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Effective Transport Parameters of Porous Media from Microstructure Images.

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Transport in porous media is central in chemical engineering. Effective transport properties are required for evaluating and improving many processes and applications, typical example are catalysts, or porous membranes in separation processes. A widely used model to describe transport in porous media is the Dusty-gas model. This model accounts for permeation, Knudsen-diffusion and binary diffusion. The model parameters are commonly determined from experiments, for instance, performed in a Wicke-Kallenbach cell [1]. The parameters derived in this way are spatially averaged effective parameters.

In this contribution we present an approach to calculate transport parameters of the Dusty-Gas model from a cross sectional image of a porous material. This reduces the currently large experimental effort, since only once a visualization of the microstructure is needed. For a structure this characterisation by a single high-resolution image is less demanding than multiple experimental series to derive the parameter as in conventional procedures. In addition, the transport properties of very thin layers, of materials that are difficult to study in the Wicke-Kallenbach cell, or of virtually designed materials for which structural information is available from simulations but no physical sample has yet been synthesized, can be determined. The presented approach can be applied to any porous material permeated by a gas (or multiple gases), e.g. membranes, filters in general, bulk material, column internals, etc.

The method applied here is asymptotic homogenization, which allows structural information on the micro scale to be lumped into effective transport properties. The key idea of asymptotic homogenization is based on expressing the real physical problem as a representative mathematical problem (the so-called cell problem). The solution of the cell problem is directly related to the effective transport properties on a macroscopic scale. By variation of characteristic geometric properties of a porous structure, various kinds of pore structures can be covered. The resulting basic functions are integrated to calculate the effective transport properties of the up-scaled model. We applied this approach to porous media to derive the dusty-gas model parameters, namely permeability, Knudsen-diffusion and binary diffusion coefficient. In our present work, as well as in our previous work [2], we compare the model predictions based on cross sectional images with experimental data and literature data to validate our results. A remarkable agreement between experiment and simulation is achieved.

Time Block Preference

Time Block B (14:00-17:00 CET)

References

[1] E. Wicke and R. Kallenbach, "Die Oberflächendiffusion von Kohlendioxyd in aktiven Kohlen,"Kolloid-Zeitschrift, vol. 97, no. 2, pp. 135–151, Nov. 1941, doi: 10.1007/BF01502640.

[2] J. H. Matthies et al., "Up-scaling transport in porous polymer membranes using asymptotic homogenization,"Int. J. Numer. Methods Heat Fluid Flow, Nov. 2019, doi: 10.1108/HFF-04-2019-0326.

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