IJSRM
INTERNATIONAL JOURNAL OF SCIENCE AND RESEARCH METHODOLOGY
An Official Publication of Human Journals

Human Journals
Research Article
November 2020 Vol.:17, Issue:1

A Research Methodology for Upscaling and Modeling of Reactive Transport from Pore-Core-Large Darcy Scale of Porous Media

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Submission: 22 October 2020
Accepted: 28 October 2020
Published: 30 November 2020

HUMAN JOURNALS
www.ijsrm.humanjournals.com

Keywords: Groundwater processes, pore-core-large Darcy scale models, upscale chemical reaction rates, dispesivity, reactive contaminant transport, numerical modeling and simulation, rainfall- runoff

ABSTRACT

Groundwater processes are complex and include physical-chemical-biological and microbiological ones. In pore-core scale, this is its infancy age. Some of them needs to be provided first in pore-core scale. Pore-scale simulation provides more versatility in choice of parameters, a greater variety of quantitative data and frequency of observation, and more importantly, easier design of numerical experiments. Since the experimental measurements are time-consuming and expensive, the use of numerically-simulated porous media is conceptually appealing. Moreover, We need to upscale different parameter and coefficients from pore-core to large Darcy scale, for example, the chemical reaction rates, dispersivity coefficients etc. In our knowledge, this the first attempt to write a computer program, being able to include pore-core-large scale phenomena as a whole system. We will make use to some existing packages making interface to them by our program. There is agreement by some others authors that if pore core experiments are in good agreement with numerical modeling at this scale then there are good chances ore probability that this upgraded numerical models are the right ones for describing large scale models. But We also need to upgrade to these models first. Reactive contaminant transport in (variably) porous media are the most difficult processes to deal with them likely the atmospheric moving boundary conditions and rainfall- runoff ones.

INTRODUCTION

The objective of this research was to enhance our understanding of and obtain quantitative relation between Darcy-scale on parameters and pore-core scale flow of the real parameters, using a three-dimensional multidirectional pore-network computer model. This helps to upscale from a simplified but reasonable representation of microscopic physics to the scale of interest in practical applications. Following Raoof and Hassanizadeh, 2014 (1) upscaled transport parameters are obtained by fitting the solute on of classical advection –dispersion - reaction equation with adsorption to the average concentration on breakthrough curves at the outlet of the pore network. Transport of reactive and adsorptive solutes in soils and aquifers plays an important role in a variety of fields, including study of leaching of agrochemicals from soil surface to groundwater, uptake of soil nutrients by plant roots, and remediation of contaminated soils and aquifers. In practical applications of modeling in porous media, we are interested in describing solute transport phenomena at larger scales than the scale at which generic underlying processes take place (e.g., the pore scale). Commonly, at the field or in lab experiments, reactive transport coefficients are employed which are obtained from experimental data. Measurement of the reaction coefficients usually employs well-mixed batch or flow-through reactors (Lasaga, 1998). In batch systems, the assumption is that the aqueous phase is stirred rapidly enough so that concentration gradients are eliminated; this removes the effect of subscale transport by diffusion and/or advection within the pore spaces. In such cases, reaction is surface-controlled and depends only on the uniform chemistry of the aqueous solution. In natural systems, however, reactions are inevitably subject to the influence of transport via advection, molecular diffusion, and/or dispersion. As such, the adsorption rates are an outcome of the coupling between reaction and hydrodynamic processes (Li *et al.*, 2007b).

MATERIAL AND METHODS

We present a methodology for using a pore-network model to investigate scaling effects in adsorption, dispersion, reactions, core-scale attachment and detachment rate coefficients rates. Our objective was to find a relation between macroscopic (Darcy-scale) and local-scale transport coefficients for an adsorbing reactive solute.

Pore network modeling Under Variably Saturated Conditions

Modeling under variably saturated conditions. In this study, after construction of a pore network, drainage simulations are performed to determine the pore level distribution of water. For each saturation level, steady-state flow is calculated, and the equation of mass balance is solved to obtain BTCs of solute concentration and to calculate the dispersivity values. We consider capillary-controlled displacement [Wilkinson and Willemsen, 1983] in a strongly water wet porous media saturated with water. To simulate drainage process in our network, the displacing air is considered to be injected through an external reservoir that is connected to every pore body on the inlet side of the network. The displaced water escapes through the outlet face on the opposite side. Impermeable boundary conditions are imposed along the sides parallel to the main direction of flow. At every stage of the process, air invades accessible pore bodies and throats with the lowest entry capillary pressure. We assume that the wetting phase is hydraulically connected everywhere. This means that there will be no trapping of the wetting phase, as it can always escape along the edges.

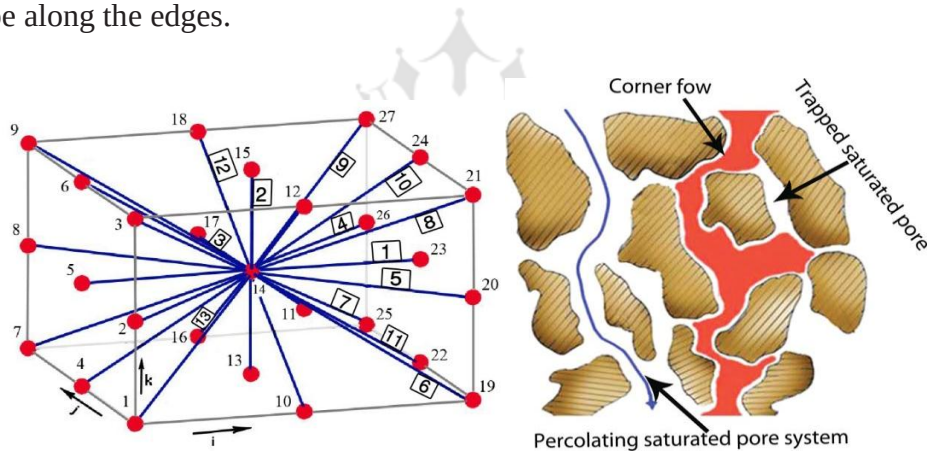

Figure No. 1: In the left schematic of a 26-connected network. Numbers inside the squares show tube directions and others are pore body numbers**.** In the right schematic representation of variably saturated porous medium. **[Raoof and Hassanizadeh, 2009]**

Fluid flow within drained pores is used to calculate the flow across the network, we need to calculate flow of water in saturated pores as well as along edges of drained pores. The conductance of each edge within a drained pore needs to be determined as a function of the thickness of the wetting film residing in the edge. This thickness depends on the radius of curvature of the fluid-fluid interface, which is calculated based on the applied capillary pressure

[Raoof and Hassanizadeh, 2012]. The formulations for calculating the flow within each pore element and determining relative permeability of the network at different saturation levels are described in Raoof and Hassanizadeh [2012]. Simulating Solute Transport in pore network modeling applying the discretization method mentioned, the unknown concentrations will be either $\mathbf{c_i}$ and c_{ij} of saturated pore bodies and saturated pore throats, respectively, or the concentrations $c_{CU,i}$ and $c_{ij,k}$ of corner unit of drained pore bodies and edges of drained pore throats, respectively. To illustrate the formulation, we provide mass balance equations for a system of two drained pores bodies connected by an angular drained pore throat (as shown in **Figure 1**), as the most general case. We assume that the flow is from corner unit j toward corner unit *i* through edges of drained angular pore throat *ij*. The effect of molecular diffusion is neglected. For a given corner unit (with concentration $c_{CU,i}$ and volume $V_{CU,i}$), we can write the following mass balance equation:

$$V_{CU,i}\,\frac{d}{dt}\left(c_{CU,i}\right) = \sum_{j=1}^{N_{in}^{throat}} \sum_{k=1}^{N_{ij}^{edge}} c_{ij,k} q_{ij,k} + \sum_{n=1}^{N_{in}^{CU}} c_{CU,n} q_{i,n} - Q_{CU,i} c_{CU,i} \quad (3)$$

where the first term on right-hand side is due to the mass arriving via N_{ij}^{edge} edges of N_{in}^{throat} throats with flow toward corner unit *i*; the second right-hand side term accounts for the mass arriving from N_{in}^{CU} neighboring corner units (within the same pore body), which are flowing toward the corner unit *i* ; and the last term shows the mass leaving the corner unit. $Q_{CU,i}$ is the total water flux leaving (or entering) corner unit i. Note that, in the case of saturated pores, the second term on the right-hand side of equation (3) vanishes and also the value of N_{ij}^{edge} in the first term will be equal to one, since there is no edge flow present. The mass balance equation for an edge element k within drained pore throat *ij* may be written as (assuming that corner unit *j* is the upstream node):

$$V_{ij,k}\,\frac{dy}{dt}\left(c_{ij,k}\right) = |q_{ij,k}|c_{CU,j} - |q_{ij,k}|c_{ij,k} \quad (4)$$

where $V_{ij,k}$,$q_{ij,k}$, and $c_{ij,k}$ are the volume, volumetric flow rate, and concentration of kth edge of pore throat *ij*, respectively. Here also, the diffusion is neglected. Combination of equations (3) and (4) results in a linear set of equations to be solved for c_i, c_{ij}, $c_{CU,i}$, and $c_{ij,k}$. Since we discretize pore bodies and pore throats on the basis of their saturation state, the number of

unknowns is different for simulations under different saturation levels. After obtaining the solution, BTCs at a given distance from the inlet were found based on flux-averaged concentrations of pores located at that position. The normalized average concentration, $\overline{c}(x,t)$, is given by

$$\overline{c} = \left[\frac{\sum_i^{N_t^x} c_i(x,t)Q_i}{\sum_i^{N_t^x} Q_i}\right]\frac{1}{c_0} \qquad i = 1,2,3,\ldots,N_t \qquad (5)$$

where c_0 is solute concentration at the inlet and N_t^x denotes the total number of pore-body elements that are centered at the longitudinal coordinate *x*.

$$\theta\frac{\partial\overline{c}}{\partial t} + \rho^b\frac{\partial\overline{s}}{\partial t} + \theta\overline{v}\frac{\partial\overline{c}}{\partial x} + \theta\overline{v}\frac{\partial\overline{c}}{\partial y} + \theta\overline{v}\frac{\partial\overline{c}}{\partial z} = \theta D_L\frac{\partial^2\overline{c}}{\partial x^2} \qquad (6)$$

In figure 2 below We have constructed the flowchart of computer program in MATLAB for pore - core - large Darcy scale of upscaled model of reactive transport in (variably) saturated porous media.

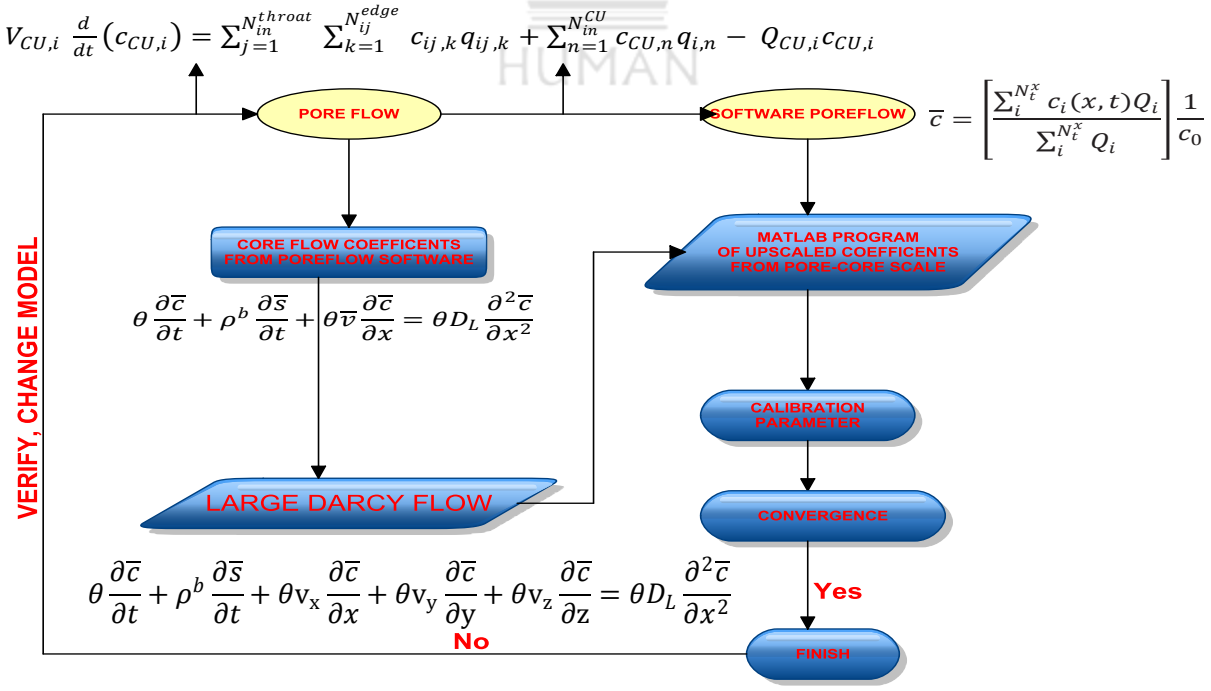

Figure No. 2: Flowchart of computer program in MATLAB for pore - core - large Darcy scale of upscaled model of reactive transport in (variably) saturated porous media (**Dulian Zeqiraj**)

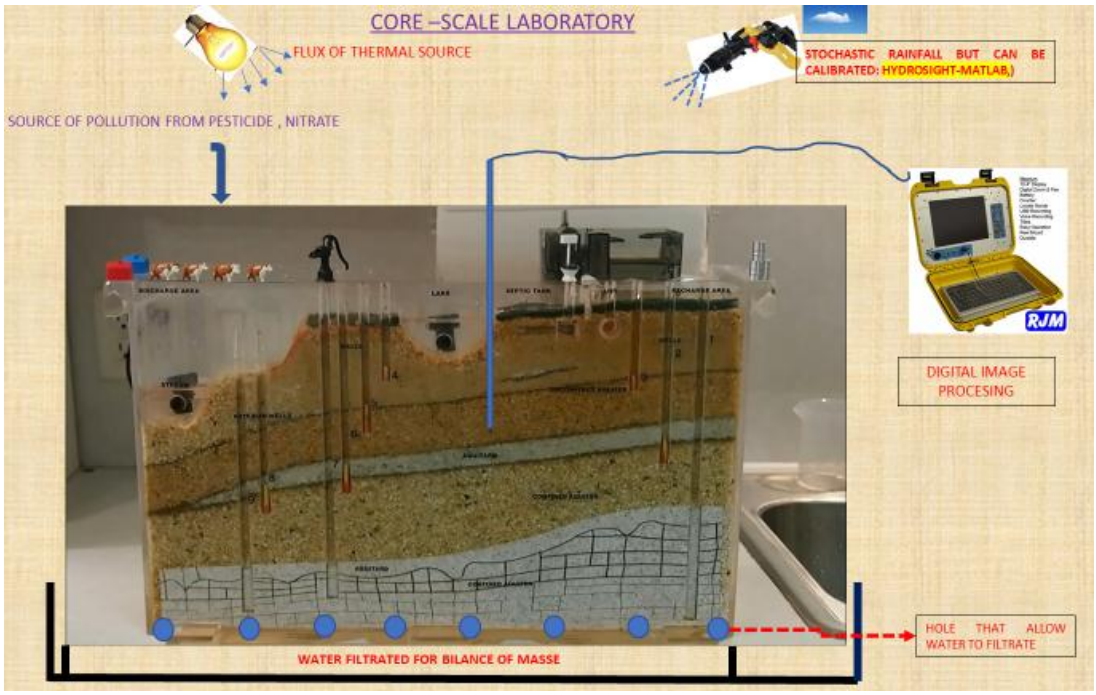

Figure No. 3: An invented core scale laboratory to compare numerical solution with experimental test, author Dulian Zeqiraj, supplementary result in video at

RESULTS AND DISCUSSION

We have formulated a versatile computer programing approach for upscaling the different coefficients that take place in the process of modeling contaminant reactions in porous media from pore -core to large Darcy scale. The program is versatile because it allows for different types of models in case of non-convergence of initial values of coefficients of pore scale. The program is simple in the sense that it needs more sophisticated Bayesian update averaging models in case of non-satisfactory results of each of existing available models. That is for future work and for further investigation of core sample experiments.

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