

REACTOR enhancements

Please look in general enhancement for non-program specific enhancements

Version 2.9-156 (10/06/2025)

Version 2.9-155 (17/02/2025)

Version 2.9-154 (21/11/2024)

Version 2.9-152 (12/09/2024)

Version 2.9-148 (18/09/2023)

Version 2.9-146

Version 2.9-144

- The Kinetic fitting model has replaced the macro equation model with in-built function of the same form. This removes inaccuracies introduced by translating the floating point values into the equation modelling environment.
- The reaction model has been upgraded to give the user the option of using either the free format equation model or the in-built mode

Version 2.9-142

- New Development environment libraries
- Restructure on-line help

Version 2.9-140

- An issue with the number of phase being saved in the datafiles has been resolved
- An issue relating to the input limits on the kinetics model bounds has been resolved
- Issues relating to kinetic simulator failing to converge have been resolved
- The Runge-kutta function in the kinetics simulator has been modified to handle the situation where component composition would become less than zero.

Version 2.9-136

- An issue with reaction model editor has been resolved

Version 2.9-132

- Minor editor bug fixes and code updates
- Optimisation bounds (Min,Max) were becoming corrupted). Fixed
- An issue with the user defined kinetic script not compiling correctly has been resolved

Version 2.9-130

- Minor internal bug fixes and code updates
- Component names were not correctly reported when no physical properties file was specified

Version 2.9-125

- Reactor flow sheeting environment has been enhanced with the Treeview facility
- The code has been restructured to aid maintainability and reduce memory requirements

Version 2.9-100

- The kinetic model decimation function can now be based on normalise difference or actual differences between sample data and derived model
- Kinetic model evaluation graph can now be based on experimental data sample time
- An issue relating to numerical overflow in the virtual CPU (user mode/kinetics model) have been resolved
- Issue relating to the feed data editor have been resolved
- Issue relating to the experimental data editor have been resolved
- An issue relating to the physical properties interface has been resolved
- Minor editor bugs have been resolved and general editor upgraded to in-house style

Version 2.9

- An issue relating to the physical properties interface has been resolved

Version 2.1

- An issue with the kinetic model not excluding selected reaction has been resolved.
- An issue with the kinetic report not correctly identifying reversible reaction has been resolved.
- An issue with reaction separation accessing non-existent splitter information has now been resolved.
- Model discrimination can now only be used in batch mode.
- An Excel copy/paste interface implemented in the experimental data editor.

Version 2.0

- An issue with "add separator" in the stochastic optimisation has been resolved.
- An issue with the inclusion of re-mix connections in optimisation /simulation has been resolved.
- An issue with feed-separation connection not being shown on the flowsheet has been resolved.
- The kinetic model section has been enhanced to include a non-isothermal (PBS and UBS) options to calculate heat of reactions.

Version 1.8

- Fenske-Gillian-Underwood implemented in the separators section.
- Iso-thermal temperature optimisation implemented.
- Individual feed optimisation implemented.
- Sample times can are no longer uniform but are now experiment based
- User can now include or exclude specific reaction.
- Bound for NLP optimiser now user configurable.

Version 1.7

- Reactor internal details (tube length, diameter, void fraction) can be specified, for detail reactor design.
- The catalyst pellet shape model has been extended to 3 dimensions.

- Evaporative crystallisation has been implemented. The evaporation profile can be optimised independently of, and simultaneously with feed and temperature profiles for batch and semi-batch crystallisation problems.
- Catalyst deactivation has been implemented. The effect of catalyst deactivation over a period of time can be simulated and investigated.
- A problem with feed editor units has been corrected.
- A problem with thermal equilibrium flag in batch mode has been corrected.

Version 1.6

- Composition/reactor length profiles added
- New Non-adiabatic method of temperature optimisation added. Similar to UBS but uses continuous heat exchange, instead of discrete exchangers. Heat exchanger area and temperature of surroundings are optimisable parameters
- Catalyst effects added. Can optimise catalyst composition profiles, and location of active material within supporting pellet.
- PBS mode optimisation rewritten and vastly simplified. Temperature profiles are now fully user-definable, rather than just optimisable. Profiles are now defined using 6 continuous parameters.
- More continuous variables added to NLP optimiser.
- Addition pre-defined objectives implement for batch and crystallisation modes.

Version 1.5

- Loading a simulated case, then re-simulating gave different temperature profiles. This has now been resolved.
- Improvements have been made to the non-isothermal temperature optimisation system
- Problem with saving catalyst data resolved
- Enhancement to non-isothermal models
- Multiple Run Mode: Multiple optimisation runs can be performed, without user intervention, to exploit the stochastic optimisation process.
- NLP Optimisation: A non-linear optimiser has been added to complement the existing stochastic optimiser.
- Batch Reactor Optimisation: Feed flow rate, product take-off, recycling, temperature profiles and cycle time, can be optimised for batch reactors.
- Reaction-Separation Systems: Reaction and separation systems can now be optimised simultaneously. Separation tasks and task orders for each separator can be individually optimised.
- User Defined Objective Functions: The optimisation objective can be programmed by the user, to supplement the pre-programmed options of yield, selectivity and conversion.
- User Defined Constraints: Simultaneous optimisation with constraints is possible, for example to minimise cost while achieving a user specified conversion or yield.
- Interactive Flowsheet Editor: The flowsheet display has been made fully interactive, and can be used to modify, as well as view, the optimised flowsheet.

Version 1.4

- Non-isothermal Reactor Design: Targets can be obtained for maximum selectivity, yield or conversion for non-isothermal reactors.

- Optimised Temperature Profiles: The temperature profile through a reactor can be optimised. Control over the complexity of the temperature profiles is maintained to avoid impractical designs being suggested.
- Adiabatic Beds: Adiabatic beds can be used with temperature control between the beds using heat transfer, intermediate feed injection, recycling and splitting.