Electrical Charge on a Nanofiltration Membrane

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Abstract

Nanotechnology applications have become useful in the optimization of filtration membranes. The extended Nernst-Planck (ENP) equation is a complex mathematical model that can be manipulated to calculate and predict flux, rejection, or electric charge across a membrane. Using the MATLAB® software, a program can be created to calculate these theoretical values that will guide the fabrication of membranes with optimized performance as well as shed light on the understanding of experimental data. With this knowledge, progression with nanofiltration membranes will be quickened, and we can sooner be able to use them for more practical applications of filtering water such as the purification and reuse of drinking water.

Introduction

The ENP equation is a complex equation using the ionic diffusion, electric field gradient, and convection of a membrane to solve flux, or the ability of a particular species to pass through the membrane, such that flux is equal to the convection minus the diffusion and electric field gradient. As such, the equation does not have any relation to the mechanistic structure of the membrane, but rather the performance of the membrane.

As a complex differential equation needing the Runge-Kutta method to be solved, manipulation of the ENP equation can be quite time consuming and difficult. Therefore, it is quite appropriate to create a program that will solve for the various variables needed to progress in nanofiltration membrane optimization.

The Runge-Kutta is a method of integration that involves a recursive method of averaging the derivative at several points, then adding this new number to a sum variable until the last point of integration is reached. There are multiple versions of the Runge Kutta with varying levels of accuracy. This alone may require many iterations, so using a computer will not only save time, but allow for a more accurate version of the Runge Kutta, and likewise attain a most accurate result.

Using the Model to Write Program

Using the MATLAB software, it is essential to write the ENP equation and its associated equations into the .m file. The ENP equation solutions must fall under the restrictions stated by the electro-neutrality condition and the under zero current condition. Using the Runge-Kutta method of solving the system of differential equation for the potential and concentration gradients, we are able to move between the flux, the electric potential across the membrane, as well as solve for the rejection of ions within a few more steps.

Future Progress

We were not able to complete the program using the ENP equation but have made some progress with it. As such, the first step is to continue the work we have done, and find a way to complete an efficient and accurate method of programming the ENP equation into MATLAB, or some other programming software application.

A logical next step to take is to continue working with the extended Nernst Planck equation to allow one to solve for any of the many variables of the model. Practically speaking, what is necessary is to find out how to reach the desired settings of the nanofiltration membrane, especially the charge across the membrane. Eventually, with work, nanofiltration will be used more and more for drinking water filtration, to medical uses throughout the world. Naturally this will be expedited by the use of computers wherever possible, such as the math calculations assigned.

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