The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5 – 9 June 2022, Oslo, Norway

RESOLVING DISPERSION COEFFICIENTS IN REDUCED ORDER CHROMATOGRAPHY MODELS

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Key Words: *chromatography, advection-diffusion-reaction, reduced order model calibration*

Packed bed liquid chromatography is extensively used in biotechnology and other industries as a key unit operation in downstream processing, i.e., the separation and purification of valuable product molecules from unwanted side products. The system involves a cylindrical column that is packed with porous particles with functionalized inner surfaces to which molecules from a liquid solution mixture competitively adsorb. Different binding affinities of each molecule species result in their separation as they are advected along the column.

Chromatography modeling is increasingly applied in academia and industry for guiding experimental work through process design, optimization and uncertainty analysis [1]. Existing models (such as the General Rate Model) are strongly simplified by neglecting radial concentration gradients in the column and assuming identical radially symmetric particles. Furthermore, they assume spatially constant velocities and porosities [2]. The simplifying assumptions reduce the dimensionality and complexity of the problem manifold, making them very quick to solve. However, the effects of geometric inhomogeneities are lumped together using a dispersion coefficient which is typically calibrated using experimental data. The 2D General Rate Model allows for more fine grained specification of the column velocities and porosities with the caveat of multiple axial and radial dispersion coefficients to be fitted. Particle resolved models, on the other hand, can inherently describe the complex geometry of a chromatography column. These simulations can generate novel insight into flow and transport patterns within the complex interstitial region as well as within the particles themselves. However, these simulations are tedious to setup at every step: packing generation, meshing, solution, and post-processing. Furthermore, solving these systems requires tremendous compute resources in the order of thousands of cores for a few days.

In this project, we aim to obtain the best of both worlds. The vast amount of data generated by the high definition simulations is extremely difficult to obtain experimentally. Using this data to calibrate several successively simpler reduced order models, we can resolve the effects of specific inhomogeneities on the dispersion coefficients. Once calibrated, the reduced order models can then be used in process design, optimization and scale-up.

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