CHEMICAL ENGINEERING

DISAT - Multiphase flow and transport in porous media for environmental applications: CFD modelling, machine learning and experimental validation

Funded By	Dipartimento DISAT
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Context of the research activity	Porous media are omnipresent in chemical engineering. Packed-bed catalytic chemical reactors, filters, metallic and ceramic foams, aquifers are common examples. Very often multiphase flows are established in porous media, involving solid particles, liquid droplets or gas bubbles, carried by a continuous liquid phase. In this PhD project we aim at developing and validating (with experiments) an innovative modelling framework, based on CFD and machine learning, to describe these complex systems.
	The ambition of this project is to develop a computational model capable of describing multiphase flows in porous media for environmental applications [2]. The multiphase flow is constituted by solid particles (or liquid droplets or gas bubbles) carried by a continuous liquid phase, through the pores and voids, left by the stationary grains constituting the porous media. The computational model will be based on computational fluid dynamics (CFD) and population balances, and will start from our previous work on this topic [3]. These simulations are however computationally very demanding, and even resorting to high-performance computing (HPC) facilities, result in very long computational times. In order to be able to simulate very large geometries, representing for example a large portion of a porous medium or a laboratory scale column, where usually experiments are performed, a surrogate model, built with machine learning, must be developed [4-8]. The modelling activities start by building reliable digital replicas of the porous media [1] and will then focus on the developments needed to account for the multiphase flow nature of the flow and for the effects of particle aggregation, breakage, attachment and detachement, within the porous medium. The experimental data needed for validating the model will be produced thanks to the extisting collaboration with DIATI. [1] Agostini, E., Boccardo, G., Marchisio, D. An open-source workflow for open-cell foams modelling: Geometry generation and CFD simulations for momentum and mass transport (2022) Chemical Engineering Science, 255, art. no. 117583

Objectives	[2] Boccardo, G., Tosco, T., Fujisaki, A., Messina, F., Raoof, A., Aguilera, D.R., Crevacore, E., Marchisio, D.L., Sethi, R. A review of transport of nanoparticles in porous media: From pore- to macroscale using computational methods (2020) Nanomaterials for the Detection and Removal of Wastewater Pollutants, pp. 351-381. [3] Icardi, M., Pasquale, N.D., Crevacore, E., Marchisio, D., Babler, M.U. Population Balance Models for Particulate Flows in Porous Media: Breakage and Shear-Induced Events (2023) Transport in Porous Media, 146 (1-2), pp. 197-222. [4] Marcato, A., Boccardo, G., Marchisio, D. A computational workflow to study particle transport and filtration in porous media: Coupling CFD and deep learning (2021) Chemical Engineering Journal, 417, art. no. 128936 [5] Marcato, A., Boccardo, G., Marchisio, D. From Computational Fluid Dynamics to Structure Interpretation via Neural Networks: An Application to Flow and Transport in Porous Media (2022) Industrial and Engineering Chemistry Research, 61 (24), pp. 8530-8541. [6] Marcato, A., Santos, J.E., Liu, C., Boccardo, G., Marchisio, D., Franco, A.A. Modeling the 4D discharge of lithium-ion batteries with a multiscale time-dependent deep learning framework (2023) Energy Storage Materials, 63, art. no. 102927 [7] Marcato, A., Marchisio, D., Boccardo, G. Reconciling deep learning and first-principle modelling for the investigation of transport phenomena in chemical engineering (2023) Canadian Journal of Chemical Engineering, 101 (6), pp. 3013-3018. [8] Marcato, A., Santos, J.E., Boccardo, G., Viswanathan, H., Marchisio, D., Prodanovic, M. Prediction of local concentration fields in porous media with chemical reaction using a multi scale convolutional neural network (2023) Chemical Engineering Journal, 455, art. no. 140367

Skills and competencies for the development of the activity	The PhD candidate must be familiar with the theory of transport phenomena and computational fluid dynamics. The computational tools employed are openfoam, Yade and Blender, and libraries from keras, tensorflow pytorch. The PhD candidate must have basic programming skills in C++ and python.