

Simulation of ion-exchange chromatography for teaching purpose using Bioprocess Library for Modelica

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An important process step in the biopharmaceutical industry is ion-exchange chromatography. It is used to separate the protein product from other proteins and various impurities in the starting material.

The ion-exchange chromatography step is a mature technology and here is modelling done with different complexities. Here we use a simplified model based on basic binding reaction between a protein and the resin and we use a series of compartments to model the column convection, taken from the literature. Further, the model is extended with an empirical proportional relation between the difference between isoelectric point and pH-resin, and the binding strength.

Despite the model simplicity it captures in a qualitative way several operational situations well, and useful for educational purpose. Examples are:

- Separation of proteins with different isoelectric points
- Impact of slope of the desorption gradient
- Impact of salt concentration in the incoming sample of material
- Impact of change of binding strength due to pH
- Impact of column binding capacity on break-through curves

The modelling is done in Modelica with use of Bioprocess Library and compiled model in the form of an FMU is simulated in a Python environment using Jupyter notebook. The simulations are done using package PyFMI, or alternatively with FMPy, with a simplified common command line interface FMU-explore.

The Jupyter notebooks combine explaining text with code snippets and results in diagrams. It is easy for the students to go back and change parameters and see what happens. Students can also continue the notebook in an explorative way.

In a teaching situation it is of interest to minimise installation requirements. We have experience of using Google Colab virtual machines to run these notebooks from a web-browser and requires no installation. You need a gmail-address though. The simulations can be run from any computer, chrome-book, tablet or even a smartphone.