Innovative process simulation software not only for electromembrane processes

M. Bobák,*, D. Šnita, J. Hrdlička, V. Pelc, T. Kotala

ABSTRACT

An effective tool is required for a successful and effective development and design of technologies. It is often necessary to propose several conceptual designs for the particular application. To assess and compare all designs, the process simulation software is usually used. Especially, for the cases of complex technologies which consist of several unit operations. There are several commercial products allowing comprehensive design, simulation, and optimization, such as Aspen HYSYS® AspenTech (commercial product) or DWSim (open source). Nevertheless, none of them includes directly electromembrane unit operations such as electrodialysis and electrodeionization. Custom unit operations have to be added in the form of user models implemented in various program or scripting languages e.g. Fortran or Python. Our objective is to develop a useful process simulator consisting of: (i) user-friendly graphic interface; (ii) set of solvers for differential algebraic equations; (iii) program for the calculation of dissociation equilibria including the database of chemical compounds and dissociation constants; and (iv) set of unit operations including electrodialysis, electrodeionization, reverse osmosis, different filtrations, simple mixers, splitters, tanks, heat exchangers, pumps, etc.

Keywords: Model; Simulation; Process simulator; Membrane; Unit operation; Electrodialysis; Electrodeionization

*Corresponding author.

Presented at the MELPRO 2014 Conference Membrane and Electromembrane Processes, 18–21 May 2014, Prague, Czech Republic

1944-3994/1944-3986 © 2014 Balaban Desalination Publications. All rights reserved.