Congress on Numerical Methods in Engineering
Lisboa, June 29 to July 02, 2015

RESUMO N° 296

OPTIMAL FINITE DIFFERENCES SCHEME FOR THE PREDICTION OF THE TIME LAG IN GAS MEMBRANE PERMEATION

Haoyu Wu, hwu055@uottawa.ca
University of Ottawa, Canada

Neveen Al-Qasas, nalqa027@uottawa.ca
University of Ottawa, Canada

Boguslaw Kruczek, bkruczek@uottawa.ca
University of Ottawa, Canada

Jules Thibault, Jules.Thibault@uottawa.ca
University of Ottawa, Canada

Keywords: Membrane Characterization, Time Lag Method, Variable Numerical Scheme, Finite Differences

Membrane-based pressure driven processes are used in an increasing number of applications. To characterize membrane permeation properties, the time-lag method is currently being used. The determination of the time lag allows finding the membrane diffusion coefficient for a target solute. Our group has undertaken an experimental research program to devise new and improved methods to rapidly and accurately determine membrane properties. Numerical simulations are also performed to gain a deeper understanding on the flow of molecules across the membrane. Numerical simulations offer the opportunity to obtain solution for Fick's diffusion equation under various boundary conditions at which analytical solutions are hard to obtain including membranes having nonlinear sorption behaviours.

This paper is mainly concerned with the selection of the optimal finite differences scheme for solving the Fick's diffusion equation that leads to the accurate determination of the membrane time lag. The pressures as a function of time at both membrane interfaces are predicted from the concentration gradients. The concentration gradient at the upstream side of the membrane is very steep, especially at short permeation time, and to accurately extract membrane properties, it is important to predict very well the concentration gradient at that interface.

In this paper, simulation results for the prediction of concentration profiles and gradients are compared with benchmark analytical equations to assess the precision of numerous numerical schemes tested where the effect of mesh size and time step are quantified. Results show a variable mesh size is required to predict accurately the concentration gradient. The choice of a variable mesh size scheme is important as a compromise must be struck between the smallest mesh size and the time step as it greatly impacts on the computation time. Results also showed that both the implicit and explicit schemes gave similar results.