Doctoral Dissertation - Summary

Ph.D. Program in Chemical Engineering – XXXV Cycle

Deep neural networks as data-driven models for flow and transport in porous media

Porous media systems are relevant in many research fields of chemical engineering: packed bed catalytic reactors, filters, subsurface applications like carbon capture and storage, and batteries. The microscale modelling, i.e. pore-scale, of a representative volume of the porous structure is a state-of-the-art methodology to obtain the accurate evaluation of transport related properties, such as reaction rates or filtration efficiencies. Computational fluid dynamics (CFD) has been widely employed to this end. Nevertheless, these microscale simulations are computationally expensive, in fact, high performance computing (HPC) systems and long computation times are usually required to numerically solve the transport equations. Thus, these models can hardly be integrated in multiscale modelling, or optimization workflows, where fast response models are needed. Machine learning, and in particular deep learning techniques, can be employed to train data-driven models as surrogates of CFD simulations. Starting from a CFD based dataset, neural networks can be trained to obtain accurate predictions of the quantities of interest, resulting in a fast surrogate model to employ in the above-mentioned examples.

This methodological dissertation is a benchmark for the use of neural networks as surrogate models for flow and transport in porous media. Two main applications have been studied: the filtration of colloids in packed beds, and the discharge of the cathode side of lithium-ion batteries. Even though these applications are governed by very different transport equations, both reactive problems were successfully modelled by neural networks, which is the main novelty of this work. In fact, main efforts of this kind of machine learning coupling in the literature are addressed to the prediction of the permeability of porous media, which is a geometry related factor, but fewer have tackled more complex problems of common interest in chemical engineering with machine learning techniques.

For the filtration case study two categories of data-driven models have been developed: networks for the prediction of integral properties, and networks for the prediction of local fields. The dataset for the training of those models has been created by the solution of the transport equation on bi-dimensional and three-dimensional sphere packings by means of a finite volume method. In the first case, simple fully connected neural networks have been trained for the prediction of both the permeability and the filtration rate starting from hand selected geometrical parameters, and operating conditions. Another approach implemented for the prediction of the same objectives is the use of convolutional neural networks (CNN), which are appropriate models for porous media applications since they allow images of the porous structure as inputs, in this way the choice of most relevant geometrical features is performed by the network itself. Instead, multiscale convolutional neural networks have been employed for the prediction of local concentration fields in porous media. In this case the dimensionality of the model is not reduced, resulting in a

complete surrogation of the CFD simulations, thus the trained model gains interpretability compared to the previous ones.

The lithium-ion batteries case study allowed us to face a transient problem: in order to do that, the time-dependent discharge of the cathode side of a lithium-ion battery has been modelled by a modified multiscale neural network. For this application, an autoregressive approach has been conceived and an appropriate training strategy has been tailored in order to obtain accurate fields of concentration and potential in the solid phase of the electrodes, both of which exhibit an evolution in time during the discharge process. This method turned out to be a reliable and accurate surrogate model for the prediction of discharge curves, also on new cathodes geometries not originally investigated with the physics-based CFD model.

This dissertation proves the feasibility of training robust neural networks models for different applications of flow and reactive transport in porous media. The guidelines presented in this work are meant to be employed to build accurate surrogate models for multiscale models and optimization workflows not only for porous media as proven here, but in general for complex reactive and transport systems of interest for chemical and process engineering.