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REX Suite version 3.2

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This document summarizes important additions in REX Suite 3.2
Additions are documented since REX Suite 3.1

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1. New Features

The REX Library has been redesigned completely to include both chemistry and experimental data. The Library content is now shown in the Projects->Library node. Data from previous versions of the Library are not converted automatically into the new one. You may publish any project to the Library.

Mass Density is a new option for Concentrations in the Units Configuration node. By using this feature, you can work with mass units throughout your project. This feature is mostly intended for bioreaction models.

Stoichiometric coefficients can be also estimated for the reactions. By enabling this feature in the Estimation node, the Stoichiometry tab is shown in the Estimation->Parameters node, where you can define the bounds for the stoichiometric coefficients.

Bioreactor models with intracellular and extracellular reactions can now be modeled. This feature is activated when the Bio Cell model is enabled in the Chemistry node.

The Chemistry->Cells node is shown only when Bio Cell models are enabled. Likewise, the Chemistry->Catalyst node is only shown when the Detailed Catalyst Model is enabled in Chemistry node.

LHHW Site constants can now be optimized by setting bounds in the Estimation->Parameters node.

Model equations are displayed in Chemistry->Rate Equations and Estimation->Results->Rate Equations nodes. Reaction Stoichiometry, Reaction and Compounds Rates, LHHW Sites and Pseudo-Compound formulas are shown in an easy-to-read form.

In the Solution Options node, a new option “Significant Figures for Initialization Values” allows you to change the number of significant figures reported for the compound profile values and kinetic parameters. In general, having more significant figures improves

initialization leading to faster execution. The default is now increased to seven digits instead of five.

The manual entry of Data Points in the Measurements->Sets node is improved. You can add a new row by entering data in any column on the row with the (*) symbol.

In the Reactor node, the Constant option is deprecated for Temperature, Pressure, Volume and Flow. To enforce constant value in estimation mode, use the “Interpolated” option and enter constant values in the experimental set. For Optimization mode, use Constant-Optimized and then fix the bounds in the Design Values node. (The Constant option has been preserved only for Flow in a Recycle reactor)

For batch reactor with Catalyst Mass as reaction basis, catalyst mass is interpolated using the experimental values entered in Experiments->Measurements->Sets node.

The Notes node was redesigned to have a more compact format.

A new Focus option (Right-click on Projectname node) allows zooming on a particular project when you have many projects in your workspace.

The ‘Backward’ reaction is now renamed as ‘Reverse’ reaction.

Column Flow Type in the Flows node is not shown anymore.

Catalyst Surface Area option for for Rate Basis in the Units Configurations node is deprecated.

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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.