

How Do We Couple Pore- to Darcy-scale Flow and Reactive Transport in A General Way?

Xiaofan Yang*, Beijing Normal University, Beijing 100875, China
Xuhui Meng, Huazhong University of Science and Technology, Wuhan 430074, China
Yuhang Tang, Lawrence Berkeley National Laboratory, Berkeley, CA 94720
Zhaoli Guo, Huazhong University of Science and Technology, Wuhan 430074, China
George Em Karniadakis, Brown University, Providence, RI 02912

Key words: reactive transport, multiscale modeling, porous media

Introduction

Using emerging understanding of biological and environmental processes at fundamental scales to advance predictions of the larger system behavior requires the development of multiscale approaches, and there is strong interest in coupling models at different scales together in a hybrid multiscale simulation. This research aims to extend and apply a recently-developed multiscale universal interface (MUI, [1]) to dynamically couple pore-scale and Darcy-scale models (both solved using the lattice Boltzmann method, LBM, [2, 3]) to study flow and reactive transport in porous media. The MUI for porous media (MUIporous) provides a set of lightweight C++ scripts (boundary coupling, data exchange, and kriging) to manage a complex multiscale simulation in a concurrent way. After validation of the boundary coupling schemes, MUIporous performance will be initially tested against a simple homogeneous problem previously described in [4], then extended to heterogeneous problems with dynamic pore structure change due to precipitation. The current work will address both scientific questions and multiscale methodology challenges: 1) How does the heterogeneity affect mixing-controlled reactive transport in porous media? and 2) How to best generalize hybrid multiscale methodologies in a high-performance computing environment?

Methodology

We consider a 2D fully-saturated porous media domain, which is divided into two sub-domains Ω_p (pore-scale domain) and Ω_d (Darcy-scale domain) with an interface Γ_I . Let \mathbf{n}_p and \mathbf{n}_d denote the outward unit normal vectors and $\boldsymbol{\tau}$ as the tangential vector.

Pore-scale equations The incompressible flow and solute transport in the pore-scale porous media are described by the incompressible Navier-Stokes equations and the convection-diffusion equation (CDE). The equations are numerically solved by the pore-scale LBM explained in [2].

Darcy-scale equations The flow in the Darcy scale can be described by the continuity equation and the Darcy's law; while the solute transport is described by a volume-averaged convection-diffusion equation. The equations are numerically solved by the pore-scale LBM explained in [3].

Coupling boundary conditions In order to couple the two sub-domains, suitable boundary conditions need to be imposed on the interface Γ_I . As for the fluid flow, the following coupling conditions should be satisfied.

1. Continuity of the normal component of the velocity

$$\mathbf{u} \cdot \mathbf{n}_p = \bar{\mathbf{u}} \cdot \mathbf{n}_d. \quad (1)$$

2. Continuity of the normal stress across Γ_I

$$-\mathbf{n} \cdot \mathbf{T}(\mathbf{u}, P) \cdot \mathbf{n} = \bar{P}, \quad (2)$$

where $\mathbf{T}(\mathbf{u}, P) = \nu(\nabla\mathbf{u} + \nabla^T\mathbf{u}) - P\mathbf{I}$.

3. Beavers-Joseph-Saffman condition is imposed on the tangential component of the fluid velocity as

$$\frac{\nu\alpha_{BJ}}{\sqrt{K}}(\mathbf{u})_{\boldsymbol{\tau}} - [\mathbf{T}(\mathbf{u}, P) \cdot \mathbf{n}]_{\boldsymbol{\tau}} = 0. \quad (3)$$

For solute transport, two coupling conditions are imposed on Γ_I .

1. Continuity of the solute concentration

$$C = \bar{C}. \quad (4)$$

2. Continuity of the solute flux across the interface

$$\mathbf{n}_p \cdot (\mathbf{u}C - D\nabla C) = \mathbf{n}_d \cdot (\bar{\mathbf{u}}\bar{C} - D\phi\nabla\bar{C}). \quad (5)$$

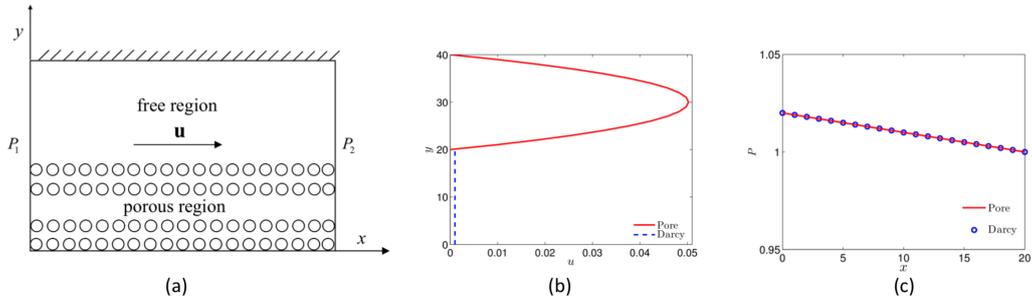


Figure 1: Case 1: (a) computational domain; (b) velocity comparison; (c) pressure comparison

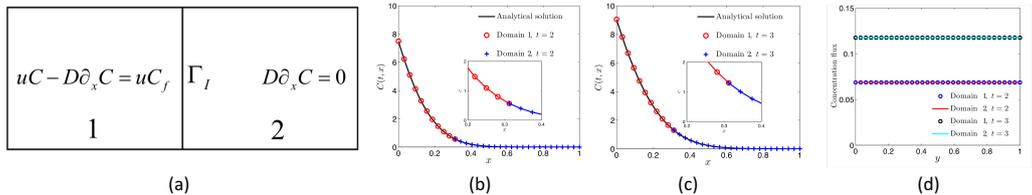


Figure 2: Case 2: (a) computational domain; (b) concentration profiles at t_1 ; (c) concentration profiles at t_2 ; (d) concentration flux at both t_1 and t_2

Results

In this section, we present 4 numerical examples for validations and applications, including Case 1 - flow through a domain which includes a free flow region and a porous one; Case 2 - convection-diffusion process in a square domain; Case 3 - mixing-controlled reaction in homogeneous porous media; Case 4 - reaction with precipitation in heterogeneous porous media.

Validation 1: Flow coupling Case 1: The computational domain and problem setup are illustrated in Figure 1(a). As we can see in Figure 1(b), the velocity profile is parabolic in the free flow region, while it is a plug in the porous region. The velocity slip for the tangential velocity mentioned in Eq. (3) can be observed. However, the pressure at the coupling interface is plotted in Figure 1(c), which clearly shows the consistency between scales indicating the coupling is successful.

Validation 2: Solute transport coupling Case 2: The computational domain and problem setup are illustrated in Figure 2(a). We compare both concentration and flux consistencies at the interface in different moments. Excellent results can be seen in Figure 2(b-d).

Application 1: Mixing controlled reaction in homogeneous porous media Case 3: Previously introduced in [4], a mixing-controlled bi-molecular reaction is a good example to test the hybrid multiscale modeling approach while using pore-scale model in the mixing zone and Darcy-scale model in the rest of the domain. Figure 3 shows the results obtained from the current MUIporous code, which are well-compared with pore-scale simulations.

Application 2: Reaction with precipitation in heterogeneous porous media Case 4: A heterogeneous porous media sample is divided by pore- and Darcy-scale subdomains. Mixing-controlled reaction is conducted just as in Case 3. MUIporous is still running. However, we have performed pore-scale and Darcy-scale simulations individually and found huge difference between the two (Figure 4), which will provide an interesting example for MUIporous. Also we will add precipitation in this case in order to dynamically change the pore

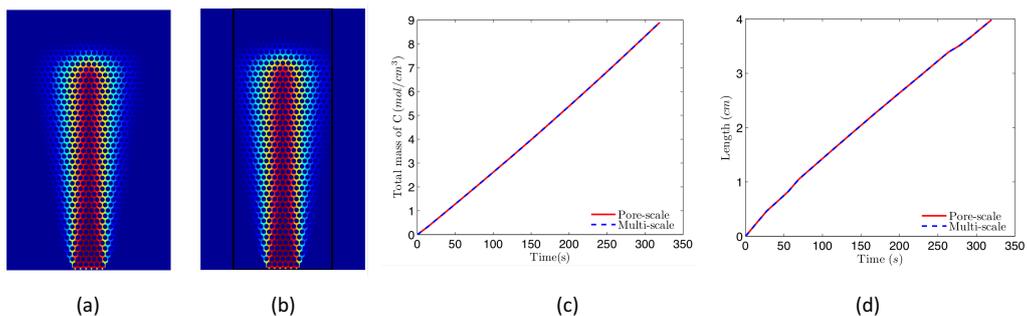


Figure 3: Case 3: (a) pore-scale simulation; (b) MUIporous simulation (pore-scale subdomain bounded by black box); (c) total mass of product C comparison; (d) mixing length comparison

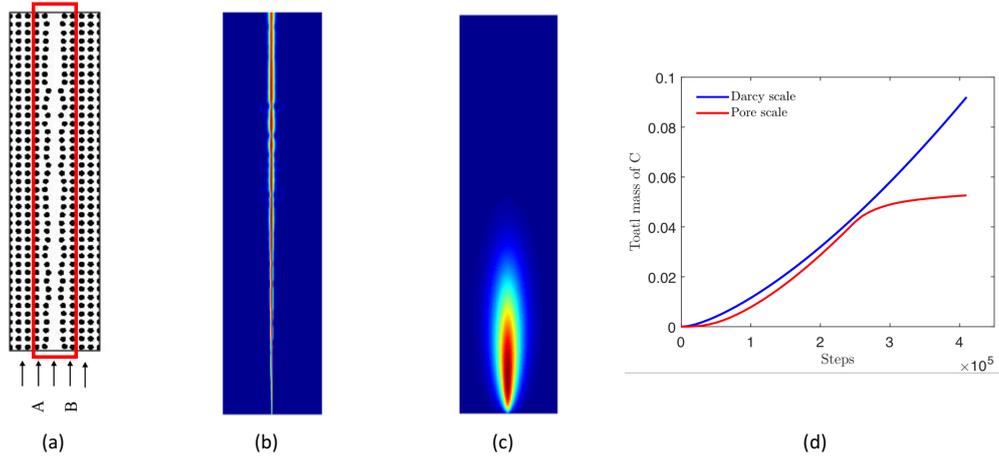


Figure 4: Case 4: (a) computational domain (pore-scale subdomain bounded by red box); (b) pore-scale simulation; (b) Darcy-scale simulation; (c) total mass of product C comparison

structure, which will enforce the adaptivity of the pore-scale subdomains.

References

- [1] Y.-H. Tang, S. Kudo, X. Bian, Z. Li, G.M. Karniadakis. Multiscale Universal Interface: A concurrent framework for coupling heterogeneous solvers. *J. Comp. Phys.*, **297**, 13–31, (2015).
- [2] X.H. Meng, Z.L. Guo. Multiple-relaxation-time lattice Boltzmann model for incompressible miscible flow with large viscosity ratio and high Péclet number. *Phys. Rev. E*, **92**, 043305, (2015).
- [3] X.H. Meng, Z.L. Guo. Localized lattice Boltzmann equation model for simulating miscible viscous displacement in porous media. *Int. J. Heat Mass Trans.*, **100**, 767–778, (2016).
- [4] T.D. Scheibe, K. Schuchardt, K. Agarwal, J. Chase, X. Yang, B.J. Palmer, A.M. Tartakovsky, T. Elsethagen, G. Redden. Hybrid multiscale simulation of a mixing-controlled reaction. *Adv. Water Res.*, **83**, 228–239, (2015).