BatchReactor

Simulation of Batch Reactors

Reducing production costs, responding to environmental or safety regulations, saving time in scale-up phases and new products launch... BatchReactor allows chemists and process engineers to rely on a dedicated tool to achieve these challenges. BatchReactor offers a comprehensive list of features allowing simulation of almost all batch reactors in chemicals, bio-based industries, pharmaceuticals…

BatchReactor demonstrates to be very useful for:

- evaluating the possibility of a new production in an existing reactor,
- running 'what if' studies such as loss of the cooling system,
- developing a strategy to control the reactor,
- reproducing lab experiments to pilot plant and production,
- operators training,
- evaluating the VOC emissions,
- keeping the knowledge gained on a synthesis by archiving its model,
- reducing batch times and product waste...

- **A detailed modeling of the reactor** (heating/cooling system, condenser…).
- **A reactional model fitted on available experimental results.**
- **A thermophysical model suited to the problem to be addressed.**
- **A reliable description of the production recipe.**
- **A scale-up tool for the vessel and the mixing device.**
- **A user-friendly interface, fast calculations and easily exploitable results.**

ProSim

Software & Services In Process Simulation

We guide You to efficiency

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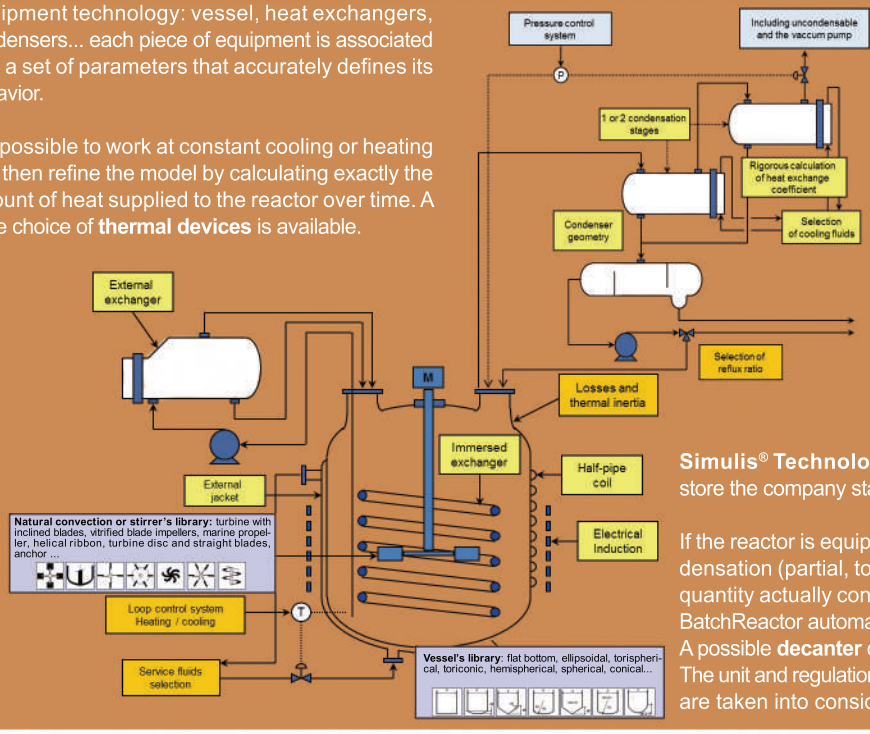
www.prosim.net
info@prosim.net

A very detailed representation of the reactor and associated equipment

Equipment technology: vessel, heat exchangers, condensers... each piece of equipment is associated with a set of parameters that accurately defines its behavior.

It is possible to work at constant cooling or heating and then refine the model by calculating exactly the amount of heat supplied to the reactor over time. A large choice of **thermal devices** is available.



The equipment can be selected in the standard libraries or can be configured:
- vessel bottoms: flat, hemispherical...
- industrial or laboratory reactors
- agitators (simple or multiple): turbines, impellers...
- immersed exchanger: coil...
- wall exchangers: half-pipe coil, external jacket
- external exchangers with circulation
- walls materials: glass-lined steel...
- thermal fluids

Simulis® Technologies allows users to manage the equipment and store the company standard equipment.

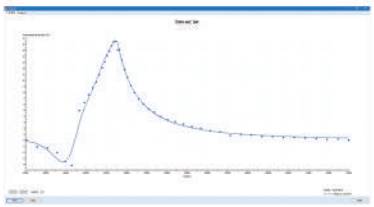
If the reactor is equipped with a **condenser**, it is possible to set the condensation (partial, total or sub-cooled) but also to calculate exactly the quantity actually condensed over time. For shell and tube condensers, BatchReactor automatically calculates heat exchange coefficients.
A possible **decanter** can also be modeled .
The unit and regulation control systems (PID...) for the various parameters are taken into consideration by BatchReactor.

Various reaction models and powerful kinetic fitting tool

Instantaneous, equilibrium, balanced, reversible or irreversible reactions can be described. Combined with the consideration of kinetic reaction laws (Arrhenius, Langmuir Hinshelwood…) they give BatchReactor all its power. Other laws (e.g. biological) can be described thanks to the user mode: there is practically no limitation concerning kinetic models.

If not available, **Simulis® Kinetics** provides the parameters of the kinetic laws and/or the reactions heat required to model the reactor from experimental data obtained in the laboratory: concentration versus time; calorimetric (exchanged heat obtained from laboratory reactors).

Depending on the available tests, kinetic parameters can be fitted: pre-exponential factors, activation energies and orders of reactions. These parameters are obtained together with their confidence intervals to assess the relevance of the model.



Kinetic parameters identification from experimental data

A flexible and efficient thermodynamic package

For thermophysical properties, several modeling levels are possible. In the case of a liquid single-phase reactor, bulk properties may be sufficient. For multiphase systems or a more detailed analysis, BatchReactor automatically calculates the thermophysical properties of the phases in the reactor over time by taking advantage of the powerful thermophysical properties and phase equilibria calculator server developed by ProSim:

- a property database of **more over 2300 pure components** built from AIChE's DIPPR® database.
- an extensive set of **thermodynamic models** for calculating mixtures properties and phase equilibria.
- a set of **services**: estimation of properties, private databases...

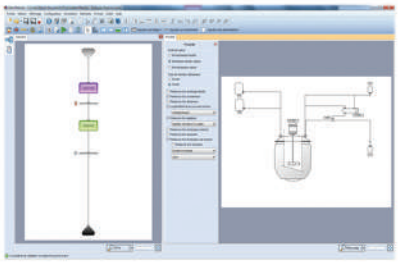
*[Refer to **Simulis® Thermodynamics** flyer]*

Test alternative synthesis routes and new production strategies

The manufacturing recipe or operating mode can be described with successive steps. The description of complete scenarios is then possible.

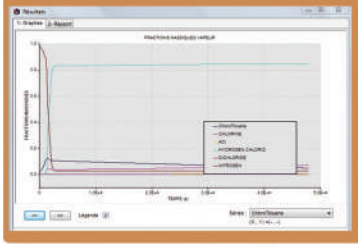
At each step, different operating conditions can be defined:
- isothermal (at fixed temperature or profile) with or without heating/cooling device description.
- adiabatic or with a given heat duty.
- with heat duty depending on the parameters of the thermal device.

At each step, it is possible to modify any of the operating parameters:
- feeds and/or withdrawals (open, closed, flow...).
- temperature, flow of thermal fluid.
- parameters of the mixing device.
- reflux, condensation system, turning off or on a decanter...
- chemical reactions...



Steps are chained automatically with the detection of events described by the user which can be operation duration, but also: temperature, pressure, concentration in the reactor, production quantity, etc.

Easy-to-use interface, fast calculations and easily exploitable results



The intuitive graphical user interface allows to describe easily the different parameters of all models even the most complex.
Thanks to robust and efficient numerical methods, BatchReactor is particularly useful to solve complex cases: highly non-ideal mixtures, processes with discontinuities (mixing interruption, valve opening or closing...).
The time-evolution of all the process variables is calculated: concentration, temperature, pressure, heat of reaction, production yield and composition...
During the simulation, values are displayed graphically making it a practical didactic tool. The results are provided in graphical format, exportable text, tables and graphics.

www.prosim.net | info@prosim.net
Immeuble Stratège A - 51, rue Ampère - 31670 Labège - FRANCE - Tel: +33 (0)5 62 88 24 30
325 Chestnut Street, Suite 800 - Philadelphia, PA 19106 - USA - Tel: +1 215 600 3760