nanomaterials

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Supplementary Data

Rejection Mechanism of Ionic Solute Removal by Nanofiltration Membranes: An Overview

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(1) Input the numerical parameters: number of discretization points, N, grid expansion factor, maximum number of iterations, normalized residuals target and the under-relaxation factor. If the grid expansion factor is higher than one, the distance between consecutive grid nodes expands by this factor from the membrane/solution interfaces to the center of the membrane active layer. If the mesh expansion factor is equal to one, the grid is uniform.
(2) Input the membrane pore radius, r_p, equivalent membrane thickness, Δx_e, membrane volume charge density, c_X and pore dielectric constant, ε_p.
(3) Input the operating parameters: permeate flux, J_v, temperature, T, number of ionic species, N_c, ions diffusivities, $D_{i,\infty}$, concentration of the ions in the feed-solution, $c_{i,b}$, parameters of the mass-transfer correlation, feed Reynolds number, and characteristic length of feed-channel, L.
(4) Initialize the variables $c_{i,m}$, $c_{i,j}$, $c_{i,p}$, Ψ_j, Ψ_p and ε The concentrations, $c_{i,m}$, $c_{i,j}$ and $c_{i,p}$, are initialized with the bulk concentration, $c_{i,b}$, and the initial values for Ψ_j, Ψ_p and ε are taken as zero.
(5) Compute the coefficients of the coupled linearized system of equations.
(6) Solve the previous linear system of equations using LU decomposition with partial pivoting. These calculations are accomplished using the subroutine SGEVS contained in the LAPACK package, which is a collection of Fortran subroutines for solving dense linear algebra problems.
(7) Under-relax the computed solutions.
(8) Update the coefficients of the coupled linearized system of equations using the under-relaxed variables.
(9) Compute the normalized residuals.
(10) Repeat the steps 5–9 until the normalized residuals are bellow a given target.