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REX Suite version 3.1

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This document summarizes important additions in REX Suite 3.1
Additions are documented since REX Suite 3.0

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1. New Features

In the Kinetics node, we eliminated the need to specify which reactions are LHHW. The LHHW detection is now done automatically if an adsorption site is assigned to a reaction. The *Rate Equation* and *Notes* column have been removed.

Visualization of the LHHW sites is improved. A new pane now shows the algebraic expression of the LHHW sites in the *LHHW Sites* tab of the Chemistry->Kinetics-> Parameters node.

For single phase projects, molar concentrations can now be reconciled. In past versions, this was only possible for multiphase reactors. The concentration measurements can be loaded in the phase tab of the Measurements->Sets node and selected for reconciliation in the weights node. The predicted values are shown in the Results->Model Data Comparison, Results->Profiles node, and also in the Excel report.

In Optimization mode, constraints for the concentrations in a single phase reactor can be now enforced. The molar concentrations are displayed in Results->Profiles node and in the Excel report.

For a single phase reactor, the direct initialization of the phase concentration variables can now be done in the Initialization Values node.

The content of *Parameter Relationships* and *Order Relationships* are merged into a new *Relationships* node. This new node has tabs where relationships can be enforced as it was in previous versions.

Relationships can also be added among the pre-exponential and activation energies of the LHHW Sites. This is now available in the *LHHW Sites* tab of the new *Relationships* node.

The *Custom View* node for Estimation Results has been redesigned. You may now draw flexible charts with any variable in the x and y axis. For example, you may draw a chart of a

compound yield vs temperature.

A new *Custom View* node is now available in Optimization mode with similar features to the one for Estimation.

The Reactor node has been redesigned. This allows you to define the reactor type, phases and other specifications for the reactor in one place. The old Phases node has been removed.

For single phase CSTR reactors, you may now define Intermediate Separation streams by entering a percentage of the phase removed. In that case, all compounds are removed by the same percentage specified for the phase.

User-defined conversions can be added to the objective function for Optimization mode.

In Estimation mode, the values of derived quantities are now reported at the integration(collocation) points. This allows for better charting of these variables in the Model-Data Comparison charts. Also, the values of PseudoCompounds and Derived Quantities are reported for all the collocation points in the Results->Profiles node and in the Excel report.

The Chemistry tree has been rearranged: Units Configuration node is located first, and the PseudoCompound node is placed just after the Compounds node.

The Checkmodel feature now classifies messages as Warnings and Critical issues. Model runs are disabled until all Critical issues are fixed. An override of this check is available in the Advanced Options tab of the Solution Options node.

Abbreviation for compounds, reactions, pseudocompounds and derived quantities are deprecated. The names defined for them are used throughout the project.

Longer names (up to 40 characters) can be used for Compounds, Reactions, PseudoCompounds, Derived Quantities, Sets and Cases.

When deleting any row, the default option in the confirmation message box is changed to OK.

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2. Changes and Bug fixes

In addition to the above, this version also includes improvements to the installation and minor bug fixes.