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Fluid-fluid porometry, pore network simulation

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Abstract
Pore network modeling used for the simulation of drainage through a porous medium is carried out. A comparison with the results of the parallel tubes model is investigated to better extract the pore-size distribution derived from the fluid-fluid porometry.

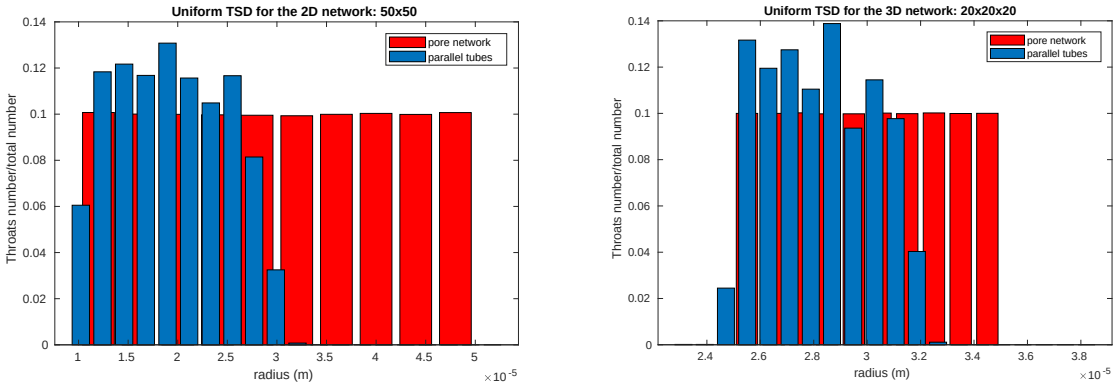
Keywords, Membrane, pore size distribution, porometry, pore network simulation

INTRODUCTION
Characterization of the pore-size distribution(PSD) of a porous material has been widely investigated among the scientific community. Direct methods based on imaging technics such as microtomography and indirect methods based on the analysis of some macroscopic results such as fluid-fluid porometry are used to determine the PSD of the porous medium. Fluid-fluid porometry uses the parallel tubes model for determining the PSD, this model does not correspond to a wide range of membranes. Thus, pore network modeling represents a good alternative for modeling the membranes. The comparison of the PSD given by the two models can be done through the simulation of drainage.

METHODS
A membrane saturated with a wetting fluid is subjected to a pressure gradient of a non-wetting fluid (drainage) and the pressure gradient is slightly increased while the volumetric flow-rate is mesured at the outlet of the membrane for each step. Assuming the parallel tubes model, the PSD can be determined by considering the Young-Laplace and Poiseuille equations[1]. The Young-Laplace equation relates the pressure difference between the two fluids to the radius of the cylinder, whereas the Poiseuille equation expresses the volumetric flow-rate as a function of the pressure difference which provides the number of tubes having the required radius for the non-wetting fluid to penetrate according to the Young-Laplace equation. The Erbe method[2] gives a statiscal expression for determining the PSD.
Pore network modelling allows representing the porous medium as a network of interconnected nodes called pores[3], which are connected by throats. In our case, the network is structured and pores and throats are modeled by spheres and cylinders respectively, the pore radii are assumed to be larger than those of throats both being randomly taken from a chosen distribution. For the throats, the distribution is called TSD (Throat size distribution). The simulation method of drainage is an invasion percolation technique, which is a quasi-static method[4]. It is based on tracking the interfaces and invading the throats when the pressure difference between the two fluids is larger than the capillary pressure given by the Young-Laplace equation. In the case of drainage, as the throats radii are smaller than the pore ones, the invasion is controlled by the throats[5]. The assumption of this method is that viscous forces are insignificant in comparison to capillary forces. Thus, in the invasion process, the pressure is considered as uniform for the two fluids in the medium. After equilibrium is reached, the distribution of the two fluids within the pore network is determined. When the non-wetting fluid reaches the outlet, the volumetric flow-rate is computed from the mass conservation applied to all the invaded pores together with the use of Poiseuille's equation, both leading to a linear system for the pressure in all the invaded pore cluster. Once solved, the volumetric flow-rate at the outlet can be determined.

RESULTS
To avoid the effects of variance of the radii randomly chosen for a given distribution, results of volumetric flow-rate and pressure are averaged. A first test was performed to determine the minimum number of pressure steps required to get results independant from the pressure step. Another test was applied to find a minimum size of the network so that the results are not influenced by the size of the network. The comparison between the TSD chosen initially and the one given by the parallel tubes model through the Erbe method is represented

on the following histograms for both 2D square and 3D cubic networks. The 2D and 3D networks are composed of 50x50 pores and 20x20x20 pores respectively. Uniform and normal distributions were considered.



(a) 2D network

(b) 3D network

Figure 1: Comparison between the TSD initially chosen and the one found through the parallel tubes model

The shape of the TSD obtained from the parallel tubes model is nearly the same as the one chosen initially for either the uniform or the normal distributions for both the 2D and 3D networks. However, the TSD given by the parallel tubes model is not spread over the whole distribution. In addition, the TSD obtained for the 3D network is seen to be more spread over the distribution domain for the uniform and normal distributions in comparison to the 2D network. The spreading of the TSD is directly related to the percolation threshold that represents the pressure at which the non-wetting fluid has reached the outlet. Below this threshold the volumetric flow-rate is zero and thus the distribution function is also zero.
A radius threshold r_c can be defined from the expression of the percolation threshold p_c:
$p_c = \int_{r_c}^{r_{max}} f(r)\,\mathrm{d}r = 1 - F(r_c)$
The function F is the cumulative distribution function.
For a uniform distribution, the radius threshold is obtained as: $r_c = r_{max}(1 - p_c) + r_{min}p_c$;
where r_{max} and $_{rmin}$ are the maximum and minimum distribution limits respectively.
For a normal distribution, the radius threshold is expressed from the mean radius r_{moy} and the standard deviation σ: $r_c = r_{moy} + \sqrt{2}erf^{-1}(1 - 2p_c)$; where erf^{-1} is the inverse of the error function.
It is known that the percolation threshold for an infinite 2D square network is equal to 0.5, for an infinite 3D cubic network, it is equal to 0.249 (i.e. 0.25). While, the radius threshold is obtained for the different networks:

	2D network	3D network
Uniform distribution	$r_c = \frac{1}{2}(r_{max} + r_{min})$	$r_c = \frac{3}{4}r_{max} + \frac{1}{4}r_{min}$
Normal distribution	$r_c = r_{moy}$	$r_c = r_{moy} + \frac{\sqrt{2}}{2}\sigma$

Table 1: Radius threshold for the two distributions and the two networks

The analytical results for the radius threshold are in good agreement with the results of the pore-network modelling. The spreading of the distribution is indeed larger for 3D networks than 2D network, this is as a result of the coordination number which is larger for 3D networks, so that invasion has more chance to occur and reach the outlet for lower pressure values.

CONCLUSION

Parallel tubes model does not represent well all types of membranes, especially those with low coordination number for which the radius threshold is smaller than the expected one, thus attributing the role of larger throats to the smaller ones.

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