CFD-Simulation of Preparative Chromatographic Columns: Effect of the Distributor and the Column Design on the Separation Performance

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Abstract

The development of new highly selective functional sorbents and gels has established preparative chromatography as a standard separation method for complex mixtures in biotechnology and live-science applications in recent years. However, improper column design and/or design of the liquid distributor may significantly reduce the separation efficiency of large scale preparative chromatographic columns. A classical way to optimize the design of chromatographic systems is to experimentally determine the breakthrough curves and/or the separation performances for pilot-scale setups and to scale up the pilot scale design. Alternatively, computational fluid dynamics (CFD) can be used for this optimization process.

Introduction

The development of new highly selective functional sorbents and gels has established preparative chromatography as a standard separation method for complex mixtures in biotechnology and live-science applications in recent years [1,2]. Due to typically high pressure drops per unit height of column packing and good separation achievable with even short column lengths, the scale-up of preparative chromatographic columns results in low height to diameter (h/D) ratios, thus increasing the need for good column design. Improper column construction and/or design of the liquid distributor may significantly reduce the separation efficiency of large scale preparative chromatographic columns (Fig.1). A classical way to optimize the design of chromatographic systems is to experimentally determine the breakthrough curves and/or the separation performances for pilot-scale setups and to scale up the pilot scale design. Alternatively, computational fluid dynamics (CFD) methods can be used for this optimization process.

CFD – Modeling

Within this work, the geometries of typical full-scale chromatographic column designs were implemented for fluid dynamic computations using the commercially available CFD code FLUENT™. Experimental data for the pressure drop of the column filling were used to define resistance coefficients in the flow model. For the distributor systems, the k-ε turbulence model was applied, and the column packing was modeled as a porous medium. Physical and thermodynamic data of typical solvent mixtures used as mobile phase were implemented. Symmetries were used to reduce the computational effort, thus leading to a computational domain which is one fourth of the whole distributor/column/collector geometry.

The CFD model was then used to investigate the performance of the liquid distributor with regard to flow velocity distribution and pressure drop. Through the definition of two or more species an unsteady CFD model was set up to investigate breakthrough curves (Fig. 2). To achieve this, the steady flow field was calculated using the properties of the mobile phase only. Then the solver was switched to unsteady calculation and a sudden concentration change of a second species (same fluid properties) was initiated. Binary diffusion was allowed, and the concentration of this second species at the collector exit with time was recorded to gain the response function at the outlet.

Results and Discussion

It could be shown that the separation efficiency of chromatographic columns could be enhanced by reducing the liquid holdup and backmixing effects of the distributor systems and by feeding liquid across the whole cross-section of the column. The performance of a detrimental design is shown in fig. 3. A large annular zone with a significantly longer residence time can be seen which would result in negative separation effects (peak widening). The concentration of a second component with time (unsteady CFD model) can be seen in fig.4, showing the weak performance of the modeled column. Radial mixing effects in the chromatographic column seem to be of minor importance. The influence of the pressure drop of the distributor is rather low because of typically high pressure drops of the column.

Conclusions

Computational fluid dynamics has shown to be a valuable tool for the optimization of preparative chromatographic columns. The effect of the liquid distributor on the product front and its residence time distribution can be easily analyzed. Proper distributor design involves feed distribution across the whole cross-section of the column to prevent a core / annulus – like residence time structure in the column.

In the future, an extension of the flow through the column packing by integration of species retention in the porous medium may lead to more detailed model of the multicomponent separation performance of chromatographic columns.

References

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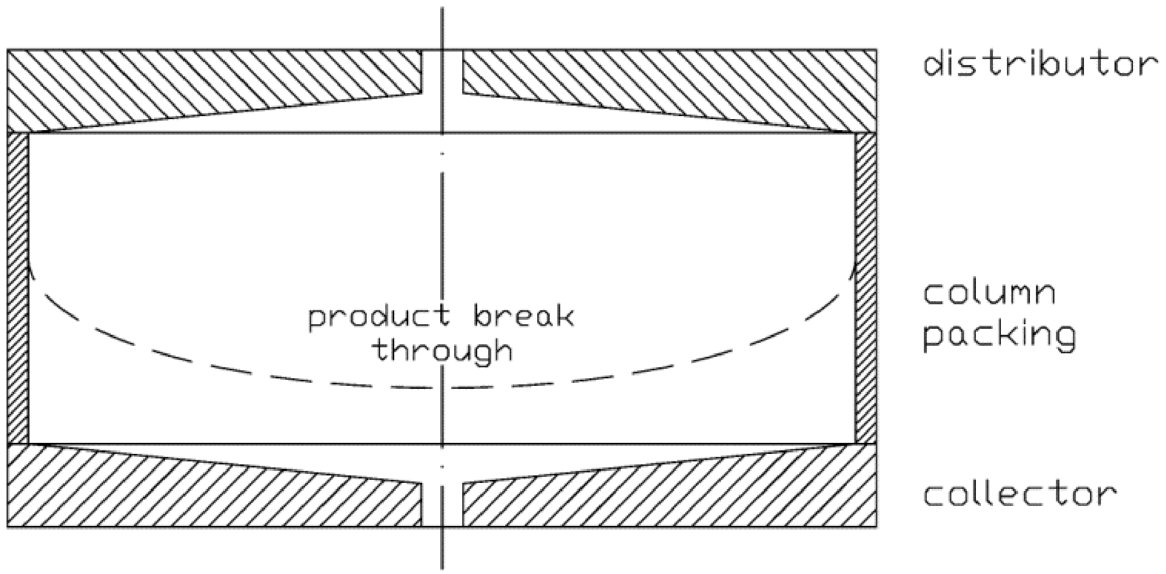

Fig. 1: Typical product breakthrough in preparative chromatography.

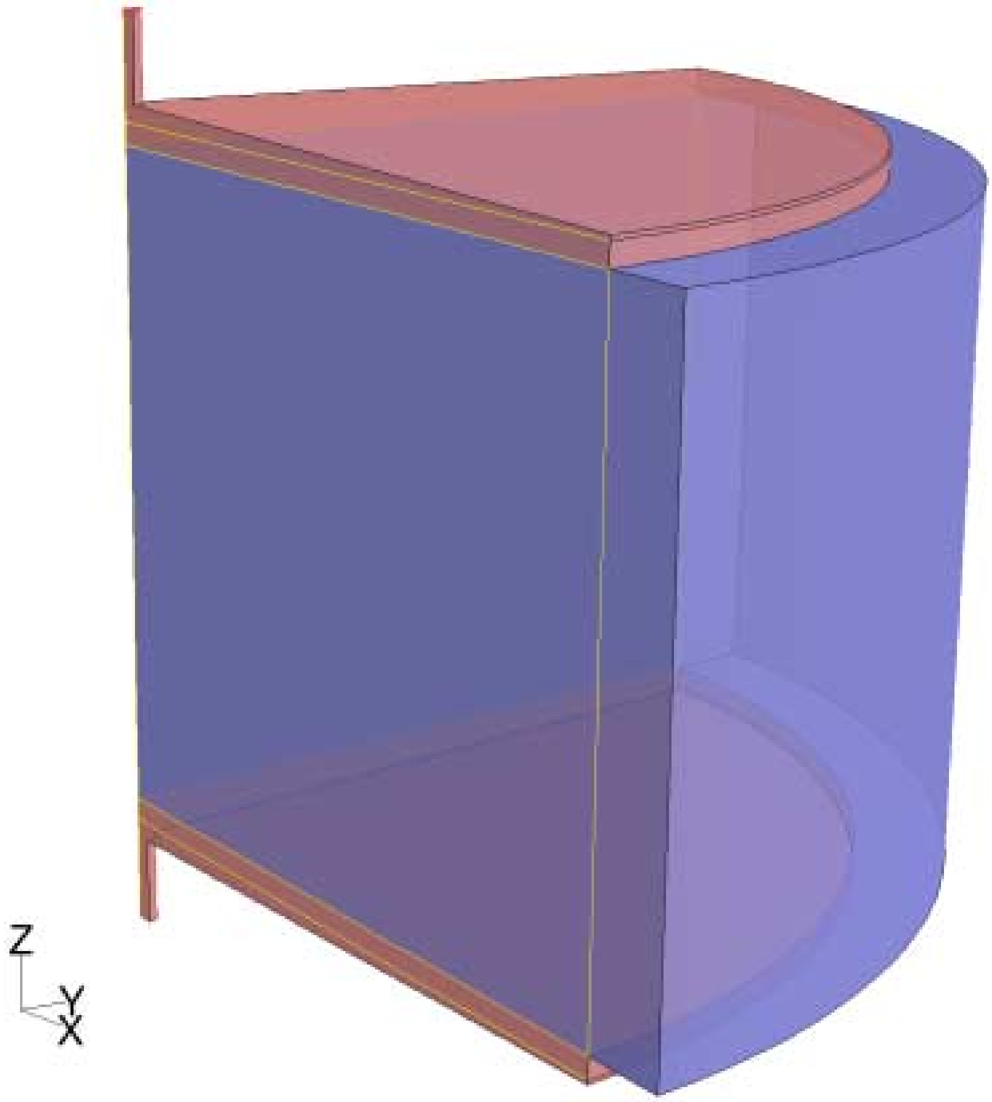

Fig. 2: Computational domain (the blue coloured volume indicates the column, the red coloured volumes indicate distributor and collector).

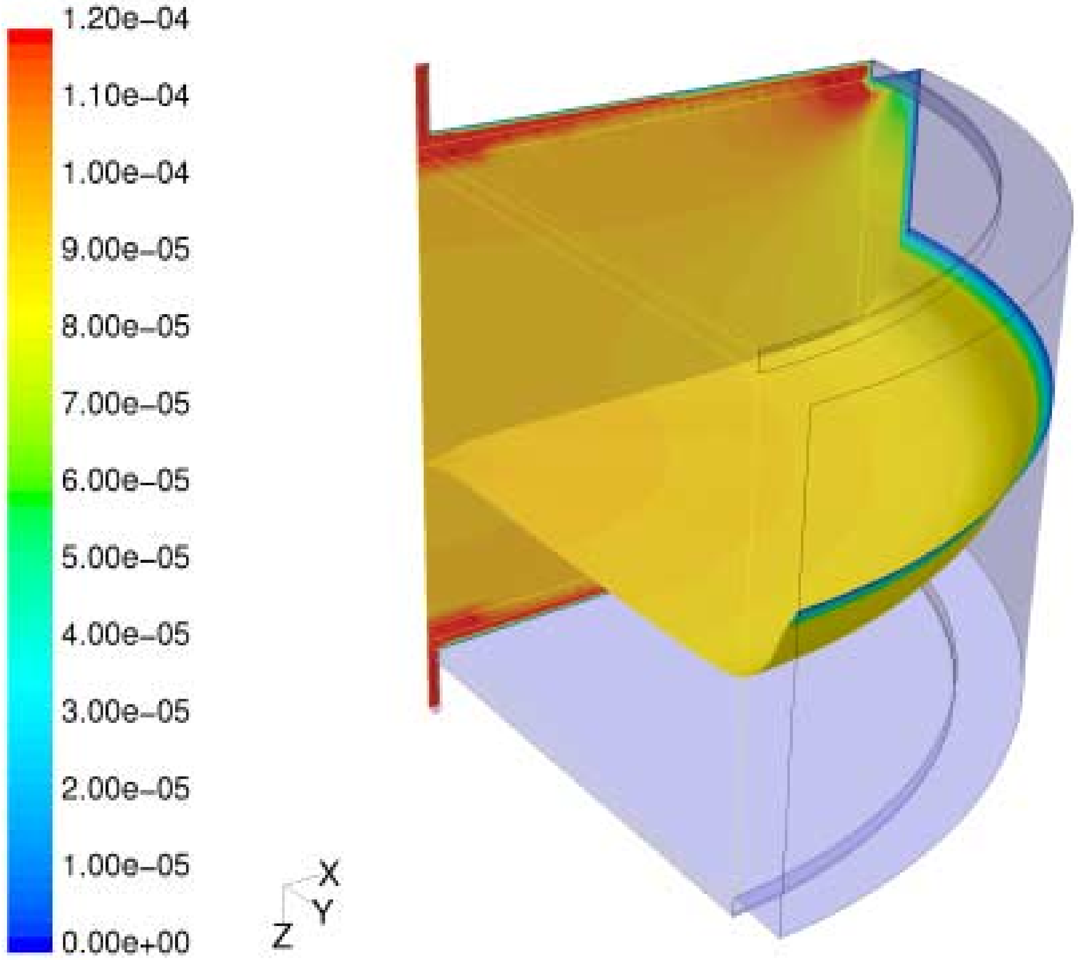

Fig. 3: Contour plot of velocity magnitude – the plane indicates the 50% concentration level of a step function moving through the column after 1000 s.

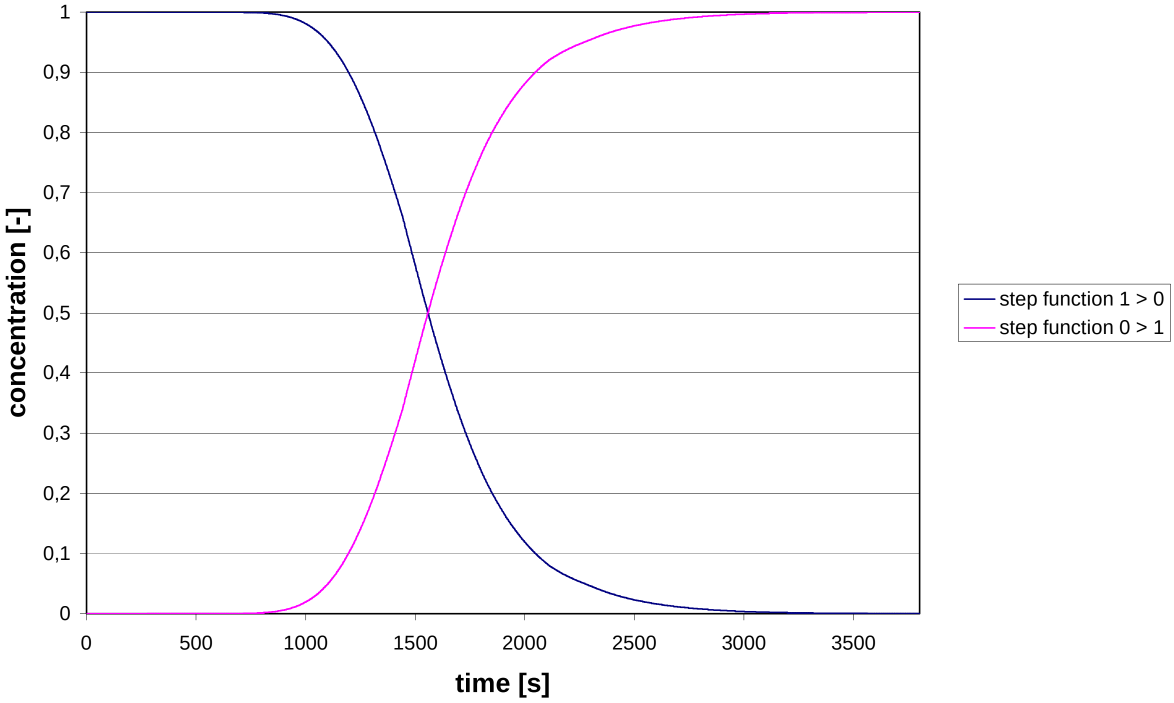

Fig. 4: Concentration at collector outlet calculated from transient CFD simulation of step function at distributor inlet.