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Innovative process simulation software not only for electromembrane processes

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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

1. Introduction

Modeling and simulation belong to the standard professional skills for chemical engineers nowadays. Simulations are widely used in both academic research and industrial practice. Modeling became an integral part of the research and development of new technologies as well as their optimization. Models are a very important tool as they can represent the real systems under relevant assumptions by the set general descriptors. Usually, only the key system properties are studied in order to evaluate the system under different conditions. Nevertheless, models allow the investigation of the specific particular system

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properties in great level of detail. All depends on the model formulation, relevant assumptions, and its appropriate implementation.

There are many simulation tools allowing more or less simplification of model formulation as well as performing the simulation tasks. These tools comprise the equation solvers, commands in common or specific scripting languages, and input and output data files. Simulation products also offer the presentation of the results in graphical form. Simulation programs could be separated into following groups:

(1) Equation-oriented programs based on the input of a set of model equations.
(2) Block-oriented programs based on the graphical representation of the functional blocks representing the mathematical operations and functions such as addition, subtraction, derivation, etc. Blocks are interconnected by the signals representing either the real signals of the control device or the material or energy streams. Example of such a tool is SimuLink®.
(3) Module-oriented are the programs similar to block-oriented. The only difference is that the blocks are models of unit operations or typical processes from internal databases. These models–modules are similarly interconnected by material and energy streams. Example of such a tool is Aspen HYSYS, Aspen Plus, UniSim, or open source DWSim.

The third group of tools is often called process simulators. Models and more generally process simulation environment are effective tools required for a successful and effective development and design of the technologies. Process simulations are beneficial at the initial stage of conceptual design. It allows to propose several variants of technologies and to compare their feasibility. 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. Disadvantage of the current process simulators is the lack of some unit operations even those considered to be robust mature processes. This drawback is frequently compensated by the implementation of the user-defined models often coded in Fortran, Python, or similar scripting language.

The lack of the specific unit operations and corresponding models is the case of electromembrane processes. None of the commonly used process simulators includes directly electromembrane unit operations such as electrodialysis and electrodeionization.

Our objective is to develop a useful process simulator consisting of: (i) user-friendly graphic interface (GUI); (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.

2. Software design

Developed software tool is based on MatLab© Mathworks engineering environment and uses inhouse developed tool including GUI and a set of solvers for algebraic and differential equations DER-PAR®[1]. Generally, there are three types of process simulator implementations. The first is based on sequential modular approach [2] used in e.g. Aspen Plus®. The second approach is equation oriented [3], which is implemented in e.g. PSE's gPROMS®. The third is simultaneous modular approach.

Sequential modular strategy is based on the solution of the flow sheet step by step according to identified calculation sequence. Calculation starts from the stream with known input parameters or the starting stream has to be initialized as a tear stream. The recycle loops have to be decomposed into sequences. The calculation is then iterative and solved by an appropriate convergence algorithm. The sequential modular approach is the first used and is mainly used for steady-state simulations.

Equation-oriented approach is based on the solution of all model equations simultaneously. Thus, it has to incorporate robust solvers for system of linear or nonlinear algebraic or differential algebraic equations depending on whether the simulation is steady state or dynamic. The equation-oriented strategy is mainly used for dynamic process simulations. Sometimes it is known as a global method.

Simultaneous-modular approach is the combination of the previous strategies. There are two levels of the solving: (i) rigorous models of units solved unit by unit and (ii) more complicated structures which are solved globally.

Developed tool is based on the global method (equation oriented) allowing both the steady state and dynamic simulations.

The process simulation software generates automatically the following types of equations:

(1) Balances
(2) Equations of state

(3) Electroneutrality
(4) Chemical equilibria
(5) Phase equilibria
(6) Transport equations
(7) Additional equations
(8) Definitions
(9) Local equations concerned with nodes
(10) Local equations concerned with streams
(11) Global equations.

Complex system of equation is created by a preprocessor module based on flow sheet topology analysis and various input parameters for streams and units operations. Nodes in flow sheet or process flow diagram represent unit operations described by particular mathematical models. Models are describing not only the unit operations (electrodialysis, electrodeionization, reverse osmosis, mixer, heat exchanger, etc.), but also the process streams (models of mixtures, dissociation equilibria, conductivity, pH, enthalpy, etc.).

Fig. 1 represents a basic functional scheme of the process simulator. The procedure of solving of the process task is following. User will draw in GUI the scheme of desired process. Scheme is analyzed in real time and translated into the data structure containing information about the topology and setup of each unit operation and process stream. The data structure is given to preprocessor, which formulates the mathematical description of the studied problem. Mathematical description has to correspond to the solver applied. The task is solved and user can choose the parameters relevant for the process analysis. Software will present analyzed process data in various forms of plots or tables.

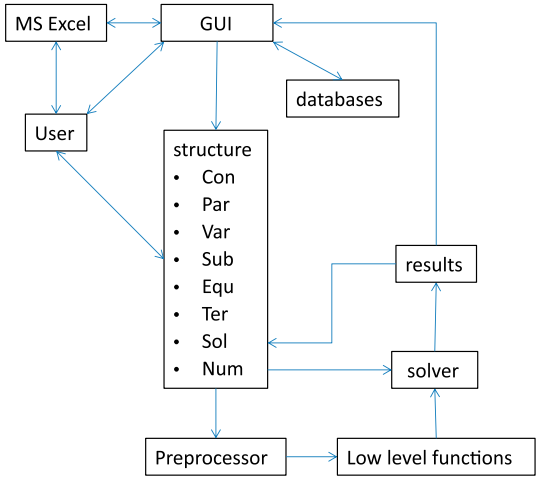

Fig. 1. Program flowchart of the developed process simulator.

3. Graphical user interface

GUI is based on a custom flow sheet developed in MatLab. GUI is composed of main program window with program menu, toolbar with functions, and flow sheet area for process drawing. Users draw the unit operations and process streams directly. This approach allows the definition of customized unit operations. The flow chart is immediately analyzed and translated into a data structure representing the topology, unit operations, and process streams. Unit operations are identified through the function selected and applied on the nodes. Thus, user can select the type of the unit operation from the menu, or program will automatically identify the appropriate unit type according to the node topology. If there are more unit operations corresponding to a particular node, system will display the menu for selection, cf. Fig. 2.

Once the unit operation is selected, user will define the parameters belonging to a particular node and model in another window. Parameters could be e.g. reactor volume, temperature, or chemical reaction specification.

For example, ED stack could be represented by one mass exchanger of certain length or by several shorter mass exchangers in a series. Fig. 3 shows the example of a flow sheet.

In the left bottom corner is the incident matrix representing the relations between process streams and unit operations.

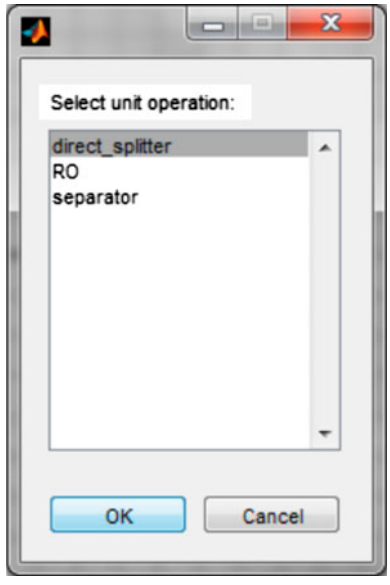

Fig. 2. Menu for selection of unit operation type.

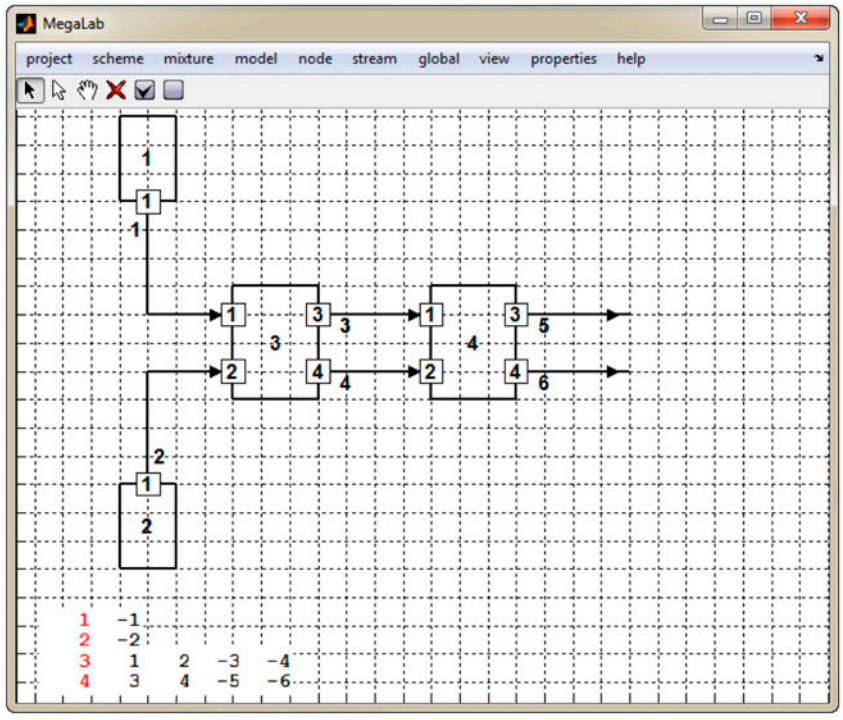

Fig. 3. User created flow sheet.

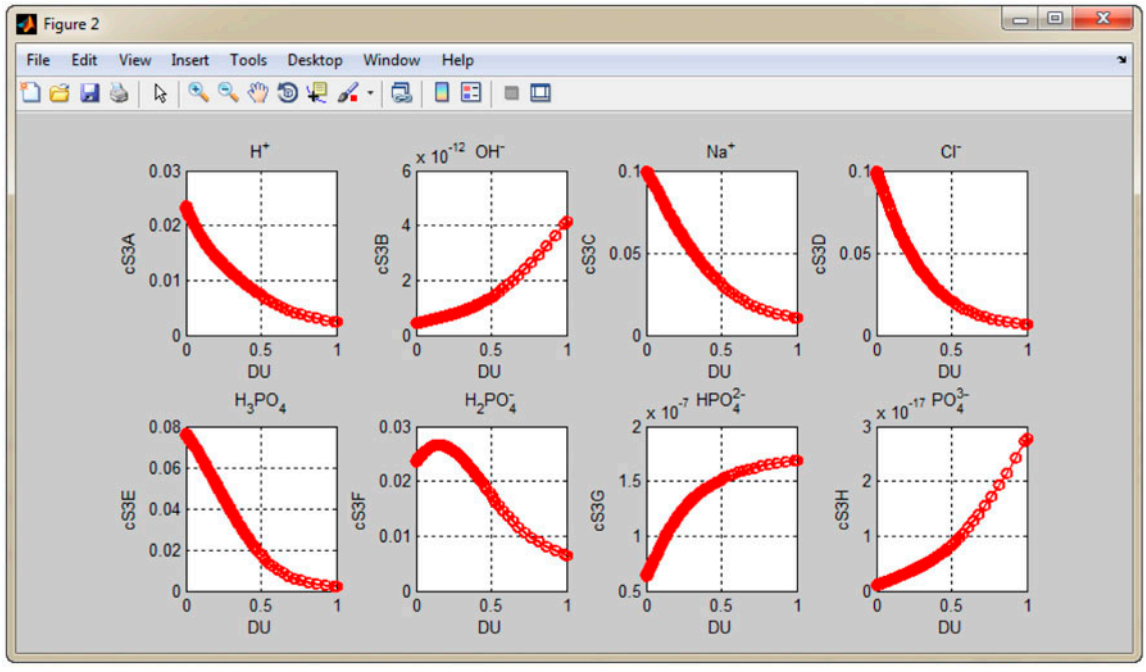

Fig. 4. Graphical output showing the concentrations of the selected components in the output stream from the diluate compartment of the electrodialyzer.

4. Solvers, data analysis, and databases

Process simulator incorporates solvers for mathematical models in the form of linear, nonlinear, and differential algebraic systems of equations. The software uses ODE solvers provided by MatLab and also DERPAR® [1] solver developed on ICT Prague and implemented in MatLab. DERPAR [4] is continuations algorithm predictor–corrector. The solver uses continuation to overcome the convergence problems of Newton's method. In addition, DERPAR® allows a complex analysis of dynamic systems by, for example, bifurcation diagrams.

The set of tools was developed for the analysis and processing of input and output data. Tools translate user input to the form acceptable for solvers and also present the results in the form of plots and tables. An example of the output is in the Fig. 4.

Software also includes following databases

(1) Chemistry—mixtures, components, and reactions
(2) Topology—nodes and stream
(3) Unit operations—mixer, splitter, reactor, exchanger, etc.
(4) Results—for users
(5) Files—for IT's

5. Conclusions

We have developed a novel process simulator, which is primarily focused on the simulation of integrated processes including membrane and electromembrane unit operations. The implementation is as general as possible to allow the simulation of a wide variety of systems encountered in industry. Software is based on global equation-oriented approach and it can be used for the analysis of both steady-state and dynamic problems. The future work is focused on the implementation of a broad range of unit operations to allow simulate large, complex processes.

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