Run Files Faster with Column and Recycle Auto-Restarts

As a rate-based modelling tool, ProTreat® simulations solve many times more equations than the old school equilibrium stage models. This is inherent in rate modelling and is necessary for rigorous, reliable, and predictive models. Often, this may mean that for every small variation in the simulation, one has to re-run and re-converge the simulation, which always involves additional computing time. However, there is good news! Starting from ProTreat® v6.3, there are ways to setup auto-restarts for columns and recycle blocks that greatly decrease the time to converge. Particularly, when the same base file is being used to run difference scenarios, simulations will now take a small fraction of time needed by earlier versions.

Recycles

The Recycle block is equivalent to the tear stream in other simulators and provides initial stream estimates to initiate calculations in recycle loops. Initial stream estimates are used only for the first recycle loop iteration. However, if the recycle block initial stream estimates are far away from the eventual solution, the number of recycle loops required for convergence will likely go up. However, if the option to "Use results from last run for Initial Stream Estimates" is selected, as illustrated in Figure 1, the results of a previous flow sheet simulation will be used instead of the user specified estimates. If the box is not checked, ProTreat will always use the user-specified estimates.

Columns

In the case of columns, the "Initialization" tab of the column dialog box allows you to specify how ProTreat® initializes temperature, pressure, and composition profiles throughout the column. The results of a previous column simulation will usually be a better estimate of profiles than heuristically determined ones. Selecting "Initialize from last run" as illustrated in Figure 2, will therefore, likely reduce column convergence time (compared to initializing from heuristics). The "Initialize from last run" option is also useful if you are doing a parametric study by changing a small number of process variables, such as composition and temperature of a feed stream, column weir height, or packing type.

Occasionally one may encounter a particularly stubborn-to-converge column. Here, it will be useful to "seed" the results of the difficult case using the results of a simpler column. Selecting "Initializing from another file" allows you to point to the file which
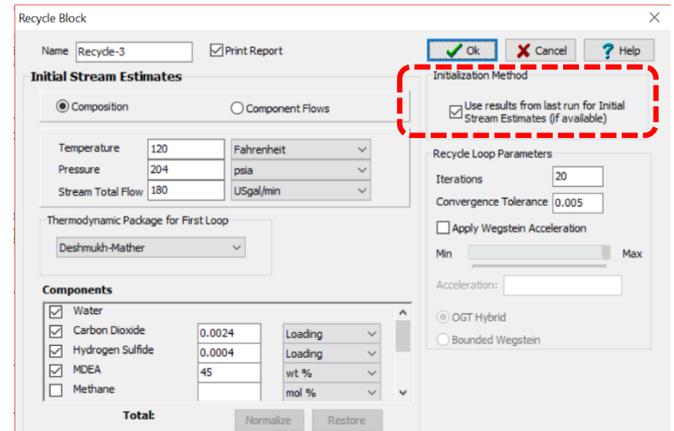
contains the results of the initializing column.

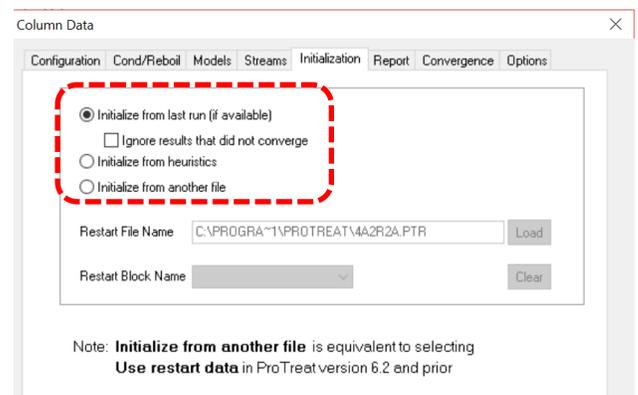**Figure 1 – Selecting Initialization Method for Recycle Blocks**

Figure 2 – Selecting Initialization Method for Columns

PROTIP: If a results (.PTR) file with the same name as the current drawing (.PTD) file does not exist, the column will initialize from heuristics. The results (.PTR) file from the last run must have the same column name, flowsheet components, and number of sections (but not necessarily the number of segments); otherwise the column will initialize from heuristics. Additionally, adding a condenser, reboiler, or Stahl column will force the column to initialize from heuristics.

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