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Didier Lasseux, Francisco J Valdés-Parada, Brian D Wood

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Editorial

Editorial: Recent developments in upscaling and characterization of flow and transport in porous media

1. Introduction

Over the past few years, developments in the theory and numerical simulation of transport phenomena in porous media, along with related experimental measurements, have advanced significantly. New technologies are responsible for the development of methods for measuring properties at unprecedented resolution within a porous material; this has also motivated the formulation of new upscaling techniques. These improvements have occurred across a range of scales of interest. Furthermore, the recent advent of machine learning methods applied to characterization and modeling seems to open another area of research that promises to have impact. This was the motivation for the edition of this special issue of *Advances in Water Resources* with focus on upscaling and characterization of flow and mass transport in porous media systems across several levels of scale. Another motivation for making this special issue came from a Workshop held at the University of Bordeaux during spring of 2019 dedicated to Michel Quintard. Many of the papers presented here deal with subjects related with his scientific contributions. As a matter of fact, some works explicitly acknowledge his scientific career.

The issue consists of 42 scientific papers spanning over a wide variety of applications and produced by many of the leading scientists in the field. The present editorial provides an overview of the contributions contained in this issue. It is organized in nine sections that summarize the different topics covered by all the articles published in this special issue.

2. Recent progress in upscaling transport phenomena in porous media

Several works were presented that use the homogenization approach in order to derive the corresponding upscaled model, departing from the governing equations at the pore-scale. [Iliev et al. \(2020\)](#) employed a two-step, double-scale homogenization method to provide macroscale models of diffusion-advection with adsorption typically encountered in filtration processes. The focus was laid upon situations for which adsorption strongly dominates diffusive/convective transfer, implying the development of eigenvalue ancillary problems in the course of upscaling. The first homogenization step, yielded a macroscopic model operating at the scale of the washcoat grains (nanoporous materials) embedded in an inert matrix. The second step resulted in a model at the scale of the filter element. The predictive capabilities of the upscaled models were assessed through comparisons with direct numerical simulations.

[Le et al. \(2020\)](#) studied the flow and transport problem of CO₂-enhanced coalbed methane recovery also by means of the homogenization technique. They considered a multiscale model that incorporated two levels of porosity that correspond to nanopores and the cleat network. This work includes a set of numerical simulations showing that the cleat permeability decreases significantly near the injection well because of the high injection pressure. In addition, [Sharmin et al. \(2020\)](#) considered two-phase (or unsaturated) incompressible flow in a thin, but long, single pore (a thin strip) with a stratified distribution of the two phases and derived an effective model starting from the Navier-Stokes equations. The upscaled model was obtained using the asymptotic homogenization method. It encompasses different regimes associated to the values of the capillary number and viscosity ratio. It also accounts for surface tension variations (Marangoni effects) which may result from the transport of a solute in one of the two phases. The upscaled model was compared to direct numerical simulations of the 2D pore-scale model. Finally, [Airiau and Bottaro \(2020\)](#) used the adjoint homogenization method to shed new light on the derivation of upscaled models for steady and creeping flow of a shear-thinning fluid in homogeneous porous media. These authors derived a Darcy-like model, where the components of the effective permeability tensor were obtained from the solution of an associated boundary-value problem in a periodic unit cell. Due to the dependence of the viscosity on the pore-scale flow, a coupled solution approach was used that translated into a strong anisotropy of the permeability tensor, even in isotropic geometries.

Not all the works corresponding to this research topic used the homogenization method to carry out their analysis. For example, [Cotta et al. \(2020\)](#) studied flow and transport in fractured porous media using the generalized integral transform technique to derive analytical and numerical-analytical solutions. A salient feature of this work is the treatment of multiporosity cases, by means of a single integral transformation process. This approach is illustrated with two examples in fractured media and unsaturated soils. In addition, [Angot et al. \(2020\)](#) used an asymptotic analysis to study single-phase inertial flow in the fluid-porous boundary. They show that the total inertial work exerted by the fluid over the solid is always positive.

3. Non-equilibrium modeling for transport in homogeneous and heterogeneous porous media

This research subject comprises stochastic modeling and upscaling of transport processes. [Engdahl and Bolster \(2020\)](#) proposed to use a

newly developed multi-domain spatial Markov model to study three-dimensional, heterogeneous and variably-saturated porous media in the catchment zone. They found that this new modeling approach improves the mass transport predictions with respect to a single-domain approach. [Gouze et al. \(2020\)](#) carried out Lagrangian upscaling of mass transport in dual porous media consisting of mobile and immobile domains. These authors proposed to separate the advective and diffusive transport processes taking place in each domain. They found good agreement in reproducing two-dimensional time-dependent random walk simulations but the same success was not achieved in three-dimensional structures. On a similar subject, [Sherman et al. \(2020\)](#) studied reactive dispersion within a non-homogeneous, non-periodic porous material. To handle these features, an extended version of the spatial random walk models was proposed using Bernoulli CTRW. The macroscopic model, which is parametrized from subsequent statistics extracted from pore-scale simulations, correctly portrayed the dynamics of the solute plume. This opens a way of including the spatial heterogeneity of Lagrangian statistics in real heterogeneous systems. [Tartakovsky and Barajas-Solano \(2020\)](#) proposed an Eulerian stochastic advection diffusion reaction macroscopic model, in which mechanical and diffusive mixing are conceptually considered as two separate mechanisms, the latter being only responsible for the mixing-controlled reaction. This resulted in an effective dispersion coefficient that is the sum of mechanical dispersion and effective diffusion coefficients. The macroscopic model was successfully compared to experimental results reported in the literature.

[Massoudieh and Dentz \(2020\)](#) followed a more particular approach and proposed to use an integro-differential equation to upscale multi-species and nonlinear reactive transport in heterogeneous porous media. This non-local equation allowed to predict breakthrough curves away from the source on the basis of ergodic cross-sectional velocity distributions and the velocity correlation using a Copula function. The results were validated by comparison with direct numerical simulations. In a similar trend of ideas, [Puyguiraud et al. \(2020\)](#) investigated reactive mixing between two solutes transported in a (2D) porous medium using the concept of dispersive lamella, *i.e.*, an effective dispersion coefficient that is approximated by the average spatial variance of the solute distribution (assumed to be Gaussian) evolving from a point-like injection. On this basis, the macroscopic spatio-temporal evolution of the reaction product concentration was found to be well-captured as shown by comparison with direct numerical simulations of the pore-scale problem.

4. Field-scale modeling of flow and transport in porous media

This topic was covered by two works. In the first one, [Murad et al. \(2020\)](#) developed a three-scale model for one-phase flow in systems embedding a matrix, conduits and enlarged fractures, as in karstified formations. Starting from the classical compressible version of Darcy's law at the finest scale, a model reduction was applied yielding a 3D (matrix), 2D (fracture) 1D (conduit) coupled system. This model could finally be upscaled once employed on a grid discretizing a field-scale domain. This yielded the concept of karst-index, similar to that of well-index employed for flow around wells. The second paper is the one from [Koohbor et al. \(2020\)](#), who focused more on simulations and proposed an efficient hybrid numerical scheme that combines finite differences for space discretization and the method of lines for temporal integration to perform the solution of Richards equations in discretely fractured porous media. In order to improve robustness and efficiency of the numerical schemes, these authors proposed to include mass lumping. This solution scheme was applied to study water infiltration in fractured soils and it was validated by comparison with standard numerical techniques.

5. Current methods for computing effective parameters in porous media

A considerable of attention was brought to this topic. In a quite general framework, [Torquato \(2020\)](#) reported on methods to determine transport coefficients, namely, formation factor, mean survival time, NMR longitudinal relaxation time and principal viscous relaxation time, as well as intrinsic permeability, for hyperuniform and nonhyperuniform structures. Accent was laid upon the relationships between the microstructure and the coefficients. Questions on how data can be consistently treated to determine effective properties were addressed by several authors. For instance, [Thovert and Mourzenko \(2020\)](#) analyzed the impact of boundary conditions in the computation of the effective coefficient related to a diffusive process in heterogeneous porous media. With this analysis, means to assess the level of confidence associated with the prediction of this coefficient were obtained. Criteria to anticipate the risk of serious artifacts were devised as well as ways to limit them. In addition, [Azizmohammadi and Sedaghat \(2020\)](#) proposed a sampling method to determine the representative elementary volume (REV) size in fractured rock environments. These authors determined the values of the components of the permeability tensor and analyzed its anisotropy using multiscale random sampling and upscaling, considering the fluid stress orientation and the fracture roughness. Due to the non-homogeneous nature of the fractures geometry, the permeability tensor was position-dependent and the degree of anisotropy of this tensor changed with the REV size, as expected.

A special focus was laid by [Ling and Battiato \(2020\)](#) upon the determination of the permeability tensor resulting from the upscaling of one-phase steady incompressible Stokes equations. They proposed a computational algorithm, called τ -SIMPLE, that allows computing this quantity from the solution of the associated closure problem present in the homogenization approach. The idea in their algorithm is to introduce an artificial time scale to satisfy the global constraint in the SIMPLE iteration and it was applied to predict permeability in two- and three-dimensional geometries. As an extension out of the creeping flow regime, [Aguilar-Madera et al. \(2020\)](#) carried out the solution of the closure problems associated to inertial flow in homogeneous porous media that lead to the prediction of the intrinsic permeability and Forchheimer tensors using digital images from real systems. The latter was found to exhibit a dependence on the average velocity with an exponent ranging from 1.7 to 4.2 depending on the topology and it was verified to be anisotropic not only in terms of the geometry but also in terms of the flow paths.

Many other works addressed the determination of the effective permeability (or hydraulic conductivity) at large scales, for heterogeneous media. For instance, [Bellin et al. \(2020\)](#) adopted a stochastic approach to identify parameters and compute the effective conductivity from measured values of the hydraulic head for the case of steady flow from a source. These authors found that the ratio of the equivalent conductivity with respect to the geometric mean corresponds to an harmonic mean near the source. They derived the head variance and the autocorrelation between the head near the source and at arbitrary distances. In the work by [Colecchio et al. \(2020\)](#), scale-independent analytical results for the variance of the effective hydraulic conductivity were obtained by means of an energy dissipation formulation. The analysis was performed under steady conditions considering two-dimensional domains for lognormal and binary media, considering an ample range of coarsening scales and heterogeneities. Convergence was found to be slower in the binary case than in the lognormal system. With a similar purpose in mind, [Mourlanette et al. \(2020\)](#) developed a method to estimate the effective permeability of a geological heterogeneous formation employing a non-structured grid. The power averaging technique was employed in which the permeability was mapped onto the unstructured mesh and further averaged with a power exponent field calibrated from numerical upscaling experiments. The method, which allows very significant

computational speed-up, was consistently compared with a refined conventional approach.

An extension to two-phase flow was considered by Soraganvi et al. (2020). They investigated the prediction of large-scale effective unsaturated conductivity in heterogeneous isotropic or anisotropic porous media. The effective coefficients obtained from numerical simulations on random heterogeneous samples were compared to predictions from stochastic spectral perturbation theory, geometric and harmonic means, and to a probabilistic semi-empirical power average model. The latter was shown to provide satisfactory estimates of the principal components of the unsaturated effective conductivity. The macro dispersion was further analyzed in terms of the effective coefficient and spreading lengths using numerical simulations.

6. Advanced methods for imaging, segmenting, and characterizing complex porous media

This topic was illustrated by the work of Tinet et al. (2020) who addressed the reconstruction of the pore-space of nanoporous materials (clays). They used two variants of the directional aggregation multiple-point statistics method from 2D images that could be obtained from FIB-SEM or TEM imaging. The choice of the method was found to be conditioned by the available data. It was shown that the reconstruction consistently provides the means to determine the intrinsic permeability, the effective diffusion and longitudinal dispersion coefficients, a key parameter being the distance between two successive 2D images in the reconstruction process.

7. Coupled phenomena and multiphase flow in porous media

Many research works were reported in this special issue that contributed to shed light on various aspects related to these topics. A new upscaling approach, called LMDTM and applied to MHD flow in a non-Darcian medium between parallel plates subject to Hall current, was proposed by Ewis (2020). The accuracy of the results was tested by comparisons with finite-differences solutions. The novelty of this approach relies on the fact that solution multiplicity and linearization is avoided. Sweijen et al. (2020) investigated the coupled unsaturated flow and deformation of a packed bed of swelling particles using pore-scale simulations of liquid invasion inside the grains. It was shown that the swelling coefficient is a key parameter in the swelling and particles rearrangement that are otherwise controlled by the time scales of unsaturated flow and absorption.

Dissolution mechanisms during saturated or unsaturated flow were investigated at the pore-scale by Esteves et al. (2020) who studied reactive transport by means of pore-network modeling taking into account changes in porosity and permeability due to calcite dissolution reactions at the mineral surface. Still at the pore-scale, Etancelin et al. (2020) studied dissolution and diffusive transport processes by coupling a Lagrangian formulation with the superficial velocity used in the volume averaging method. This approach takes advantage of the quality of particle tracking for transport, the quality of particle distributions from remeshing and the computation of diffusion by adaptation of the remeshing kernel. At the Darcy scale, Meng et al. (2020) investigated 2D density-driven flow with dissolution in porous media, combining a linear stability analysis at the Darcy scale and lattice Boltzmann simulations at the pore-scale. Distinct behaviors were observed that are governed by the interplay between the density contrast between the fluids, the chemical reaction rate and the porosity and permeability evolution due to dissolution.

Two-phase flow is another problem that was extensively addressed in this special issue. Alamooti et al. (2020) performed pore-scale numerical simulations of two-phase flow in different pore-trapping situ-

ations in order to analyze the recirculation in the trapped phase for several displacement scenarios, fluids configurations and dynamic parameters. The contrast between drainage and imbibition mechanisms was highlighted. A new computational method that couples graphical processing units for the lattice Boltzmann method with an up-scaling technique was developed by An et al. (2020). This approach was applied to study two-phase flow at a scale-level of centimeters in three applications involving a sandstone sample. This type of volumetric lattice-Boltzmann technique lead to accurate predictions at a lower computational cost than performing routine lattice-Boltzmann simulations.

With the aim of providing a description of two-phase flow at the Darcy scale, Schreyer and Hilliard (2021) proposed a macroscopic model using the hybrid mixture theory. The model reveals to be compliant with the existing two-phase Cahn-Hilliard equation, the Korteweg stress tensor, Darcy's law and a generalized form of Richards equation. In addition, macroscopic interfaces could be captured by the model. Considering stratified heterogeneous media, Ghosh et al. (2020) studied two-phase flow in a porous column with varying porosity and permeability in a periodic manner. The resulting flow equations were derived using the homogenization technique and the model predictions were validated by direct numerical simulations at the pore-scale finding good agreement. In addition, Cheng and Rabinovich (2020) carried out the upscaling process of capillary pressure curves for situations associated to two-phase flow driven by gravity and capillary forces. These authors proposed an upscaling method that relies on optimization, which yielded Brooks and Corey functions that reproduced microscale results, albeit at a considerable computational cost. Kassa et al. (2020) derived a dynamic capillary-pressure model for two-phase flow in porous media that takes into account temporal variations in wettability by adding a time-dependent term to the standard capillary pressure function. In this way, the relevance of unsteady wettability for determining the capillary pressure over time scales, that range from months to years, was evidenced. Heterogeneous low-permeability matrix-fracture systems were considered by Wang et al. (2020), who provided a methodology to estimate the fracture-matrix two-phase flux assuming negligible capillary effects in the fracture and using a steady-flow approximation. Comparison with reference solutions proved good agreement, validating the approach.

Finally, a study dedicated to three-phase flow at the Darcy scale was reported by Schäfer et al. (2020). They analyzed relative permeabilities using the total differential model and the mechanistic model, both recently reported in the literature, to further carry out comparisons with experimental data. The latter model was found to better predict the mobilities and relative permeabilities, to the cost, however, of requiring some preliminary calibration.

8. Multiscale experimental analysis in porous media

Two studies of flow in tight connection with experimental measurements were reported. In the work by Omirbekov et al. (2020), foam flow experiments were performed in porous media and a simplified upscaled model was employed to predict the seepage velocity to pressure gradient relationship. Poor agreement was achieved and this was explained by the compressibility of the foam at high pressure and trapping effects at low capillary numbers. In addition, an experimental study of thermal effects on capillary pressure and relative permeability curves during quasi-steady and dynamic two-phase drainage/imbibition processes was reported by Philippe et al. (2020). While barely no effects were observed in the former case, relative permeabilities increase and residual saturation decrease were noticed while increasing the temperature under dynamic conditions. This suggests the importance of flow rate in conjunction to temperature effects for the recovery of heavy DNAPL, for instance.

9. The use of machine learning and neural networks in representations for parameterization in upscaled models in porous media

This new methodology was addressed in the work by Zhou et al. (2020) who developed a convolutional neural network approach to correlate the hydraulic conductivity field and the longitudinal macro-dispersivity in heterogeneous porous media. Robustness of the deep learning technique was assessed in the case of moderate heterogeneity, showing the potential efficiency of the method to estimate macroscale dispersion from permeability fields.

10. Information theory as it applies to upscaling and upscaled representations in multiphase porous media

This topic was addressed by two papers. In the work by Dell'Oca et al. (2020), information theory was used to evaluate the information shared between the Darcy flux fields and those of the hydraulic conductivity. The latter was treated as a spatial random field. In this way, flow was evaluated over several realizations of hydraulic conductivity subject to uniform mean flow. These authors found consistent trends in the variation of the average information in relation to the lower scale size as well as in the manner of information sharing between pairs and triplets of the Darcy flux components. Finally, Wood and Taghizadeh (2020) reviewed key concepts of information theory and explored how they can be applied to define a representative volume and also to systematically reduce the amount of information in upscaling processes and applied them to several examples. Among the contributions made by the authors in this work, are the distinction between microscale and macroscale variables, and also between empirical and probabilistic entropy. In addition, they extended the notion of typical sequence by requiring that they are also typical in the probabilistic sense.

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Didier Lasseux*

I2M, UMR 5295, CNRS, Université Bordeaux, 351, Cours de la Libération, 33405 Talence CEDEX, France

Francisco J. Valdés-Parada

División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana-Iztapalapa, Av. San Rafael Atlixco 186, col. Vicentina, 09340, Mexico

Brian D. Wood

School of Chemical, Biological, and Environmental Engineering, Oregon State University, Corvallis, OR 97330, USA

*Corresponding author.

E-mail address: didier.lasseux@u-bordeaux.fr (D. Lasseux)

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