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Thin Porous Media

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Theoretical, numerical, and experimental research related to thin porous media is of great importance to various industries. Thin porous media definition here includes both geometrically thin porous layers, i.e., whose thickness is much smaller than in-plane dimensions, and physically thin porous layers, i.e., whose thickness is only around one order of magnitude larger than its mean pore size (Qin and Hassanizadeh 2015).

Hygiene products, filters, fuel cells, membranes, paper, textiles, biological materials, and manufacturing thin composite parts are some examples. In several of these applications, porous materials are used as very thin and highly porous layers, often as stack of thin layers creating interfaces, and are typically deformable and inhomogeneous both in their structure and in surface energy properties, hence difficult to characterize. Such characteristics present major challenges in experimental studies, theoretical modeling, and numerical simulations.

Some critical challenges are the validity of the established geosciences models based on Darcy's law, the consistent definition of the representative elementary volume, the characterization and modeling of the heterogeneities of these materials (both pore structure and surface chemistry) and of their interfaces, the definition of a pore scale model for thin porous media.

This special issue builds on the InterPore Industry Workshop on Thin Porous Media that was organized in Prague on May 13, 2014 as part of the 5th International Conference of the

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Interpore Society that brought together researchers from various disciplines interested in thin porous media.

The contributions included in this special issue span a wide range of aspects of thin porous media research, from experimental measurements of time-dependent imbibition or drainage to measurements of effective diffusion coefficients and of water amount in thin media such as paper materials; from modeling of drainage in single-layer or dual-layer structures to estimating permeability of thin porous media and modeling transport and separation of carbon dioxide–alkane mixtures in carbon molecular sieve membranes at molecular scale; from the liquid molding process for making polymer composites to predicting water saturation in the gas diffusion layer of fuel cells; from modeling the gas evacuation process underneath a moving resin film in a prepeg for making polymer composites to solving the flow and deformation problems in thin poroelastic plate. Although it should be clear that all aspects of thin porous media could not be addressed, the contributions in this special issue provide interesting progress across several areas. At the same time, some other aspects still remain open problems for the research in this field. Among others, these include the characterization and modeling of the heterogeneities of these thin porous media, the definition of two-phase flow pore scale models capable of describing the structural and surface energy complexity of the thin porous media, and the definition of upscaling methods to effectively describe the thin porous media in the continuum scale.

In the following, we briefly describe the scope of each contribution.

Rashapov and Gostick measured experimentally the in-plane effective diffusion coefficients in GDL (gas diffusion layers) as a function of compression and hydrophobic polymer loading, using a convenient method based on the transient diffusion of oxygen from air into an initially nitrogen purged porous sample. As expected, the effective diffusivity decreased with higher compressions and higher polymer loadings. Interestingly, when plotted against compressed porosity, the effective diffusivity of untreated and treated materials for a given type of sample collapsed on top of each other, despite the simultaneous impact of PTFE loading and compression. A percolation model was fitted through one of the tested materials, and a reasonable agreement was observed for lower compression, but a fit to the entire data could not be achieved. Within the tested compression range, a clear percolation threshold was not observed, this being attributed to the damage of fiber structure and introduction of cracks at increased compressions. This confirms the general inability of theoretical tortuosity models to describe GDLs.

Continuing with on the topic of GDL, Medici and Allen modeled, with a two-dimensional pore network model, water injection experiments in hydrophobic GDL in a Hele-Shaw style test. Interestingly, the material properties of the pore network realizations, i.e., pore size distribution, contact angle, and thickness, were based on independent measurements of the porous materials tested. The pore length was the only tuned parameter, the same pore length for a given material led to excellent agreement between experiments and simulations within the tested Ca range. In view of the stochastic nature of thin porous media structure, a new scaling of the dissipated energy during percolation in thin porous media in a time-dependent manner was used to compare the numerical simulations against the experiments. Specifically, the use of the wetted area in these percolation experiments was possible as there is no significant difference in the water distribution profile along through the thickness of such thin GDL materials.

Belgacem et al. modeled liquid water injection into an hydrophobic thin porous medium formed by the assembly of a fine layer and a coarse layer, inspired from a situation considered in relation to the water management problem in polymer electrolyte membrane fuel cell (PEMFC). They used a pore network model and a variant of the invasion percolation (IP) algorithm, which allows multiple independent injection points and the coalescence between liquid paths originating from different liquid injection points. The computational challenge of dealing with the very large network of the fine layer was approached with extrapolation methods based on data available on smaller networks. This interesting approach requires future validation with extensive pore network simulations on larger networks. While in this work a simple sharp interface was assumed between the two layers, the authors interestingly suggest to further consider in future the role of such interface if treated as a transition region of a certain thickness having specific properties.

Lundstrom et al. studied the stationary incompressible fluid flow in a thin periodic porous medium which are similar to the well-known Hele-Shaw flows. The authors employed the homogenization method and asymptotic analysis to present an in-depth theoretical/mathematical treatment of this particular flow example. The medium under consideration is a bounded perforated 3D domain confined between two parallel plates. The distance between the plates is delta, and the perforation consists of epsilon-periodically distributed solid cylinders which connect the plates in the perpendicular direction. Both parameters (delta and epsilon) are assumed to be small in comparison with the planar dimensions of the plates. By constructing asymptotic expansions, three cases are analyzed: delta $\ll$ epsilon, delta proportional to epsilon, and delta $\gg$ epsilon. For each case, a permeability tensor is obtained by solving local problems. In the intermediate case, the cell problem is 3D, whereas they are 2D in the other cases, which is a considerable simplification. The dimensional reduction can be used for a wide range of epsilon and delta with maintained accuracy. This is illustrated by some numerical examples.

Firouzi and Sahimi studied transport and separation of carbon dioxide–alkane mixtures in carbon molecular sieve membranes (CMSM) under sub- and supercritical conditions. Non-equilibrium molecular dynamics (NEMD) simulations were performed; pressure gradient across membranes was imposed through a dual control volume system. N-alkanes were generated and inserted into the control volume system using configurational biased Monte Carlo method. The membranes were produced using a 3D molecular pore network (MPN) model based on the Voronoy tessellation, producing pores of irregular shapes and sizes. Authors reported two main findings: optimal pressure drop for separation of mixtures of CO_2 and n-alkanes under supercritical conditions, and increased separation efficiency as the size of the alkane increased.

To address challenges associated with characterization and multiphase flow simulations in highly porous thin materials, Riasi et al. developed the pore topology method (PTM), a fast, algorithmically simple method that reduces the complexity of the 3D void space geometry to its topologically equivalent medial surface, and used it as a solution domain for single- and multi-phase flow simulations. The authors showed that PTM produces a voxel-wide, fully connected surface that preserves the topology of the void space, and is as close as possible to the center of the void space in all directions. The use of the medial surface as a solution domain was demonstrated for permeability calculations and quasi-static drainage and imbibition simulations for porous media samples ranging from 25 to 95% porosity. Agreement of results with analytical solutions and direct numerical simulations is encouraging, and future work will focus on increasing the reconstructive power of medial surfaces.

Processing of composite materials typically involves wetting of thin fabrics made from reinforcing fibers, such as glass, with a resin injected from a side. Use of prepegs is an important technique to make thin parts out of polymer composites. Cender et al. present a novel method to model the evacuation of gas trapped underneath a moving resin film while the prepeg placed in a bag is compressed within an autoclave. The pulse-decay method was employed to model suction of gas underneath a moving resin film in a porous fabric. Dimensionless analysis showed how the initial pressure, boundary conditions (vacuum pressure at $x = 0$ and with or without a reservoir volume at $x = L$), and the Klinkenberg parameter affected the predicted decay of gas pressure. By comparing the experimental data to a set of dimensionless master curves, the intrinsic permeability, Klinkenberg parameter, and porosity were determined. Resin saturation was inferred by monitoring the area of resin saturating the initially dry side of the fabric. By mapping the gas flow parameters to the observed area fraction of resin, a complete and repeatable characterization method was demonstrated.

Poroelasticity deals with a class of problems involving a fluid flowing within a porous medium where the fluid flow and solid deformation interact with each other. Iliev et al. study the numerical solution of boundary value problems found in thin poroelastic plates. They consider the biharmonic equation for vertical displacement and non-stationary equation for pressure in the porous medium. The computational algorithm is based on the finite element approximation in longitudinal coordinates and the finite difference approximation in time. The standard stability conditions for two-level schemes with weights are formulated. The computational implementation of such schemes is based on solving a system of coupled equations: fourth-order elliptic equation for displacement and second-order elliptic equation for pressure. Unconditionally stable splitting schemes are constructed with respect to physical processes, when the transition to a new time level is associated with solving separate problems for the desired displacement and pressure.

The issue concludes with two review articles. Michaud presented a review of the modeling strategies adopted by the polymer composites processing community while studying and predicting multi-phase flows in LCM (liquid composite molding) molds. The literature essentially ranged along two distinct modeling approaches. One was treating the flow as a standard two-phase (resin–air) flow with graded saturation during flow while using the usual saturation-dependent parameters such as relative permeability and capillary pressure. The other approach was that of treating the flow as a saturated flow, with a sharp-front dividing the resin wet and dry region of the fiber preform. In this, the gradual saturation behind the front was modeled using a sink term in the continuity equation, accounting for the delayed impregnation of fiber bundles of the fiber preforms. The author concluded that though both of these approaches have their merits and drawbacks, a significant amount of progress has been made toward having a complete understanding of the mold-filling process.

Finally, Tomozeiu reviewed spectroscopic methods for studies of water-based ink–substrate interactions. Optical techniques, such as VIS reflectometry, IR-ATR, and spectroellipsometry, are compared to electrical impedance spectroscopy (EIS) and analyzed in terms of their applications, performance metrics, and limitations. The review is inspired by applications arising in printing industry and offers detailed descriptions of equipment, measurement specifics, and result interpretation specific to these techniques.

The special issue provides a snapshot of the range of issues and contemporary understanding of thin porous media, and issues shared among different scientific and engineering fields. We thank both the contributing authors and the reviewers for their professional and constructive efforts to improving the quality of the contributions. We are also grateful for professional and timely assistance of the Editorial office of Transport in Porous Media.

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