Flow and transport in highly heterogeneous formations: high-resolution large-scale numerical simulations

IGOR JANKOVIC
Civil, Structural and Environmental Engineering Department, University at Buffalo, 231 Jarvis Hall, Buffalo, New York 14260-4400, USA
ijankovic@eng.buffalo.edu

Abstract: High-resolution numerical simulations of flow and transport in porous media were performed to examine the performance of the first-order dispersion model and newly introduced "self-consistent" model (Dagan, 2003; Fiori, 2003). Simulations were performed using the Analytic Element Method that allows for large contrasts in hydraulic conductivity between neighbouring inclusions. Numerically obtained results agree well with those obtained using the self-consistent model. The agreement is favourable for both the velocity variances and the dispersion coefficients at all levels of heterogeneity. The agreement between numerically obtained results and the first-order results is limited to moderate levels of heterogeneity.

Key words: analytic element method; dispersion; inhomogeneities; self-consistent model

INTRODUCTION

The topic of this paper is contaminant spreading (dispersion) in groundwater caused by heterogeneity in the hydraulic conductivity of aquifer formations. The goal is to investigate the transport phenomena using accurate numerical models and to evaluate the performance of a few dispersion models.

The most common dispersion model limits the variations in hydraulic conductivity to a small value; only mild heterogeneity is allowed. One of the aims of the present study is to investigate the validity of this approximation. Recently, Dagan & Lessoff (2001) have derived an approximate solution of flow and transport for a bimodal medium of arbitrary conductivity contrast, but of small volume fraction of one of the phases (dilute limit). This model has been extended to media of finite volume fractions by Dagan & Fiori (2003) and Fiori & Dagan (2003) as well as to formations of distributed conductivity ("self-consistent" model; Dagan, 2003; Fiori, 2003).

HETEROGENEITY MODEL

The conceptual model behind numerical simulations of flow and transport is a multi-indicator permeability model (Dagan, 1979, 1981, 2003) that contains an arbitrary number of inclusions (inhomogeneities) that are embedded into a homogeneous background. The geometry of inhomogeneities is limited in this study to two-dimensional
(2-D) circular shapes. Inclusions may also be shaped as 3-D spheroids (rotational ellipsoids) and ellipses in 2-D. Intersections of inhomogeneities are not allowed. The flow through this medium of piecewise constant conductivity satisfies Darcy's law and is incompressible, i.e. potential flow. The vorticity in this type of flow is concentrated along the boundaries of inclusions. However, within these limitations, the underlying flow problem can be solved analytically, regardless of the conductivity of inclusions, their actual shape, size and locations.

The flow solutions behind numerical simulations are based on the Analytic Element Method of Strack (1989). The actual solutions used in the present study are available in Jankovic & Barnes (1999); Barnes & Jankovic (1999); Strack et al. (1999). Based on the principle of superposition, the velocity potential is expressed as a sum of velocity potential due to uniform flow, and disturbance velocity potentials as a result of individual inclusions. The disturbance potentials are constructed by requiring continuity of head and flow across the boundaries of inclusions. The velocity potential satisfies the governing Laplace equation and continuity of flow exactly everywhere; continuity of head across the boundaries of inclusions is met in an approximate, but highly precise fashion. The velocity components are obtained analytically (without interpolation) for any location by differentiating the expressions for velocity potentials.

The flow solutions used here are limited to circular (2-D) and spheroid (3-D) inclusions. However, within this limitation, precise solutions can be obtained for any levels of heterogeneity.

In order to infer transport statistics that are representative of an infinite domain, the inclusions are placed in a domain that was shaped as a large circle (2-D) that was submerged in an unbound homogeneous medium. On a large scale, the large body of inclusions behaves like a single large inhomogeneity. The analytical solution for a uniform flow past the single inhomogeneity of such geometry yields uniform velocity inside the domain. The velocity differs from that at infinity and can be used to infer the effective conductivity of the medium. Both 2-D simulations (presented here) and 3-D simulations (to be presented elsewhere) were conducted with 50 000 inhomogeneities.

In order to infer transport statistics that are representative of an infinite domain, the inclusions are placed in a domain that was shaped as a large circle (2-D) that was submerged in an unbound homogeneous medium. On a large scale, the large body of inclusions behaves like a single large inhomogeneity. The analytical solution for a uniform flow past the single inhomogeneity of such geometry yields uniform velocity inside the domain. The velocity differs from that at infinity and can be used to infer the effective conductivity of the medium. Both 2-D simulations (presented here) and 3-D simulations (to be presented elsewhere) were conducted with 50 000 inhomogeneities.

Particles are released and tracked inside the circular domain. Following the particle tracking, various transport statistics are computed. These include: spatial moments of particle positions; probability density function of hydraulic conductivity and each component of velocity; their two-point covariance function in the direction of flow and normal to it; covariance of Lagrangean velocities; and probability density function of travel times to various break-through locations. Hundreds of simulations were conducted on a massively parallel supercomputer cluster at the Center for Computational Research, University at Buffalo. Most simulations took seven days to complete, some over a month. Simulations range from mildly heterogeneous domains to highly heterogeneous domains with the variance of the logconductivity ($\sigma_Y^2$) equal to 10, and from very sparsely populated systems to systems where inhomogeneities cover 95% of the volume (packing density, $n$, equal to 0.95). Simulations are performed with inhomogeneities of constant and varying conductivity. The results presented here are obtained with the lognormally distributed conductivity. Following the analytic nature of the flow solution, all the results are presented in dimensionless forms. For example, the dispersion coefficients are made dimensionless with respect to the mean velocity and size of inhomogeneities.
The results show that it is possible to obtain accurate flow and transport solutions for the multi-indicator conductivity model, regardless of the variance of logconductivity. Figure 1 shows a portion of the domain that contains 50 000 circular inclusions with packing density of 0.95. The variance of the logconductivity, $\sigma_l^2$, was 10. The
variances of Lagrangean velocities are presented in Fig. 2 (longitudinal component of the velocity) and Fig. 3 (transverse component of the velocity). The results agree very well with those obtained using the self-consistent dispersion model (Fiori, 2003) up to a packing density of 0.6, which predicts considerably smaller variances than the first-order solution. Beyond the packing density of 0.6, the match deteriorates because of the influence of high-order terms from the flow solution which are not included in the self-consistent model.

Dispersion coefficients were computed as half the rate of change of second-order spatial moments of concentration distribution. Typical results are presented in Fig. 4. The travel times needed to obtain constant values of dispersion coefficients (linear growth of moments) were influenced mainly by the variance of the logconductivity. The results were consistent, both qualitatively and quantitatively, with those obtained using the self-consistent model: the setting time necessary to obtain constant dispersion coefficients was orders of magnitude larger than that predicted using the

Fig. 2 Longitudinal velocity variances $\sigma_{11}^2$ as functions of logconductivity variance $\sigma_i^2$ for four levels of packing density $n$; $U$ is the intensity of the uniform flow; velocity fields used in the computations are Lagrangean velocity fields.

Fig. 3 Transverse velocity variances $\sigma_{22}^2$ as functions of logconductivity variance $\sigma_i^2$ for four levels of packing density $n$; $U$ is the intensity of the uniform flow; velocity fields used in the computations are Lagrangean velocity fields.
first-order solutions for large values of logconductivity. In cases with large logconductivity variances, the constant of dispersion coefficient value was never reached.

The dispersion coefficients computed using the numerical laboratory and the self-consistent model show very good agreement for a large range of logconductivity variance and packing density.

CONCLUSIONS

Numerical simulations of flow in transport in groundwater were performed to check the performance of the first-order dispersion model and self-consistent model. The results show good overall agreement with the self-consistent model. The main discrepancy between the numerical results and the first-order results is in setting times. According to numerical experiments, the setting time (time to reach constant dispersivity values) is underestimated in the first-order theory. This finding is supported by the self-consistent model.

REFERENCES


