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REX Suite version 4.0

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This document summarizes additions in REX Suite 4.0
Additions are documented since REX Suite 3.9

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1. New Features

A Charts Node is provided in the Experiments Tree to graph Measurement values

New nodes: Estimation->Results->Model Data and Optimization->Results->Profiles.
Flexible charts for compound moles, concentration, yield, conversion and selectivity:

- Any variable can be selected for the X axis
- Different series types can be displayed in the same chart. For example, Compound moles/yield chart with respect to Initial Temperature
    - Display All, or just Experimental/Calculated for Estimation mode
    - Select First/Last points instead of entire series
    - Values child node to efficiently select/export to Excel.

Estimation / Optimization Results:

- Export to Excel action in most nodes of this tree.
- When running from any of the Results nodes, the values are updated after the run without the need to manually refresh.
- Legacy tree contains deprecated Chart nodes

Default Upper bound values for Mass Action PreExponential and Activation Energy have been set to 1e9 and 100 respectively, irrespective of units chosen. Initial PreExponential value is set to 0.1. In previous versions, they were all set to zero and so values had to be entered by the user.

Two initialization methods to help convergence in newly created projects. Either of these options could be useful in the early stage of getting a feasible simulation.

- *Autoinitialize Parameters* option in Estimation->Solution Options node.
  This feature does an internal initialization of Preexponential and Activation Energies. This option is enabled by default for new projects, so when estimating them with Warmstart = Experimental Data, the user entered values for preexponential and activation energies in Estimation->Parameters node are ignored as it uses the internally calculated parameters. After getting a feasible solution, you must execute the *Initialize from Results->All* action: this will automatically switch off the *Autoinitialize Parameters* option and you can rerun starting from the last solution point as usual.
- *Initialize Parameters* action in Estimation->Parameters node.

This method calculates preexponential values for the mass action Preexponential and Activation Energies to be used and displays the initial estimates in the node. Also, compound profile values are updated in the Initialization Values node. When executing this action, the previous option of *Autoinitialize Parameters* is automatically switched off. You can also run with *Warmstart=Use Provided Initial Values* to start with the calculated compound profiles values.

For Conopt4 solver, the default for *Upper bound solution values and equation levels* option is changed to 1E+15

Model run is now enabled in all subnodes of the Results node.

A REX Cleanup tool is now packaged with the installer to assist in cleaning up partial installations

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2. Changes and Bug fixes

Issues related to French regional format have been resolved in Experiments nodes as well as Solver node

The automatic correction of names that contain invalid characters (such as #,@...) has been restored

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