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Numerical and experimental study of fouling in microfluidic channels and microfiltration membranes

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Introduction: Macroscopic description shows limitations in the modeling of the fouling. These limitations are mainly due to a misunderstanding of the phenomena occuring at pore scale. It is therefore necessary to investigate more accurately particle interactions as the ability to predict the fouling of a membrane remains a great scientific and industrial challenge. In this study, we first performed pore-scale 3D numerical simulations, validated by experiments in regular geometries mimicking the tortuosity and connectivity of the pores of a membrane. We then reconstructed the 3D model of a commercial membrane thanks to X-Ray tomography and compared the numerical results to dead end experimental microfiltrations of latex particles in defined operating conditions. This double investigation experimental/numerical allowed us to analyze local fouling phenomena and to improve the description of complex interactions between hydrodynamics and the physico-chemical effects.

Materials and methods: Microsystems were implemented using the standard soft-lithographic technique of manufacturing a wafer then the microsystem itself. Production consists of manufacturing 2 PDMS « loaves », one engraved and one virgin, which are then joined in order to close the microsystems contained on the engraved side. Each microsystem was designed with a common base (thickness = 50 µm, length = 25.4 mm, width of main channel = 1.7 mm). Three different geometries with 20 micrometers channels were used (Figure 1) to test the effect of the connectivity (FP20) and the tortuosity (FQ20) Filtration experiments in microfluidic with spherical latex particles in polystyrene of 4,9 µm were performed and the quantification of the fouling dynamics was investigated by image analysis.

The same latex particles were filtered through a cellulose ester membrane (d_{pore} = 5 µm) in a conventional mounting using an AMICON cell. An X-Ray tomography was performed at the European Synchrotron Radiation Facility (ESRF - Grenoble) in order to obtain data on the 3D structure of this membrane. The 3D reconstruction was performed using the iMorph software. GeoDict (ITWM Fraunhofer) was then used to simulate: (i) experiments in microfluidic in order to validate the approach and for a better understanding of the experimental results and (ii) filtrations on a reconstituted membrane for a better understanding of the capture phenomenon.

Results: Experiments performed in microfluidic were compared to numerical simulations (Figure 2). Thus the surface properties of the microchannels parallel to the flow were modified. The walls were subjected to higher shear stresses and were considered non-adhesive in order to take into consideration the phenomenon of re-entrainement of particles observed experimentally., The sensitivity of four physical parameters was tested numerically: the particle diameter, the flow velocity and the two adhesion parameters namely the Hamaker constant and the coefficient of restitution as collisions between a particle and the membrane play a major role in the phenomenon of capture by adhesion. The ratio between the kinetic energy of a particle and its Hamaker constant can determine in which capture mechanism the system is likely to be operating. It was also possible to highlight the effects induced by geometrical parameters such as tortuosity and the connectivity of the pores and the ones due to operating conditions such as ionic strength, flow and concentration. In the coupled approach filtration on microfiltration membrane – numerical simulation, the comparison helped to identify different fouling mechanisms depending of the size of the particles. For a particle diameter bigger than 1.25 µm, the results show that fouling decreases with an increase of the particle size. Indeed, the particles become bigger than the pore size and are captured on the surface thereby putting up a lower resistance to the flow. It is especially the case for the 4 µm, 5 µm and 6 µm particle sizes. So more particles with a diameter higher than 4 µm must be injected to observe an effect on the

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permeability of the simulated membrane (S ≈ 630 μm²). Then a maximal fouling appears for particles between 1 μm and 1.25 μm. This particle diameter is slightly smaller than the pore size and around the size of the cut-threshold. The presence of this minimum may be due to a change of the fouling mechanism. In order to better understand this phenomenon, it is interesting to analyze the distribution of the captured particles in the depth of the membrane. In Figure 3, the Cumulative Distribution Function (CDF) is represented over the relative depth. The particles with a size bigger than 1.5 μm do not penetrate the membrane and stay on the surface. So only intermediate and complete pore blocking can occur. For smaller particles there is real penetration. However, simulations show limits in the description of the filtration cake: simulations lead to very large deposit porosity and therefore to permeability deposits much larger than those measured experimentally. Progress towards a better description of hydraulic resistance of deposits will have to be made to consider using predictive simulations.

Conclusion: Simulations have been performed for i) microfluidic devices allowing a direct observation of the fouling at pore scale and ii) commercial membranes to compare the ability to predict fouling in a “real” case study. The comparison with experiments in microfluidic devices permitted to evaluate the ability of simulation to depict the way particles attach and accumulate in a porous structure. It has been noted that the adhesion parameters and the possibility of particles rebound plays an important role. The parameters of the simulation can then be adapted in order to reach a good qualitative description of the accumulation. The comparison with experiments done with commercial membranes have been performed. The reconstruction of the membrane described the structural complexity within the numerical simulation of the flow and the particle fouling during filtration. Simulation therefore quantified the fouling mechanisms and their consequences in term of permeability for different particle/size ratios and adhesion parameters. However, simulation shows important limitations in giving us a correct description of the permeability of the fouling mechanism.

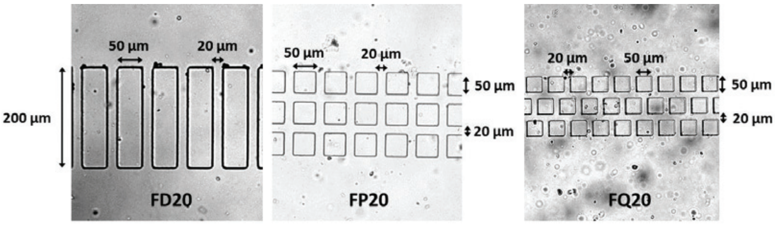

Figure 1. Experimental microsystems studied

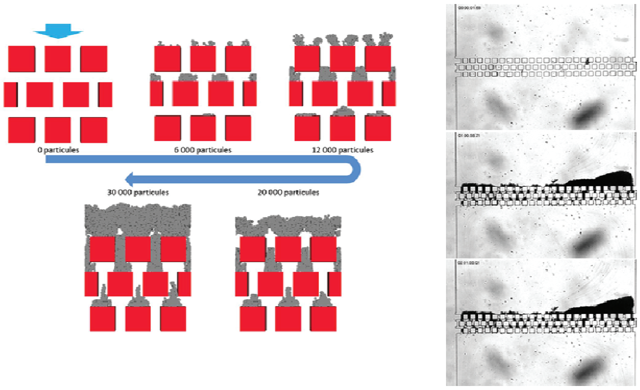

Figure II. Comparison of the fouling structure in microfluidics channels (left: numerical simulations - right: experiments

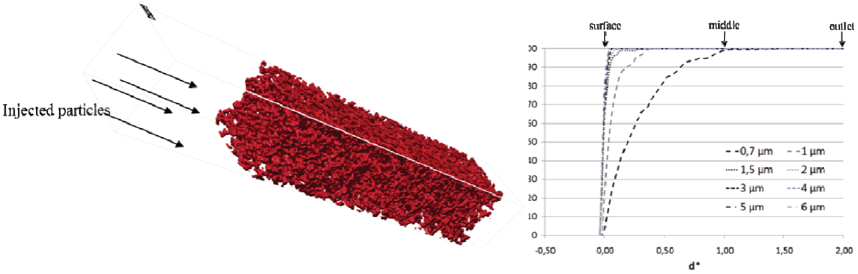

Figure 3. Cumulative Distribution Function (CDF) of the captured particles as a function of the penetration distance within the membrane

Keywords: fouling, numerical simulation, microfluidic, X-ray tomography