Direct upscaling of kinetically controlled reactive transport with mobile-immobile mass transfer

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1 - Abstract

Mass transfer processes are known to strongly influence the migration of passive tracers and contaminants through porous media but the effect of such processes on reactive transport systems has not been studied as thoroughly in the passive case. Mobile-immobile diffusion can delay solute arrival times and prolonging taking of tracers which will affect the extent of mixing and the apparent reaction rates within the transport domain. This study investigated the effect of the most basic effects that mass transfer processes will have on several variations of a reactive transport system and evaluates the behavior of the systems at multiple scales using highly-resolved numerical models. In particular, we consider the importance of correctly accounting for the portion of the domain within which reactions are able to occur. The “reactive domain” may include the entire model or only the mobile or immobile portions of the domain. Sometimes a reaction rate is a function of how long one or more of the solutes have been exposed to another solute, a particular mineral, or how long it has been immobile (Fig. 4). Some examples include colloid filtration and biodegradation, both of which are important to remediation. There are many applications where the observed behavior of the system is similar to that of a single continuum but more complex reactions that are functions of the concentration and exposure time [3] can also be explicitly modeled. We solve the transport equation and then the kinetic reaction terms directly from the raw data as a forward process.

2 - Mobile-immobile mass transport with reactions

Mass transfer processes are known to strongly affect transport in porous media [1]. Most of the research on this subject has focused on passive tracers and only recently have the effects of reactive transports in the domain been considered [2]. Most of these methods are based on a single mobile continuum that accurately represents complex flow and transport processes ignoring their ability to empirically account for the detailed, pore-scale processes. There is still no full understanding of the link between the pore-scale and transport-scale processes.

3 - Model components and design

Pore-scale flow and transport is simulated with the partial bounce-back Lattice-Boltzmann method [2]. All of the simulations shown here use the same steady-state velocity field (Fig. 3). It varies in the kinds of simulations that are allowed to occur which include advection-diffusion, mass transfer and reactions. Table 1 summarizes the elements of each model is designed to simulate but more complex reactions that are functions of the concentration and exposure time [3] can also be explicitly modeled. We solve the transport equation and then the kinetic reaction terms directly from the raw data as a forward process.

4 - High resolution flow and transport simulations

To understand the upscaling response of reactive transport processes, we need a strong understanding of how these processes manifest physically. Since we are able to solve using the pore-scale, the models provide knowledge of the actual parameter distributions (Fig. 13) that can be used to obtain the obtained statistics of the “reality” to an upscaled equivalent that might be found in the laboratory from the effluent end of a column. Sometimes a reaction rate is a function of how long one or more of the solutes have been exposed to another solute, a particular mineral, or how long it has been immobile (Fig. 4). Some examples include colloid filtration and biodegradation, both of which are important to remediation. There are many applications where the observed behavior of the system is similar to that of a single continuum but more complex reactions that are functions of the concentration and exposure time [3] can also be explicitly modeled. We solve the transport equation and then the kinetic reaction terms directly from the raw data as a forward process.

5 - Model results and simple upsampling

Since many analyses are conducted using breakthrough curves we see them as our starting point. We then evaluate making measurements and alternating ap- plications to evaluate simulation to an upscaled model. A representative of the physical process is the model. The mobile-immobile mass and reactive transport results can create unique test results that are difficult to describe and may be difficult to identify in field studies so further research is needed.

A note on graphical computing:

The figures in this paper are created using various graphical software tools. Some of the figures are created using Adobe Illustrator, others are created using MATLAB, and still others are created using Python. Some of the figures are created using 3D modeling software, while others are created using 2D vector graphics software. Each figure is created with the tools that best suit the needs of the figure and the requirements of the paper. The figures are then compiled into the final document using Adobe InDesign.

6 - Exposure time dependency and mixing

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7 - References


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Table 1 - Model types currently being simulated with the direct downscaling framework. Models 6, 7, and 8 are similar to B5 but have immobile diffusion and reactions. Table 2 summarizes the elements of each model is designed to explicitly simulate but more complex reactions that are functions of the concentration and exposure time [3] can also be explicitly modeled. We solve the transport equation and then the kinetic reaction terms directly from the raw data as a forward process.

Table 2 - Model types currently being simulated with the direct downscaling framework. Models 6, 7, and 8 are similar to B5 but have immobile diffusion and reactions. Table 2 summarizes the elements of each model is designed to explicitly simulate but more complex reactions that are functions of the concentration and exposure time [3].