Brad Cross

From: Brad Cross
Sent: Friday, May 06, 2011 11:40 AM
To: 'bssmith@tceq.state.tx.us'
Cc: James Beach; David O'Rourke; 'sreinert@epwu.org'
Subject: FW: El Paso Model Information
Attachments: Modman.pdf; MT3DMS_manual.pdf; image002.png; image004.png; image006.png; image008.png; image001.png; image002.png; image003.png; image004.png

Good Morning Bryan,

As a follow-up to our telephone discussion this morning, below you will find a brief summary of both the MODFLOW and MT3D programs. We have also attached user guides for both programs should you desire additional information.

Should you have any further questions on the use of the models, please do not hesitate to let us know.

Thanks!

Brad

MODFLOW is a public domain code that simulates the three-dimensional movement of groundwater through porous earth material described by the partial differential equation:

$$\frac{\partial}{\partial_x}\left(K_{xx}\,\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial_y}\left(K_{yy}\,\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial_y}\left(K_{zz}\,\frac{\partial h}{\partial z}\right)-W=S_s\,\frac{\partial h}{\partial t}$$

Where

K_{xx}, K_{yy}, and K_{zz} are values of hydraulic conductivity along the x, y, and z coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity;

h is the potentiometric head;

W is a volumetric flux per unit volume and represents sources and/or sinks of water;

Ss is the specific storage of the porous material;

t is time.

This equation, together with specification of flow and/or head conditions at the boundaries of an aquifer system and specification of initial head conditions, describes a groundwater flow system under nonequilibrium conditions in a heterogeneous and anisotropic medium, provided the principal axes of hydraulic conductivity are aligned with the coordinate directions. MODFLOW uses a block-centered finite-difference approximation to solve the partial differential equation for each grid cell and time step defined in the model.

MT3D is a public domain three-dimensional transport model commonly used in contaminant transport modeling and remediation assessment studies. (MT3DMS refers to a recent update that incorporates changes for Multiple Species).

MT3D can be used to simulate changes in concentration of contaminants in groundwater considering advection, dispersion, diffusion, and some basic chemical reactions, with various types of boundary conditions and external sources or sinks. It is designed for use with any block-centered finite difference flow model, such as MODFLOW. The partial differential equation describing the fate and transport of contaminants of species k in three-dimensional, transient groundwater flow systems can be expressed as follows:

$$\frac{\partial(\theta C^k)}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C^k}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(\theta v_i C^k) + q_s C_s^k + \sum R_n$$

Where

C^k is the dissolved concentration of species k;

Θ is the porosity of the subsurface medium;

t is time;

x_i is the distance along the respective Cartesian coordinate axis;

D_{ij} is the hydrodynamic dispersion coefficient tensor;

v_i is the seepage or linear pore water velocity; it is related to the specific discharge or Darcy flux through the relationship, $v_i = q_i/\Theta$;

q_s is the volumetric flow rate per unit volume of aquifer representing fluid sources (positive) and sinks (negative);

C_s^k is the concentration of the source or sink flux for species k;

$\sum R_n$ is the chemical reaction term;

More detailed information on the derivation and manipulation of the fate and transport equation is contained in Chapter 2 of the documentation and user's guide for MT3D, which is attached to this email. A link to the original documentation of MODFLOW, including details of the groundwater flow equation and the finite-difference application, is included in the electronic manual for MODFLOW, also attached.