Title: **Multiscale modelling of fluid flow and particle transport in porous media for engineering applications: from catalytic packed-bed chemical reactors to aquifers**

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Abstract: In this lecture the simulation of porous media, with particular attention to two specific applications, namely catalytic packed-bed chemical reactors and aquifers, will be discussed. Being the problem of fluid flow and and particle transport inherently multiscale in nature, a multiscale approach is used here. Packing of solid objects of increasing complexity (in two and three dimensional geometries) are created, in order to reproduce realistic porous media. Different strategies and tools are used and tested: from in-house random-placing codes to open-source computer graphics codes, implementing the well known bullet physics library (i.e. Blender). Once the geometries are defined, fluid flow is simulated by solving (at the pore-scale) the steady-state mass and momentum balance equations. This is done by using the finite-volume method, implemented in commercial (e.g. Fluent) and open-source (e.g. openFoam) computational fluid dynamics codes. This analysis includes both Newtonian and non-Newtonian fluids. Then particle (and solute) transport is simulated by solving the advection-diffusion equation (again at the pore-scale) in order to describe both particle hydrodynamic dispersion and deposition. Great emphasis is given to the various numerical issues involved in finite-volume discretization, that can generate large errors and undermine the quality of the final results. Simulation data are then treated with well-known macro-scale laws, as well as analyzed with homogenization theory, in order to derive better models to be used at the macro-scale. Our work has generated so-far the following important results: (1) guidelines for the usage of the finite-volume discretization when applied to complex geometries, such as those required in porous medium simulations (2) extension of the Darcy–Forchheimer Law to non-Newtonian fluids, (3) development of correlations for the "equivalent particle diameter" for packing of non-spherical particles,(4) new correlations for particle deposition in porous media, (5) confirmation of the validity of existing correlations for hydrodynamic dispersion (based on the Fickian diffusion hypothesis).

Future work includes the investigation of transport of polydisperse particles (characterized by a wide particle size distribution), as well as the investigation of particle-particle and particle-grain interactions.