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Pore network modelling of single phase flow in functionalized porous materials: permeability prediction and validation

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Capillarity driven lab-on-chips (LOC) are small cheap devices dedicated to perform diagnostics autonomously. To operate the chips, fluids flow in functionalized porous channels. Performance of the LOC however depends on the microporous fluid flow characteristics of the device. Pore-network (PN) models are a powerful tool to investigate transport phenomena at the pore scale while avoiding expensive and time consuming computational fluid dynamics (CFD) direct simulations. High resolution imaging techniques allow topologically representative PNs to be extracted on which fluid flow can be simulated. In this work, 1 µm resolution X-Ray computed tomography (CT) scans were executed on functionalized porous matrixes of poly-methyl methacrylate (PMMA). The reconstructed images were binarized to isolate the pore space. A watershed algorithm was applied to obtain divided pores as a basis for the material PN. The PN was composed by nodes representing the pores interconnected by channels with simplified geometry, representing the pores throats. Two different channels geometries were considered: cylindrical channels with the diameter computed as the average between pore and pore throat equivalent diameters, and bi-conical shaped channels. The latter were represented as stacks of 1 pixel thick cylinders with diameter varying smoothly from the pore to the pore throat.

The obtained PNs were employed to simulate single phase flow and compute the material permeability by means of the Darcy's law and verified by measured values and CFD simulations. The effect of different parameters on the obtained permeability was investigated. In particular, the study focused on the number of seeds used for the watershed algorithm, the channel geometry as well as the pore shape, that was taken into account through the sphericity parameter.

A higher number of watershed seeds led to a more accurate solution, since a more precise pores space subdivision is generated, but to longer computational times as well. Cylindrical channels were found to produce permeability values around 250% higher than the bi-conical ones at the same number of seeds. As a result when cylindrical channels were used, a permeability value comparable to both the CFD and experimental ones was obtained with a number of seeds about five time higher with respect to bi-conical channels. Eventually, considering pore sphericity was proved to reduce permeability dependency on both the number of seeds and the channels geometry. When bi-conical channels were used and pore sphericity was taken into account, permeability values comparable to the CFD and experimental results were obtained with a number of seeds eight times smaller, than when cylindrical channels with no sphericity corrections were employed. This corresponded to a reduction of computational time of about 60%. The developed PN model, therefore, allows material permeability to be computed with good accuracy in significantly shorter time with respect not only to direct CFD, but also to other PN models (shape). In a next step, the main focus will be on the application of the extracted PN to study multi-phase capillary flow.

References

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