MANCHESTER 1824
The University of Manchester

REACTOR enhancements

This document summarises REACTOR enhancements and bug fixes by release version, with the most recent changes listed first.

For enhancements that are not specific to REACTOR, see the general enhancements document.

Version 2.9-160 (08/06/2026)

- The zoom slide control in the flowsheet environment has been changed from a linear scale to an exponential scale, giving a more intuitive response.
- The input data table reports have been enhanced to display all data and can now be copied to Excel with correct alignment.

Version 2.9-144

- The kinetic fitting model has replaced the macro equation model with an in-built function of the same form. This removes inaccuracies introduced by translating 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-build model

Version 2.9-142

- New Development environment libraries
- The online help has been restructured.

Version 2.9-140

- An issue with the number of phases being saved in the data files 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 cases 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. This has been 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

- The REACTOR flowsheeting 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 normalised differences or actual differences between sample data and the derived model.
- The kinetic model evaluation graph can now be based on the experimental data sample time.
- An issue relating to numerical overflow in the virtual CPU (user mode/kinetics model) has been resolved.
- Issues 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 has been 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 non-isothermal (PBS and UBS) options to calculate heats of reaction.

Version 1.8

- Fenske-Gillian-Underwood implemented in the separators section.
- Iso-thermal temperature optimisation implemented.
- Individual feed optimisation implemented.
- Sample times no longer must be uniform and can now be experiment based.
- Users can now include or exclude specific reactions.
- Bounds for the NLP optimiser is now user configurable.

Version 1.7

- Reactor internal details (tube length, diameter, void fraction) can be specified for detailed 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.
- Additional predefined objectives have been implemented 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 optimisations 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.