SAND2017-2879J

Manuscript Details

Manuscript number	ADWR_2017_99
Title	Application of a hybrid multiscale approach to simulate hydrologic and biogeochemical processes in the river-groundwater interaction zone
Article type	Research Paper

Abstract

The groundwater-surface water interaction zone (GSIZ) plays an important role in riverine and watershed ecosystems as the exchange of waters of variable composition and temperature (hydrologic exchange flows) stimulate microbial activity and associated biogeochemical reactions. Variable temporal and spatial scales of hydrologic exchange flows, heterogeneity of the subsurface environment, and complexity of biogeochemical reaction networks in the GSIZ present challenges to incorporation of fundamental process representations and model parameterization across a range of spatial scales (e.g. from pore-scale to field scale). This paper presents a novel hybrid multiscale simulation approach that couples hydrologic-biogeochemical (HBGC) processes between two distinct length scales of interest. Our multiscale simulation approach is tested and demonstrated on a two-dimensional (2D) domain that intersects the aquifer and the adjacent Columbia River within the 300 Area of the U. S. Department of Energy's Hanford Site. This domain is characterized by temporally dynamic intrusion of river water, aquifer contaminant plumes that interact with hydrologic exchange flows, and complex biogeochemistry driven by mixed sources of organic carbon. Microbial activity and biogeochemical reactions are focused in a relatively thin zone (1-2 m thick) immediately underlying and adjacent to the river, comprising recent riverbed sediments and referred to here as the alluvium layer. Within this layer, it has been hypothesized that biogeochemical reactions are strongly impacted by flow variations associated with permeability heterogeneity, and therefore may require unusually high spatial resolution of processes and material properties within the alluvium (microscale domain), relative to the full model domain (macroscale domain). Use of a fine grid over the full macroscale domain would be computationally inefficient and perhaps infeasible for three-dimensional domains of larger size. Additionally, the biogeochemistry within the alluvium layer is more complex than that of the rest of the macroscale domain, warranting use of different BGC reaction networks in the two domains. One approach to address these challenges is the application of a hybrid multiscale method that loosely couples high-fidelity simulations in the microscale domain with low-fidelity simulations in the macroscale domain. In the hybrid multiscale modeling workflow demonstrated and tested here, simulations at both scales employ the PFLOTRAN code. However, at the microscale, a grid with finer resolution is employed together with a complex BGC reaction network, while at the macroscale a simplified reaction network is utilized with a coarsely-resolved model grid. A scripted workflow using the Swift computational workflow environment is used to execute, monitor and couple microscale and macroscale simulations. The coupling is loose and is accomplished through iterated input-output file transfers. The approach, previously demonstrated for coupling pore- and continuum-scale reactive transport simulations, is applied here to couple multiple scales of continuum models over a field-scale domain. We test the accuracy and efficiency of our hybrid multiscale simulation by comparison with equivalent single-scale models, and then apply the multiscale model to numerically investigate the potential impacts of small-scale heterogeneity and different BGC reaction models.

Keywords	hybrid multiscale simulation; loose coupling; groundwater-surface water interaction; hydrologic-biogeochemical processes
Taxonomy	Biogeochemistry, Multiscale Analysis, Subsurface Hydrology, Groundwater
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February 6th 2017

Dear Prof. D'Odorico, Prof. Sander:

Please find enclosed a manuscript entitled "Application of a hybrid multiscale approach to simulate hydrologic and biogeochemical processes in the river-groundwater interaction zone" by Xiaofan Yang et al., which we wish to submit for publication in *Advances in Water Resources*. The manuscript was prepared using Microsoft Word and creates a 36-page document in 1.5-spaced format.

This paper presents a novel hybrid multiscale simulation approach that couples hydrologic-biogeochemical (HBGC) processes between two distinct length scales of interest in the river-groundwater interaction zone. Our multiscale simulation approach is tested and demonstrated on a two-dimensional (2D) domain that intersects the aquifer and the adjacent Columbia River within the 300 Area of the U. S. Department of Energy's Hanford Site. This domain is characterized by temporally dynamic intrusion of river water, aquifer contaminant plumes that interact with hydrologic exchange flows, and complex biogeochemistry driven by mixed sources of organic carbon. Microbial activity and biogeochemical reactions are focused in a relatively thin zone (1-2 m thick) immediately underlying and adjacent to the river, comprising recent riverbed sediments and referred to here as the alluvium layer. Within this layer, it has been hypothesized that biogeochemical reactions are strongly impacted by flow variations associated with permeability heterogeneity, and therefore may require unusually high spatial resolution of processes and material properties within the alluvium (microscale domain), relative to the full model domain (macroscale domain). Use of a fine grid over the full macroscale domain would be computationally inefficient and perhaps infeasible for three-dimensional domains of larger size. Additionally, the biogeochemistry within the alluvium layer is more complex than that of the rest of the macroscale domain, warranting use of different BGC reaction networks in the two domains. The current multiscale approach loosely couples high-fidelity simulations in the microscale domain with low-fidelity simulations in the macroscale domain.

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Regarding the choice of referees, we will leave to your better judgment the selection of individuals that you feel can best offer constructive feedback on our manuscript. Researchers that we feel are especially well-qualified include

Prof. Albert Valocchi (University of Illinois at Urbana-Champaign, valocchi@illinois.edu),

Prof. Matthew Balhoff (University of Texas at Austin, balhoff@mail.utexas.edu),

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Prof. Ciaran Harman (Johns Hopkins University, charman1@jhu.edu).

On behalf of my co-authors, I wish to thank you for your time and consideration of our manuscript. We look forward to hearing from you in due course.

Yours sincerely,

Xiaofan Yang
Hydrology Technical Group
Energy and Environment Directorate
Pacific Northwest National Laboratory

Application of a hybrid multiscale approach to simulate hydrologic and biogeochemical processes in the river-groundwater interaction zone

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Submitted to *Advances in Water Resources*

Abstract

The groundwater-surface water interaction zone (GSIZ) plays an important role in riverine and watershed ecosystems as the exchange of waters of variable composition and temperature (hydrologic exchange flows) stimulate microbial activity and associated biogeochemical reactions. Variable temporal and spatial scales of hydrologic exchange flows, heterogeneity of the subsurface environment, and complexity of biogeochemical reaction networks in the GSIZ present challenges to incorporation of fundamental process representations and model parameterization across a range of spatial scales (e.g. from pore-scale to field scale). This paper presents a novel hybrid multiscale simulation approach that couples hydrologic-biogeochemical (HBGC) processes between two distinct length scales of interest.

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Key words: hybrid multiscale simulation; loose coupling; groundwater-surface water interaction; hydrologic-biogeochemical processes

1. Introduction

The groundwater-surface water interaction zone (GSIZ), the region of the subsurface below or adjacent to a river or stream into which surface water exchanges occur, has been recognized as an ecologically and biogeochemically active zone that plays a critical role in river ecosystems [Findlay, 1996; Brunke and Gonser, 1997; Smith, 2005; Larned et al., 2015]. It is also a key element of the earth critical zone (land surface-soil-water-atmosphere interaction zone) [http://criticalzone.org/national/]. Movement of surface water into and out of the GSIZ (referred to as hydrologic exchange flows [Harvey and Gooseff, 2015]) leads to mixing of waters containing variable levels of dissolved oxygen (DO), dissolved organic carbon (DOC), nutrients, contaminants, and other solutes, and thereby gives rise to complex coupled hydrologic-biogeochemical (HBGC) processes [Boano, 2014;Cardenas, 2015]. Among those processes, microbially-mediated aerobic respiration of organic carbon, nitrification and denitrification are considered to be important [Findlay,1995; Bencala, 2000; Pinay et al., 2015], and can be related to other redox-sensitive reactions. Field experiments [Packman et al., 2004; Kessler et al., 2012; Fox et al., 2014], column experiments with hyporheic zone sediments [Doussan et al., 1997; Gu et al., 2007; Yan et al., 2016; Liu et al., 2017] and numerical modeling studies [Mayer et al., 2002; Storey et al., 2003; Lautz and Siegel, 2006; Fleckenstein et al., 2010; Brunner et al., 2010; Frei et al., 2012; Gu et al., 2012; Janssen et al., 2012; Han et al., 2014; Krause et al., 2014; Chen et al., 2015; Liggett et al., 2015] have all been useful in improving our understanding of solute transport and biogeochemical turnover processes in the GSIZ. A number of studies have successfully used numerical models to simulate results of field studies and laboratory experiments [Boano et al., 2009; Fleckenstein et al., 2010; Frei et al., 2012; Gu et al., 2012; Janssen et al,. 2012; Han et al., 2014; Krause et al., 2014; Trauth et al., 2013; Trauth et al.,2014], by providing detailed understanding of the controlling mechanisms and dynamic distributions of the processes within the GSIZ. However, three major issues pose challenges to field-scale numerical modeling of HBGC processes in the GSIZ. Firstly, hydrogeological structures in the GSIZ are often complex and exhibit strong physical and biogeochemical heterogeneity that can greatly impact HBGC processes. Secondly, river discharge (and therefore river stage) can vary over a range of temporal scales from hourly to multi-year, leading to dynamic hydrologic exchange flows and complexities in microbiological responses that introduce computational challenges. Finally, because of multiple scales of physical and biogeochemical heterogeneity in

natural systems, HBGC processes in the GSIZ often require scale-dependent parameterizations and/or process representations, and the interactions among processes at different scales are poorly understood and difficult to predict.

In summary, coupled HBGC processes in the GSIZ exhibit multi-scale and multi-physical features (different mathematical representations of physical, biological and chemical processes at distinct scales) that motivate the development of multiscale modeling approaches. Single-scale simulations at low fidelity are computationally efficient, but require high levels of parameterization that may inadequately represent impacts of microscopic physical/chemical processes and their linkages to macroscopic phenomena [Wood, 2009; Gray et al., 2013]. Single-scale simulations at high fidelity may offer higher predictive potential, but at high computational expense [Molins, 2015; Yang et al., 2016]. In recent years, hybrid multiscale methods [E et al., 2003; Ingram et al., 2004; Mehmani and Balhoff, 2015] have begun to be applied to study of flow and transport processes in subsurface systems with multiscale heterogeneity. Scheibe et al. [2015a] provide a review of several classes of multiscale methods including hybrid multiscale methods, with discussion of recent applications to subsurface flow and reactive transport simulation. Conceptually, hybrid multiscale methods describe the flow and reactive transport processes using different mathematical models and parameters at each scale, and define coupling schemes between models at different scales (e.g., Tartakovsky and Scheibe, 2011) to ensure process continuity and exchange model parameters (e.g. reaction rate), states, and boundary conditions. It is obvious that the coupling scheme between scales is the core and major challenge of this method. Key factors to be considered include the consistency between models, data exchange and I/O control, and computational efficiency. A variety of different hybrid methods have been developed and applied, such as the hybrid mortar method [Balhoff et al., 2008; Mehmani and Balhoff, 2014; Tang et al., 2015], iterative boundary coupling [Battiato et al., 2011], non-iterative coupling of Smoothed Particle Hydrodynamics (SPH, Tartakovsky et al., 2010), and the hybrid multiscale finite volume (h-MsFV) method [Tomin and Lunati, 2013; Tomin and Lunati, 2015; Barajas-Solano and Tartakovsky, 2016]. A hybrid loose coupling method based on the heterogeneous multiscale method of E et al. [2003] was developed by our team and previously applied to coupled pore- and Darcy-scale simulation of reactive transport [Scheibe et al., 2015b, 2015c]. The loose coupling method employs user-specification of input and output files passed to and from each at-scale simulator, together with functional descriptions

(subdomain determination and upscaling/downscaling schemes) used for data exchange between scales, in a Swift-controlled high-performance computing workflow environment [Wilde et al., 2011]. The script-based multiscale modeling framework was tested using a mixing-controlled reaction in a homogeneous porous media system [Scheibe et al., 2015b], in which microscale (pore-scale) and macroscale (continuum-scale) reactive transport models were loosely coupled. Most of the previous hydrogeologic applications of hybrid multiscale methods have been used to couple flow and reactive transport from pore scale to continuum scale in synthetic porous media, with limited focus on field-scale applications. In the current study, we apply the same loose-coupling modeling framework to simulate field-scale groundwater-river water mixing and its impacts on HBGC processes (carbon and nitrogen biogeochemistry) in the GSIZ.

The current study is based on a field research site at the 300 Area of the U. S. Department of Energy's (DOE) Hanford Site [Zachara et al., 2013]. The site is located in a semi-arid region and is bordered by the Columbia River (Figure 1a). Interest in field-scale models applied over domains hundreds of meters in size is motivated by the existence of contaminant plumes near the river [Hammond and Lichtner, 2010]. The plumes are impacted by river water intrusion that can extend significant distances inland [Johnson et al., 2015], and by biogeochemical processes that are relatively high in the GSIZ [Moser et al., 2003]. Modeling coupled hydrologic and biogeochemical processes in this context is challenging because 1) biogeochemical activity is enhanced in a relatively thin zone of recent river alluvium (1-2 meters thick) immediately underlying the river (referred to as the alluvial layer, Figure 1b) relative to the surrounding aquifer materials; 2) hydrobiogeochemical processes may be strongly impacted by small-scale physical and biogeochemical heterogeneity within the alluvial layer; and 3) the biogeochemical reactions in the alluvial layer are more complex than those in the surrounding aquifer. Therefore, a more sophisticated level of simulation may be required for accuracy in the thin alluvial layer (higher resolution and complex biogeochemical reaction network) while maintaining a simpler model in the rest of the model domain for computational efficiency. Hybrid multiscale simulation offers a potential approach to meet these competing objectives. The loose coupling approach used in our previous studies was adapted to this problem. In this application both model scales (the alluvial layer – microscale domain -- and the rest of the system –macroscale domain, Figure 1c) are simulated using the open-source PFLOTRAN flow and reactive transport simulation code [Lichtner et al., 2013]. However, at the microscale a computational grid with

finer resolution is employed together with a more complex biogeochemical reaction network, while at the macroscale a simplified reaction network is utilized with a coarsely-resolved model grid. Table 1 summarizes the attributes of the microscale and macroscale models. Customized scripts were developed for coupling schemes and exchange of data between scales. The entire multiscale simulation framework is executed in the Swift-based environment on high performance computing clusters.

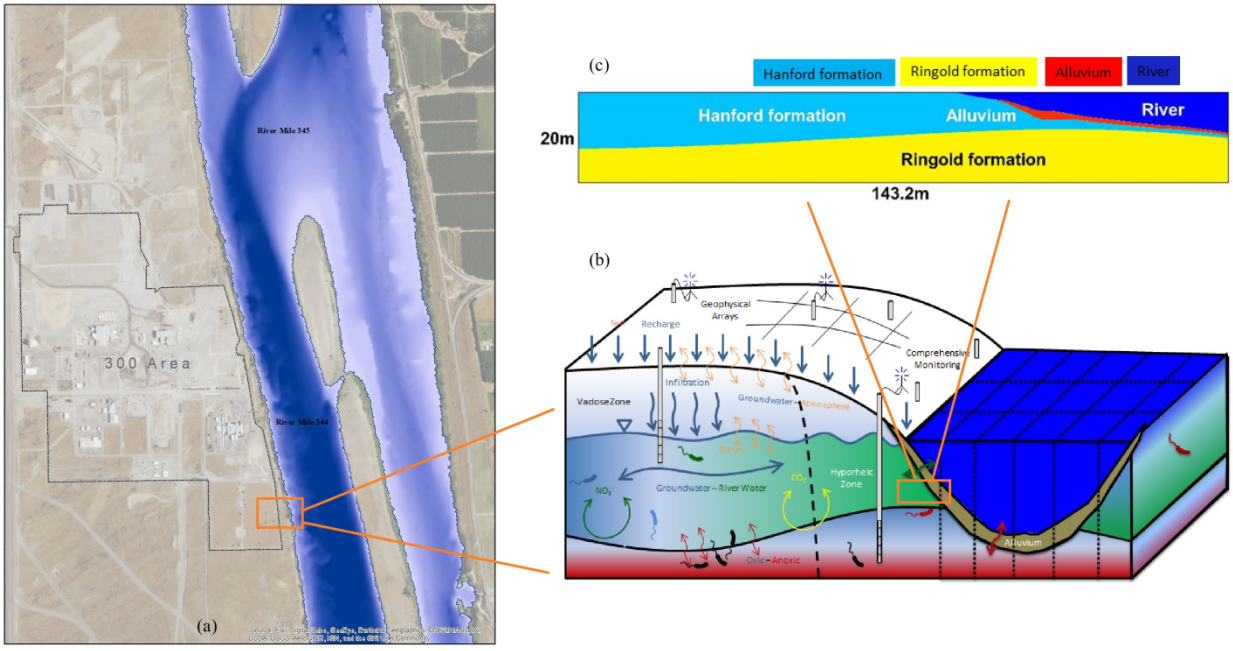


Figure 1. Schematic diagrams of the modeling domain: (a) Hanford 300A study site; (b) the GSIZ; (c) the current 2D modeling domain.

Table 1. Multiscale modeling framework for flow and reactive transport

Scale\Model	Facies	Formation	Flow model	BGC model	Grid	Solver
Macro-scale	Subsurface	Hanford+Ringold	Richards Equation	Gu et al. 2012	Coarse	PFLOTRAN
Micro-scale	Riverine	Alluvium	Richards Equation	Song et al. 2017	Fine	PFLOTRAN

The rest of the paper is organized as follows: Section 2 introduces the modeling domain and setup (including hydrogeological properties assigned in the domain and the biogeochemical reaction network models); Section 3 explains the hybrid multiscale simulation framework and its execution; Section 4 presents results and discussion followed by concluding remarks.

2. Hanford 300A Site Model Configuration

The hybrid multiscale modeling framework simulates subsurface flow and reactive transport. Subsurface flow is simulated on a 2D cross-sectional domain (Figure 2), with dynamic head boundary conditions specified from observations of river water stage (river boundary) and interpolation of observations from inland wells (aquifer boundary). Reactive transport simulations are based on a combination of previously published (Gu et al., 2012) and newly developed (Song H.-S., et al., 2017) biogeochemical network models describing aerobic respiration and denitrification. The 2D computational domain is that same as that used by our team to investigate the impact of dam operation and hydropeaking on HBGC processes (Song X. et al., 2017). We use this 2D domain here for simplicity, and to facilitate comparisons with independent simulation outputs (such as a single-scale simulation with uniformly fine grid resolution). We recognize that this 2D system could be represented at high resolution over the entire domain without undue computational demand, and therefore does not require the hybrid multiscale approach. However, this test system allows us to develop, test and demonstrate our approach prior to application to larger 3D domains for which the computational efficiency of the hybrid method would be more advantageous.

2.1. Computational domain and setup

The 2D model domain is shown in Figure 2. The dimensions of the domain are 143.2 m by 20 m, with the elevation ranging from 90 m to 110 m. A sloping bank represents the geometry of the groundwater-river water interface. The modeling domain comprises three stratigraphic formations with different hydrogeological properties [Williams et al., 2000; Williams et al., 2008; Zachara et al., 2012]: alluvium layer (recent fluvial deposits with low permeability), Hanford formation (gravels with high permeability) and Ringold formation (ancient semi-consolidated fluvial deposits with low permeability). The boundaries and shapes of the formations are based on previous field surveys and measurements at the extensively-studied

300A site. As mentioned above, the alluvium is a thin layer (1-2 m thick) adjacent to the river, but with disproportionate impact on flow and biogeochemical reactions. Both homogeneous and heterogeneous property distributions are considered for the aquifer properties in the current study. For homogeneous scenarios, hydraulic conductivity is assumed to be constant within each formation with values as listed in Table 2. For heterogeneous scenarios, the spatial distributions of the hydraulic conductivities in the modeling domain were defined using geostatistical models explained in Section 2.3. Four sets of hypothetical well observation points (marked by red dots in Figure 2) are located in the alluvium layer and the Hanford formation.

Figure 2. Computational domain (143.2 m x 20 m) and hydrostratigraphic formations: blue – Hanford formation; yellow – Ringold formation; red – Alluvium; dark blue – River water. Four sets of observation points are marked in red and located in the Hanford and Alluvium layers for comparison. In the current multiscale modeling framework, the Hanford and Ringold layers are defined as macro-scale domains while the thin Alluvium layer is defined as micro-scale domain.

Table 2. Parameters used in homogeneous scenarios

Parameters\Formations	Hanford	Ringold	Alluvium
Porosity	0.2	0.43	0.43
Permeability	7.387e-9	1.055e-12	3.864e-11

2.2. Geostatistical model of physical heterogeneity

Hydrogeological properties vary naturally through space as a result of the complex geologic processes through which aquifers evolve. The heterogeneity of hydraulic conductivity (K) exerts control on the movement of water and solutes in groundwater and through surface water-groundwater interfaces. Hydraulic conductivity can vary by several orders of magnitude over short distances. However, there is rarely sufficient data to deterministically prescribe these

heterogeneous spatial distributions. Accordingly, it has become common practice to use stochastic approaches to incorporate spatial heterogeneity in hydraulic properties into numerical models of subsurface fluid flow and transport [e.g., Gelhar, 1986; Wagner and Gorelick, 1989; Rubin, 2003]. Various geostatistical simulation approaches can be used to generate multiple realizations of heterogeneous fields of hydraulic conductivity, which are treated in this context as spatial random functions. Gaussian geostatistical simulation is commonly used for continuous data; it assumes that the data, or a transformation of the data, is multivariate Gaussian and stationary (i.e., the mean, variance, and spatial structure (semivariogram) is constant in the spatial domain) [Rubin and Journel, 1991; Deutsch and Journel, 1998].

The Hanford, Ringold, and recent alluvium geological units are each associated with different erosional and depositional processes and therefore exhibit different characteristics of heterogeneity [Hou et al., 2017]. The statistical moments of hydraulic conductivity (K) for the Hanford and Ringold formations are inferred based on previous reports focused on the Columbia River and Hanford Reach [Newcomb and Brown, 1961; Newcomb et al., 1972; Cass et al., 1981; Williams et al., 2000; Vermeul et al., 2003, 2009; Last et al., 2006; Thorne et al., 2006; Fritz and Arntzen, 2007; Fritz et al., 2007; Peterson et al., 2008; Williams et al., 2008; Truex et al., 2009; Bjornstad et al., 2010; USDOE, 2010; Zachara et al., 2012], and the spatial semivariogram model parameters are trained based on hydraulic conductivity measurements from an array of boreholes in Hanford 300A (an exponential semivariogram model is used here). The anisotropy angles are determined by assuming the maximum correlation direction is parallel to the interfaces between the formations. Insufficient data are available for the alluvium layer to determine the correlation length parameter, which is assumed here to be no more than 1 m since the parameter is scale-dependent [Goovaerts and Webster, 1994; Davis et al., 1997; Di Fedrico and Neuman, 1997; Dobermann et al., 1997] and the thickness of the alluvial layer is typically 1-2 meters. Table 3 summarizes the geostatistical parameters that are used for the simulations of $log_{10}(K(m/d))$.

Table 3. Geostatistical parameters for three geostratigraphic formations in the modeling domain.

Parameters\Formations	Hanford	Ringold	Recent alluvium
Mean, $\log_{10}$(m/d)	3.077	0.8787	1.978
Variance/Sill	0.71	0.41	0.55
Max correlation range (m)	9.4	9.4	1.0
Anisotropy ratio	0.1	0.1	0.1
Nugget	0	0	0
Anisotropy angle (radians)	-0.052	-0.052	0.157

Figure 3 shows two representative realizations (for the alluvium and the entire domain, respectively) of the heterogeneous 2D field of $log_{10}(K)$ generated based on the above parameters using the R geostatistical package geoR. To systematically evaluate the performance of the numerical model and understand how spatial heterogeneity (K) may affect the flow and transport processes in the study domain, multiple realizations are generated reflecting uncertainty in the specific configuration of the K field while honoring the global distribution and spatial correlation structure of the data. A small number of selected realizations are employed and tested in the current multiscale modeling study. Further studies using additional realizations and sensitivity analysis of parameters are continuing and will be reported in future manuscripts.

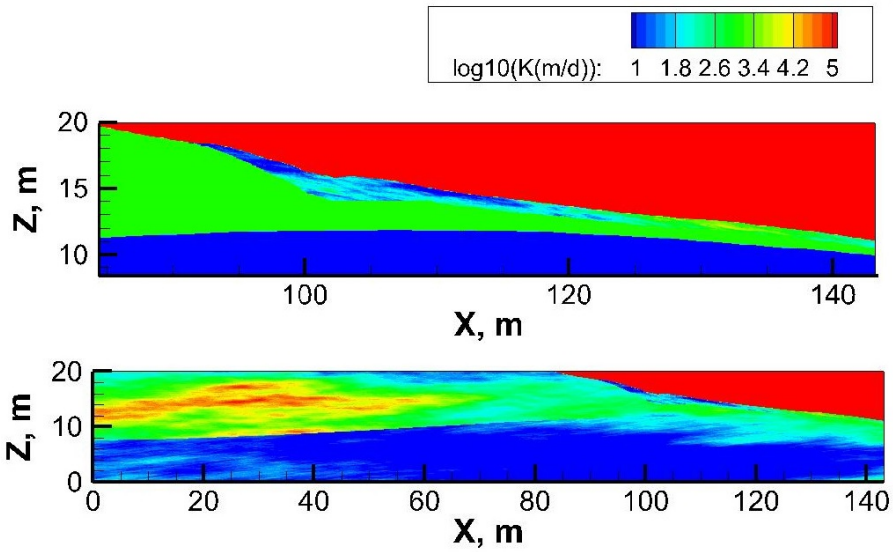


Figure 3. Two example realizations of the 2-D heterogeneity field of $\log_{10}$ hydraulic conductivity (m/d).

2.3. Subsurface flow model

In PFLOTRAN, the groundwater model simulates variably saturated flows by solving the Richards equation described as follows:

$$\frac{\partial \varphi s \rho}{\partial t} + \nabla \cdot \mathbf{q}\rho = Q \tag{3.1}$$

where φ denotes the porosity for each stratigraphic formation, s is the saturation, ρ is the fluid density, t is the time, $\mathbf{q}$ is the Darcy velocity and Q is the source/sink term. For variably saturated flow, the unsaturated soil hydraulic conductivities (Section 2.2) are accounted for using the van Genuchten soil water retention model [van Genuchten, 1980]. The residual and saturated moisture contents and the associated parameters are determined from in situ soil characteristics.

Hydrostatic heads are applied to the entire modeling domain as initial conditions. Transient hydrostatic (variable head) boundary conditions are interpolated from observations and assigned to the inland (West) and river (East) boundaries (Figure 4) over a period of 2500 hr (short-term) for the current modeling application. Longer-term simulations with different objectives are described in Song X. et al. [2017]. The river stage varies 2 m or less over the short-term study period. The top and bottom boundaries of the domain are treated as no flow boundaries. Recharge is not considered in the model.

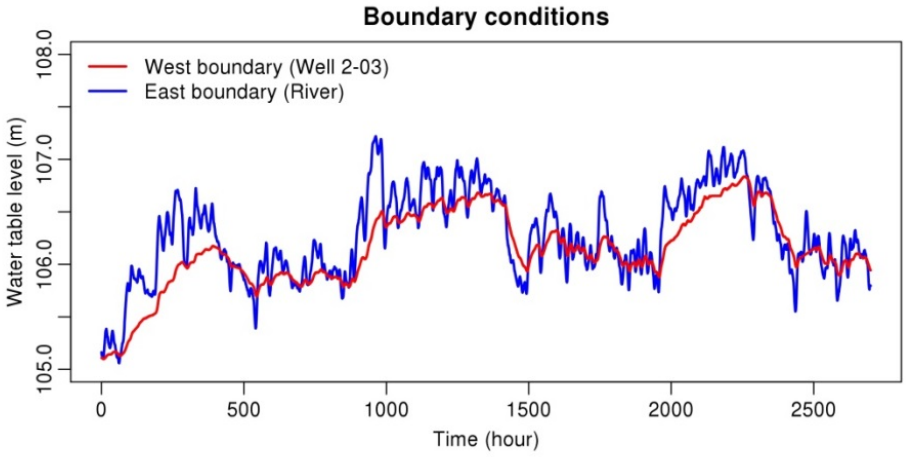


Figure 4. Boundary conditions: seasonal river stage calibrated from field measurement and monitored data from wells.

A standard finite volume method is used for discretization in PFLOTRAN (see user manual for details). The grid resolution of the domain is initially uniform (0.1 m x 0.05 m) then nested (finer resolution in alluvium) for multiscale simulations, which will be further explained in Section 3. A time step of 1 hr was selected to ensure numerical stability. All numerical simulations were conducted using National Energy Research Scientific Computing Center (NERSC) supercomputers (Edison and Cori).

2.4. Reactive transport and biogeochemical models

Solute transport in PFLOTRAN is represented by the advective-dispersive equation based on the simulated transient flow field:

$$\frac{\partial \varphi C_i}{\partial t} + \nabla \cdot (\mathbf{q}_i C_i - \varphi s \tau D \nabla C_i) = Q_{ci} \qquad (3.2)$$

where C_i is the concentration of each species, D is the dispersion coefficient and Q_{ci} is the source/sink term. The dispersion coefficients are constant in all directions with an assumed value of 1e-9 m^2/s. The boundary conditions for the transport (inland and river) are based on averaged sampling data from field measurements [Stegen et al., 2016].

As introduced in Section 1, two different biogeochemical (BGC) models were employed concurrently: one for the alluvial layer [Song H.-S. et al., 2017] and second simpler model for the rest of the domain [Gu et al., 2012]. Both BGC models represent aerobic respiration and denitrification but utilize different reaction networks and reaction rates/coefficients.

Gu et al. [2012] developed a general Monod-type model to describe aerobic respiration

$$CH_2O + O_2 \rightarrow CO_2 + H_2O \tag{3.3}$$

and denitrification

$$1.25CH_2O + NO_3^- + H^+ \rightarrow 0.5N_2 + 1.25CO_2 + 1.75H_2O \tag{3.4}$$

The reactants and products being monitored in the simulations include H^+, CO_2, CH_2O, O_2, NO_3^- and N_2. The source term for the reactive transport of the species is calculated as:

$$Q_{ci} = R_i \mathbf{q}_i \tag{3.5}$$

where the reaction rates R_i are calculated using multiple Monod kinetics. The above model was previously used to study flow and reactive transport under hyporheic exchanges in the riparian zone, and has been tested and proved to be informative. Therefore we have adopted this model for use in the Hanford and Ringold formations, with the associated parameters as described in Gu et al. [2012].

The model of Song H.-S. et al. [2017] is based on laboratory experiments using 300A alluvium sediments, and thus more specifically represents the microscale domain in the current study. This new model places a focus on the description of microbial regulation as a key component of biogeochemical modeling. Microbes regulate metabolism by controlling enzyme levels and activities so that, when alternative electron donors and acceptors are available in environment, they often preferentially use one over another instead of using them all simultaneously. Detailed regulatory modeling will require information on molecular details, which are largely unknown, however, except for specific processes. Consequently, in most of the biogeochemical modeling studies, microbial regulation has been accounted for using empirical inhibition kinetics (e.g., Trauth et al., 2014; Gu et al., 2007). The cybernetic modeling approach developed Ramkrishna and coworkers provides an alternative way to account for microbial regulation [Ramkrishna and Song, 2012]. The cybernetic approach views organisms as teleonomic systems that regulate metabolism to promote a certain metabolic objective in a varying environment. This postulate leads to analytic forms of regulation rules (called the cybernetic control laws), which can be

derived from an optimal control theory [Young and Ramkrishna, 2007]. In a previous study, Song and Liu [2015] demonstrated how the cybernetic modeling could be successfully applied to model denitrifying organisms. In the extension to microbial communities, Song H.-S. et al. [2017] provided two versions of the cybernetic model: genetically structured and simplified models. Below, we provide a summary of the simplified cybernetic model.

Based on data from the laboratory column experiments [Li et al., 2016], the microbially mediated biogeochemical processes are modeled by accounting for aerobic respiration and denitrification as follows:

Oxidative respiration:

$$CH_2O + O_2 \rightarrow CO_2 + H_2O \tag{3.6}$$

NO_3^- reduction to NO_2^-:

$$CH_2O + 2NO_3^- \rightarrow 2NO_2^- + CO_2 + H_2O \tag{3.7}$$

NO_2^- reduction to N_2:

$$CH_2O + 4/3NO_2^- + 4/3H^+ \rightarrow 2/3N_2 + CO_2 + 5/3H_2O \tag{3.8}$$

In equation (3.8), multi-stage reduction from NO_2^- to N_2 is lumped into a single reaction by assuming relatively fast dynamics of nitrogen oxide intermediates such as NO and N_2O.

Microbial biomass production can be written as follows:

$$CH_2O + 1/5NH_4^+ \rightarrow 1/5C_5H_7O_2N + 3/5H_2O + 1/5H^+ \tag{3.9}$$

Microbes obtain energy for growth and maintenance through aerobic or anaerobic respiration depending on what electron acceptors are available in environment. To account for this coupling, each of the energy-producing reactions, equations (3.6) – (3.8), is combined with biomass synthesis reaction, equation (3.9), as follows:

$$CH_2O + f_{O_2}O_2 + \frac{1}{5}(1-f_{O_3})NH_4^+ \rightarrow f_3CO_2 + \frac{1}{5}(1-f_{O_2})C_5H_7O_2N \tag{3.10}$$

$$CH_2O + 2f_{NO_3^-}NO_3^- + \frac{1}{5}(1-f_{NO_3^-})NH_4^+ \rightarrow 2f_{NO_3^-}NO_2^- + f_{NO_3^-}CO_2 + \frac{1}{5}(1-f_{NO_3^-})C_5H_7O_2N \tag{3.11}$$

$$CH_2O + \frac{4}{3}f_{NO_2^-}NO_2^- + \frac{1}{5}(1-f_{NO_2^-})NH_4^+ \rightarrow \frac{2}{3}f_{NO_2^-}N_2 + f_{NO_2^-}CO_2 + \frac{1}{5}(1-f_{NO_2^-})C_5H_7O_2N \tag{3.12}$$

where f_{O_2} , $f_{NO_3^-}$, and $f_{NO_2^-}$ are parameters that denote the fraction of energy-producing pathway. Due to our focus on simulating carbon and nitrogen flows, H^+ and H_2O are omitted in

the equations above. Equations (3.10) - (3.12) share the same electron donor (CH_2O), but involve different electron acceptors (i.e., O_2 for aerobic respiration, NO_3^- and NO_2^- for anaerobic respiration), thus representing three alternative pathways for the production of biomass ($C_5H_7O_2N$).

The reactants and products in the simulations include $C_5H_7O_2N$, CO_2, CH_2O, O_2, NO_3^-, NO_2^-, and N_2. Hereafter, we use *DOC* (dissolved organic carbon), *DIC* (dissolved inorganic carbon) and *BM* (biomass) to denote CH_2O, CO_2 and $C_5H_7O_2N$ for simplicity.

Dynamic mass balances of key variables in simulation can be written based on stoichiometric equations (3.10) - (3.12) as follows:

$$\frac{d}{dt}\begin{bmatrix}[DOC]\\ [O_2]\\ [NO_3^-]\\ [NO_2^-]\\ [N_2]\\ [DIC]\\ [BM]\end{bmatrix}=\begin{bmatrix}-1 & -1 & -1\\ -f_{O_2} & 0 & 0\\ 0 & -2f_{NO_3^-} & 0\\ 0 & 2f_{NO_3^-} & -4f_{NO_2^-}/3\\ 0 & 0 & 3f_{NO_2^-}/2\\ f_{O_2} & f_{NO_3^-} & f_{NO_2^-}\\ (1-f_{O_2})/5 & (1-f_{NO_3^-})/5 & (1-f_{NO_2^-})/5\end{bmatrix}\begin{bmatrix}r_{O_2}\\ r_{NO_3^-}\\ r_{NO_2^-}\end{bmatrix}[BM] \qquad (3.13)$$

where r_{O_2} , $r_{NO_3^-}$, and $r_{NO_2^-}$ denote microbes' carbon uptake rates through three reaction pathways (equation (3.10) - (3.12)), respectively. Finally, mass balances of *BM* and *DOC* are modified to account for biomass degradation and the resulting impact on DOC concentration,

$$\frac{d[BM]}{dt}=\left(\frac{1-f_{O_2}}{5}r_{O_2}+\frac{1-f_{NO_3^-}}{5}r_{NO_3^-}+\frac{1-f_{NO_2^-}}{5}r_{NO_2^-}-k_{\deg}\right)[BM] \qquad (3.14)$$

$$\frac{d[DOC]}{dt}=-\left(r_{O_2}+r_{NO_3^-}+r_{NO_3^-}-5k_{\deg}\right)[BM] \qquad (3.15)$$

where $k_{\deg}$ denotes the rate of biomass degradation [1/day].

Three biogeochemical reactions considered above can be modeled as being catalyzed by distinct enzymes as follows:

$$r_{O_2}=e_{O_2}r_{O_2}^{kin},\quad r_{NO_3^-}=e_{NO_3^-}r_{NO_3^-}^{kin},\quad r_{NO_2^-}=e_{NO_2^-}r_{NO_2^-}^{kin} \qquad (3.16)$$

where e_{O_2} , $e_{NO_3^-}$, and $e_{NO_2^-}$ denote the relative level of enzymes that catalyze aerobic respiration and two-step denitrification reactions, respectively, and $r_{O_2}^{kin}$, $r_{NO_3^-}^{kin}$, and $r_{NO_2^-}^{kin}$ are unregulated reaction rates that can be represented by Monod kinetics, i.e.,

$$r_{O_2}^{kin} = k_{O_2} \frac{[DOC]}{K_{d,O_2} + [DOC]} \frac{[O_2]}{K_{a,O_2} + [O_2]}$$

$$r_{NO_3^-}^{kin} = k_{NO_3^-} \frac{[DOC]}{K_{d,NO_3^-} + [DOC]} \frac{[NO_3^-]}{K_{a,NO_3^-} + [NO_3^-]} \quad (3.17)$$

$$r_{NO_2^-}^{kin} = k_{NO_2^-} \frac{[DOC]}{K_{d,NO_2^-} + [DOC]} \frac{[NO_2^-]}{K_{a,NO_2^-} + [NO_2^-]}$$

While enzyme levels are determined by solving dynamic enzyme balance equations in the original formulation of the cybernetic modeling, they can be determined through a direct linkage to the cybernetic control laws [Young and Ramkrishna, 2007]:

$$e_{O_2} = \frac{r_{O_2}^{kin}}{r_{O_2}^{kin} + r_{NO_3^-}^{kin} + r_{NO_2^-}^{kin}}, \quad e_{NO_3^-} = \frac{r_{NO_3^-}^{kin}}{r_{O_2}^{kin} + r_{NO_3^-}^{kin} + r_{NO_2^-}^{kin}}, \quad e_{NO_2^-} = \frac{r_{NO_2^-}^{kin}}{r_{O_2}^{kin} + r_{NO_3^-}^{kin} + r_{NO_2^-}^{kin}} \quad (3.18)$$

The above equation implies that microbes control the synthesis of enzymes in proportion to their relative contribution to a chosen objective (i.e., the carbon uptake rate). This formulation enables the model to simulate the dynamic shift among three electron acceptors (i.e., O_2, NO_3^- and NO_2^-) without having to rely on empirical inhibitive kinetics.

Key parameters of denitrification, including $f_{NO_3^-}$, $f_{NO_2^-}$, $k_{NO_3^-}$ and $k_{NO_2^-}$ and $k_{\deg}$, are determined through model fit to the batch denitrification data [Li et al., 2016], which was collected using the sediment obtained from the Columbia River hyporheic zone at the US DOE's Hanford Site. More details of the lab sediment experiments are reported in previous studies [Li et al., 2016]. Literature data are used for the half saturation constants associated with *DIC* (i.e., K_{d,NO_3^-} and K_{d,NO_2^-}) and electron acceptors (i.e., K_{a,NO_3^-} and K_{a,NO_2^-}) [Rittmann and McCarty, 2001; Yan S. et al., 2016]. Parameters associated with oxidative respiration are determined by assuming the relation to anaerobic respiration, i.e., 1) oxidative respiration is energetically more favorable than NO_3^- reduction (i.e., $f_{O_2} = f_{NO_3^-}/3$, $k_{O_2} = 3k_{NO_3^-}$) and 2) half saturation constants are the same (i.e., $K_{d,O_2} = K_{d,NO_3^-}$, $K_{a,O_2} = K_{a,NO_3^-}$). This parameter setting leads to the sequential

utilization of three alternative electron acceptors, i.e., O_2, NO_3^-, NO_2^-, and in batch reactor simulation. Model parameters used for simulations here are summarized in Table 4 and are based on fitting model results to the experimental data, which shows good agreement [Song H.-S. et al., 2017].

Table 4. Parameter values of the biogeochemical model used to simulate the interaction between environment and microbial growth through aerobic respiration and denitrification.

Parameter	Aerobic respiration	NO_3^- reduction	NO_2^- reduction
Fractional of energy-producing pathway [-]	$f_{O_2} = 0.217$	$f_{NO_3^-} = 0.65$	$f_{NO_2^-} = 0.99$
Reaction rate constant [mmol/mmol BM/day]	$k_{O_2} = 84.78$	$k_{NO_3^-} = 28.26$	$k_{NO_2^-} = 23.28$
Half saturation constant of electron donor [mM]	$K_{d,O_2} = 0.25$	$K_{d,NO_3^-} = 0.25$	$K_{d,NO_2^-} = 0.25$
Half saturation constant of electron acceptor [mM]	$K_{a,O_2} = 0.001$	$K_{a,NO_3^-} = 0.001$	$K_{a,NO_2^-} = 0.004$
Biomass degradation rate [1/day]	$k_{\text{deg}} = 0.242$		

3. Hybrid Multiscale Modeling Approach

3.1. A loose-coupling framework

The hybrid multiscale modeling framework follows the loose-coupling method presented in Scheibe et al. [2015b; 2015c]. In the current framework, the computational domain is divided into hierarchical macroscale and microscale subdomains that are simulated using different models. The at-scale simulations are conducted sequentially and loosely-coupled by customized scripts. In the current study, as shown in Figure 2 and Table 1, the microscale subdomain (alluvial layer) is simulated using the Richards equation with fine grid resolution and the cybernetic BGC model [Song H.-S. et al., 2017], and the macro-scale subdomain including the Hanford and Ringold formations are simulated using the Richards equation with coarse grid resolution and the BGC model developed by Gu et al. [2012]. The concept of the loose-coupling method is to use script-based functional operators to perform numerical upscaling/downscaling, exchange data (file based) and convert between input and output files from at-scale simulators

where the two domains overlap. Advantages of the loose-coupling method include (1) it does not require modification of the at-scale simulators and (2) ease of programming. Potential disadvantages are 1) numerical errors or instabilities introduced by the sequential coupling, and 2) inefficiencies introduced by passing data through I/O files rather than direct message passing. The workflow of the loose-coupling framework for the current application is presented in Figure 5, which includes the following steps:

1. The macroscale simulator (PFLOTRAN) is applied over the full computational domain. Flow and reactive transport simulation using BGC model by Gu et al. [2012] are executed for a specified period of time. Configuration files describing the initial model configuration (initial condition, boundary condition and parameters) are provided to start the simulation at the beginning of the workflow.
2. A serial python script –Lifting Operator (LO) –executes the downscaling step (interface coupling and model updating) and constructs microscale simulator (PFLOTRAN) input files. The LO script provides algorithms to reconstruct initial conditions for micro-scale subdomains based on macro-scale quantities from Step 1. Since the size of the micro-scale subdomain is fixed in the current application, no adaptivity control (to dynamically determine the micro-scale subdomains) is needed.
3. The microscale simulator (PFLOTRAN) is then applied only to the alluvial layer subdomain with the cybernetic BGC model [Song H.-S. et al., 2017] and finer grids, and is executed for the same period of time as the previous macroscale simulation.
4. A serial python script – Restriction Operator (RO) –performs numerical upscaling (interface coupling and averaging) and constructs macroscale input files for the next time step based on outputs from the microscale simulations.
5. Repeat the procedure until the entire simulation period is completed.

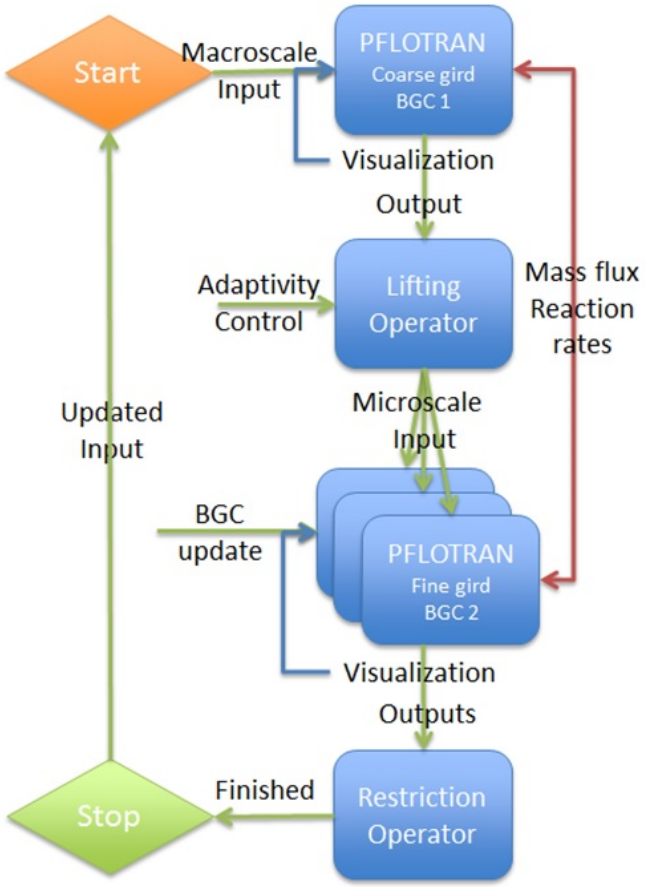


Figure 5. Swift-managed flowchart and execution for the current application

3.2. *Coupling strategies*

The challenge in all hybrid methods based on physical domain decomposition is how to ensure consistency between the macroscale and microscale subdomains [Scheibe et al., 2015a; Mehmani and Balhoff 2015]. For flow and reactive transport problems, it is critical to ensure consistency of flow and concentrations of multiple chemical species and their flux at the interface (in this case, the bottom boundary of the alluvium layer). There are two critical issues for coupling in the current application: (1) multi-grid matching and (2) consistency of the BGC models. Since the heterogeneity and unique HBGC processes in the alluvium (microscale subdomain) require simulations with higher resolution, we refine the grids in the microscale subdomain relative to the coarser grids used in the macroscale subdomain. Different ratios of grid resolutions (macro- to micro-) were tested: 1:1, 1:0.5 and 1:0.25. To match the values (velocity, concentration and their fluxes) on the nodes of the nested grids, the loose-coupling

method uses an interpolation/extrapolation scheme for the dependent variable along the interface. From macro-scale to micro-scale subdomain, the nodal values of the coarse grid are distributed evenly to the fine nodes. On the other hand, the nodal values simulated on the fine grids are averaged to coarse grids. A prediction-correction procedure is enforced in each time step. For example, for flow simulations, at the beginning of each time step, we use the velocity from the last time step at the interface. Thereafter the flow and transport equations in the macro-scale subdomain can be solved. Then we pass the interfacial pressure to the micro-scale subdomain, and solve the governing equations to correct the micro-scale velocity. We repeat this procedure iteratively until convergence. The same procedure is conducted for transport simulations. The two BGC models presented in Section 2.4 are different in terms of species and reaction rates. In Gu et al. [2012], the species (reactants and products) include H^+, CO_2, CH_2O, O_2, NO_3^- and N_2. In the cybernetic model [Song et al., 2017], the reactants and products being monitored in the simulations include $C_5H_7O_2N$, CO_2, CH_2O, O_2, NH_4^+, NO_3^-, NO_2^-, and N_2. The number of reactions and species are slightly different in two models. For variable data exchange, we only pass those that co-exist in both models. The reaction rates are calculated in each time step, then passed and updated between scales.

3.3. Simulation cases

To validate and apply the above Swift-managed workflow to the 2D modeling domain, we set up a series of simulation cases using increasingly complex scenarios. A list of the cases is summarized in Table 5.

1. Case 1 is designed to validate that the multiscale coupling algorithm is working correctly. In this case, we compare results from the hybrid multiscale simulation (including multiple nested grid ratios) with equivalent single-scale (single-domain) simulations using a uniform grid resolution, homogeneous properties and one BGC model (Gu et al., 2012). Since both the multiscale and single-scale models use the same property distributions and BGC model, the only difference is the multiscale coupling and subgrid resolution, and all solutions should be comparable.
2. Following successful validation, Case 2 simulations are designed to evaluate the potential impacts of sub-grid heterogeneity within the alluvial layer only. We apply

several realizations of the statistical heterogeneity model (Section 2.2) to the alluvium only (microscale subdomain) and compare with the homogeneous case (Case 1).

3. Case 3 is designed to evaluate the potential impacts of applying an alternative and more complex BGC model in the alluvium layer. The BGC model of Song H.-S. et al. [2017] is applied in the alluvium while maintaining use of the Gu et al. [2012] BGC model in the larger domain. Again, results are compared to Case 1 which uses the Gu et al. [2012] model everywhere.
4. Case 4 applies the full combination of nested multiscale grids, heterogeneities in all formations, and different BGC model in the alluvial layer. This reflects the full level of complexity that is enabled by the hybrid multiscale coupling, and the results are evaluated to determine whether representing this level of complexity could reveal different behaviors from the simpler cases above.

Table 5. A list of simulation cases

Scale\Case	Case 1	Case 2	Case 3	Case 4
Macro-scale	Coarse/fine grid Homogeneous BGC model 1	Coarse grid Homogeneous BGC model 1	Coarse grid Homogeneous BGC model 1	Coarse grid Homogeneous BGC model 1
Micro-scale	Coarse/fine grid Homogeneous BGC model 1	Fine grid Heterogeneous BGC model 1	Fine grid Homogeneous BGC model 2	Fine grid Heterogeneous BGC model 2

4. Results

4.1. Case 1: Validation

The hybrid multiscale model was applied to simulate HBGC processes in the 2D domain over a 2500 hr time period. The instantaneous velocity (with streamlines) and reaction product (N_2) species concentration contour plots at a selected time (384 hours) are shown in Figure 6. Intrusion of river water into the various subsurface formations is clearly evident. The

geostratigraphic formations strongly impact the flow paths, with the fastest flow paths occurring in the high-permeability Hanford formation. The purpose of Case 1 is to validate the multiscale coupling methodology by comparing results to equivalent single-scale simulations. For this case, a uniform fine (high-resolution 0.05 m horizontal x 0.025 m vertical) grid was used for the single-scale model, whereas the multiscale model used variable nested grids.

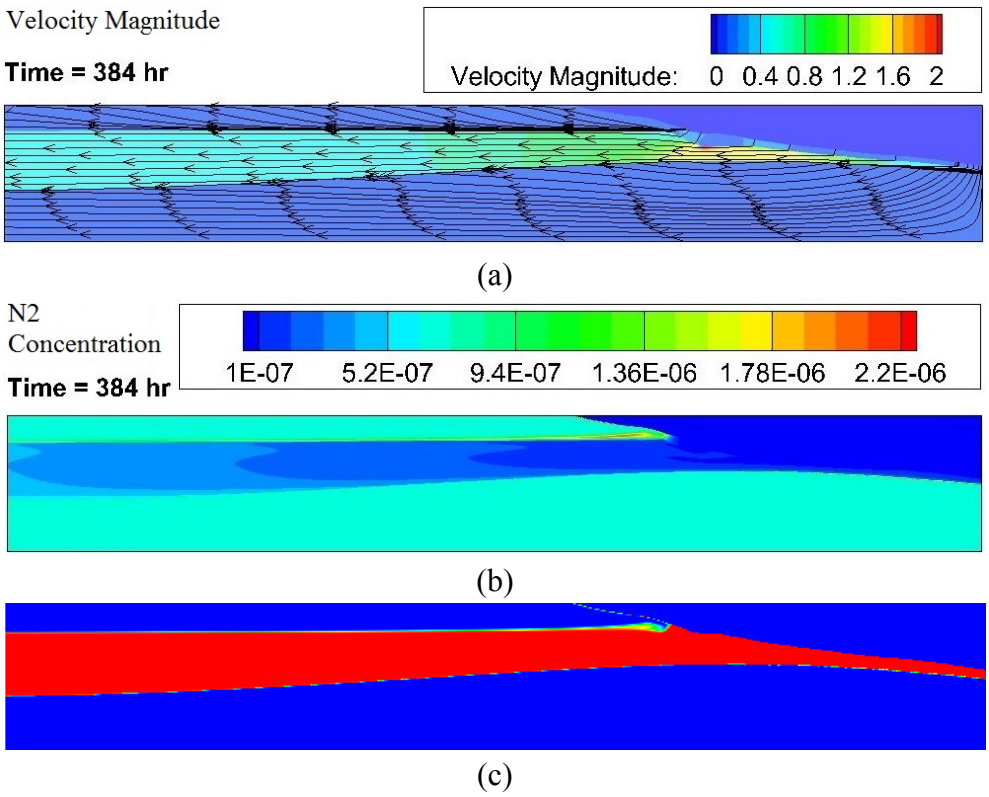


Figure 6. Instantaneous contour plots of (a) velocity magnitude, (b) concentrations of N_2 and (c) tracer.

Figures 7-9 present the comparisons from different perspectives. Instantaneous contour plots of velocity magnitude are shown in Figure 7, which shows minimal differences between the single-scale and multi-scale simulations. To further quantify the results, velocity distributions (histograms) are shown in Figure 8 for a series of simulations with different computational grids (Figure 8). The hybrid multiscale result with a uniformly fine grid is indistinguishable from that of the equivalent single-scale model, indicating minimal error introduced by the coupling process. Employment of a coarse (0.1 m horizontal x 0.05 m vertical) grid everywhere introduces errors of up to 6%. The nested grid used in the multiscale simulation (coarse-to-fine ratio equals

to 0.25) provides results that are more accurate than the coarse grid, but still have small errors relative to the uniform fine grid. This is expected from the loosely-coupled multiscale method, and represents the tradeoff between accuracy and computational demand. In cases where a uniform fine grid is not computationally feasible, the multiscale method provides higher accuracy than a uniform coarse grid, but with a relatively modest increase in computational demand. To evaluate impacts on predictions of biogeochemical reactions, multiple species concentration histories at one of the hypothetical observation locations (Well 2M in the alluvium in Figure 2) are presented in Figure 9. Again the results obtained from the single- and multi-scale simulations (based on uniform fine grids and BGC model from Gu et al. 2012) are indistinguishable, which validates the loose coupling of reactive transport.

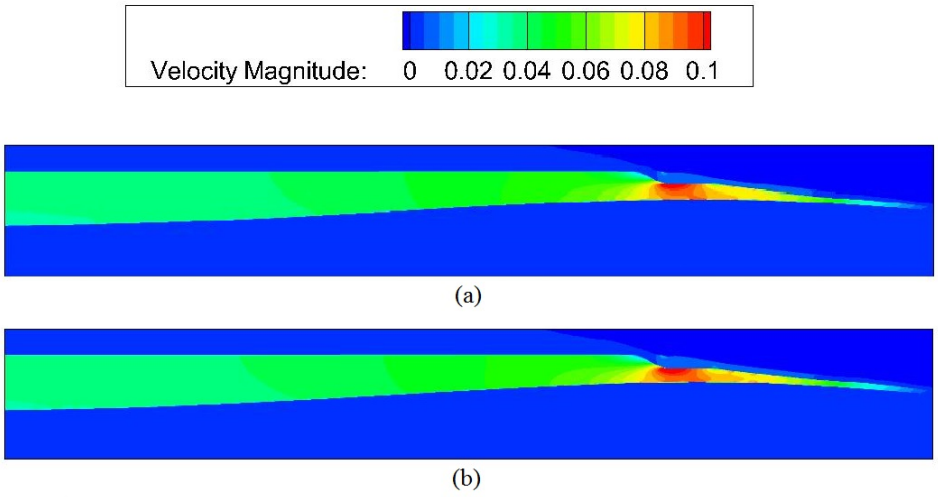


Figure 7. Comparisons of velocity magnitude contour plots (t = 384 hr): (a) single-scale simulation using uniform fine grids; (b) hybrid multi-scale simulation using nested grids.

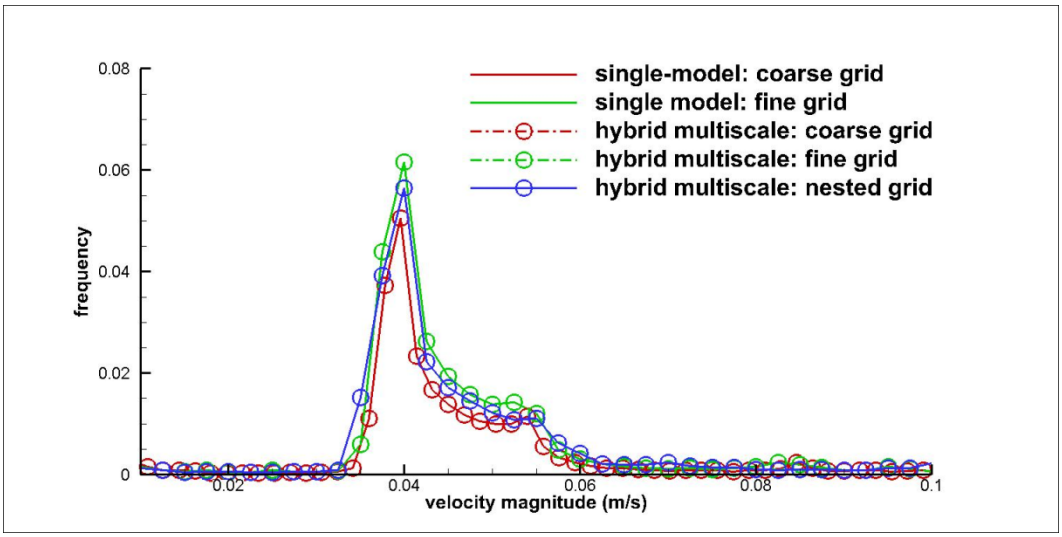


Figure 8. Comparisons of velocity histograms between single- and multi-scale models.

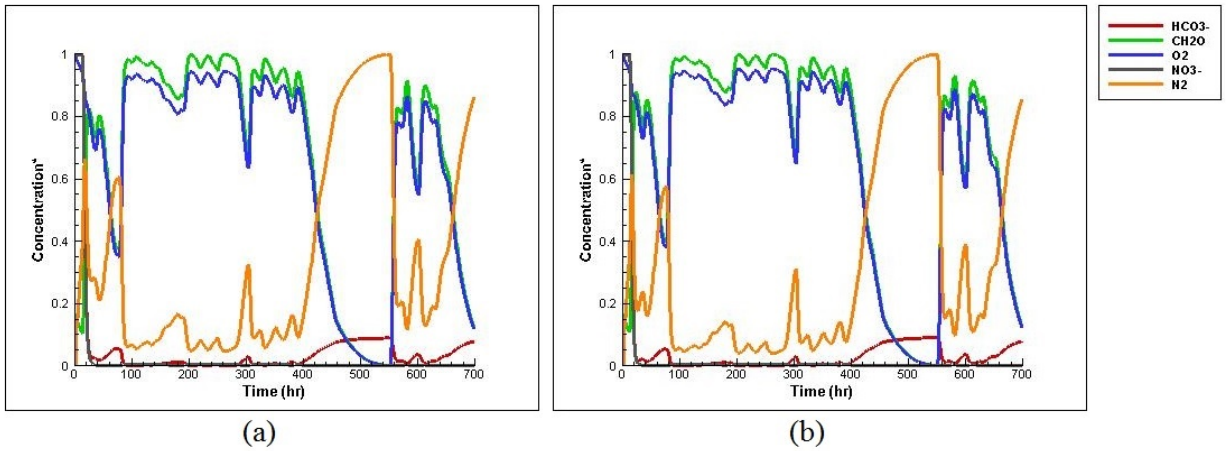
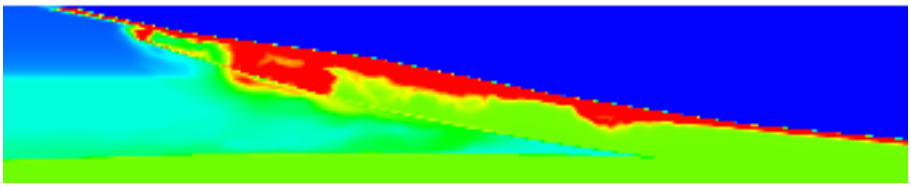


Figure 9. Comparisons of species concentration time histories (using the same setup) between (a) single-scale model and (b) hybrid multi-scale model.

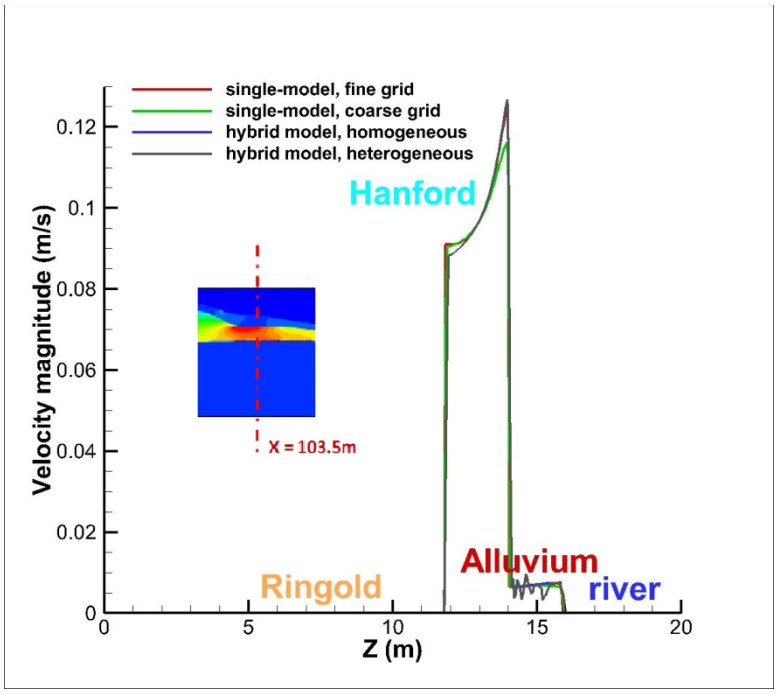
Finally, we present the results of computing cost in terms of CPU hrs (Table 5). For uniform (fine or coarse) grids, the hybrid simulations use more CPU time than the corresponding single-scale models due to computational overhead associated with model coupling and data/file exchange. However, for the nested grid in multiscale hybrid simulations, the computing cost was significantly reduced relative to single-scale simulations on uniform fine grids. These results demonstrate that the loosely-coupled hybrid multiscale simulation method is a feasible approach for investigation of the impacts of detailed processes and property distributions within microscale subdomains.

4.2. *Case 2: Impact of micro-scale heterogeneity*

Having established confidence in the numerical coupling algorithm based on Case 1 comparisons, we now apply our hybrid multiscale model approach to more complex cases. We consider these additional cases as numerical experiments to evaluate the potential impact of small-scale heterogeneity and complex biogeochemistry within the alluvial layer. Case 2 tests the potential impacts of permeability heterogeneity in the alluvial layer by replacing the homogeneous properties used in Case 1 with heterogeneous distributions (using a geostatistically-generated realization). Figure 10 shows the altered flow field in the alluvium and associated velocity profiles along a selected transect as shown in the figure. Comparisons between homogeneous and heterogeneous cases are provided along the transect (red dashed line). While the overall results are similar for all cases, variable velocities are observed in the alluvium layer for the multiscale case, indicating that the microscale heterogeneity impacts flow fields within the microscale subdomain but not in the macroscale domain. Figure 11 shows the time history of the considered biogeochemical species at hypothetical observation location 2M (Figure 2). In comparison to Figure 9 (Case 1), the overall trends are similar but there are some significant differences, suggesting that physical heterogeneity in the alluvium alone can impact the system biogeochemistry through formation of preferential flow paths and low-flow zones.



(a)



(b)

Figure 10. Case 2: (a) distribution of river water (as a tracer) within the alluvium at a selected time point (t = 384 hr), showing the impacts of alluvial heterogeneity; (b) comparisons among velocity magnitude profiles (along the red dashed line across the domain) for single-scale and multiscale models on different grids and with homogeneous and heterogeneous alluvium properties.

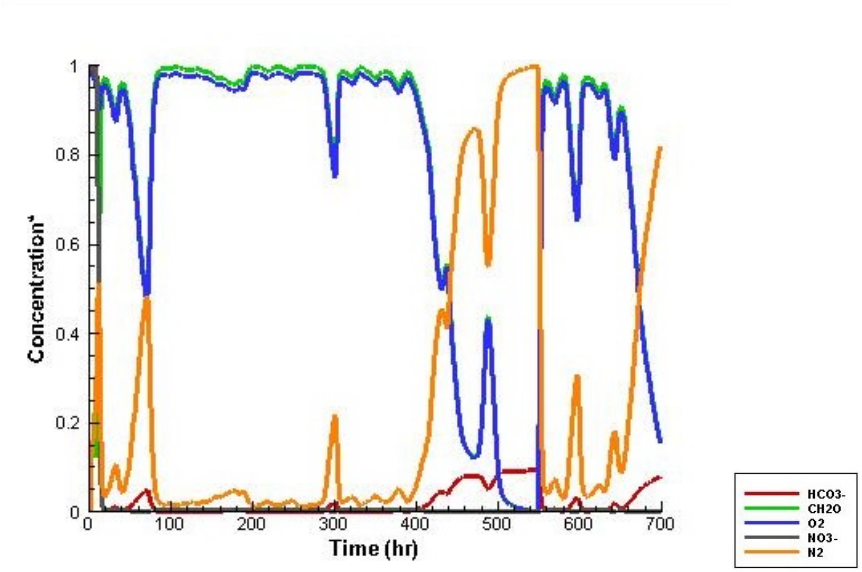


Figure 11. Impact of small-scale permeability heterogeneity in the alluvium on biogeochemical reaction outcomes; compare to Figure 9.

4.3. *Case 3: Impact of alternative BGC model in the alluvium*

In Case 3, we employ the more complex biogeochemical model of Song H.-S. et al. [2017], developed specifically for alluvial sediments, in the microscale subdomain while keeping the more general model of Gu et al. [2012] used in the macro-scale subdomain. Since there are two pathways in the model by Song H.-S. et al. [2017], there exist additional species and intermediate products that are not simulated in the macroscale domain. This inconsistency induces some potential numerical instability in the loose coupling algorithm. For comparison purposes, we consider only those species simulated in both biogeochemical models. Figure 12 again shows the time histories of the species concentrations at hypothetical observation point 2M. Comparison to Case 1 results (Figure 9) indicate significantly lower simulated concentrations of N_2 (reaction product) among other differences, which suggests that the application of a more complex reaction network within the biogeochemically active alluvial layer can lead to significant differences in model prediction. However, since we do not have direct observational information for comparison, we cannot confidently state that this prediction is in fact better. What is clear is that the multiscale hybrid approach enables the use of more complex representations of biogeochemistry (Case 3) and physical heterogeneity (Case 2) which could have significant impacts on model predictions. Additional model testing and experimental data are needed to confirm the significance of these differences.

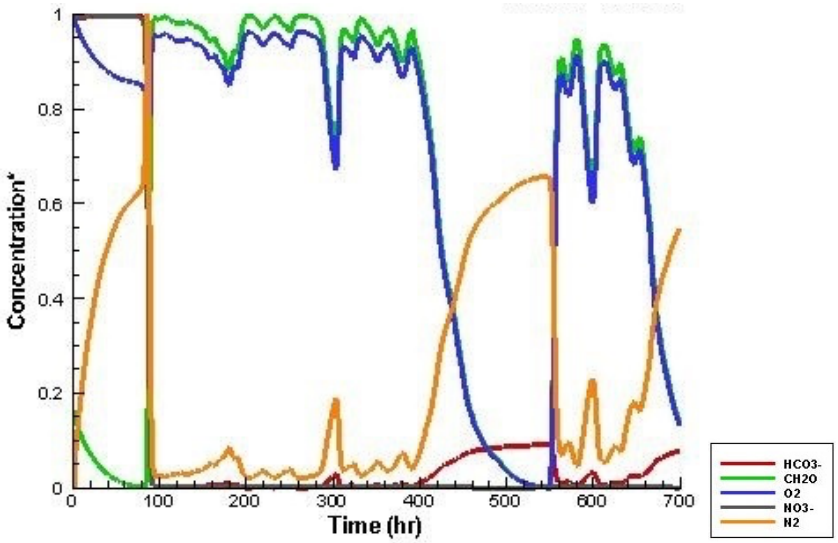
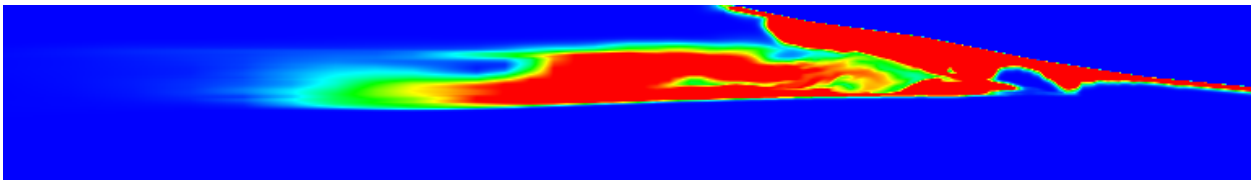


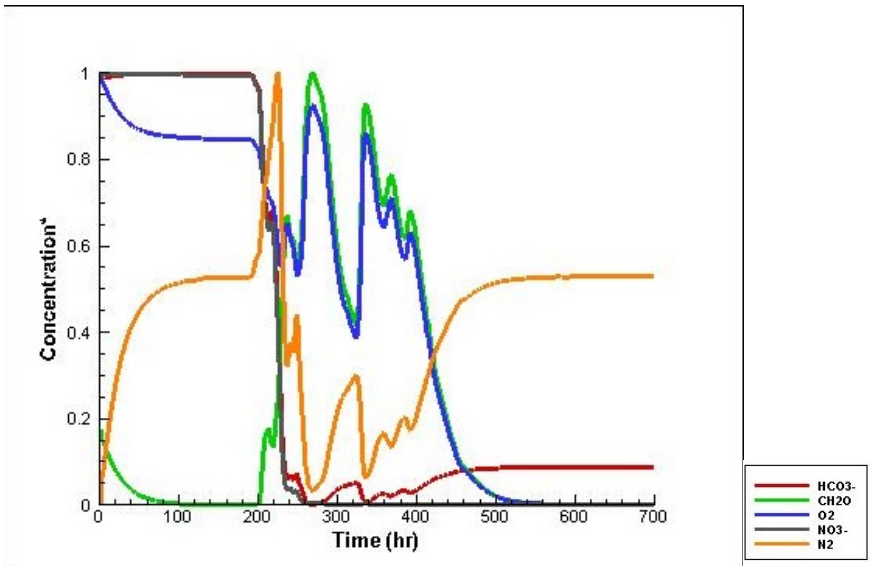
Figure 12. Impact of using an alternative biogeochemistry model in the alluvium; compare to Figure 9.

4.4. *Case 4: A complete simulation*

This final case combines the complexities of Cases 2 and 3, and in addition incorporates a realization of physical heterogeneity (hydraulic conductivity) in the Hanford and Ringold formations (macroscale domain). Figure 13a shows a snapshot of tracer (river water) distribution at a selected time (t = 276 hr), and Figure 13b shows the corresponding time history of biogeochemical species at the hypothetical observation point 2M. The complex flow pattern interacts with the biogeochemical processes (mostly in the alluvial layer) to create transient species behaviors that differ significantly from the homogeneous scenarios (Case 1). Again, additional model testing and experimental data are needed to confirm the significance of these differences. However, our numerical experiments demonstrate that multiscale physical heterogeneity and complexity of the biogeochemical reaction model are key factors that can strongly impact predictions of hydrobiogeochemical processes in the GSIZ.



(a)



(b)

Figure 13. Case 4: (a) instantaneous contour plot of tracer transport (t = 276 hr); (b) BGC species concentration time histories.

5. Summary and Conclusions

We used a hybrid multiscale modeling approach to simulate hydrologic-biogeochemical processes (HBGC) in the groundwater-surface water interaction zone (GSIZ) at the US DOE Hanford 300A site. A 2D modeling domain [Song X. et al., 2017] was studied and decomposed into macroscale and microscale subdomains based on the spatial configuration of hydrogeological formations [Hou et al., 2016]. Enhanced biogeochemical activity associated with groundwater-river water exchange has been observed in a heterogeneous thin alluvial layer that is adjacent to the river. Resolution of these processes was enabled by utilizing a fine grid and complex biogeochemical model in the microscale domain, coupled to a coarser grid and simpler biogeochemical model in the macroscale domain. A hybrid multiscale method was implemented in a script-based high-performance computing workflow to loosely couple microscale and macroscale models, both implemented using the same reactive transport simulator, through upscaling/downscaling methods and file-based data exchange.

The hybrid multiscale model algorithm was successfully validated by comparing results to a single-scale simulation with uniformly fine grid, homogeneous facies properties and uniform BGC models. Comparisons demonstrate that the hybrid multiscale simulation approach provides greater process fidelity than a coarsely-resolved single-scale model while maintaining higher computational efficiency than a finely-resolved single-scale model. A series of numerical experiments demonstrated potential impacts of incorporating microscale heterogeneity and complex biogeochemistry on model predictions; further testing and validation against experimental results are needed to confirm these outcomes. The use of stochastic simulation methods to represent heterogeneous properties also can enable future study of model uncertainties associated with microscale heterogeneity.

Our results demonstrate that hybrid multiscale models can be successfully implemented in field-scale simulations with complex subsurface sediment structures and complicated HBGC processes. The 2D model system used here for method demonstration and testing does not require the computational efficiency of the multiscale approach, but the same method can easily be extended to 3D domains of much larger size for which this efficiency will be required. Further developments of the hybrid multiscale models, especially refinement of the coupling methods, are needed to ensure robustness and generalizability. Research is continuing in (1) development

of a generalized hybrid multiscale modeling framework using a universal coupling interface and (2) intercomparison and community benchmarking of alternative hybrid multiscale modeling approaches.

Acknowledgement

This research was supported by the U. S. Department of Energy (DOE) Office of Biological and Environmental Research (BER), Subsurface Biogeochemical Research (SBR) program, through the PNNL SBR Scientific Focus Area project and the Interoperable Design of Extreme-scale Application Software (IDEAS) project. Computations described here were performed at the National Energy Research Supercomputing Center (NERSC), which is supported by the DOE Office of Science under contract DE-AC02-05CH11231.

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