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Determination of stability criteria for a semi-analytical model of solute transport

By:
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Management Perspective

Simulation of groundwater flow and contaminant transport is a routine method of analysis in hydrogeology. In many cases, the computational models that are used to predict groundwater flow and transport are robust for only a limited range of conditions, and a method of predicting the failure of a given model is required in order to ensure the reliable performance of the model. This paper describes the determination of stability criteria for RADT, an existing model of solute transport during divergent radial tracer tests. RADT has proven to useful in predicting tracer breakthrough and in estimating the formation properties that are manifest in tracer test data. The stability criteria that are determined in this paper reduce the frequency of the failure of RADT, thereby adding considerable value to the model.

Determination of stability criteria for a semi-analytical model of solute transport

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Abstract

Stability criteria are determined for RADT, a semi-analytical model of solute transport during divergent radial tracer tests. These stability criteria differentiate the conditions where RADT successfully returns solute concentration from the conditions that lead to the failure of the model. The criteria are determined in an experimental manner by relating the parameters that form input to RADT to the observed conditions at failure. Two criteria are obtained where both reflect advection and dispersion of the solute and assume critical values that are regulated by the input parameters.

Introduction

Re-use of an existing computational model in an extended algorithm (e.g., an inverse analysis routine) is an effective method of software development that avoids the formulation of redundant models and reduces development time and cost. Examples of this approach are presented by Piggott et al. (1992) and Piggott et al. (1994). Implementation of a model in this manner requires that the model is not prone to failure, or is designed to terminate in a controlled manner when failure is imminent. For example, an inverse analysis algorithm is likely to be of little value if the failure of a component model routinely aborts the analysis. Many research calibre models do not perform without fault over the full range of input parameter values, so methods of reducing the probability of failure of these models are very desirable.

This paper describes the determination of stability criteria for RADT, which is based on a semi-analytical solution for solute transport in a divergent radial flow field (Novakowski, 1992). Particular solutions for solute concentration in the formation and in observation wells are obtained using the Laplace transform method in conjunction with a numerical inversion scheme (De Hoog et al., 1982). The particular solutions consist of algebraic combinations of exponential and Airy functions. Airy functions are a solution to a particular Bessel equation in which the first order term with respect to the spatial coordinate is not present (Abramowitz and Stegun, 1964). Thus, the stability of the solution in real space is dependent on the precision of the numerical inversion scheme and the Airy functions. Moench (1991) provides a detailed comparison of solutions based on different implementations of the scheme for Laplace transform inversion and of the Airy functions. The range of Peclet numbers (a relative measure of solute transport by advection and dispersion) over which the solution remains viable is dependent primarily on the precision of the computer and the robustness of the implementation of the Airy functions. Peclet numbers as large as 220 were achieved using the De Hoog et al. (1982) algorithm and a non-commercial implementation of the Airy functions, when executed on a personal computer.

With extended use, it was determined that RADT fails under conditions that do not display the anticipated relation to the magnitude of the Peclet number (Novakowski and Lapcevic, 1994). Specifically, Peclet numbers as low as 100 occasionally cause failure. Figure 1 shows the record of the solute concentration returned by RADT for input parameters that are consistent with transport in a single fracture in rock (P.A. Lapcevic, personal communication, 1994). The results span the range of values of time where RADT returns solute concentrations, in other words, the model fails at all values of time that are less than 4.5×10^2 s or greater than 7.3×10^5 s. Two sets of results are shown in Figure 1. The first set of results was generated on a DOS-based personal computer and displays a consistent variation at large values of time. The second set of results was generated on a UNIX-based workstation and displays spurious fluctuations that are characteristic of advection-dominated solute transport (Huyakorn and Pinder, 1983).

Occasional failure of RADT is easily managed in manual type-curve matching of tracer test data; however, automated type-curve matching (inverse analysis) using RADT requires that the frequency of failure is nominal. Thus, the purpose of this paper is to describe the determination of stability criteria that predict the failure of RADT and can be used to achieve the required reduction in the frequency of failure. These criteria are developed using an experimental approach that requires no knowledge of RADT other than the identity of the input parameters.

Determination of the Stability Criteria

The stability criteria were determined by linking RADT to an algorithm that supplies input parameters to the model and then decreases or increases the time at which solute concentration is requested until RADT terminates with an error message. The times at which solute concentrations are requested are output and the time at failure is approximated by the last value recorded prior to failure. The algorithm generates the required sequence of times using

$$t_{i+1} = a\,t_i \tag{1}$$

where a < 1 for a descending series of times and a > 1 for an ascending series. Values of a = 0.99 and a = 1.01 provide adequate resolution of the time at failure, and a value of t_i for which RADT successfully returns solute concentration is used to initialize the sequence.

The list of formation parameters that regulate solute concentration includes the dispersivity, porosity, and thickness of the formation, α, θ_f, and b; the distance between the injection and observation wells, r; the injection rate, q; and details of the construction of the injection and observation wells, r_s and r_o, V_s and V_o, and γ_s and γ_o. For transport in a single fracture, the coefficient of molecular diffusion of the tracer, D*, and the tortuosity and porosity of the adjacent formation, τ and θ_m, also regulate solute concentration. The role of these parameters in defining solute concentration is described in Novakowski (1992).

Inference of the conditions associated with the failure of RADT involved defining reference input parameter values, perturbing each of these values, and observing the time at failure for the reference and perturbed parameter values. For example, two values of the time at failure, t_1 and t_2, were recorded for two values of the dispersivity of the formation, α_1 and α_2, where the remaining parameters retained the reference values. It was then possible to resolve a series of scaling relations that predict the failure of RADT by inspection of the results obtained for each of the input parameters. Not all of the input parameters influence the failure of RADT; for example, no dependence on the details of the construction of the source and observation wells was detected.

This experimental approach detected a unique series of scaling relations for failure at small and large values of time. For small values of time, the resulting scaling relations are

$$\frac{t_1}{t_2} = \frac{\alpha_2}{\alpha_1}\ ,\ \frac{t_1}{t_2} = \frac{r_1^3}{r_2^3}\ ,\ \frac{t_1}{t_2} = \frac{\theta_{f,1}}{\theta_{f,2}}\ ,\ \frac{t_1}{t_2} = \frac{b_1}{b_2}\ , \text{ and } \frac{t_1}{t_2} = \frac{q_2}{q_1} \tag{2}$$

where the subscripts denote the two values of the time at failure and the two corresponding values of the indicated input parameter. These relations may be rewritten as

$$t_2 = t_1\frac{\alpha_1}{\alpha_2}\ ,\ t_2 = t_1\frac{r_2^3}{r_1^3}\ ,\ t_2 = t_1\frac{\theta_{f,2}}{\theta_{f,1}}\ ,\ t_2 = t_1\frac{b_2}{b_1}\ , \text{ and } t_2 = t_1\frac{q_1}{q_2} \tag{3}$$

and expressed in the simpler form

$$t \sim \frac{1}{\alpha}\ ,\ t \sim r^3\ ,\ t \sim \theta_f\ ,\ t \sim b\ , \text{ and } t \sim \frac{1}{q}\ . \tag{4}$$

The relations in (4) may then be compiled as

$$\frac{r^3\,\theta_f b}{\alpha\, q\, t} = C_{small} \tag{5}$$

where C_{small} denotes the critical value of the measure for failure at small values of time. If time is expressed in dimensionless form as the cumulative number of pore volumes of fluid injected into the formation

$$t_d = \frac{q\,t}{\pi\, r^2\,\theta_f b}\ , \tag{6}$$

then (5) may be restated as

$$\frac{r}{\alpha}\frac{1}{t_d} = C_{small}\ . \tag{7}$$

The analogue to (5) for large values of time was determined to be

$$\frac{\alpha^2\,\theta_f b}{q\,t} = C_{large} \tag{8}$$

by applying the same sequence of operations to the observed scaling relations. The average radial penetration of the tracer into the formation, R, is determined by relating the accumulated volume of fluid injected into the formation, qt, to the accumulated pore volume of the formation, $\pi R^2 \theta_f b$, as

$$R = \sqrt{\frac{qt}{\pi \theta_f b}} \tag{9}$$

and therefore (8) may be restated as

$$\frac{R}{\alpha} = C_{large} \; . \tag{10}$$

Decreasing values of time increase (7) toward a critical value that corresponds to failure, thus (7) forms the required stability criterion for small values of time when stated in the form

$$\frac{r}{\alpha}\frac{1}{t_d} < C_{small} \; . \tag{11}$$

Similarly, increasing values of time increase (10) toward a critical value and therefore the required stability criterion for large values of time is

$$\frac{R}{\alpha} < C_{large} \; . \tag{12}$$

Equations (11) and (12) are dimensionless and reflect advection and dispersion of the solute. Advection is represented in (11) through dimensionless time and dispersion is represented through the local Peclet number, r/α. In (12), advection is represented by the penetration of the tracer into the formation and dispersion is represented through the global Peclet number, R/α.

Additional experimentation indicated that the critical values of the stability criteria vary in accordance with two stability parameters. The forms of the stability parameters were determined by repeating the experimental approach adopted in the determination of the stability criteria. The stability parameter that regulates the critical value of the stability criterion for small values of time has the form

$$P_{small} = \frac{\alpha b q}{r^3 D^* \tau \theta_f \theta_m^2} \tag{13}$$

and the stability parameter that regulates the critical value of the stability criterion for large values of time has the form

$$P_{large} = \frac{\alpha\sqrt{D^*}\sqrt{\tau}\sqrt{\theta_i\theta_m}}{\sqrt{b}\sqrt{q}} . \tag{14}$$

Figure 2 shows the variation of the critical values of the stability criteria with the values of the stability parameters. Both variations may be adequately approximated by a bi-linear relation to yield

$$\begin{aligned} C_{small} &= 3.08\times10^{8}\, P_{small} \quad \text{for} \quad P_{small} < 3.07\times10^{-5} \\ &= 9.47\times10^{3} \quad \text{for} \quad P_{small} > 3.07\times10^{-5} \end{aligned} \tag{15}$$

for small values of time and

$$\begin{aligned} C_{large} &= 4.39\times10^{2} \quad \text{for} \quad P_{large} < 2.17\times10^{-3} \\ &= 2.02\times10^{5}\, P_{large} \quad \text{for} \quad P_{large} > 2.17\times10^{-3} \end{aligned} \tag{16}$$

for large values of time. Equations (15) and (16) may be used to test the values of the input parameters and determine the likelihood of the failure of RADT. Here, the stability parameters are determined using (13) and (14), and the critical values of the stability criteria are determined using (15) and (16) and compared to the current values determined using (11) and (12). In application, the critical values of the stability criteria are factored to further reduce the probability of failure. Thus, (11) and (12) are replaced by

$$\frac{r}{\alpha}\frac{1}{t_d} < F_{small}\, C_{small} \tag{17}$$

and

$$\frac{R}{\alpha} < F_{large}\, C_{large} \tag{18}$$

where F_{small} and F_{large} are specified such that $0 < F_{small} < 1$ and $0 < F_{large} < 1$.

A prototype inverse analysis implementation of RADT has been developed using (17) and (18) to limit the input of parameter values that are likely to cause failure. Enforcing the stability criteria sufficiently reduced the frequency of failure that inverse analyses can be completed over a useful range of solute transport regimes. Values of $F_{small} = 0.8$ and $F_{large} = 0.8$ were used in these analyses.

Conclusions

Robust performance is a requirement for a computational model that is to be implemented in an extended algorithm (e.g., an inverse analysis routine). While it is not critical that the component model return the target result over the full range of input parameter values, it is necessary that the conditions that lead to the failure of the component are recognized such that the performance of the extended algorithm is not degraded by the failure of the component.

This paper described the determination of stability criteria for RADT, a semi-analytical model of solute transport during divergent radial tracer tests. These stability criteria define the conditions where RADT successfully returns solute concentration. Both of the criteria represent advection and dispersion of the solute and assume critical values that are regulated by various of the parameters that form input to RADT.

The form of the stability criteria may be specific to the Laplace transform solutions reported in Novakowski (1992) and to the implementation of these solutions in RADT. The criteria may also be specific to the computer, operating system, and compiler used to determine the results. However, the analyses reported in this paper were performed using a DOS-based personal computer and were confirmed using a UNIX-based workstation, with only a marginal difference in the critical values of the stability criteria. Thus, there is evidence that the form of the stability criteria, and the method of derivation of these results, may be of general interest.

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Figure Captions

Figure 1. Variation of solute concentration with time for a tracer test performed on a single fracture in rock.

Figure 2. Variation of the critical values of the stability criteria with the stability parameters.

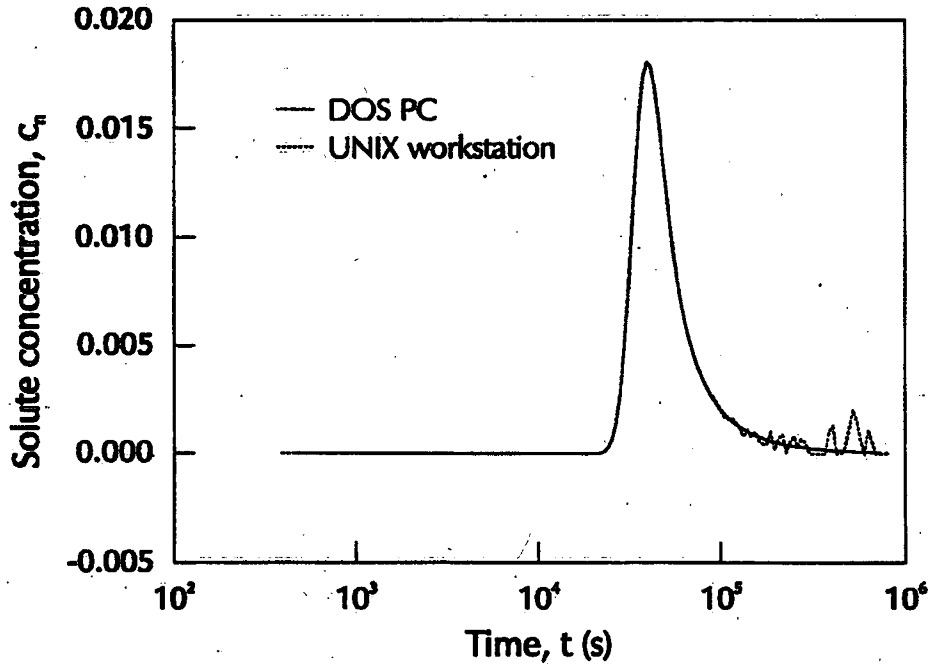

Figure 1
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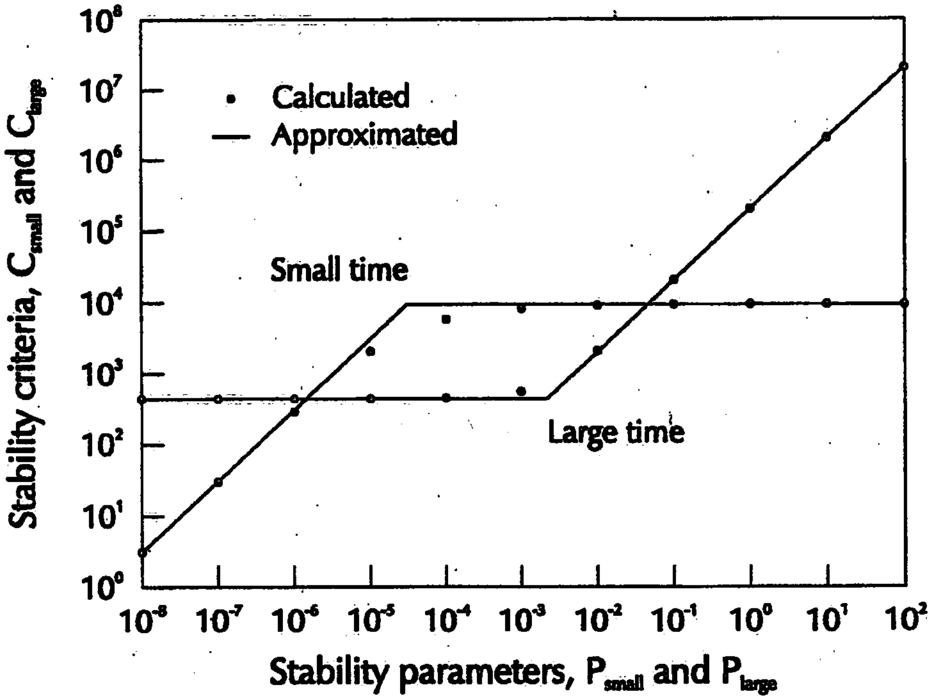

Figure 2
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