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REX Suite version 2.6
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This document summarizes important additions in REX Suite 2.6
Additions are documented since REX Suite 2.5

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1. New Features

The weights node has been completely redesigned to facilitate the automatic weighting of new or modified experimental data, without affecting the weights of old data. You can also generate automatic weights for a customized combination of sets and variables.

The Set Variance method for weighting has been eliminated. Projects from previous versions that have that option selected are converted to the Hybrid weighting option. There is no change however to the weighting factors, so model results will not be affected.

For a Multiphase system with Liquid and Gas phases, the Henry model is enhanced to also allow loading solubility parameters of volatile species with respect to several solvents. The old method of using Henry solubility with respect to the whole liquid mixture is still available.

When a LHHW Site is defined as estimated in Estimation node, but one or more reactions associated to that Site are not included as estimated, the Site parameters are kept fixed during an estimation run.

You can now compare projects to find the differences between them. To open the Compare Projects tool, please go to :
Start->Program Files->Optience Corporation->REX Suite-> Compare Projects.
A Help document with examples is also available for this feature. You may access it by pressing F1 in any node or grid of the Compare Projects, or locate it in C:\Program Files\Optience Corporation\REX UIs\Compare Projects.chm

An alternative way to change the order of appearance for rows by relocating them with the mouse is available in Compounds, Reactions, Profile/Order Relationships, Experiments and Case Design nodes. This procedure is explained in the Frequently Asked Questions section of the Help.

A new Custom View node in the Estimation->Results tree facilitates the manipulation of experimental and predicted values for all variables and all sets at the datapoints. Layout changes and special filtering of data can be performed.

The Check Atom Balance node is moved inside the Estimation->Experiments tree to facilitate the reviewing of experimental data.

In Charts of Estimation->Results, when enabling Parity Plots, auxiliary lines can be displayed to identify points at which the model prediction is higher or lower than a given error percentage.

The Steady State column in the Compounds node is not shown anymore. The steady state condition is now automatically detected and enforced for the Catalyst Complex species when dealing with a Detailed Catalyst model.

Units can be defined for PseudoCompounds and Derived Quantities. The user-defined units are shown for these variables in other grids and charts where they are displayed.

In the Units Configuration node, an additional way to perform automated units conversion of the experimental data and kinetic parameters is available.

For Detailed Catalyst model in Mode Estimation, surface fractions of free sites and adsorbed species are shown in Model Data Comparison node.

Sorting of rows is enabled in the Estimation->Results node, by clicking the column header.

In node Estimation->Results-> Parameters / LHHW Sites, you may hide the compounds orders for the reactions in order to have a more compact view of the PreExponential factors and Activation Energies.

In the charts of the Yield-Conversion node, Ignore Zero Measurements also hides the experimental 100% conversion values resulting from zero compound measurements.

In Optimization mode, the initialization for the variables that are Control Optimized is improved. When there are one or more variables selected as Optimize in Control Profiles, a new Initial Control Profile subnode appears under Initialization Values, containing initial values for those variables.

In any REX node, you can open the related HELP page by pressing F1 key. It is no longer necessary to be in an active grid before pressing the F1 key.

In Projects->ProjectName node, the default tab was changed to now show the Solution Summary.

The Layout of nodes can be saved when enabling Save Layout in the Top Menu, inside View->Layout.

REX 2.6 can import REX files exported from REX 2.1 or newer. You may also restore REX databases exported from version REX 2.1 or newer.

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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.