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Fluid Mixing and Reactions in Uniform and Tortuous Flow Fields

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1. Introduction

Interacting fluids in porous media are present in many natural systems. The effective reaction rates in dissolved species moving through geologic media (over short and medium time-scales) can depend significantly on the topological features of the pore network. The degree of mixing is influenced by the spatial variation in the flow rates; itself governed by the tortuosity of channels and the abundance of manifold bifurcations. Understanding and being able to predict such processes is of primary importance to water resource engineers.

This paper reports on recent 2-D lattice Boltzmann and lattice gas cellular automata simulations that capture these features. The work represents an initial phase of a larger study to identify the link between macroscopic effective continuum measures (in particular, *dispersion* and *reaction rates* used in large-scale groundwater models) and local features of the pore network.

2. Lattice Methods for Groundwater Flow

Lattice gas cellular automata (LGCA) and lattice Boltzmann models (LBM) are mesoscopic idealisations of discrete mobile systems that can reproduce flow fields and transport processes in fluids. The approach discretises time and space, such that particles move on a regular lattice at a constant speed in a pre-defined limited set of direction. LGCA *hop* (or propagate) and *scatter* (or collide) operations [1] can be represented by integer arithmetic leading to efficient codes that can take advantage of multi-processor computer hardware. The core algorithm takes the form

```
initialise density and speed
while t<t_max
  propagate
  collide
  bounceback
  calculate density, speed and equilibrium distribution
  increment t
end
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Pan *et al* [2] provide an overview of recent developments in parallel LB models of two-phase flow. For the 2-D LGCA used here, each lattice node has four links to other nodes, which can contain many particles. In the absence of boundaries and diffusion, each particle will travel to a linked node in time Δt [3].

In order to calculate macroscopic parameters, such as density and velocity, an averaging of the motion of many particles is necessary. LBM, originally developed by McNamara and Zanetti [4] to overcome the statistical noise inherent in LGCA, use continuous values for the number of particles moving in each direction. This has the effect of carrying out the spatial averaging during the model's run. Our solutions use coupled LBM-LGCA simulations. A common lattice is shared between the two simulations: (i) flow and (ii) reactive transport. The flow field, representing water movement, is generated using a 9-directional LBM (known as the LBGK approach). This is then used to bias the diffusion of particles within a multi-particle LGCA model, which represent groundwater-transported reacting species. When type A and type B particles met on a node, particles of species C are created.

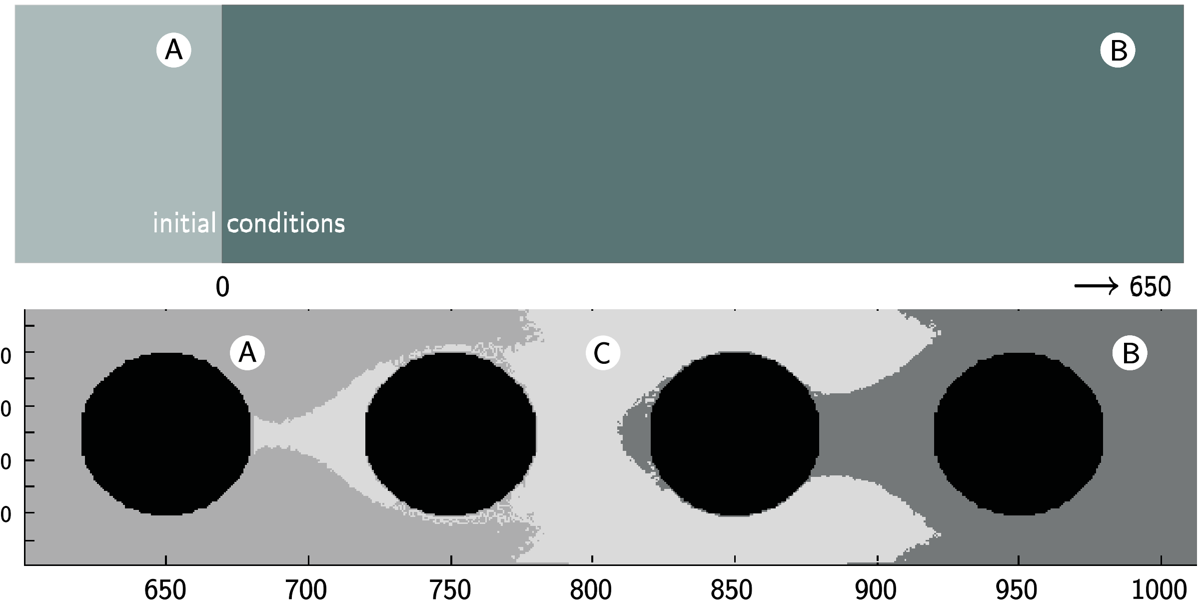

FIGURE 1. Simulation of flow (left-to-right) and diffusion in a 2-D tube with periodic obstacles. Upper plot shows the initial conditions, lower plot gives the distribution of the species A, B and C.

PARAMETER	VALUE	UNITS
diffusion coefficient (D)	0.2	$L^2.T^{-1}$
tube width (obstructed case)	98	L
tube length	1850	L
discharge	9.65	$L^2.T^{-1}$
average velocity	0.14	$L.T^{-1}$

3. The Modelled Systems

Two flow regimes have been considered: (i) slug flow (uniform velocity across the width, over its entire length) in a 2-D tube and (ii) laminar, viscous, incompressible flow in a 2-D tube with periodic circular obstructions. The *average* velocities, diffusion coefficients and discharges of the two cases were set equal. Both systems were modelled with and without the reaction $A + B \rightarrow C$. Key parameters for these simulations are given above (all data given in terms of unit length and time).

4. Evolution of the Systems

In Figure 2, we observe the effect of the tortuosity of the flow on the chemical reaction rate and the time to reach the *ergodic limit*. The variance (σ^2) of the concentration versus distance is a measure of the spreading of the solute caused by mixing. Early in the simulations, the shape of the reactant cloud is determined mainly by the flow field, but when diffusion starts to dominate, σ^2 increases linearly with time [5]. This appears to occur after approximately 200-300 lattice spacings or 2-3 obstructions for both reactive and non-reactive cases.

The dispersivity of the medium is given by $\sigma^2/2x$, and is calculated from the gradient of the curves in Fig. 2 after they have reached an equilibrium state. Based on the non-reactive case (species A), a dispersivity of 15.7 may be derived for the flow system modelled compared with a diffusion coefficient of 0.2. This quantity is of the same order of magnitude as the obstructed channel dimensions (as would be expected). The average velocity was also separately determined by examining the velocity of travel of the species centroids. This gave values of 0.14 in agreement with the average velocity determined from the discharge and channel geometry.

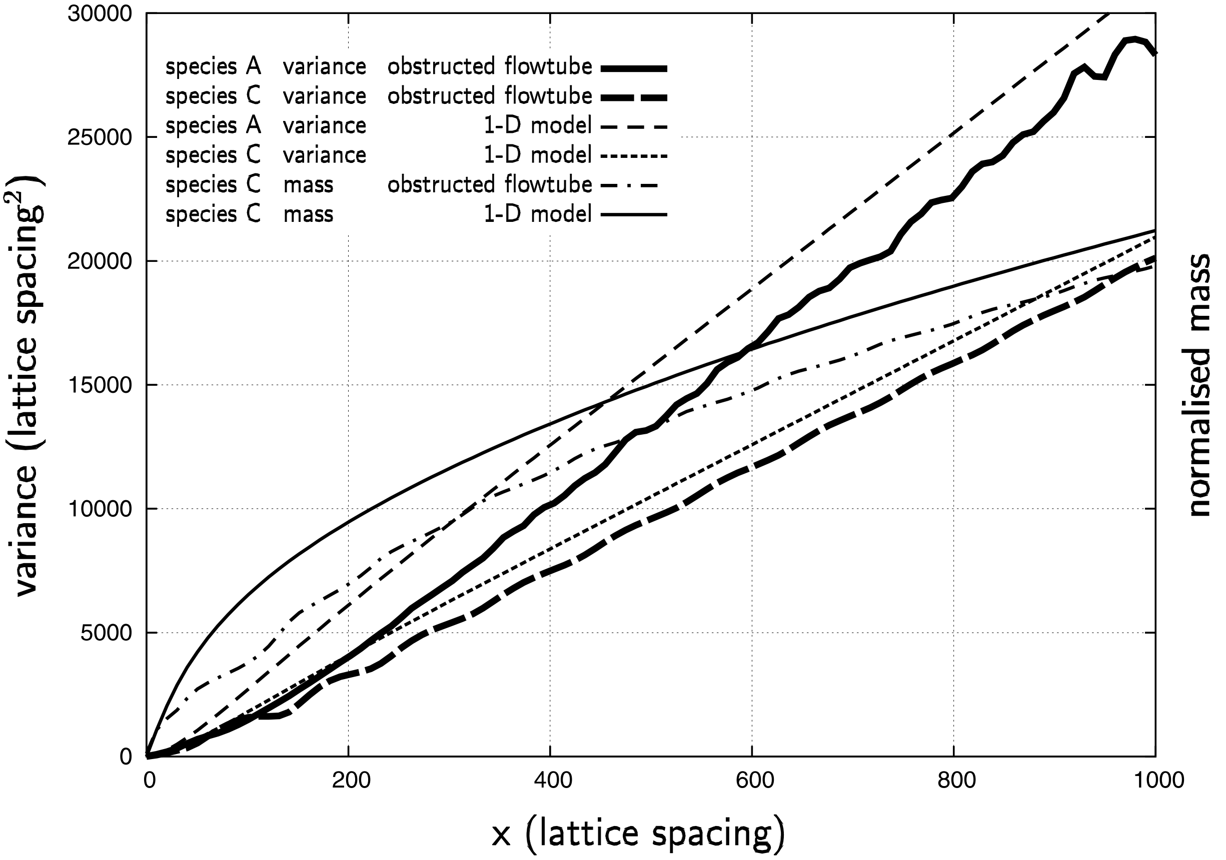

FIGURE 2. Variance and mass of the solutes during reactive transport within an obstructed (LG) and 1-D (analytical) tube.

5. COMPARISON WITH CONTINUUM MODELS

It is of interest to model an idealised 1-D representation of the obstructed flow case and compare this with the full 2-D simulation. This gives insights into any limitations of using a simple advection-dispersion equation to represent pore scale flow and reactive transport.

We thus present data based on the analytical model of Gramling *et al.* [6] employing a dispersivity of 15.7, an average velocity of 0.14 and a discharge of 9.65. In Figure 2 it is seen that the variance of the 1-D case closely matches that of the 2-D model for both the non-reactive case as expected, and for the reactive case. If concentration-time plots are are compared for the two simulations in Figure 3, it is seen that the 2-D cases are skewed more than the 1-D simulations.

Examination of the mass of Species C produced with time, plotted in Figure 2, indicates that the 1-D continuum model over predicts mass production. It is seen that this overprediction is due to incorrect modelling during the non-ergodic conditions (over the first 200-300 lattice spacings). Beyond this, the rate of mass production is correctly predicted, but there is a constant absolute error in the total mass.

6. CONCLUSIONS

A single pore tube flow scenario has been simulated and the effect of obstructions (representative of soil particles) has been investigated by making comparisons with an equivalent simple 1-D advection dispersion continuum model. Dispersivities derived from the 2-d model are significantly higher than the inherent diffusion coefficient and of similar order to the width of the obstructed flow field.

Modelling of reactive flow indicates that the simple 1-D continuum model over-predicts production of the reaction product and predicts reduced skewness in the reaction product plume shape.

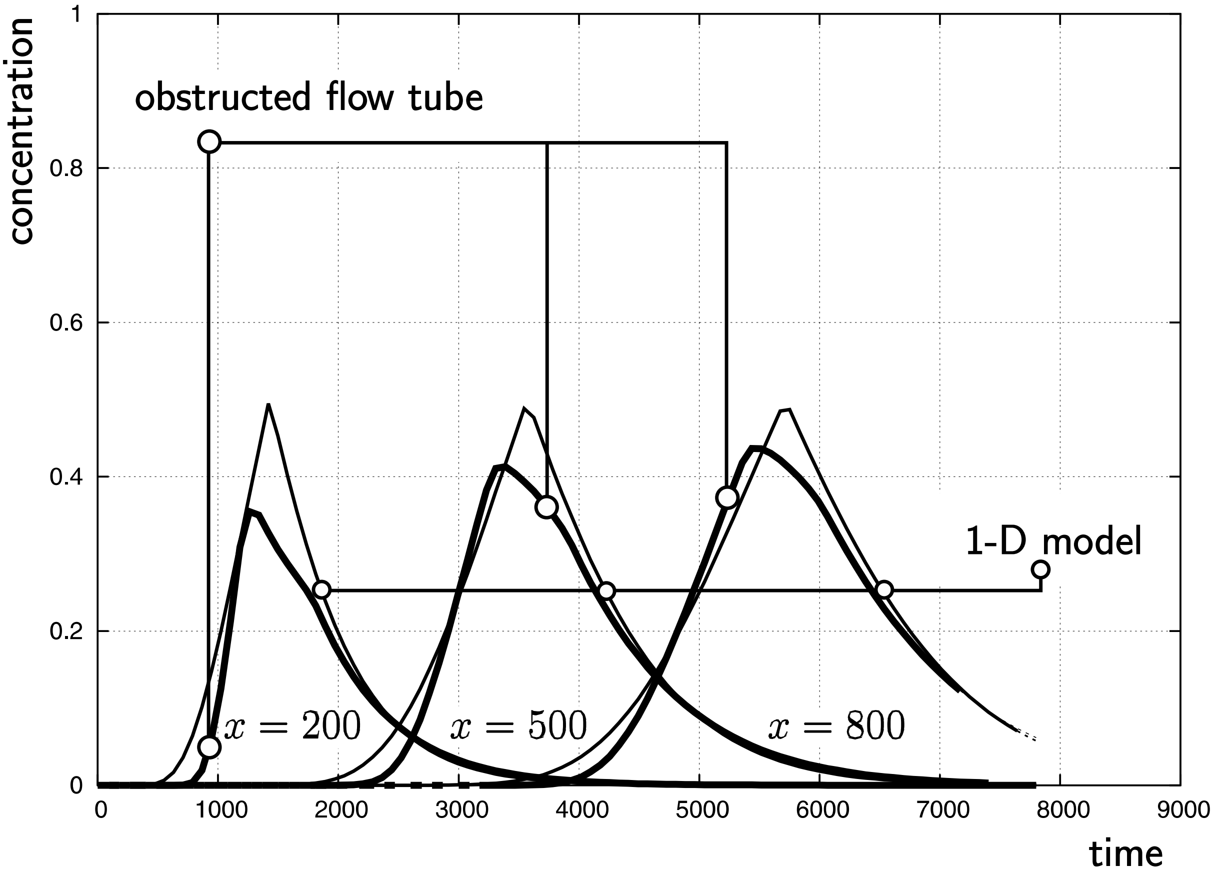

FIGURE 3. Mass of species C versus time, generated at three locations.

This paper represents a snapshot of work in progress focussing on a single parameter set. Further parametric studies will be undertaken investigating

(i) the relationship between macroscale non-reactive dispersivity and obstruction size, flow velocity and diffusion coefficient

(ii) the relationship between skewness, dispersion and mass production rate of reaction product with obstruction size, flow velocity and diffusion coefficient

(iii) the influence of reaction probability on matching the modelled systems. In the systems presented in this paper, the reaction probability was unity.

Future work will investigate large scale pore networks in 2-D and 3-D and additionally explore transverse dispersion processes.

REFERENCES

[1] Rothman, D H & Zaleski, S, *Lattice-Gas Cellular Automata: Simple Models of Complex Hydrodynamics*, Cambridge University Press, **1997**.

[2] Pan, C, Hilpert, M and Miller, C T, Lattice-Boltzmann simulation of two-phase flow in porous media, *Water Resources Research*, 40, **2004**.

[3] Haslam, I, Smith, C C and Crouch, R S, Lattice Gas simulations of reactive flow in porous media: Preliminary findings, *ACME2004 Conference*, University of Cardiff, **2004**.

[4] McNamara, G and Zanetti, G, Use of the Boltzmann equation to simulate lattice gas automata, *Phys Rev Lett*, 61, **1988**, 2332-2335.

[5] Rutherford, J C, *River Mixing*, John Wiley, **1994**.

[6] Gramling, C M, Harvey, C F and Meigs, L C, Reactive Transport in Porous Media: A Comparison of Model Prediction with Laboratory Visualization, *J Environ. Sci. Technol.*, (36)11, **2002**, 2508-2514.