CFD Simulations to Improve Protein Separation Introducing a Permeable Surface with Periodic Grooves

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Introduction: Flow field-flow fractionation (FlFFF) is a size-based separation technique suitable for macromolecules. The separation is based on an ultrafiltration membrane that retains the solutes when a cross-flow is applied. Selectivity of two solutes is equal to the ratio of their diffusion coefficients. We investigate the possibility to increase selectivity using microstructured membranes (fig. 1).

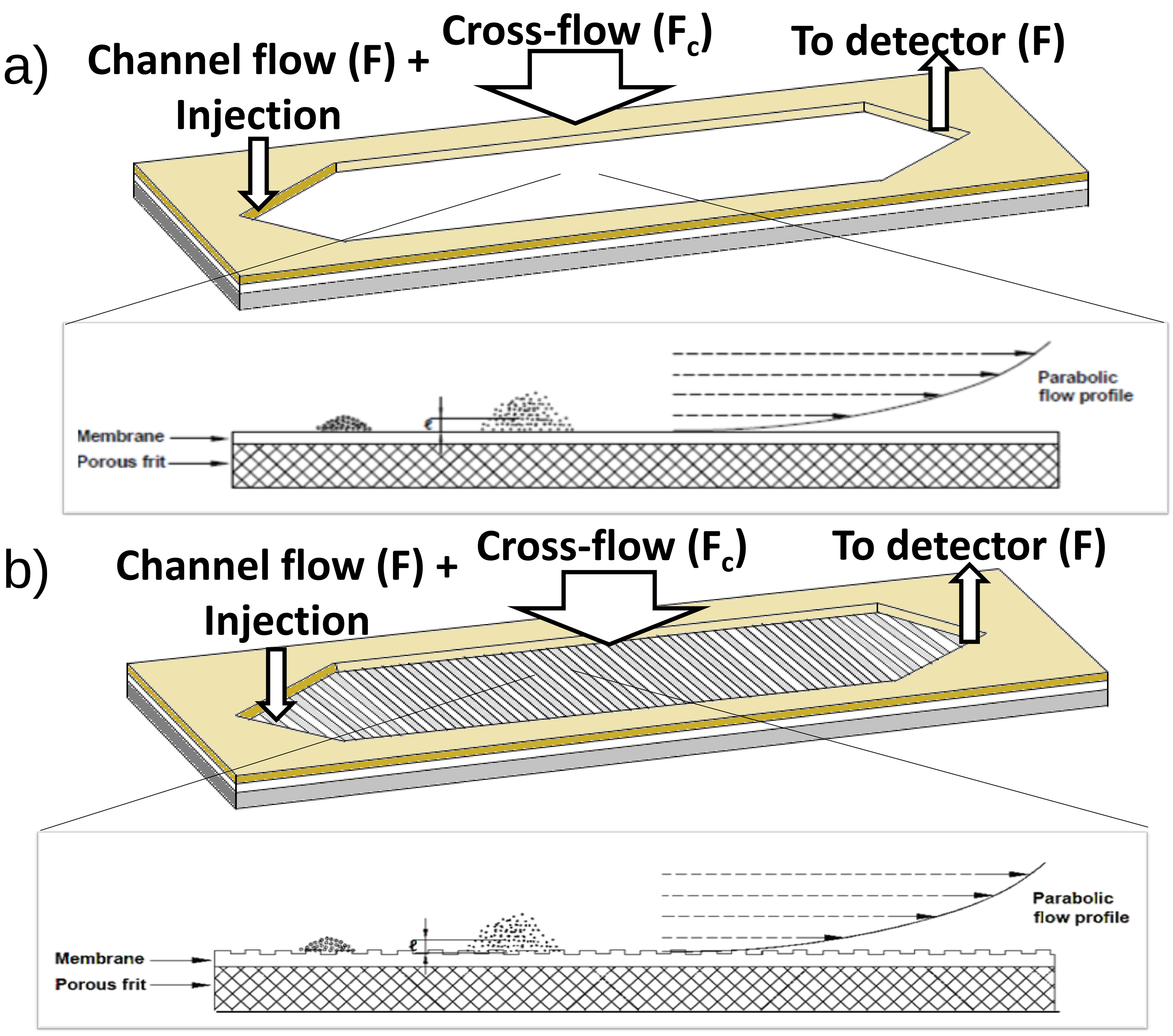

Figure 1. FlFFF channel with a) a flat b) a patterned membrane

Computational Methods: Single-phase laminar flow was used and the boundary conditions (inlet, outlets) were set to define channel flow and cross flow (fig. 2). The study of the flow profile was solved as stationary state problem and this output was used to solve the time dependent problem of protein migration. Transport of diluted species (convection and diffusion) was used to simulate proteins.

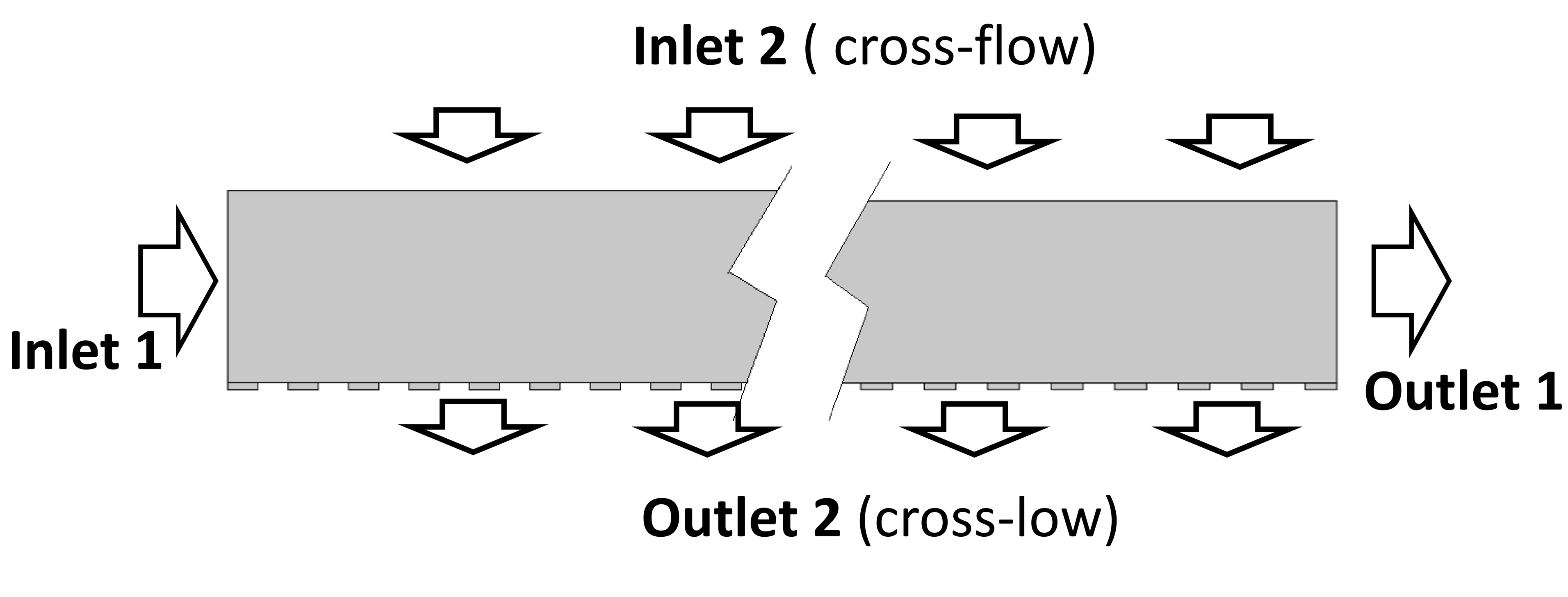

Figure 2. Two dimensional model

Equations:

- Laminar flow, incompressible, stationary

$$\rho(u\cdot\nabla)u = \nabla\cdot[-pI+\mu(\nabla u+(\nabla u)^T)]+F$$
$$\rho\nabla(u)=0$$

- Transport of dilutes species, convection and difussion, time dependent

$$\frac{\partial c_i}{\partial t}+\nabla\cdot(-D_i\nabla c_i+uc_i)=R_i$$
$$N_i=-D_i c_i+uc_i$$

Results: Results of a 6 cm length, 2 cm width and 280 µm height FlFFF channel for two proteins abundant in blood plasma. F = 1.25 / Fc = 2 mL/min

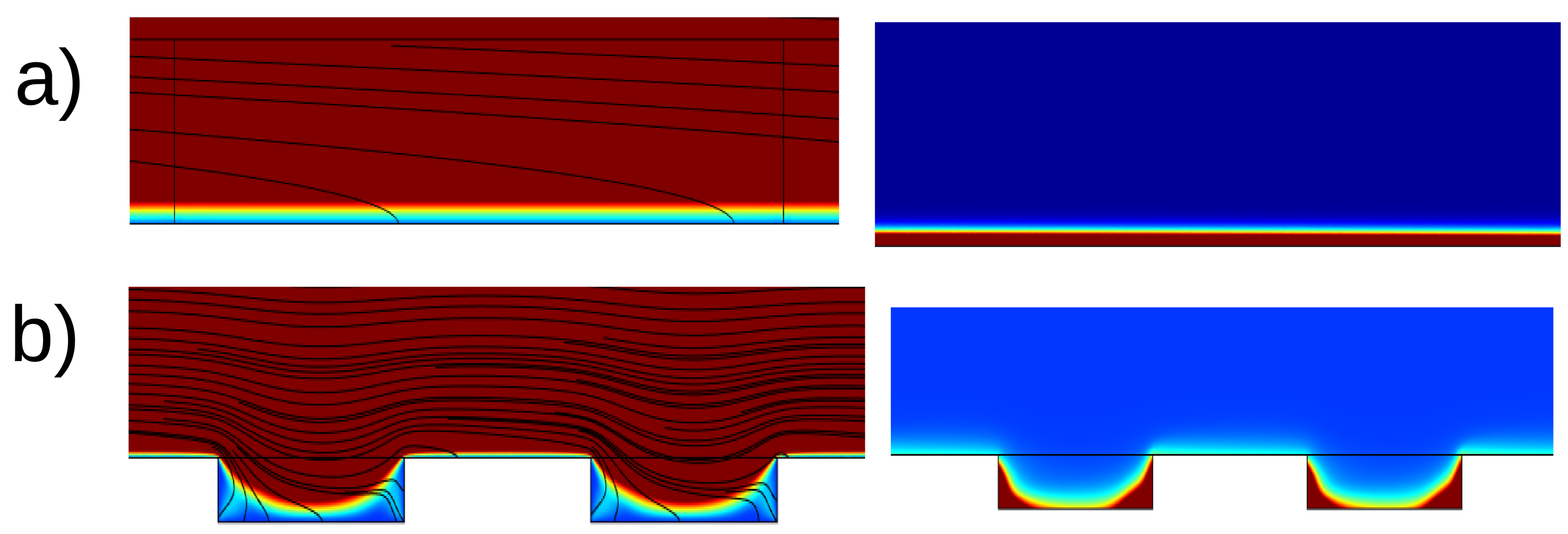

Figure 3.Flow profile and concentration profile over a)a flat UF membrane b) a patterned membrane

	Protein	Retention time (s)	Selectivity
Flat membrane	Bovine Serum Albumin (D =6.1·10^{-11} m^2/s)	320	1.43
	γ-globulin (D =4.3·10^{-11} m^2/s)	460	
Patterned membrane with grooves c = 100 µm r = 100 µm h = 10 µm	Bovine Serum Albumin (D =6.1·10^{-11} m^2/s)	670	2.27
	γ-globulin (D =4.3·10^{-11} m^2/s)	1520	

Table 1. Retention time and selectivity (see fig.4)

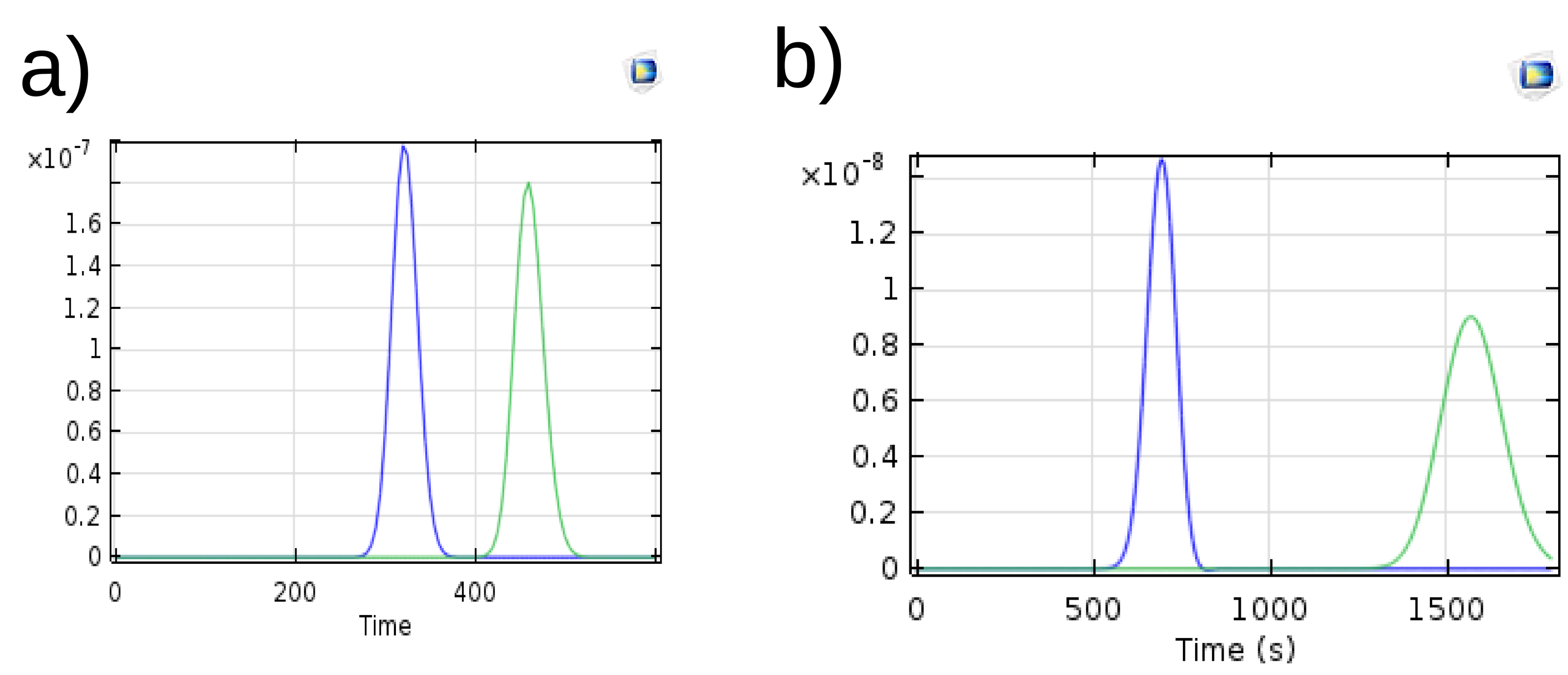

Figure 4. Protein concentration vs time in the outlet of the channel with a) a flat and b) a patterned membrane

Conclusions: Microstructured membranes result to higher selectivity and could improve the separation of the FlFFF technique (Table 1).

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