species | Species Concentration | Species Liq Concentration]

Liquid Mass

Source Temporal Variation [Constant | Tabular],

Constant

Liquid Source Rate {real},
Units [*M/T*],
Source Start Time {real},
Units [s | min | h | day | wk | yr],
Source End Time {real},
Units [s | min | h | day | wk | yr],
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

where unit of M is [kg | gm | lbm]; and unit of T is [min | h | day | s | wk | yr].

Tabular

Table number {integer},
,
,
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

Line n M {integer} "line(s) of source tables input follows."
Line m Time {real},
Units [s | min | h | day | wk | yr],
Liquid Mass Source Rate {real},
Units [M/T],

where unit of M is [kg | gm | lbm]; and unit of T is [min | h | day | s | wk | yr].

Species

Source Temporal Variation [Constant | Tabular],

Constant

Species Source Rate {real},
Units [1/s | 1/min | 1/h | 1/day | 1/wk | 1/yr],
Source Start Time {real},
Units [s | min | h | day | wk | yr],
Source End Time {real},
Units [s | min | h | day | wk | yr],
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

Tabular

Table number {integer},
,
,
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

Line n M {integer} "line(s) of source tables input follows."
Line m Time {real},
Units [s | min | h | day | wk | yr],
Species Mass Source Rate {real},
Units [M/T],

where unit of M is [kg | gm | lbm]; and unit of T is [min | h | day | s | wk | yr].

Species Concentration

Source Temporal Variation [Constant | Tabular],

Constant

Species Concentration Source Rate {real},
Units [1/L^3 T],
Source Start Time {real},
Units [s | min | h | day | wk | yr],
Source End Time {real},
Units [s | min | h | day | wk | yr],
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

where unit of T is [min | h | day | s | wk | yr]; and unit of L is [m | cm | mm | in | ft | yd].

Tabular

Table number {integer},
,
,
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

Line n M {integer} "line(s) of source tables input follows."
Line m Time {real},
Units [s | min | h | day | wk | yr],
Species Mass Concentration Source Rate {real},
Units [M/L^3 T],

where unit of M is [kg | gm | lbm]; unit of T is [min | h | day | s | wk | yr]; and unit of L is [m | cm | mm | in | ft | yd].

Species Liquid Concentration

Source Temporal Variation [Constant | Tabular],

Constant

Species Liquid Concentration Source Rate {real},
Units [1/L^3 T],
Source Start Time {real},
Units [s | min | h | day | wk | yr],
Source End Time {real},
Units [s | min | h | day | wk | yr],
I Start {integer},

I End {integer},
J Start {integer},
J End {integer},

where unit of *T* is [min | h | day | s | wk | yr]; and unit of *L* is [m | cm | mm | in | ft | yd].

Tabular

Table number {integer},
,
,
I Start {integer},
I End {integer},
J Start {integer},
J End {integer},

Line n	M {integer} "line(s) of source tables input follows."
Line m	Time {real}, Units [s	min	h	day	wk	yr], Species Mass Concentration Source Rate {real}, Units [*M*/*L*^3 *T*],

where unit of *M* is [kg | gm | lbm]; unit of *T* is [min | h | day | s | wk | yr]; and unit of *L* is [m | cm | mm | in | ft | yd].

7.15 *Output Control Card*

The Output Control card is used to specify reference node output and plotting output.

Format:

Line 0	"~Output Control"
Line 1	N {integer} "line(s) of output control input to follow."
Line n	Field Variable Output Time (for "output" and "plot" file) {real}, Units [s	min	h	day	wk	yr],
Next Line	I-index of Reference Node 1 {integer}, J-index of Reference Node 1 {integer}, I-index of Reference Node 2 {integer}, J-index of Reference Node 2 {integer}, I-index of Reference Node 3 {integer}, J-index of Reference Node 3 {integer}, I-index of Reference Node 4 {integer}, J-index of Reference Node 4 {integer}, Reference Node Output Frequency (Time Steps per Output) {integer},
Next Line	N {integer} "line(s) of output control input to follow."
Line n	"plot" file field variable (see Table 4)
Next	N {integer} "line(s) of output control input to follow."

Line
Line n reference node field variable (see Table 4)

Table. List of field variable available for “plot” file and reference node record.

Field Variable Name in Input File	Name Used in Reference Node Record
Hydraulic Head	HH
Species Concentration	C
Porosity	PR
Storativity	ST
Aquifer Top-Surface Elevation	AT
Aquifer Bottom-Surface Elevation	AB
X-Dir. Liquid Velocity	U
Y-Dir. Liquid Velocity	V
X-Dir. Species Velocity	UC
Y-Dir. Species Velocity	VC
Species Liq Concentration	CL
Species Sol Concentration	CS
Species Fix Concentration	CF
Species Fue Concentration	CP

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Appendix

A. Input File of One-Dimensional Groundwater Flow

```
~Simulation Title and Notes
Test for 1-D Boussinesq Equation
Sergey L. Kivva
IPMMS, Kiev
Wednesday, October 21, 1998
10:28:20 AM
0 line(s) of simulation title notes follows.
~Solution Schemes
false,false,false,
true,false,
3.0,h,
0.1,h,
1.500,
0.1,h,
true,
~Numerical Control
30,Maximum Residual,
1.0E-08,
Arithmetic Mean,Harmonic Mean,
~Grid Geometry
cartesian
100,1,
10.,cm,1.,cm,
0.,cm,
100 line(s) of grid geometry input follows.
Node  1,  .05,cm,
Node  2,  .15,cm,
Node  3,  .25,cm,
Node  4,  .35,cm,
Node  5,  .45,cm,
Node  6,  .55,cm,
Node  7,  .65,cm,
Node  8,  .75,cm,
Node  9,  .85,cm,
Node 10,  .95,cm,
Node 11, 1.05,cm,
Node 12, 1.15,cm,
Node 13, 1.25,cm,
Node 14, 1.35,cm,
Node 15, 1.45,cm,
Node 16, 1.55,cm,
Node 17, 1.65,cm,
Node 18, 1.75,cm,
```

Node 19, 1.85,cm,
Node 20, 1.95,cm,
Node 21, 2.05,cm,
Node 22, 2.15,cm,
Node 23, 2.25,cm,
Node 24, 2.35,cm,
Node 25, 2.45,cm,
Node 26, 2.55,cm,
Node 27, 2.65,cm,
Node 28, 2.75,cm,
Node 29, 2.85,cm,
Node 30, 2.95,cm,
Node 31, 3.05,cm,
Node 32, 3.15,cm,
Node 33, 3.25,cm,
Node 34, 3.35,cm,
Node 35, 3.45,cm,
Node 36, 3.55,cm,
Node 37, 3.65,cm,
Node 38, 3.75,cm,
Node 39, 3.85,cm,
Node 40, 3.95,cm,
Node 41, 4.05,cm,
Node 42, 4.15,cm,
Node 43, 4.25,cm,
Node 44, 4.35,cm,
Node 45, 4.45,cm,
Node 46, 4.55,cm,
Node 47, 4.65,cm,
Node 48, 4.75,cm,
Node 49, 4.85,cm,
Node 50, 4.95,cm,
Node 51, 5.05,cm,
Node 52, 5.15,cm,
Node 53, 5.25,cm,
Node 54, 5.35,cm,
Node 55, 5.45,cm,
Node 56, 5.55,cm,
Node 57, 5.65,cm,
Node 58, 5.75,cm,
Node 59, 5.85,cm,
Node 60, 5.95,cm,
Node 61, 6.05,cm,
Node 62, 6.15,cm,
Node 63, 6.25,cm,
Node 64, 6.35,cm,
Node 65, 6.45,cm,

Node 66, 6.55,cm,
Node 67, 6.65,cm,
Node 68, 6.75,cm,
Node 69, 6.85,cm,
Node 70, 6.95,cm,
Node 71, 7.05,cm,
Node 72, 7.15,cm,
Node 73, 7.25,cm,
Node 74, 7.35,cm,
Node 75, 7.45,cm,
Node 76, 7.55,cm,
Node 77, 7.65,cm,
Node 78, 7.75,cm,
Node 79, 7.85,cm,
Node 80, 7.95,cm,
Node 81, 8.05,cm,
Node 82, 8.15,cm,
Node 83, 8.25,cm,
Node 84, 8.35,cm,
Node 85, 8.45,cm,
Node 86, 8.55,cm,
Node 87, 8.65,cm,
Node 88, 8.75,cm,
Node 89, 8.85,cm,
Node 90, 8.95,cm,
Node 91, 9.05,cm,
Node 92, 9.15,cm,
Node 93, 9.25,cm,
Node 94, 9.35,cm,
Node 95, 9.45,cm,
Node 96, 9.55,cm,
Node 97, 9.65,cm,
Node 98, 9.75,cm,
Node 99, 9.85,cm,
Node 100, 9.95,cm,
1 line(s) of grid geometry input follows.
Node 1, 0.50,cm,
~Inactive Nodes
0 line(s) of inactive Nodes input follows.
~Aquifer Surfaces
1 line(s) of aquifer top-surface input follows.
20.,cm,1,100,1,1,
1 line(s) of aquifer bottom-surface input follows.
0.,cm,1,100,1,1,
~Rock or Soil Types
0 lines(s) of rock or soil types notes follows.
1 line(s) of rock or soil types input follows.

Sand,1,100,1,1,
~Mechanical Properties
1 line(s) of mechanical properties input follows.
Sand,0.03,0.03,,gm/cm^3,1.0,,m,,m,
~Hydraulic Properties
1 line(s) of hydraulic properties input follows.
Sand,0.05,0.05,hc:cm/h,1.e+20,s,
~Species Properties
1 line(s) of species properties input follows.
Sand,Solute,1.1574074E-9,m^2/s,0.0,gm liq./gm sol.,,s,,,,
~Liquid Boundary Conditions
1 line(s) of liquid boundary conditions input follows.
X-Direction: West Surface,Dirichlet @ Boundary,tabular,Head_W,,1,1,1,1,
31 line(s) of Head_W table input follows.
Head_W, .00,h, .0000,cm,
Head_W, .10,h, .5964,cm,
Head_W, .20,h, 1.0770,cm,
Head_W, .30,h, 1.4703,cm,
Head_W, .40,h, 1.7962,cm,
Head_W, .50,h, 2.0691,cm,
Head_W, .60,h, 2.2999,cm,
Head_W, .70,h, 2.4965,cm,
Head_W, .80,h, 2.6652,cm,
Head_W, .90,h, 2.8107,cm,
Head_W, 1.00,h, 2.9370,cm,
Head_W, 1.10,h, 3.0471,cm,
Head_W, 1.20,h, 3.1434,cm,
Head_W, 1.30,h, 3.2279,cm,
Head_W, 1.40,h, 3.3023,cm,
Head_W, 1.50,h, 3.3681,cm,
Head_W, 1.60,h, 3.4262,cm,
Head_W, 1.70,h, 3.4777,cm,
Head_W, 1.80,h, 3.5235,cm,
Head_W, 1.90,h, 3.5641,cm,
Head_W, 2.00,h, 3.6003,cm,
Head_W, 2.10,h, 3.6324,cm,
Head_W, 2.20,h, 3.6610,cm,
Head_W, 2.30,h, 3.6865,cm,
Head_W, 2.40,h, 3.7091,cm,
Head_W, 2.50,h, 3.7292,cm,
Head_W, 2.60,h, 3.7470,cm,
Head_W, 2.70,h, 3.7628,cm,
Head_W, 2.80,h, 3.7767,cm,
Head_W, 2.90,h, 3.7889,cm,
Head_W, 3.00,h, 3.7996,cm,
~Species Boundary Conditions
0 line(s) of species boundary conditions input follows.

~Initial Conditions
101 line(s) of initial conditions input follows.
Hydraulic Head, .099750,cm,0.0,1/m,0.0,1/m, 1, 1,1,1,
Hydraulic Head, .297750,cm,0.0,1/m,0.0,1/m, 2, 2,1,1,
Hydraulic Head, .493750,cm,0.0,1/m,0.0,1/m, 3, 3,1,1,
Hydraulic Head, .687750,cm,0.0,1/m,0.0,1/m, 4, 4,1,1,
Hydraulic Head, .879750,cm,0.0,1/m,0.0,1/m, 5, 5,1,1,
Hydraulic Head,1.069750,cm,0.0,1/m,0.0,1/m, 6, 6,1,1,
Hydraulic Head,1.257750,cm,0.0,1/m,0.0,1/m, 7, 7,1,1,
Hydraulic Head,1.443750,cm,0.0,1/m,0.0,1/m, 8, 8,1,1,
Hydraulic Head,1.627750,cm,0.0,1/m,0.0,1/m, 9, 9,1,1,
Hydraulic Head,1.809750,cm,0.0,1/m,0.0,1/m, 10, 10,1,1,
Hydraulic Head,1.989750,cm,0.0,1/m,0.0,1/m, 11, 11,1,1,
Hydraulic Head,2.167750,cm,0.0,1/m,0.0,1/m, 12, 12,1,1,
Hydraulic Head,2.343750,cm,0.0,1/m,0.0,1/m, 13, 13,1,1,
Hydraulic Head,2.517750,cm,0.0,1/m,0.0,1/m, 14, 14,1,1,
Hydraulic Head,2.689750,cm,0.0,1/m,0.0,1/m, 15, 15,1,1,
Hydraulic Head,2.859750,cm,0.0,1/m,0.0,1/m, 16, 16,1,1,
Hydraulic Head,3.027750,cm,0.0,1/m,0.0,1/m, 17, 17,1,1,
Hydraulic Head,3.193750,cm,0.0,1/m,0.0,1/m, 18, 18,1,1,
Hydraulic Head,3.357750,cm,0.0,1/m,0.0,1/m, 19, 19,1,1,
Hydraulic Head,3.519750,cm,0.0,1/m,0.0,1/m, 20, 20,1,1,
Hydraulic Head,3.679750,cm,0.0,1/m,0.0,1/m, 21, 21,1,1,
Hydraulic Head,3.837750,cm,0.0,1/m,0.0,1/m, 22, 22,1,1,
Hydraulic Head,3.993750,cm,0.0,1/m,0.0,1/m, 23, 23,1,1,
Hydraulic Head,4.147750,cm,0.0,1/m,0.0,1/m, 24, 24,1,1,
Hydraulic Head,4.299750,cm,0.0,1/m,0.0,1/m, 25, 25,1,1,
Hydraulic Head,4.449750,cm,0.0,1/m,0.0,1/m, 26, 26,1,1,
Hydraulic Head,4.597750,cm,0.0,1/m,0.0,1/m, 27, 27,1,1,
Hydraulic Head,4.743750,cm,0.0,1/m,0.0,1/m, 28, 28,1,1,
Hydraulic Head,4.887750,cm,0.0,1/m,0.0,1/m, 29, 29,1,1,
Hydraulic Head,5.029750,cm,0.0,1/m,0.0,1/m, 30, 30,1,1,
Hydraulic Head,5.169750,cm,0.0,1/m,0.0,1/m, 31, 31,1,1,
Hydraulic Head,5.307750,cm,0.0,1/m,0.0,1/m, 32, 32,1,1,
Hydraulic Head,5.443750,cm,0.0,1/m,0.0,1/m, 33, 33,1,1,
Hydraulic Head,5.577750,cm,0.0,1/m,0.0,1/m, 34, 34,1,1,
Hydraulic Head,5.709750,cm,0.0,1/m,0.0,1/m, 35, 35,1,1,
Hydraulic Head,5.839750,cm,0.0,1/m,0.0,1/m, 36, 36,1,1,
Hydraulic Head,5.967750,cm,0.0,1/m,0.0,1/m, 37, 37,1,1,
Hydraulic Head,6.093750,cm,0.0,1/m,0.0,1/m, 38, 38,1,1,
Hydraulic Head,6.217750,cm,0.0,1/m,0.0,1/m, 39, 39,1,1,
Hydraulic Head,6.339750,cm,0.0,1/m,0.0,1/m, 40, 40,1,1,
Hydraulic Head,6.459750,cm,0.0,1/m,0.0,1/m, 41, 41,1,1,
Hydraulic Head,6.577750,cm,0.0,1/m,0.0,1/m, 42, 42,1,1,
Hydraulic Head,6.693750,cm,0.0,1/m,0.0,1/m, 43, 43,1,1,
Hydraulic Head,6.807750,cm,0.0,1/m,0.0,1/m, 44, 44,1,1,
Hydraulic Head,6.919750,cm,0.0,1/m,0.0,1/m, 45, 45,1,1,

Hydraulic Head,7.029750,cm,0.0,1/m,0.0,1/m, 46, 46,1,1,
Hydraulic Head,7.137750,cm,0.0,1/m,0.0,1/m, 47, 47,1,1,
Hydraulic Head,7.243750,cm,0.0,1/m,0.0,1/m, 48, 48,1,1,
Hydraulic Head,7.347750,cm,0.0,1/m,0.0,1/m, 49, 49,1,1,
Hydraulic Head,7.449750,cm,0.0,1/m,0.0,1/m, 50, 50,1,1,
Hydraulic Head,7.549750,cm,0.0,1/m,0.0,1/m, 51, 51,1,1,
Hydraulic Head,7.647750,cm,0.0,1/m,0.0,1/m, 52, 52,1,1,
Hydraulic Head,7.743750,cm,0.0,1/m,0.0,1/m, 53, 53,1,1,
Hydraulic Head,7.837750,cm,0.0,1/m,0.0,1/m, 54, 54,1,1,
Hydraulic Head,7.929750,cm,0.0,1/m,0.0,1/m, 55, 55,1,1,
Hydraulic Head,8.019750,cm,0.0,1/m,0.0,1/m, 56, 56,1,1,
Hydraulic Head,8.107750,cm,0.0,1/m,0.0,1/m, 57, 57,1,1,
Hydraulic Head,8.193750,cm,0.0,1/m,0.0,1/m, 58, 58,1,1,
Hydraulic Head,8.277750,cm,0.0,1/m,0.0,1/m, 59, 59,1,1,
Hydraulic Head,8.359750,cm,0.0,1/m,0.0,1/m, 60, 60,1,1,
Hydraulic Head,8.439750,cm,0.0,1/m,0.0,1/m, 61, 61,1,1,
Hydraulic Head,8.517750,cm,0.0,1/m,0.0,1/m, 62, 62,1,1,
Hydraulic Head,8.593750,cm,0.0,1/m,0.0,1/m, 63, 63,1,1,
Hydraulic Head,8.667750,cm,0.0,1/m,0.0,1/m, 64, 64,1,1,
Hydraulic Head,8.739750,cm,0.0,1/m,0.0,1/m, 65, 65,1,1,
Hydraulic Head,8.809750,cm,0.0,1/m,0.0,1/m, 66, 66,1,1,
Hydraulic Head,8.877750,cm,0.0,1/m,0.0,1/m, 67, 67,1,1,
Hydraulic Head,8.943750,cm,0.0,1/m,0.0,1/m, 68, 68,1,1,
Hydraulic Head,9.007750,cm,0.0,1/m,0.0,1/m, 69, 69,1,1,
Hydraulic Head,9.069750,cm,0.0,1/m,0.0,1/m, 70, 70,1,1,
Hydraulic Head,9.129750,cm,0.0,1/m,0.0,1/m, 71, 71,1,1,
Hydraulic Head,9.187750,cm,0.0,1/m,0.0,1/m, 72, 72,1,1,
Hydraulic Head,9.243750,cm,0.0,1/m,0.0,1/m, 73, 73,1,1,
Hydraulic Head,9.297750,cm,0.0,1/m,0.0,1/m, 74, 74,1,1,
Hydraulic Head,9.349750,cm,0.0,1/m,0.0,1/m, 75, 75,1,1,
Hydraulic Head,9.399750,cm,0.0,1/m,0.0,1/m, 76, 76,1,1,
Hydraulic Head,9.447750,cm,0.0,1/m,0.0,1/m, 77, 77,1,1,
Hydraulic Head,9.493750,cm,0.0,1/m,0.0,1/m, 78, 78,1,1,
Hydraulic Head,9.537750,cm,0.0,1/m,0.0,1/m, 79, 79,1,1,
Hydraulic Head,9.579750,cm,0.0,1/m,0.0,1/m, 80, 80,1,1,
Hydraulic Head,9.619750,cm,0.0,1/m,0.0,1/m, 81, 81,1,1,
Hydraulic Head,9.657750,cm,0.0,1/m,0.0,1/m, 82, 82,1,1,
Hydraulic Head,9.693750,cm,0.0,1/m,0.0,1/m, 83, 83,1,1,
Hydraulic Head,9.727750,cm,0.0,1/m,0.0,1/m, 84, 84,1,1,
Hydraulic Head,9.759750,cm,0.0,1/m,0.0,1/m, 85, 85,1,1,
Hydraulic Head,9.789750,cm,0.0,1/m,0.0,1/m, 86, 86,1,1,
Hydraulic Head,9.817750,cm,0.0,1/m,0.0,1/m, 87, 87,1,1,
Hydraulic Head,9.843750,cm,0.0,1/m,0.0,1/m, 88, 88,1,1,
Hydraulic Head,9.867750,cm,0.0,1/m,0.0,1/m, 89, 89,1,1,
Hydraulic Head,9.889750,cm,0.0,1/m,0.0,1/m, 90, 90,1,1,
Hydraulic Head,9.909750,cm,0.0,1/m,0.0,1/m, 91, 91,1,1,
Hydraulic Head,9.927750,cm,0.0,1/m,0.0,1/m, 92, 92,1,1,

Hydraulic Head,9.943750,cm,0.0,1/m,0.0,1/m, 93, 93,1,1,
Hydraulic Head,9.957750,cm,0.0,1/m,0.0,1/m, 94, 94,1,1,
Hydraulic Head,9.969750,cm,0.0,1/m,0.0,1/m, 95, 95,1,1,
Hydraulic Head,9.979750,cm,0.0,1/m,0.0,1/m, 96, 96,1,1,
Hydraulic Head,9.987750,cm,0.0,1/m,0.0,1/m, 97, 97,1,1,
Hydraulic Head,9.993750,cm,0.0,1/m,0.0,1/m, 98, 98,1,1,
Hydraulic Head,9.997750,cm,0.0,1/m,0.0,1/m, 99, 99,1,1,
Hydraulic Head,9.999750,cm,0.0,1/m,0.0,1/m,100,100,1,1,
Leaky Hydraulic Head,0.0,m,0.0,1/m,0.0,1/m,1,1,1,1,
~Sources & Sinks
0 line(s) of sources & sinks input to follow.
~Output Control
3 line(s) of output control input follows.
0.,h,
1.,h,
3.,h,
1,1,10,1,90,1,100,1,1,
3 line(s) of output plot control input follows.
Hydraulic Head,
Species Liq Concentration,
Porosity,
4 line(s) of output display control input follows.
Hydraulic Head,
Species Concentration,
Storativity,
X-Dir. Liquid Velocity,

B. Input File of Two-Dimensional Groundwater Flow

~Simulation Title and Notes
Test for 2-D Boussinesq Equation
Sergey L. Kivva
IPMMS, Kiev
Monday, November 9, 1998
10:28:20 AM
0 line(s) of simulation title notes follows.
~Solution Schemes
false,false,false,
true,false,
2.0,h,
0.05,h,
1.500,
0.05,h,
true,
~Numerical Control
30,Maximum Residual,
1.0E-08,
Arithmetic Mean,Harmonic Mean,

~Grid Geometry
cartesian
30,20,
15.,cm,10.,cm,
0.,cm,
30 line(s) of grid geometry input follows.
Node 1, .250,cm,
Node 2, .750,cm,
Node 3, 1.250,cm,
Node 4, 1.750,cm,
Node 5, 2.250,cm,
Node 6, 2.750,cm,
Node 7, 3.250,cm,
Node 8, 3.750,cm,
Node 9, 4.250,cm,
Node 10, 4.750,cm,
Node 11, 5.250,cm,
Node 12, 5.750,cm,
Node 13, 6.250,cm,
Node 14, 6.750,cm,
Node 15, 7.250,cm,
Node 16, 7.750,cm,
Node 17, 8.250,cm,
Node 18, 8.750,cm,
Node 19, 9.250,cm,
Node 20, 9.750,cm,
Node 21,10.250,cm,
Node 22,10.750,cm,
Node 23,11.250,cm,
Node 24,11.750,cm,
Node 25,12.250,cm,
Node 26,12.750,cm,
Node 27,13.250,cm,
Node 28,13.750,cm,
Node 29,14.250,cm,
Node 30,14.750,cm,
20 line(s) of grid geometry input follows.
Node 1, .250,cm,
Node 2, .750,cm,
Node 3, 1.250,cm,
Node 4, 1.750,cm,
Node 5, 2.250,cm,
Node 6, 2.750,cm,
Node 7, 3.250,cm,
Node 8, 3.750,cm,
Node 9, 4.250,cm,
Node 10, 4.750,cm,

Node 11, 5.250,cm,
Node 12, 5.750,cm,
Node 13, 6.250,cm,
Node 14, 6.750,cm,
Node 15, 7.250,cm,
Node 16, 7.750,cm,
Node 17, 8.250,cm,
Node 18, 8.750,cm,
Node 19, 9.250,cm,
Node 20, 9.750,cm,
~Inactive Nodes
0 line(s) of inactive Nodes input follows.
~Aquifer Surfaces
1 line(s) of aquifer top-surface input follows.
20.,cm,1,30,1,20,
1 line(s) of aquifer bottom-surface input follows.
0.,cm,1,30,1,20,
~Rock or Soil Types
0 lines(s) of rock or soil types notes follows.
1 line(s) of rock or soil types input follows.
Sand,1,30,1,20,
~Mechanical Properties
1 line(s) of mechanical properties input follows.
Sand,0.02,0.02,,gm/cm^3,1.0,,m,,m,
~Hydraulic Properties
1 line(s) of hydraulic properties input follows.
Sand,0.05,0.05,hc:cm/h,1.e+20,s,
~Species Properties
1 line(s) of species properties input follows.
Sand,Solute,1.1574074E-9,m^2/s,0.0,gm liq./gm sol.,,s,,,,,
~Liquid Boundary Conditions
2 line(s) of liquid boundary conditions input follows.
Y-Direction: North Surface,Gradient @ Boundary,tabular,Y-Bound,,1,30,20,20,
X-Direction: East Surface,Gradient @ Boundary,tabular,X-Bound,,30,30,1,20,
62 line(s) of Head_W table input follows.
X-Bound, .00,h, -1.5000,cm/cm,
X-Bound, .10,h, -1.3636,cm/cm,
X-Bound, .20,h, -1.2500,cm/cm,
X-Bound, .30,h, -1.1538,cm/cm,
X-Bound, .40,h, -1.0714,cm/cm,
X-Bound, .50,h, -1.0000,cm/cm,
X-Bound, .60,h, -.9375,cm/cm,
X-Bound, .70,h, -.8824,cm/cm,
X-Bound, .80,h, -.8333,cm/cm,
X-Bound, .90,h, -.7895,cm/cm,
X-Bound, 1.00,h, -.7500,cm/cm,
X-Bound, 1.10,h, -.7143,cm/cm,

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X-Bound,  1.20,h,    -.6818,cm/cm,
X-Bound,  1.30,h,    -.6522,cm/cm,
X-Bound,  1.40,h,    -.6250,cm/cm,
X-Bound,  1.50,h,    -.6000,cm/cm,
X-Bound,  1.60,h,    -.5769,cm/cm,
X-Bound,  1.70,h,    -.5556,cm/cm,
X-Bound,  1.80,h,    -.5357,cm/cm,
X-Bound,  1.90,h,    -.5172,cm/cm,
X-Bound,  2.00,h,    -.5000,cm/cm,
X-Bound,  2.10,h,    -.4839,cm/cm,
X-Bound,  2.20,h,    -.4687,cm/cm,
X-Bound,  2.30,h,    -.4545,cm/cm,
X-Bound,  2.40,h,    -.4412,cm/cm,
X-Bound,  2.50,h,    -.4286,cm/cm,
X-Bound,  2.60,h,    -.4167,cm/cm,
X-Bound,  2.70,h,    -.4054,cm/cm,
X-Bound,  2.80,h,    -.3947,cm/cm,
X-Bound,  2.90,h,    -.3846,cm/cm,
X-Bound,  3.00,h,    -.3750,cm/cm,
Y-Bound,   .00,h,   -1.0000,cm/cm,
Y-Bound,   .10,h,    -.9091,cm/cm,
Y-Bound,   .20,h,    -.8333,cm/cm,
Y-Bound,   .30,h,    -.7692,cm/cm,
Y-Bound,   .40,h,    -.7143,cm/cm,
Y-Bound,   .50,h,    -.6667,cm/cm,
Y-Bound,   .60,h,    -.6250,cm/cm,
Y-Bound,   .70,h,    -.5882,cm/cm,
Y-Bound,   .80,h,    -.5556,cm/cm,
Y-Bound,   .90,h,    -.5263,cm/cm,
Y-Bound,  1.00,h,    -.5000,cm/cm,
Y-Bound,  1.10,h,    -.4762,cm/cm,
Y-Bound,  1.20,h,    -.4545,cm/cm,
Y-Bound,  1.30,h,    -.4348,cm/cm,
Y-Bound,  1.40,h,    -.4167,cm/cm,
Y-Bound,  1.50,h,    -.4000,cm/cm,
Y-Bound,  1.60,h,    -.3846,cm/cm,
Y-Bound,  1.70,h,    -.3704,cm/cm,
Y-Bound,  1.80,h,    -.3571,cm/cm,
Y-Bound,  1.90,h,    -.3448,cm/cm,
Y-Bound,  2.00,h,    -.3333,cm/cm,
Y-Bound,  2.10,h,    -.3226,cm/cm,
Y-Bound,  2.20,h,    -.3125,cm/cm,
Y-Bound,  2.30,h,    -.3030,cm/cm,
Y-Bound,  2.40,h,    -.2941,cm/cm,
Y-Bound,  2.50,h,    -.2857,cm/cm,
Y-Bound,  2.60,h,    -.2778,cm/cm,
Y-Bound,  2.70,h,    -.2703,cm/cm,
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Y-Bound, 2.80,h,   -.2632,cm/cm,
Y-Bound, 2.90,h,   -.2564,cm/cm,
Y-Bound, 3.00,h,   -.2500,cm/cm,
~Species Boundary Conditions
0 line(s) of species boundary conditions input follows.
~Initial Conditions
601 line(s) of initial conditions input follows.
Hydraulic Head,19.99375,cm,0.0,1/m,0.0,1/m, 1, 1, 1, 1,
Hydraulic Head,19.96875,cm,0.0,1/m,0.0,1/m, 2, 2, 1, 1,
Hydraulic Head,19.91875,cm,0.0,1/m,0.0,1/m, 3, 3, 1, 1,
Hydraulic Head,19.84375,cm,0.0,1/m,0.0,1/m, 4, 4, 1, 1,
Hydraulic Head,19.74375,cm,0.0,1/m,0.0,1/m, 5, 5, 1, 1,
Hydraulic Head,19.61875,cm,0.0,1/m,0.0,1/m, 6, 6, 1, 1,
Hydraulic Head,19.46875,cm,0.0,1/m,0.0,1/m, 7, 7, 1, 1,
Hydraulic Head,19.29375,cm,0.0,1/m,0.0,1/m, 8, 8, 1, 1,
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Hydraulic Head,19.21875,cm,0.0,1/m,0.0,1/m, 3, 3, 8, 8,
Hydraulic Head,19.14375,cm,0.0,1/m,0.0,1/m, 4, 4, 8, 8,
Hydraulic Head,19.04375,cm,0.0,1/m,0.0,1/m, 5, 5, 8, 8,
Hydraulic Head,18.91875,cm,0.0,1/m,0.0,1/m, 6, 6, 8, 8,
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Hydraulic Head,14.04375,cm,0.0,1/m,0.0,1/m, 21, 21, 8, 8,
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Hydraulic Head,12.96875,cm,0.0,1/m,0.0,1/m, 23, 23, 8, 8,
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Hydraulic Head, 9.14375,cm,0.0,1/m,0.0,1/m, 29, 29, 8, 8,
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Hydraulic Head,19.01875,cm,0.0,1/m,0.0,1/m, 3, 3, 9, 9,
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~Sources & Sinks
0 line(s) of sources & sinks input to follow.
~Output Control

3 line(s) of output control input follows.
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1.,h,
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1,1,10,1,20,1,30,1,1,
3 line(s) of output plot control input follows.
Hydraulic Head,
Species Liq Concentration,
Porosity,
4 line(s) of output display control input follows.
Hydraulic Head,
Species Concentration,
Storativity,
X-Dir. Liquid Velocity,

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