Editorial

Branko Bijeljić^a, Matteo Icardi^b, Maša Prodanović^c

^a*Department of Earth Science and Engineering, Prince Consort Road, Imperial College London, London SW7 2BP, UK*

^b*School of Mathematical Sciences, University of Nottingham, NG7 2RD, Nottingham, UK*

^c*Hildebrand Department of Petroleum and Geosystems Engineering, The University of Texas at Austin, 200 E. Dean Keeton St, Stop C0300, Austin, TX 78712, USA*

Substantial progress has been made over last few decades on understanding the physics of multiphase flow and reactive transport phenomena in subsurface porous media. Confluence of advances in experimental techniques (including micromodels, X-ray microtomography, Nuclear Magnetic Resonance (NMR)) as well as computational power have made it possible to observe static and dynamic multi-scale flow, transport and reactive processes, thus stimulating development of new generation of modelling tools from pore to field scale. One of the key challenges is to make experiment and models as complementary as possible, with continuously improving experimental methods in order to increase predictive capabilities of theoretical models across scales. This creates need to establish rigorous benchmark studies of flow, transport and reaction in porous media which can then serve as the basis for introducing more complex phenomena in future developments.

This special issue resulted from scientific exchanges during a session at the XXII International Conference Computational Methods in Water Resources, CMWR 2016, which took place at University of Toronto. It is dedicated to development of computational and experimental techniques that provide benchmark datasets; validation studies based on experiment, analytical and numerical models; and studies providing an assessment of uncertainty in predictions across scales. It brings together a broad range of contributions dedicated to upscaling and numerical techniques (Lee et al. (2017); Boccardo et al. (2017); Dell'Oca et al. (2017); Pierce et al. (2018)); lab-scale validation of transport models (Maina et al. (2017); Mondal et al. (2017)); use of NMR to probe different flow characteristics in dissolution, density-driven convection, and tracer transport (Muljadi et al. (2017); Montague et al. (2017); Zheng et al. (2017)); validation of two-phase displacement in simple porous media (Verma et al. (2018); Chen et al. (2017)); and, last but not the least, machine learning for contaminant source identification (Vesselinov et al. (2017)).

The first two groups of papers are related to methodologies and fundamental understanding of solute and particle transport in multiscale and heterogeneous porous media, with significant results in model development, numerical advances, and practical simulation best practices. Boccardo et al. (2017) presented a contribution that clarifies several inconsistencies in the commonly used pore-to-core upscaling methods for reaction and particle deposition. Starting from a fairly general Eulerian formulation that can be extended beyond simple solute transport, a simple, though rigorous approach to quantitatively measure effec-

tive reaction rates is proposed, for arbitrary fast reaction kinetics at the solid surfaces. The approach is demonstrated for a periodic spherical packing but can be readily be extended for arbitrary pore structures. Another important conceptual advancement in the development of predictive upscaled models is the contribution by Lee et al. (2017), that deals with the upscaling of longitudinal dispersion in media with strongly heterogeneous permeability. The method allows to compute the Fickian dispersion coefficient explicitly, given the solution of three auxiliary closure problems which, we believe, offer an interesting connection with the ones naturally arising in volume averaging and homogenisation. The method has been applied for Darcy-to-field upscaling on two-dimensional block-wise permeability heterogeneities and compared with classical perturbation theory on log-normal random fields. Dell’Oca et al. (2017) propose a novel numerical tools to accurately compute transport in heterogeneous systems. The importance of this study is demonstrated by the number of papers in this issue (experiments and numerical benchmarks) dealing with such media. The adaptive technique proposed is grounded on the definition of an a-posteriori error estimator for the global (space-time) discretisation error and can therefore efficiently find the optimal mesh parameters for a given tolerance. These types of techniques have a great potential in fundamental numerical studies, where they can be directly applied to increase the fidelity of numerical simulations, as well as in more complex applications, where prior results can be used as qualitative guidelines for improved meshing/discretisation strategies. In Pierce et al. (2018) discrete fracture network transport and degradation modeling of contaminant (trichloroethane) degradation is combined with field data to illustrate the importance of small degradation rates on large scale plume extent.

Both Maina et al. (2017) and Mondal et al. (2017), present a combination of laboratory-scale tracer experiments and numerical simulations. The former focuses on the benchmarking and validation of a number of codes and models (including well-known commercial packages) to reproduce 2D controlled experiments on a heterogeneous sand packing arrangement. Results include meshes with different resolutions and concentration in different locations. In the latter, experiments in a glass-walled quasi-2D porous medium have been used in combination of a numerical model to better understand the effects of water discharge and polymer concentration on the polymer-stabilized contaminant transport. This work demonstrates how experiments and modelling can improve efficiency of polymer attachment to contaminant as a function of specific discharge.

NMR is a powerful technique capable of providing spatial and temporal characteristics of flow, transport and reaction. Zheng et al. (2017) perform NMR flow experiments examining connectivity in dual porosity beadpack to validate numerical models of transport based on coupled random walk and lattice-Boltzmann methods. Probability distributions of molecular displacements measured as a function of time (flow propagators) are successfully compared with the model accounting for fluid exchange between regions of different scales. A concept based on Euclidian distance maps has been used to relate fluid transport at different scales to the connectivity. Furthermore, Muljadi et al. (2017) analyse the same transport characteristic obtained in NMR experiments on acid dissolution of a carbonate rock for validation and calibration of a multi-scale Continuous Time Random Walk model. Pore-scale flow propa-

gators are first validated for transport in porous media of increasing degree of complexity. Based on this, evolution of propagators during reactive transport experiment is modelled from pore to core scale, which indicates a higher degree of transport heterogeneity induced by reaction. Finally, Montague et al. (2017) use the same experimental technique to observe solute transport during density driven convection in a dual permeability sand column, and compare it to a numerical model based on Navier-Stokes equations coupled to a convection-dispersion equation. This work provides further evidence that small density differences can reduce the time required for mixing by convective currents. Non-invasive imaging in three dimensions allows for an accurate characterisation of the movement of concentration across a sharp material interface to be observed and modelled accurately.

Wettability is a key property influencing fluid displacement, and Verma et al. (2018) provide rigorous accuracy assessment of two methods with the ability to simulate different wettability scenarios: namely, a popular, open-source volume-of-fluid method and a capillarity-dominated level set method. The assessment is done in simple 3D pores bounded by spheres and validated against analytically available critical curvatures, but the methods are nevertheless capable of simulating results in arbitrarily complex geometries. Chen et al. (2017) validate another method popular for its handling of fluid displacement in complex geometries, lattice Boltzmann method color model, against micromodel experiments to explore the range of validity at reservoir conditions. Numerical stability of the method requires use of higher viscosity for individual fluids (while maintaining their ratio) and that increases the inertial effects (and ultimately alters displacement patterns) compared to those observed in the experiments. Therefore, caution has to be exercised if the numerical simulation maintains only the capillary number and viscosity ratio of the fluids.

Machine learning is taking data-based modeling world by the storm, and contaminant source identification is no exception. A combination of semi-supervised machine learning clustering and decomposition methods for mixture observations can identify both the unknown number of groundwater types and the original geochemical concentration of the contaminant sources from measured geochemical mixtures with unknown mixing ratios without any additional site information Vesselinov et al. (2017).

Experimental data, theory and modelling continue to advance at a fast pace. Infrastructure supporting them (sample and data repositories, multi-user experimental facilities, numerical models and software) are developing at a fast pace as well, and are increasingly dynamically linked and interoperable. In foreseeable future, a reader of validation/benchmark studies such as documented in this special issue will be able to access and dynamically test, reuse/aggregate and extend all of the experimental and numerical data associated with it.

References

- Boccardo G., Crevacore E., Sethi R., Icardi M. A robust upscaling of the effective particle deposition rate in porous media. *Journal of Contaminant Hydrology* 2017; URL: <http://www.sciencedirect.com/science/article/pii/S0169772217300402>. doi:10.1016/j.jconhyd.2017.09.002.

- Chen Y., Li Y., Valocchi A.J., Christensen K.T. Lattice Boltzmann simulations of liquid CO₂ displacing water in a 2d heterogeneous micromodel at reservoir pressure conditions. *Journal of Contaminant Hydrology*2017;URL: <http://www.sciencedirect.com/science/article/pii/S0169772217300645>. doi:10.1016/j.jconhyd.2017.09.005.
- Dell'Oca A., Porta G.M., Guadagnini A., Riva M. Space-time mesh adaptation for solute transport in randomly heterogeneous porous media. *Journal of Contaminant Hydrology*2017;URL: <http://www.sciencedirect.com/science/article/pii/S016977221730061X>. doi:10.1016/j.jconhyd.2017.07.001.
- Lee J., Rolle M., Kitanidis P.K. Longitudinal dispersion coefficients for numerical modeling of groundwater solute transport in heterogeneous formations. *Journal of Contaminant Hydrology*2017;URL: <http://www.sciencedirect.com/science/article/pii/S0169772217300761>. doi:10.1016/j.jconhyd.2017.09.004.
- Maina F.H., Ackerer P., Younes A., Guadagnini A., Berkowitz B. Benchmarking numerical codes for tracer transport with the aid of laboratory-scale experiments in 2d heterogeneous porous media. *Journal of Contaminant Hydrology*2017;URL: <http://www.sciencedirect.com/science/article/pii/S016977221630328X>. doi:10.1016/j.jconhyd.2017.06.001.
- Mondal P.K., Furbacher P.D., Cui Z., Krol M.M., Sleep B.E. Transport of polymer stabilized nano-scale zero-valent iron in porous media. *Journal of Contaminant Hydrology*2017;URL: <http://www.sciencedirect.com/science/article/pii/S016977221730102X>. doi:10.1016/j.jconhyd.2017.11.004.
- Montague J.A., Pinder G.F., Gonyea J.V., Hipko S., Watts R. Visualization and simulation of density driven convection in porous media using magnetic resonance imaging. *Journal of Contaminant Hydrology*2017;URL: <http://www.sciencedirect.com/science/article/pii/S0169772217300426>. doi:10.1016/j.jconhyd.2017.07.005.
- Muljadi B.P., Bijeljic B., Blunt M.J., Colbourne A., Sederman A.J., Mantle M.D., Gladden L.F. Modelling and upscaling of transport in carbonates during dissolution: Validation and calibration with NMR experiments. *Journal of Contaminant Hydrology*2017;URL: <http://www.sciencedirect.com/science/article/pii/S0169772217300980>. doi:10.1016/j.jconhyd.2017.08.008.
- Pierce A.A., Chapman S.W., Zimmerman L.K., Hurley J.C., Aravena R., Cherry J.A., Parker B.L. DFN-M field characterization of sandstone for a process-based site conceptual model and numerical simulations of TCE

transport with degradation. Journal of Contaminant Hydrology2018;URL: <http://www.sciencedirect.com/science/article/pii/S0169772217301109>. doi:10.1016/j.jconhyd.2018.03.001.

Verma R., Icardi M., Prodanovi M. Effect of wettability on two-phase quasi-static displacement: Validation of two pore scale modeling approaches. Journal of Contaminant Hydrology2018;URL: <http://linkinghub.elsevier.com/retrieve/pii/S0169772217300992>. doi:10.1016/j.jconhyd.2018.01.002.

Vesselinov V.V., Alexandrov B.S., OMalley D. Contaminant source identification using semi-supervised machine learning. Journal of Contaminant Hydrology2017;URL: <http://www.sciencedirect.com/science/article/pii/S0169772217301201>. doi:10.1016/j.jconhyd.2017.11.002.

Zheng Y., Shikhov I., Gbayan L.K., Arns J.Y., Arns C.H. About the connectivity of dual-scale media based on micro-structure based regional analysis of NMR flow propagators. Journal of Contaminant Hydrology2017;URL: <http://www.sciencedirect.com/science/article/pii/S0169772217301080>. doi:10.1016/j.jconhyd.2017.11.001.