

## MODELING AND DESIGNING DOUBLY POROUS MATERIALS : AN APPROACH BY HOMOGENIZATION

Hai-Bang LY<sup>1,2</sup>, Vincent MONCHIET<sup>1</sup> and Daniel GRANDE<sup>2</sup>

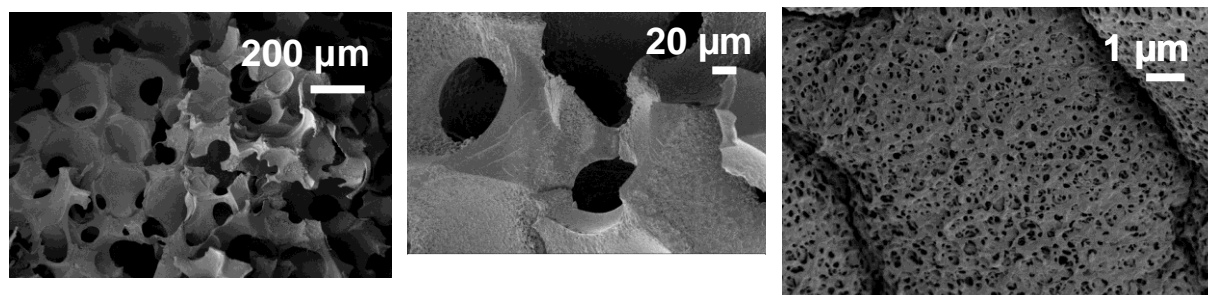
<sup>1</sup>Laboratoire de Modélisation et de Simulation Multi-Echelle, UMR 8208 CNRS-Université Paris-Est Marne-la-Vallée - 5, Boulevard Descartes, 77454, Marne-la-Vallée Cedex 2, France

<sup>2</sup>Institut de Chimie et des Matériaux Paris-Est, UMR 7182 CNRS - Université Paris-Est Créteil Val-de-Marne - 2, rue Henri Dunant, 94320 Thiais, France

**Key Words:** *Porous media, Permeability, Homogenization, Fast Fourier transform, Finite Element method, Modeling, Designing*

Doubly porous materials have nowadays offer new perspectives for the preparation of sustainable materials. The role of each porosity level is different and associated with different transfer processes. Macropores, would allow macromolecules flow through the materials, while a microporous (or submicro) network would be dedicated to the passage of smaller molecules, thus acting as a second transport mechanism, or in the case that macropores are totally clogged [1]. Investigating the physical behavior of these complex systems requires not only controlled chemical syntheses but also mechanical modelling tools.

To finely estimate the transport properties of such materials, the development of models and up-scaling methods has been considered. Indeed, the determination of the permeability of porous media is important in several practical problems related to mechanics and civil engineering (biomechanic, petroleum, flow in micro and nano systems, etc.). The modelling of flow through doubly porous materials raises a number of fundamental and practical questions such as the role of each porosity on the macroscopic permeability, also the optimization of microstructure to specific applications. The morphology of the microstructure is well defined in controlling the interconnectivity of the porous media : macropores may be interconnected to each other or through the microporous network. The development of adapted numerical tools to simulate the fluid flow in multiporous materials then appears to be of key importance.



**Figure 1** : SEM images of the microstructure in case of micropores are interconnected to each other.

The determination of the permeability in connection with microstructure geometry has been addressed with homogenization techniques, either based on the series of asymptotic expansions methods [6], [7] either on volume average methods applied to random microstructures [8]. These approaches provide the elementary cell problem which has to be solved to determine the macroscopic permeability. Standard numerical tools based on Finite Element Methods (FEM) or Finite Volume methods have been employed to compute the permeability [2], [3], [4], [5]. More recently, alternative methods based on Fast Fourier Transform (FFT) have been adapted to handle the problem of fluid flow in porous media [9], [10]. Later, the homogenization approaches have been extended to the case of doubly porous media [11], [12], [13]. Particularly, in [12] and [13], the authors considered the fluid flow in granular aggregates for which grains are also porous, i.e. contains a network of smaller interconnected pores. In such situation, there is a dominant flow at the larger pores level and the fluid flow at the lower pore level only introduce a small correction in the macroscopic permeability. Furthermore, the grains seem to be impervious when the micropores are very much smaller than the macropores and they could be not considered in the calculation of permeability. However, for porous material constituted of isolated macropores in a microporous solid, the role of smaller pores is primordial in the calculation of macroscopic permeability. Between these two limit cases, there is a range of various situations for which both the micropores and the macropores have an important role on the macroscopic filtration law.

In this work, we develop a double upscaling approach to compute the permeability of doubly porous material designed in [1] (see Fig.1) by employing numerical tools based on a Fast Fourier Transform (FFT). Due to the presence of three separated scales, the micropores, the macropores and the macroscopic scale, the effective permeability is determined by a consecutive double homogenization. In a first step, we compute a microscopic permeability obtained by a first homogenization at the lower scale. The fluid flow at the intermediate scale is described by the Stokes equations in the macropores and by the Darcy law for the solid (containing the micropores) in order to finally compute the macroscopic permeability at the upper scale by a second homogenization. Each scale transition is performed with FFT based algorithms. The role of each porosity will be analysed for different pores configurations.

## REFERENCES

- [1] Droumaguet B.L. et al *Polymer* **55** **2014**, 373-379
- [2] Barrere. J et al. *CR Acad. Sci. Paris, Sér. II* **1990**, 310: 347–352
- [3] Cioranescu. D et al. *Math. Meth in the Applied Sciences* **1996**, 19 (11):857–881x
- [4] Alcocer. F.J. et al. *Physical Review E*. **1999**, 59 (1):711–714
- [5] Alcocer. F.J. et al. *Physics of Fluids* **2002**, 14 (7):2578–2581
- [6] Auriault J.L. and Sanchez-Palencia E. *J. Mécanique* **1977**; 16-4:575-603.
- [7] Sanchez-Palencia E. *Lecture Notes in Physics* **1980**, vol. 127.
- [8] Whitaker S. *AIChE Journal* **1967**, 13-3:420-427.
- [9] Monchiet V. et al. *C. R. Méca.* **2009** 337-4 : 192-197.
- [10] Nguyen T.K et al. *Eur. J. Mech. B/fluids* **2013** 37:90-98.
- [11] Quintard and Whitaker S. *J. Mécanique Théor. Appl.* **1987**, 6:691-726.
- [12] Auriault J.L. and Boutin C. *Transport in Porous Media* **1992**, 7:63 82.
- [13] Boutin C. et al. *Int. J. Solids Structures***1998** 35 :4709-4737.