# Florida HEALTH

Florida Onsite Sewage Nitrogen Reduction Strategies Study

Task D.11

Aquifer Model Combined with Complex Soil Model Development

### White Paper

June 2014

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In association with:



Otis Environmental Consultants, LLC



# Florida Onsite Sewage Nitrogen Reduction Strategies Study

# TASK D.11 WHITE PAPER

# Aquifer Model Combined with Complex Soil Model Development

#### Prepared for:

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# Section 1.0 Introduction

#### 1.0 Introduction

As part of Task D for the Florida Onsite Sewage Nitrogen Reduction Strategies (FOS-NRS) Study a combined vadose zone and saturated zone model was developed. This report, prepared by the Colorado School of Mines (CSM), documents the Task D.11 aquifer model development.

The overreaching goal of Task D.11 (and subsequent tasks) is to develop quantitative tools for groundwater contaminant transport that can be employed by users with all levels of expertise to evaluate onsite wastewater treatment systems (OWTS). Like the approach in the development of the complex soil model STUMOD-FL (Task D.8), the aquifer model is intended to fill the gap that currently exists between end users and complex numerical models by overcoming the limitations in the application of complex models while maintaining an adequate ability to predict contaminant fate and transport. While complex numerical models have strengths, they are difficult to implement for end users with little modeling experience. As part of the process in developing an effective model, different analytical solutions were compared to determine those most accurate and efficient. As part of the validation and corroboration process, the groundwater transport tools will be evaluated against field data and other robust models (Tasks D.12 and D.13). In keeping with the current development of STUMOD-FL, the aquifer model has been implemented as an Excel Visual Basic Application (Excel VBA) to make the final product readily available to and easily implemented by a wide range of users.

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## Section 2.0 Background

An analytical solution has been developed for the saturated zone module to provide a computationally efficient tool for modeling the fate and transport of groundwater contaminant plumes. This model is referred to here after as the aquifer model. The model is designed to couple with STUMOD-FL to provide the user a seamless method for estimating the concentration and mass flux of nitrogen in an aquifer receiving percolate from the soil treatment unit (STU) of an OWTS. The governing equation which describes solute transport in porous media is given by equation 2-1, the advection dispersion equation (ADE) (Fetter, 1999). The ADE is a partial differential equation that requires sophisticated methods to solve. Numerical methods are common techniques that are utilized however numerical methods, the spatial and temporal domains must be discretized, and convergence criteria and boundary conditions for the problem must be defined. Beyond the input requirements numerical methods can be unstable returning erroneous results that require trained professionals to identify.

$$\left[\frac{\partial}{\partial x}\left(D_{x}\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{y}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_{z}\frac{\partial C}{\partial z}\right)\right] - \left[\frac{\partial}{\partial x}(v_{x}C) + \frac{\partial}{\partial y}(v_{y}C) + \frac{\partial}{\partial y}(v_{y}C)\right] = \frac{\partial C}{\partial t} \quad (2-1)$$

Because the aquifer model users are expected to have a wide range of expertise in mathematical modeling, numerical methods are not suitable. Analytical solutions provide advantages over numerical techniques, because they require relatively less input data and do not suffer numerical instabilities. Several analytical solutions to equation 2-1 have been derived which consider one, two and three dimensional contaminant transport (Domenico, 1987; Galya, 1987, Wexler, 1992).

Two methods were evaluated; a vertical plane source model (VPS) and a horizontal plane source model (HPS). Both the VPS and HPS models require certain parameter values be defined prior to predicting contaminant transport. Domenico and Robbins (1987) developed a methodology whereby the parameters for the VPS model could be reasonably determined from a concentration profile. While this may be a valid approach in some situations, the transport model has been preprogrammed with default values that enable a first approximation for contaminant transport. The principal parameters that

2.0 Background

will need to be estimated are groundwater velocity (hydraulic gradient), dispersivity in three dimensions, and rate terms for nitrogen transformations.

Existing Domenico based analytical tools assume the existence of a hypothetical "mixing layer", located beneath the source. The contaminant flux from the source zone is mixed homogeneously and instantaneously over this mixing layer. This idealized mixing provides a groundwater concentration beneath the source area, which becomes a boundary condition for transport in the groundwater. Transport in the groundwater is then evaluated using the Domenico solution. The assumption of ideal mixing could be a limitation to the Domenico solution since mixing is expected to be a gradual process related to various factors such as advection, lateral dispersion, density effects, etc. An alternative model that does not require this mixing assumption is a solution presented by Galya (1987) which assumes a HPS.

Because of the stability and minimal input requirements as well as the availability of a solution that specifically considers the geometry of an OWTS, the aquifer model was designed around an analytical solution to equation 2-1. The HPS solution derived by Galya (1987) was utilized, because it considers a horizontal mass flux contaminant source. The HPS solution does not require assumptions of a mixing layer beneath the STU or estimation of concentration for the contaminant source, Figure 2.1. Other analytical solutions that are derived for a vertical contaminant source such as those derived by Domenico (1987) and Wexler (1992) require explicit assumptions concerning the dimensions of the vertical source plane and concentration at the source plane, Figure 2.2.



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## Section 3.0 Horizontal Plane Source Model

Typical OWTS distribute effluent to the STU via a gravity or pressurized distribution system. Regardless of the distribution system that is employed, a HPS model is a reasonably accurate method of describing the contaminant source area (Figure 2.1). The HPS solution was derived by Galya (1987) using the work of Carslaw and Jaeger (1959) and Crank (1975). The equations presented below are solutions to a modified form of equation 2-1 which considers one dimensional advection and three dimensional dispersion, equation 3-1. The solution method is based on a mathematical proof given by Carslaw and Jaeger (1959) which states that a solution to a three dimensional partial differential equation may be derived from individual one dimensional solutions, equation 3-2.

$$\frac{\partial c}{\partial t} + \frac{v}{R} \frac{\partial c}{\partial x} = \frac{D_x}{R} \frac{\partial^2 c}{\partial x^2} + \frac{D_y}{R} \frac{\partial^2 c}{\partial y^2} + \frac{D_z}{R} \frac{\partial^2 c}{\partial z^2} - \lambda c + \frac{M_s}{\theta}$$
(3-1)

$$C(x, y, z, t) = \frac{1}{\theta_R} \int_0^t M_s(\tau) c(x, t-\tau) c(y, t-\tau) c(z, t-\tau) T(t-\tau) d\tau$$
(3-2)

Equations 3-3 through 3-6 are the one dimensional solutions to equation 3-1 in the x, y and z dimensions which are convolved over time to describe concentration at any point within an aquifer through time. Equation 3-5 is utilized for an aquifer of infinite or substantial thickness and equation 3-6 describes an aquifer of finite thickness. Use of equation 3-5 or 3-6 is specified by the user via a numerical tag recognized by the model. The user must enter '999' for aquifer thickness to consider an aquifer of infinite thickness. Equations 3-3 and 3-4 only consider an aquifer of infinite areal extent.

$$c(x,t) = \frac{1}{2L} \left[ \operatorname{erf}\left(\frac{\left(\frac{L}{2} - x - x' + \frac{vt}{R}\right)}{4\sqrt{D_{x}t/R}}\right) + \operatorname{erf}\left(\frac{\left(\frac{L}{2} - x + x' + \frac{vt}{R}\right)}{4\sqrt{D_{x}t/R}}\right) \right]$$
(3-3)

$$c(y,t) = \frac{1}{2B} \left[ \operatorname{erf}\left(\frac{\left(\frac{B}{2} - y - y'\right)}{4\sqrt{D_y t/R}}\right) + \operatorname{erf}\left(\frac{\left(\frac{B}{2} - y + y'\right)}{4\sqrt{D_y t/R}}\right) \right]$$
(3-4)

$$c(z,t) = \frac{1}{2\sqrt{(\pi D_z t/R)}} \left[ e^{-(z-z')^2/(4D_z t/R)} + e^{-(z+z')^2/(4D_z t/R)} \right]$$
(3-5)

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PAGE 3-1 HAZEN AND SAWYER, P.C. 3.0 Horizontal Plane Source Model

$$c(z,t) = \frac{1}{H} \left[ 1 + 2\sum_{n=1}^{\infty} e^{-\left(\frac{n^2 \pi^2 D_z t}{H^2 R}\right)} \cos\left(\frac{n\pi z}{H}\right) \cos\left(\frac{n\pi z'}{H}\right) \right]$$
(3-6)

The parameters in equations 3-3 through 3-6 are defined as follows:

x, y, z = location where concentration is evaluated (z = 0 is the water table)

x', y', z' = center of contaminant source plane (define as 0 in the aquifer model)

L = length of source plane

B = width of source plane

v = groundwater seepage velocity in the x dimension

R = retardation coefficient

 $D_x$ ,  $D_y$ ,  $D_z$  = dispersion coefficients

*n* = index for infinite sum

*t* = time (assigned large value for steady state conditions)

 $\theta = \text{porosity}$ 

Ms = contaminant loading rate

C (and c) = contaminant concentration in groundwater

 $\lambda$  = degradation rate constant

T = decay function for contaminant

 $\tau$  = variable of integration for Galya's solution expressed in terms of Green's functions (time)

Equation 3-6 contains an infinite sum, however Galya (1987) presents a method to estimate the number of terms needed to accurately calculate the solution in equation 3-7. Where  $\tau$  is the integration parameter utilized in equation 3-2.

$$N_{INF} = \left(\frac{H}{\pi}\right) \left[\frac{25R}{D_z}(t-\tau)\right]^{1/2} + 1$$
(3-7)

The convolution integral given in equation 3-2 is the complete analytical solution to equation 3-1 in terms of individual one dimensional solutions presented in equations 3-3 through 3-6. A closed form solution to equation 3-2 does not exist, however, it can easily be solved via numerical integration. Numerical integration computes the sum of the area beneath the curve described by equations 3-2 through 3-6 in a piece wise fashion. Numerous techniques exist to carryout numerical integration, many of which have been designed for functions that change rapidly. A simple trapezoidal method was selected to solve equation 3-2 after comparing multiple solution techniques. The trapezoidal method affords the needed accuracy while minimizing the computational cost.

3.0 Horizontal Plane Source Model

While equation 3-2 indicates the integration must be carried out from time zero to time t, the integration limits may be reduced. Galya (1987) adapted the work of Codell and Schriber (1977) for the HPS solution and shows that the lower and upper integration limits can be calculated as given in equations 3-8 and 3-9. The upper and lower integration limits given in equation 3-8 and 3-9 minimize the number of computations required to solve equation 3-2 providing an overall savings in computation time.

$$t_1 = t - \frac{\frac{2xv}{R} + \frac{100D_x}{R}}{\left(\frac{v}{R}\right)^2 + \frac{4D_x\lambda}{R}} - \left[ \left(\frac{\frac{2xv}{R} + \frac{100D_x}{R}}{\left(\frac{v}{R}\right)^2 + \frac{4D_x\lambda}{R}}\right)^2 - \left(\frac{4x^2}{\left(\frac{v}{R}\right)^2 + \frac{4D_x\lambda}{R}}\right) \right]^{1/2}$$
(3-8)

$$t_{2} = t + \frac{\frac{2xv_{+}+100D_{x}}{R}}{\left(\frac{v}{R}\right)^{2} + \frac{4D_{x}\lambda}{R}} - \left[ \left( \frac{\frac{2xv_{+}+100D_{x}}{R}}{\left(\frac{v}{R}\right)^{2} + \frac{4D_{x}\lambda}{R}} \right)^{2} - \left( \frac{4x^{2}}{\left(\frac{v}{R}\right)^{2} + \frac{4D_{x}\lambda}{R}} \right) \right]^{1/2}$$
(3-9)

The aquifer model is designed as a steady state model though equation 3-2 can be formulated in a manner that considers transient conditions. Considering transient conditions requires a mathematical description of the contaminant mass flux to the aquifer. The only benefit of such a rigorous approach would be if the level of accuracy in model predictions needed to be exceedingly high. Adding transient capabilities to the aquifer model would require the user to define time varying mass flux of nitrogen to the aquifer. This would likely be a needless complication because most users will not have sufficient resources or the expertise to estimate mass flux with such precision. If transient conditions are to be considered or the cost of not accurately estimating nitrogen concentrations is high, numerical models should be utilized and a substantial investment made in gathering the required input data for those models.



# Section 4.0 Implementation in Excel VBA

Algorithms have been developed in Excel VBA to solve equations 3-2 through 3-9. These form the core of the aquifer model, coupled with STUMOD-FL. Auxiliary algorithms have also been developed to provide the user with a mass flux estimate and visual representations of the plume cross section in the y-z plane and x-y plane. Additionally, methods have been developed to allow the user to estimate the groundwater seepage velocity and direction using spatially located hydraulic head observations. The method developed by Xu and Eckstein (1995) to estimate dispersivity has also been included to improve the availability of the aquifer model to a wide user group.

#### 4.1 Groundwater Seepage Velocity

Groundwater seepage velocity is an important parameter in the aquifer model. It can readily be calculated using Darcy's law, given in equation 4-1, and the Dupuit approximation which assumes flow lines are approximately horizontal (Fetter, 2001). Representative saturated hydraulic conductivity and porosity values for several soil textures are available through the STUMOD-FL graphical user interface (GUI). The hydraulic gradient, however, must be estimated or calculated directly. If no additional data is available the user may wish to estimate the hydraulic gradient as the average slope of the surrounding land surface. A similar method is utilized by ArcNLET which estimates the water table as a subdued replica of the land surface (Rios et al., 2013). Alternatively the magnitude of the hydraulic gradient can be calculated using the three point graphical method (Fetter, 2001).

$$v_x = \frac{q}{n} = -\frac{K_{sat}}{n} \frac{dh}{dl}$$
(4-1)

While the three point graphical method can be quickly learned, it is cumbersome and not suited for those who have not had exposure to hydrogeology. To address this and provide the user a quick and accurate method for estimating the hydraulic gradient, an algorithm was developed to solve the three point problem using vector analysis (Fienen, 2005). This algorithm makes use of three spatially located hydraulic head observations provided by the user. The user must provide hydraulic head measured using any reference datum and the latitude longitude coordinates of each observation. Latitude and longitude are spherical coordinates and were chosen as the preferred coordinate system

because most Global Positioning Systems (GPS) typically provide location in this coordinate system. Because latitude and longitude are spherical coordinates, they must be projected onto a flat coordinate system. This is accomplished by an additional algorithm adapted from a JAVA script developed by the Woods Hole Oceanographic Institution.

Using projected coordinates the magnitude and direction of the hydraulic gradient can be calculated by observing the following. Let  $p_1=(x_1,y_1,z_1)$ ,  $p_2=(x_2,y_2,z_2)$  and  $p_3=(x_3,y_3,z_3)$  be the spatially located head measurements where the x and y points represent the latitude and longitude coordinates projected on a flat surface and z the observed hydraulic head. Then two vectors that are positioned end to end can be constructed by subtracting p1 from p2 and p1 from p3.

$$\overrightarrow{v_{1}} = \begin{bmatrix} v_{1}\hat{i} \\ v_{1}\hat{j} \\ v_{1}\hat{k} \end{bmatrix} = p_{2} - p_{1} = \begin{bmatrix} (x_{2} - x_{1}) \\ (y_{2} - z_{1}) \\ (z_{2} - z_{1}) \end{bmatrix}$$
(4-2)

$$\vec{v}_{2} = \begin{bmatrix} v_{2}\hat{i} \\ v_{2}\hat{j} \\ v_{2}\hat{k} \end{bmatrix} = p_{3} - p_{1} = \begin{bmatrix} (x_{3} - x_{1}) \\ (y_{3} - z_{1}) \\ (z_{3} - z_{1}) \end{bmatrix}$$
(4-3)

Selecting  $\overline{v_1}$  such that it always lies to the right of  $\overline{v_2}$  and calculating the cross product of  $\overline{v_1}$  and  $\overline{v_2}$  will give a vector normal to the plane containing  $\overline{v_1}$  and  $\overline{v_2}$  pointing in the positive z direction (up), equation 4-4.

$$\overrightarrow{v_{1}} \times \overrightarrow{v_{2}} = \det \begin{bmatrix} \hat{i} & \hat{j} & \hat{k} \\ v_{1\hat{i}} & v_{1\hat{j}} & v_{1\hat{k}} \\ v_{2\hat{i}} & v_{2\hat{j}} & v_{2\hat{k}} \end{bmatrix} = \begin{bmatrix} (v_{1\hat{j}}v_{2\hat{k}} - v_{2\hat{j}}v_{1\hat{k}})\hat{i} \\ (v_{2\hat{i}}v_{1\hat{k}} - v_{1\hat{i}}v_{2\hat{k}})\hat{j} \\ (v_{1\hat{i}}v_{2\hat{j}} - v_{2\hat{i}}v_{1\hat{j}})\hat{k} \end{bmatrix}$$
(4-4)

Where the unit vector of  $\vec{v_1} \times \vec{v_2}$  can be calculated by equation 4-5, where  $\|-\|$  indicates magnitude:

$$\vec{n} = \frac{1}{\|(\vec{v_1} \times \vec{v_2})\|} (\vec{v_1} \times \vec{v_2})$$
(4-5)

Defining the projection of  $\vec{n}$  onto the x-y plane as  $\vec{n}_{proj}$ , will give a vector that can be used to find the direction of the hydraulic gradient relative of North (equation 4-6). This

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vector can be thought of as the shadow of the unit normal vector,  $\vec{n}$  on the horizontal plane if illuminated from directly above.

$$\vec{n}_{proj} = \vec{n} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} \vec{n}\hat{i} \\ \vec{n}\hat{j} \\ 0\hat{k} \end{bmatrix}$$
(4-6)

The angle between the unit vector pointing in the direction of North  $\overline{\alpha_x}$  (where North is  $0^o$ ) and  $\overline{n_{proj}}$  can be calculated using equation 4-7, giving the direction of the hydraulic gradient in degrees relative of north, where <sup>T</sup> indicates the transpose, as:

$$\theta = \cos^{-1} \left( \frac{\overrightarrow{\alpha_{x}} \cdot \overrightarrow{n_{proj}}}{\| \overrightarrow{\alpha_{x}} \| \| \overrightarrow{n_{proj}} \|} \right) = \cos^{-1} \left( \frac{\overrightarrow{\alpha_{x}}^T \overrightarrow{n_{proj}}}{\sqrt{\overrightarrow{\alpha_{x}}^T \overrightarrow{\alpha_{x}}} \sqrt{\overrightarrow{n_{proj}}^T \overrightarrow{n_{proj}}}} \right)$$
(4-7)

Equation 4-7 will give the inner angle between  $\overline{\alpha_x}$  and  $\overline{n_{proj}}$  which is always less than 180° but the true angle can easily be determined by observing the sign of the x and y components of  $\overline{n_{proj}}$ . A positive value for both x and y or a positive and negative value for x and y, respectively, indicates an angle between  $\overline{\alpha_x}$  and  $\overline{n_{proj}}$  less than 180° lying in quadrant one or four. If the values of x and y are both negative or negative and positive, respectively, then the angle is greater than 180° when measured clockwise from north and the angle lies in quadrant two or three.

With the direction of the hydraulic gradient being established, it is relatively easy to then calculate the magnitude of the hydraulic gradient. The magnitude is measured off a horizontal reference plane giving the magnitude of the gradient as slope (length per length) which is familiar to many and can be utilized directly in computing the groundwater seepage velocity. Observing the unit normal vector calculated by equations 4-4 and 4-5 it is easy to see that the dip angle of the plane defined by the three head observations is equal to the angle between the unit normal vector and a vector normal to the horizontal plane. The magnitude is then calculated by equation 4-8.

$$grad = \frac{\vec{n}k}{\|\vec{n}_{proj}\|} \tag{4-8}$$

The output from this algorithm is displayed on the aquifer model GUI, Figure 4.1, providing the user the hydraulic gradient and direction in degrees relative of North. The direction is also projected onto a North arrow image imbedded within the GUI providing the user a visual that can be easily interpreted. This algorithm may be run independently of

the aquifer model if the user wishes to investigate the site specific hydraulic gradient and direction. The hydraulic gradient algorithm is automatically run as part of the aquifer model if the user provides the required inputs and selects the option to calculate the hydraulic gradient. The calculated hydraulic gradient is then utilized to calculate the groundwater seepage velocity utilizing equation 4-1.



Figure 4.1: Aquifer Model GUI Figure that allows Users to Visualize the Direction of the Local Hydraulic Gradient

#### 4.2 Dispersivity Estimates

Numerous studies have attempted to develop mathematical relationships between flow length and dispersivity. Dispersivity is an important parameter in contaminant transport because it describes the degree of spreading that will occur. Large dispersivity values will cause lower peak concentrations because the solute mass is dispersed over a larger volume. Lallemand-Barres and Peaudecerf (1978) were the first to publish a log-log plot of dispersivity and flow length which appears to suggest that dispersivity can be approximated as 1/10th the flow length. More recent work by Gelhar (1986) and Gelhar et al. (1992) show that this common assumption is perhaps flawed and could lead to excessively high dispersivity values. The work of Gelhar et al. (1992) suggests that dispersivity may reach some asymptotic value at large flow lengths and several methods have been developed to estimate dispersivity given these observations (Newman, 1990; Xu and Eckstein, 1995).

The aquifer model provides a method whereby the user can choose to allow the model to estimate dispersivity values based on flow length. The method that was selected was chosen based on a review of studies that reported dispersivity values for surficial sand aquifers similar to those in Florida (Bitsch and Jensen, 1990; Mallants et al., 2000; Sudicky et al., 1983). The relationship developed by Xu and Eckstein (2005), equation 4-9, is capable of replicating the observations from these studies and also follows the observations of Gelhar et al. (1992) that suggest dispersivity reaches asymptotic values at large distances. This method has precedence as well, as it is a method utilized by the EPA for estimating dispersivity values (http://www.epa.gov/athens/learn2model/parttwo/onsite/longdisp.html) and has been incorporated as standard practice in contaminant transport modeling for OWTS by some state environmental protection agencies (Idaho). Equations 4-10 and 4-11 determine the transverse horizontal and transverse vertical dispersivity. These relationships are based on the observations of many that contaminant plumes are generally flat and narrow with respect to longitudinal length. These relationships are not based on any physical data but are generally conservative estimates of dispersivity and yield conservative estimates. If more accuracy is required in model predictions the user is encouraged to independently evaluate dispersivity at the location under consideration.

$$\alpha_x = 0.83(\log_{10}(x))^{2.414} \tag{4-9}$$

$$\alpha_y = \frac{1}{10} \alpha_l = 0.083 (\log_{10}(x))^{2.414}$$
(4-10)

$$\alpha_z = \frac{1}{100} \alpha_l = 0.0083 (log_{10}(x))^{2.414}$$
(4-11)

#### 4.3 Mass Flux and Plume Cross Sections

The aquifer model will provide the user with estimates of concentration and mass flux as well as plume cross sections for visualization. Concentration is calculated via equation 3-2 through 3-6 as outlined in the preceding sections. Mass flux and plume cross sections are calculated via two algorithms that estimate the dimensions of the plume and calculate nitrogen concentrations at discreet points within the plume. Plume cross sections can be utilized by the user to understand the distribution of nitrogen within the aquifer down gradient of an OWTS while mass flux may be used to estimate nitrogen loads from an OWTS to a stream or lake and the likelihood of exceeding the nitrogen total maximum daily load for that water body.

The mass flux is constructed using equation 4-12, which calculates mass flux for a cross section perpendicular to the hydraulic gradient, Figure 4.2. The extent of the plume in the  $\pm y$  and z direction is determined by an algorithm that calculates the location where the plume concentration is approximately 0.0004 mg-N/L. These locations mark the maximum extent of the plume. Using lower concentrations to locate the extent of the plume is not practical because of the number of calculations that would be required significantly increase while not providing any significant improvements in accuracy. The plume is then discretized into N rows and M columns where the total number of cells across the entire cross section is 1600.



#### Figure 4.2: Illustration of Aquifer Model Mass Flux Calculated by Creating a Plane Perpendicular to the Hydraulic Gradient Discretized in N Rows and M Columns

The number of rows to columns is determined by the ratio of the plume depth to height. This is necessary to avoid errors that could arise when there is a large difference between the transverse dispersivity values. By determining the number of rows and columns based on plume width and depth the mass flux algorithm will increase the discretization along the dimension where the concentration gradient is the largest. The concentration in equation 4-12 is calculated at the center of each cell and mass flux is calculated as the product of the volumetric flux through the cell and the cell concentration. Be-

cause of plume symmetry, computation time is reduced in half by calculating the mass flux for one side of the plume and then doubling the calculated mass flux.

The plume cross sections in the y-z and x-y planes are generated using equation 4-12 in a manner similar to that described for mass flux. The x-y plume cross section is essentially an aerial view of the plume. The user must specify the 'x' location where the plume cross section is to end and the 'z' plane where the plume is to be located. The user may choose to construct a plume cross section at the water table or below the water table. The number of rows and columns that are used to generate the plume cross sections are fixed. For both the y-z and x-y cross sections there are exactly 40 rows and 40 columns. This was necessary because of the limited graphics capabilities within Excel. The one disadvantage of fixing the number of rows and columns is that the image that is generated is at times distorted. For example, a y-z cross section with a depth of 10 feet and a width of 50 feet will look square because it contains the same number of rows in the 'Z' dimension as it has columns in the 'Y' direction, Figures 4.3 and 4.4. However the width and depth or length of the plume is always reported on the cross section so the user will have an understanding of the actual dimensions of the plume.



Length, 1500 ft

Figure 4.3: Aquifer Model Plan View of the Contaminant Plume (the plume is constructed for a plane coinciding with the water table)



Figure 4.4: Aquifer Model Plume Cross Section in the y-z Plane (inputs are generic)



# Section 5.0 Integration of Aquifer Model with STUMOD-FL

The aquifer model follows the design of STUMOD-FL by utilizing a GUI to facilitate user interaction. The GUI is constructed as an addition to STUMOD-FL and is available to the user on a separate tab within the STUMOD-FL GUI (Figure 5.1). The user may choose to use the aquifer model independently of STUMOD-FL; however they will access it utilizing the STUMOD-FL GUI. The aquifer model has been integrated with STUMOD-FL such that STUMOD-FL outputs will automatically populate the correct aquifer model input fields, if STUMOD-FL is run prior to running the aquifer model. STUMOD-FL parameters and outputs that correspond with the aquifer model inputs are, saturated hydraulic conductivity, porosity, hydraulic loading rate (HLR) and concentration. Three of these are parameters defined by the user through the STUMOD-FL GUI and are simply carried over to the aquifer model GUI. Concentration of nitrogen at the water table is a STUMOD-FL output and is obtained directly from the STUMOD-FL algorithm. Concentration, hydraulic loading rate, and the dimensions of the infiltrative surface are utilized by the aquifer model to calculate mass flux of nitrogen at the water table.

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Figure 5.1: Illustration of Aquifer Model GUI

The aquifer model GUI is designed to guide the user through the other inputs that are required by grouping input fields by type. The "Input Dimensions" are parameters specific to the OWS that will be evaluated. The width and length refer to the footprint of the infiltrative surface that can easily be measured in the field as the width and length of the area where the distribution tubes have been installed. The HLR is the volumetric flow rate applied to the infiltrative surface per day divided by the area of the infiltrative surface. If STUMOD-FL is run prior to running the contaminant transport model, the HLR value is automatically populated. The latitude and longitude refer to the center of the infiltrative surface and are only utilized if the user chooses to calculate the distance to the point where concentration or mass flux will be evaluated rather than input those data directly.

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"Aquifer Properties" refer to the physical characteristics of the surficial aquifer where the OWS is constructed. The porosity and saturated hydraulic conductivity are automatically populated with values from the STUMOD-FL interface if STUMOD-FL is run prior. The values from STUMOD-FL have been determined based on soil textural classes. The aguifer thickness is the thickness of the saturated zone or the distance from the water table to the first confining unit. If the user enters the value '999' equation 3-5 is selected to calculate the concentration or mass flux for an aquifer of substantial thickness. The three dimensional dispersivity values must be input by the user or the user may select to calculate those values based on the longitudinal distance to the observation point. The method for calculating dispersivity has been described in Section 4.2. If the user chooses this method, the input fields for those parameters become inactive indicating to the user that input to those fields is no longer needed. The estimated dispersivity values are posted to the respective dispersivity input fields once the model is done running to allow the user to evaluate the dispersivity values. The user may alter the estimates after the first model run by unchecking "Estimate Dispersivity" which activates the input fields but does not alter the values.

"Groundwater Velocity" or seepage velocity can be calculated using the method described in Section 4.1. If the user does not have access to spatially located hydraulic head observations, they must specify the magnitude of the local hydraulic gradient and the option to calculate hydraulic gradient becomes inactive. If the user chooses the option to calculate the hydraulic gradient the input fields for latitude, longitude and head become active signaling to the user that inputs are required. The user may choose to calculate the direction and magnitude of the hydraulic gradient independent of a model run by clicking "Run Groundwater Model." The magnitude and direction of the hydraulic gradient is reported on the GUI and the direction is plotted relative to a North arrow imbedded within the GUI. If the user does not choose to calculate the hydraulic gradient prior to running the model, results are posted after the entire model is finished running. The ability to calculate the direction of the hydraulic gradient independent of a model run is useful, because it may indicate to the user that the local direction of flow is oriented differently than what they may have anticipated.

"Contaminant Properties" refer to the chemical characteristics of the contaminant that affect its movement within the aquifer. Nitrate is generally not retarded in the subsurface but the option to change the retardation factor is given to allow a user the flexibility of modeling the transport of other contaminants, such as ammonium, in the subsurface. This option may also be utilized to evaluate the effects of anion exclusion on nitrate transport. Retardation values less than one indicate solutes are traveling faster than the average seepage velocity. This can occur when solutes are restricted to faster moving

pore water because of charge repulsion between the soil matrix and the solute (James and Rubin, 1986; McMahon and Thomas, 1974). First order kinetics are utilized to simulate the denitrification process which is the generally accepted method (McCray et al., 2005). Also, the use of first order kinetics to represent denitrification is a conservative approach that minimizes model parameters. Concentration refers to the concentration of nitrate (as nitrogen) in the percolate at the water table. STUMOD-FL has been designed to calculate this value and is the best method for obtaining this value. This field will contain STUMOD-FL calculated concentrations at the water table if STUMOD-FL is run prior to running the aquifer model.

The user may select outputs within the "Visualization & Multiple Spatial Inputs" section. The "Multiple OWS" option is not active in this version of the aquifer model. This option is currently under development and will meet Task D.14 specifications. Two options are available to calculate mass flux using a user specified distance or a calculated distance using latitude and longitude provided by the user. The distance is measured between the center of the infiltrative surface and the location where mass flux is to be calculated such as a stream or lake. The latitude and longitude option is provided to the user in the event that the distance is substantial and the user does not have an adequate measuring device. Similarly, concentration can be calculated at a user specified point using x, y and z distances from the center of the infiltrative surface or by providing latitude and longitude. A plume cross section can be constructed in the y-z plane if the user specifies the location down gradient where the cross section is to be constructed. An aerial view of the plume may also be constructed at the water table or below the water table at the location specified by the user. Concentration, mass flux and cross section outputs are provided within the STUMOD-FL GUI on a tab adjacent to the aquifer model tab. Outputs also include plume width, depth and minimum and maximum concentrations within the plume if mass flux or plume cross sections are calculated.

The aquifer model interface has been designed to facilitate user interaction. Appropriate input fields become active or inactive based on user selection prompting the user to enter data where needed. If inputs are missing and the user attempts to run the aquifer model, they will be prompted to provide the missing inputs. Within the "Visualization & Multiple Spatial Inputs" section, the user will note that only one output can be selected at a time. For example if mass flux is to be calculated, all other output options become inactive. This design is to prevent confusion when the user chooses to view outputs. Preventing multiple outputs from being selected at the same time prevents the model from crashing or becoming inactive for extended periods of time. Some of the calculations are cumbersome and require time to complete. Progress indicators, which users familiar with

GUI's often expect, have also been included to indicate to the user that the model is indeed running and has not malfunctioned.



## Section 6.0 Summary

The aquifer model is designed to couple seamlessly with STUMOD-FL, providing the user an estimate of nitrogen concentration or mass flux through the vadose zone and into the saturated zone. While the aquifer model is designed to work in conjunction with STUMOD-FL it may be utilized independently of STUMOD-FL, though access to the aquifer model is still provided through the STUMOD-FL GUI. The option to calculate the hydraulic gradient magnitude and direction can be utilized independently of the aquifer model. This may be useful to the user if they wish to understand the local groundwater flow regime for a site to better locate an OWTS. The parameters and outputs utilized by STUMOD-FL and relevant to the aquifer model are automatically updated if STUMOD-FL is run prior to running the aquifer model. The user is provided the ability to modify these values if they choose before running the aquifer model. The user interface for the aquifer model has been designed to be intuitive and intelligent indicating to the user where inputs are needed or no longer needed and by prompting the user when input data is missing. Progress indicators allow the user to see the model is functioning correctly and has not malfunctioned.

The analytical HPS solution derived by Galya (1987) is the core of the aquifer model. Use of an analytical solution to the ADE to describe contaminant transport in aquifers greatly minimizes the required inputs and the computation time and guarantees stability in the solution. Analytical solutions, however, do not afford the flexibility to consider multi-dimensional advection or temporally varying boundary conditions. Also, the HPS solution does not consider spatial variation in hydraulic conductivity or denitrification. While numerical solutions afford this flexibility, the limitation is often the availability of input data and the numerical solution may approach that of the analytical. The anticipated lack of input data is also why the aquifer model has been designed as a steady state model, though the HPS solution is capable of considering transient conditions. The limitations of the aquifer model have been carefully considered in order to maximize the model capabilities while meeting the project specifications of an easy to use mathematical tool. The current design of the aquifer model will provide the user quantitative estimates of dispersivity, concentration, mass flux and the magnitude and direction of the hydraulic gradient in a timely and accessible manner.



## Section 7.0 References

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