Towards Large Scale Packed Bed Chromatography Simulations with OpenFOAM®

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Column liquid chromatography (CLC) is a widely used unit operation in biotech and chemical process engineering for purification of target products (e.g. proteins for pharmaceutical agents) from unwanted substances. An aqueous solution containing the mixture of molecules is forced to flow through the chromatography column which is filled with porous particles (beads). While transport through the interstitial volume between the beads is governed by advection and dispersion, molecules diffuse into the beads and are adsorbed at their inner surfaces. Separation is achieved since the different species exhibit differently strong binding, which leads to different retention times and finally to temporally separated exiting from the column (fig. 1) [1].

For numerical process analysis and optimization of CLC, most established solvers employ one- or two-dimensional general rate models [2]. In order to overcome complex packing geometries, these models rely on homogeneity assumptions, considering concentration gradients only in the column axial and in bead radial directions. Such simplified models generally produce proper numerical predictions for industrial scale applications with columns of several liters of volume. However, recent trends in separation science point towards utilization of micro scale columns with only up to milliliters of volume for investigation of sorption processes. For these applications, the available one/two-dimensional solvers are not suitable, since inhomogeneity effects like channeling and wall influence become the dominating phenomena.

We have conducted research in spatially resolved numerical simulations of chromatographic separation processes [3]. However, such simulations are currently subject to strong restrictions on numbers of beads (< 10³) and degrees of freedom because standard commercial solvers do not permit efficient scale-up to large high performance computers (fig. 2). Hence, we aim at developing a simulator which is capable of accurately and efficiently solving chromatographic separation processes in micro scale columns in three dimensions. Such a software package will include three major modules:

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1. Robust unstructured (or cartesian) mesh generator for complex geometries
2. Incompressible Navier-Stokes solver for flow profile in the interstitial column volume
3. Time-accurate convection/diffusion/reaction solver for transient mass transport of an arbitrary number of chemical species

While the first two steps can be respectably achieved with many freely available CFD codes, adding the last step requires a coupling of different physical phenomena (multiphysics modeling), which reduces the number of applicable solvers. Therefore, for our project we choose OpenFOAM as the development framework because first it already provides robust solvers for a wide range of CFD problems, second it gives us the possibility to extend the existent algorithms to our needs, and third it is freely available under GNU GPL license.

![Figure 1: CLC – schematic diagram](image1)

![Figure 2: 3D CLC simulation – flow speed](image2)

The final simulator will feature at least four requisites:

- High flexibility concerning addition of physical phenomena and development of algorithms
- Utilization of approved solvers for steady state flow profile computation (e.g. simpleFoam)
- Highly accurate implicit time integration scheme for stiff mass transport problems
- Excellent scalability on massively distributed machines

Besides user-friendliness, the last aspect will receive special attention, since realistic problems in micro scale CLC involve up to $10^5$ beads, which results in at least $10^7$ degrees of freedom. Therefore, adequate scaling on large numbers of processors is a must in order to solve the problem in reasonable time. Then, the simulator will be used to investigate inhomogeneity effects in column and bead cross sections and their impact on the resulting chromatograms.

References

