

Summary

In chemical engineering, the study of the fluid flow in porous media is of paramount importance. This is the case for instance for packed bed reactors, where the fluid regime and its distribution and interaction with the porous structure influences the yield of the end products. Nevertheless, the mathematical modeling of systems involving porous media remains a challenging task. The nature of porous media is inherently multiscale, a great variety of flow regimes are witnessed as the operating conditions change and, in many applications, more than one fluid phase is involved.

In this work, novel numerical and data-driven methodologies are proposed with the objective to improve the accuracy, extend the range of validity and decrease the computational cost of existing models that describe two-phase flow in porous media. The work is articulated in three parts.

In the *first part*, a data-driven multiscale model for two-phase flow in porous media is developed. The multiscale model consists of one model for the macro-scale and one for the micro-scale. Two-phase Darcy's law is employed to describe the macroscale. This model is derived through an averaging procedure of Navier-Stokes equations and presents some terms that need closure, the relative permeabilities. We propose a multiscale coupling where the values of the closure terms are first computed from microscale high-fidelity simulations and next are surrogated to macroscale equations at run-time through a data-driven model. With our approach, closure terms depend on the local flow regime, leading to non-linearities in Darcy's law. This, gives a more general form to the model and the possibility to reproduce situations deviating from the operating conditions for which the original equations were derived. The multiscale model is tested on 2D and 3D simplified geometries representing a packed bed.

Given the simplicity of two-phase Darcy's law, in the *second part* of the thesis a richer model to describe the macroscale is introduced; the Baer-Nunziato type model of Abgrall and Saurel. This is an Eulerian-Eulerian model and describes compressible multiphase flows. Also, this model is derived through an averaging procedure and presents coupling terms that represent the interaction between the phases. The choice of a compressible formulation is driven by applications in chemical engineering where chemical reactions provoke volume variations in the fluids involved. To account for these effects, compressible solvers must be used. However, the same workflow proposed for two-phase Darcy's law cannot be readily applied to the model of Abgrall and Saurel. Indeed, the model of Abgrall and Saurel presents stiff terms in the low-Mach regime, which is relevant for the simulation of packed beds. To alleviate this problem, we propose an all-Mach method to solve model equations efficiently.

The all-Mach scheme is based on the implicit-explicit Runge-Kutta (IMEX-RK) time integration scheme. With this scheme stiff terms are solved implicitly and non-stiff terms are solved explicitly. In this manner, the material waves are still solved accurately. Moreover, a well-balanced discretization of the non-conservative terms present in the model is introduced to preserve the equilibria states of the continuous hyperbolic system of balance laws also on a discrete level. Finally, to improve the performance of the code, an elliptic equation for the pressure is derived to replace the implicit step.

The numerical scheme is validated against several benchmark tests at high and low Mach regime giving satisfactory results. As a final task for the model of Abgrall and Saurel, a proof of the asymptotic-preserving (AP) property of the numerical scheme is proposed.

The first two parts of the thesis focus on enabling the simulation of systems with two-phase flow in porous media. Nonetheless, simulating full systems represents the first step for a proper understanding of a technology. Indeed, it is often of interest to explore the changes in the systems as the operating conditions deviate from the standard configuration. This can be done through studies where, after a proper parametrization of the problem, we repeat the simulations varying the parameters values within the ranges

of interest. In this framework, the interest is to obtain the solution of model equations on a fine grid at a low computational cost.

In the *third part* of the thesis, is proposed a super-resolution (upscaling) method based on Convolutional Neural Networks (CNNs) and tailored to applications in fluid dynamics.

The proposed procedure is succinctly sketched as follows. First, some pairs of high- and low-fidelity simulations are performed on a fine and a coarse grids for a small number of points in the parameters space. Next, the CNN is trained using a supervised loss to map the CFD solution obtained on the coarse grid (model input) to the solutions on the fine grid (model output). The advantage of this approach is evident in many-query CFD problems such as in optimization, optimal control or uncertainty quantification. In fact, after the cost to train the model and of a few simulations on a fine grid is paid once, this approach allows to obtain as many solutions of the high-fidelity flow field at the cost of the same simulations carried out on the low-fidelity grid. Moreover, residual and transfer learning are employed to make the deep architectures computationally less costly to train. Finally, the trained architectures are tested on confined flows and on flow in porous media.