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

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Abstract

In this study, we use COMSOL Multiphysics® to improve protein separations by the analytical technique asymmetrical flow field-flow fractionation (AF4). AF4 is a very mild separation technique where separation of macromolecules or nanoparticles takes place along a ribbon-like channel that exhibits a laminar parabolic flow profile. The key component of AF4 is an ultrafiltration (UF) membrane which is positioned over a porous frit in the bottom of the channel. When a flow is applied through the membrane (cross-flow), solutes are accumulating close to the membrane with average accumulation layer in different regions of the parabolic flow profile which results in different retention times. Therefore, the selectivity of solutes, which is the ratio of their retention times, depends on their diffusion coefficients and it cannot be altered with experimental parameters.

Conventionally, only flat UF membranes are used in AF4 and any surface roughness is considered harmful for the separation. However, with CFD simulations we demonstrate that a periodic "roughness", for instance perpendicular grooves on the surface of the membrane, could actually improve separation as the selectivity is increasing. A 2D model was used to describe our system. Flow profile and protein migration is predominantly homogeneous along the breadth of the channel and that enabled us to reduce the model to two dimensions. A mesh was created with very fine elements in the proximity to the bottom flat or grooved permeable surface (membrane) as protein migration takes place in this region.

To describe the flow, single phase laminar flow was used and boundary conditions (inlet, outlets) were set to define channel flow and cross flow. 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 of two different sizes, bovine serum albumin and gamma-globulin with hydrodynamic radius 3.7 nm and 5.3 nm respectively. The model was verified by varying input parameters and it was validated comparing the retention times of proteins obtained over a flat surface with the theory, as there is an exact theoretical correlation of the retention time and diffusion coefficient (or hydrodynamic radius) of the protein. The simulation experiments indicated that our model is suitable to predict protein retention times in an AF4 channel and that patterned membranes with parallel grooves could improve the separation. Physical experiments could be carried out using an engineered patterned UF membrane.

Figures used in the abstract

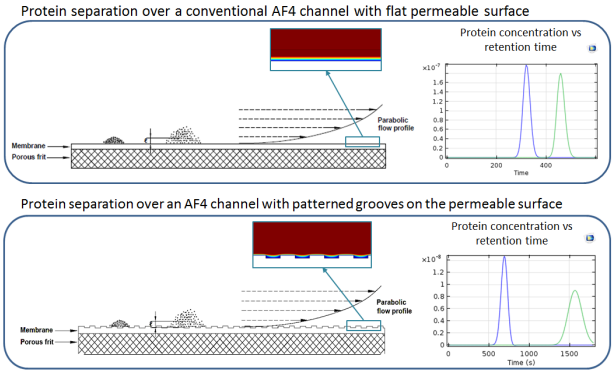

Figure 1: Migration of two proteins of different sizes along a flat and a patterned permeable surface.