Aspen Chromatography Model

The mass balance equation used in the Aspen Chromatography simulations is as follows:

$$\varepsilon_b \frac{\partial C_i}{\partial t} + K_{se}(1-\varepsilon_b)\varepsilon_p \frac{\partial \bar{C}_{i,pore}}{\partial t} + (1-\varepsilon_b)\left(1-\varepsilon_p\right)\rho_s \frac{\partial \overline{q_\imath}}{\partial t} + \varepsilon_b \frac{\partial\left(u_o^j C_i\right)}{\partial z} = \varepsilon_b\left(E_{b,i}^j\right)\frac{\partial^2 C_i}{\partial z^2} \quad (AF2.1)$$

Where ρ_s is the solid phase density, u_o^j is the mobile phase velocity within zone "j", ε_b is the bed void fraction, ε_p is the particle porosity, $\bar{C}_{i,pore}$ is the average pore phase concentration. In Eq. (AF2.1), the $\frac{\partial \overline{q_\imath}}{\partial t}$ term is the linear lumped mass transfer parameter. In Example 1 it is:

$$\frac{\partial \overline{q_\imath}}{\partial t} = MTC_{s,i}(q_i^* - q_i) \quad (AF2.2)$$

Where $MTC_{s,i}$ is the mass transfer coefficient based on the solid phase concentration and q_i^* is the equilibrium solute concentration in the stationary phase

In Example 2 it is:

$$\frac{\partial \overline{q_\imath}}{\partial t} = MTC_{l,i}(C_i - C_i^*) \quad (AF2.3)$$

Where $MTC_{l,i}$ is the mass transfer coefficient based on the liquid phase concentration and C_i^* is the equilibrium mobile phase concentration. The axial dispersion coefficient was estimated using the Chung and Wen Correlations [1].

Simulations were performed using the Aspen Chromatography simulated moving bed template. The discretization method used in the simulations was a Quadratic Upwind Differencing Scheme (QDS) with 181 elements for example 1 and 150 elements for example 2.

The integration method used was the Implicit Euler Method with fixed step sizes. The step size for the first step of each run was set to $5x10^{-6}$ and then after the first step, the step size was reduced. A MA48 linear solver was used with a maximum iterative passes of 10. The absolute variable tolerance, relative variable tolerance, and the absolute equation tolerances were set to $1x10^{-7}$. The Numerical derivative absolute perturbation, numerical derivative relative perturbation and explicit event tolerance were set to $1x10^{-5}$. The Non Linear Solver mode was set to Standard with a Mixed Newton Method. A least squares estimator was used with the solution convergence tolerance of $1x10^{-6}$ and a maximum of 400 iterations. The FEASOPT (feasible path successive quadratic programming optimizer) was used with a maximum of 100 iterations and a solution convergence tolerance of 0.0001.