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REX Suite version 3.4
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This document summarizes important additions in REX Suite 3.4
Additions are documented since REX Suite 3.3

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1. New Features

The most significant addition is the ability to model Membrane Reactors in REX. This feature is available for PFR and n-CSTR reactors. The Gas-Gas option must be selected in the Reactor node and Diffusivity parameters must be entered for the species that diffuse across the membrane.

A new variable, Specific Membrane Area (SMA) is introduced to account for the ratio between membrane area and the amount of catalyst mass or reactor volume. For a tubular reactor, you may provide a profile of SMA with reactor length in both Estimation and Optimization mode. This allows to model scenarios where we wish to have a profile with varying membrane area along the reactor length.

For batch reactor with one or more Inflow or Outflows, a new node called 'Integrated Flows' is available in the Results tree of both Estimation and Optimization modes. This shows the accumulated amount of each species that entered or left the reactor through the inflows and outflows. In Estimation mode, the "experimental" integrated values are also shown which is obtained by interpolating the experimental values of flows and concentrations entered in the Measurements→Sets node

In Estimation→Experiments→Measurements node, Compounds are disabled for the phases they do not belong to as defined in the Reactor→Phase Distribution node. Similarly, in the Weights node the compounds checkboxes are only enabled for phases where the compounds are present and for which experimental values are enabled in Measurements node.

There is a change in the integration of single phase batch outflows defined as *reaction mixture*. For experimental values, we now use interpolation of experimental phase concentrations as provided in the Measurements nodes. In previous versions, the calculation was done by using the total moles value to get the phase concentrations. This change only affects the results for the Experimental reported values for Yields, Selectivity and Conversions for the special case of single phase batch reactor. This change was needed because in early versions of REX, it was not possible to enter phase concentration

measurements for a Single phase reactor, so there was no option but to use Total moles.

In all the Rate Equations nodes, the equilibrium equation expression is shown for the reactions selected as equilibrated.

2. Changes and Bug fixes

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