COMPUTATIONAL BIOSEPARATION PROCESS DEVELOPMENT

Marcel Ottens, Delft University of Technology, The Netherlands
m.ottens@tudelft.nl

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With the increase in computational power over the last decades, the use of modeling and simulation in process design for (petro)chemical industry has become common ground. Computational tools like ASPEN are standard in the design and operational analysis of (petro)chemical plants. However, in the bio pharmaceutical field, such modeling and simulation techniques are only recently being investigated for use and (potential) implementation. Being the workhorse of purification in the biopharmaceutical industry, chromatography is a good candidate for this modeling approach. Detailed mechanistic models describing chromatographic separation behavior are available, and software to simulate chromatography is becoming more and more available (i.e. DelftChrom, CADET, etc.). A bioseparation process normally consists of multiple chromatographic and conditioning steps, hence, an extreme large design space needs to be investigated. This may lead to prohibitive simulation times, even on state-of-the-art fast computers, when only mechanistic models are used. This presentation will show the implementation of a hybrid bioseparation process design approach using a combination of mechanistic models, artificial neural networks and high throughput experimentation for process development and optimization of the production of industrial relevant biologicals.