Improving Ground-Water Flow Model Calibration With the Advective-Transport Observation (ADV2) Package to MODFLOW-2000

The Advective-Transport Observation (ADV2) Package (Anderman and Hill, 2001) allows advective-transport observations of steady-state flow fields to be used in conjunction with the hydraulic head and flow observations included in the three-dimensional ground-water flow parameter-estimation model MODFLOW-2000 (Harbaugh and others, 2000; Hill and others, 2000). In the ADV Package, advective-transport paths and times are represented using particle tracking. This allows advective-transport observations to be included in the regression with minimal increase in computational effort. Features of the package include:

- *A particle-tracking routine that duplicates the semi-analytical method of MODPATH (Pollock, 1994).*
- *Comparison of the x-, y-, and z-movements of the simulated and observed advective front at defined times. Thus, the direction and path of travel as well as the overall travel distance is included in the calibration process.*
- *Calculation of sensitivities of the particle movement to the parameters using the exact sensitivity-equation approach. Composite scaled sensitivities provide users with a quantitative measure of the information provided by the observations.*
- *Particle tracking in a forward or backward direction can be used to evaluate transport of contaminants or recharge areas.*
- *Inclusion of effects such as retardation by adjustment of the effective-porosity value.*

Effective porosity is not included as a parameter to be estimated in version 2.0 of the ADVpackage.

This publication outlines the major features of the ADV Package and gives information on obtaining the program and documentation.

The ADV Package

Observations of the advective component of contaminant transport can provide important information for the calibration of ground-water flow models. The addition of the Advective-Transport Observation (ADV2) Package to MODFLOW-2000 allows the path and speed of advective travel to be used in conjunction with formal parameter-estimation methods, which are powerful tools for model calibration (Hill, 1998; Poeter and Hill, 1997).

Applying the ADV Package

Advective-transport observations generally cannot be measured directly but can be inferred from a number of data types, such as contaminant concentrations, tracer tests, or, in some circumstances, age datings. If contaminant concentrations are used, advective-transport observations can be obtained by contouring measured concentrations and using the distribution along the plume front to determine the likely advective-front location, as shown by the triangle in figure 1. In some situations, an analytical solution can help approximate an advective-front location.

A simulated equivalent to the observation is generated by tracking a particle through the grid from the source location for the known time of ground-water movement, as shown by the blue line in figure 1. The differences in the x-, y-, and z-components between the simulated and observed advective-front locations are then used in the nonlinear regression in conjunction with the differences between the simulated and observed heads and flows to estimate optimal model parameter values.

If ground-water age dates are used, the ADV Package can be used to test hypothesized recharge areas. In this case, a particle is tracked backward from the observed age-date location, and the advective-transport observation consists of the hypothesized recharge area; regression is used to determine whether the resulting flowpath is possible with reasonable parameter values.

It is important to include the uncertainty in approximated advective-transport observations in the analysis. The weighted regression procedure used in MODFLOWP allows this uncertainty to be included explicitly.

Improving Model Calibration With the ADV Package

Application of the ADV Package to the Otis Air Force Base sewage-discharge plume (Anderman and others, 1996) illustrates the utility of the package.

Parameter sensitivities indicate the relation between changes in parameter values (e.g. hydraulic conductivity and recharge rate) and simulated values of head,

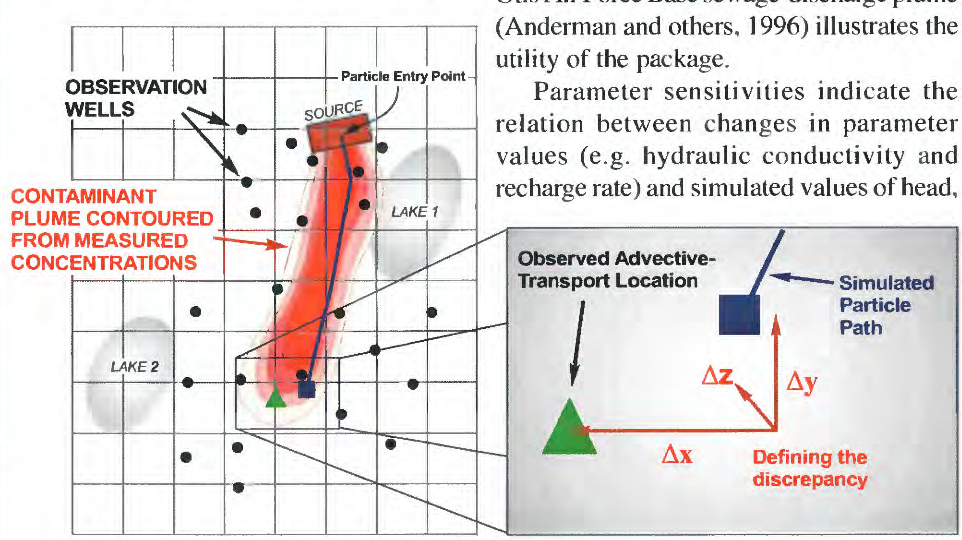

Figure 1. Conceptual representation of advective-transport observations.

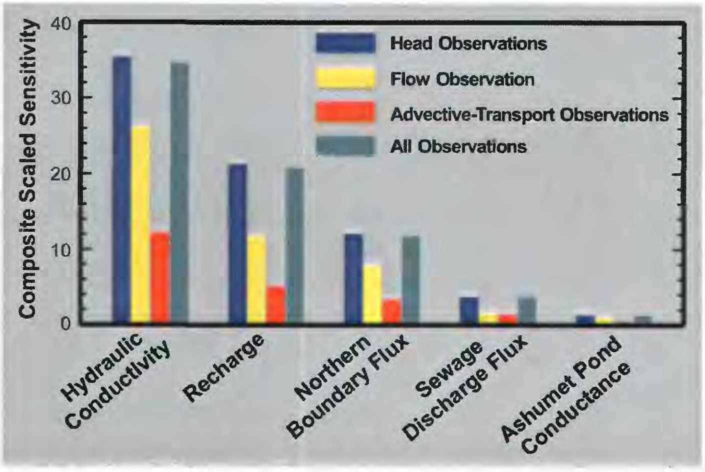

Figure 2. Composite scaled sensitivities for the Otis Air Force Base model are one measure of the information provided by different types of data.

flow, and advective transport within the model. They also provide a measure of the information about the system parameters present in the different data types and indicate how well the parameters are likely to be estimated from the available data. In the Otis Air Force Base model, sensitivities for the advective-transport observations are smaller than for the other observations (fig. 2). The additional information provided by the advective-transport observations, however, reduces parameter correlation (fig. 3), which measures if a coordinated change in parameter values produces the same model solution, such that the parameters cannot be estimated uniquely.

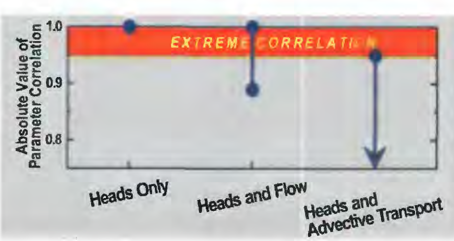

Figure 3. Range of parameter correlation for the Otis Air Force Base model with different types of data. For correlation greater than 0.95, parameters may not be estimated uniquely and predictions may be substantially in error. For the data set with heads only, all values equal 1.

Ground-water flow model validity can be judged, in part, by evaluating the reasonableness of the parameter estimates. Historically, unreasonable estimated parameter values have been perceived as a drawback of inverse modeling; in fact, they provide useful information that allows the modeler to scrutinize the model and, perhaps, explore alternative conceptual models (Poeter and Hill, 1997), resulting in a better calibrated model. In the Otis Air Force Base model, investigation of an unreasonable value of estimated recharge revealed that the model was sensitive to a) the season in which observations are obtained, and b) the heads at the downstream boundary conditions. This led to reevaluation of the data collection effort and the conclusion that probable errors in the stream elevations caused significant model error.

Advective-transport observations reflect ground-water velocities and patterns over a long period of time and provide more complete information about the ground-water flow system than flow measurements taken at a discrete point in time. This results in different estimated parameter values when different observation types are used and has a significant impact on the probable accuracy of the transport predictions of the model. This is clearly demonstrated by the Otis Air Force Base model. The plume movement simulated by a model calibrated with only hydraulic-head and flow observations significantly underpredicted the observed plume movement, as indicated by the yellow box in fig. 4. Including the advective transport in the model calibration resulted in a model that more accurately simulated subsurface flow rate and direction, as indicated by the blue box in fig. 4.

How to Obtain ADV Package Program, Documentation, and Additional Information

The ADV2 Package is included with MODFLOW-2000 at no cost and is available from the USGS at World Wide Web site *http://water.usgs.gov/nrp/gwsoftware/modflow2000/modflow2000.html*. The site includes links to download program source code, test data sets, and compiled versions for some computers.

To purchase reports documenting USGS model programs, contact:

U.S. Geological Survey
Branch of Information Services
Box 25286
Denver, CO 80225-0286

—*E.R. Anderman and M.C. Hill*

Figure 4. Improved simulated plume movement using advective-transport observations.

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