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REX Suite version 2.9
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This document summarizes important additions in REX Suite 2.9
Additions are documented since REX Suite 2.8

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1. New Features

The 95% Confidence interval for estimated kinetics parameters are now available. This feature can be enabled in the Run Estimation→Solution Options node.

Bounds on the reaction rates can now be enforced in the Estimation→Parameters node. In previous versions, only bounds on the kinetic parameters were available.

For an LHHW Site that is selected as “Estimate” in the Estimation node, its parameters are always estimated, regardless of whether it is associated with one or more reactions that are fixed. A message indicating whether the site is associated with fixed (non-estimated) reactions is shown in the Estimation node.

The maximum number of finite elements allowed is increased from 20 to 30.

When the amount of finite elements is decreased, the profile is now re-initialized using interpolation. Previously, profile re-initialization was done only when increasing finite elements.

Additional variables can be minimized or maximized in the Optimization mode. Objective function weights can be set for variables like Time, Catalyst Mass, Volume, Temperature, etc in the Objective node.

In Optimization Mode, if there are multiple cases, they are run in parallel using threads. That allows more than one case to be run at a time, leading to a reduction of the total execution time.

The following nodes have been merged together:

- Chemistry→Kinetics→Parameters and Chemistry→Kinetics→LHHW Sites merged into the Chemistry→Kinetics→Parameters node
- Estimation→Kinetics and Estimation→Kinetics→LHHW Sites merged into the Estimation→Parameters node
- Results→Parameters and Results→LHHW Sites merged into the Results→Parameters node, which now shows results for Mass Action, LHHW Sites and Confidence Interval in tabs.

In the Estimation node, the tabs are merged into a single view.

The charts shown in the Estimation→Results→Model-Data Comparison and Yield-Conversion nodes can now be customized. Right clicking on the chart allows you to select options for the Show Series combo. With this option, you may choose to show only Experimental Data, only Calculated Values or both.

When “Show Parity Plots” is enabled in Estimation→Results→Model-Data Comparison or in Yield-Conversion nodes, a correlation index is shown to quantify the model deviation from data. More details are provided in the Help section.

In the Projects node, a new column for Display Order allows you to sort the projects as desired. The ordering in the list can also be changed by dragging the individual projects to a different row. Additionally, you may drag the ProjectName nodes in the tree to reposition projects.

You may make a project inactive by right-clicking the project node. You can also see the list of inactive projects with the possibility of switching some of them to Active status.

In Compare Projects, orders for Reactions and Site Terms are compared in a new node and thus separated from the PreExponentials and Activation Energies comparison to enable easier and quicker comparison.

New GAMS version 21.1.1 is used for running the models. The Conopt2 solver is not available anymore. Old projects that had Conopt2 selected as the solver option are automatically updated to run with Conopt3.

Graphviz visualization software for Reaction Traffic is updated to version 2.30.1.

When selecting a numerical cell, the Format icon is enabled in the toolbar to choose among several numerical formats.

A ‘Show Image’ button has been added in Reaction Traffic→Options node, to go directly to the parent node that has the reaction traffic chart.

Reactions Rate units are also indicated in Units Configuration node.

In Node Chemistry→Kinetics it is now shown the reaction stoichiometry. Column for Arrhenius Type is not shown anymore.

Excel Report: Average values for LHHW sites and each term are now reported.

For a reaction where both the forward and reverse rates are fast, a test is done to advise that the reaction is fast enough to consider it as equilibrated. An equilibrium icon is shown in the Results→Parameters node in that case.

A Navigation Bar is implemented to the left of the REX windows, containing the Views available, together with the Tree for the selected view.

Problem Steps Recorder can be enabled in the Help section of the Top Menu. That will record snapshots of your steps in REX, so that you can send them to Optience for assistance.

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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.