



Setting Convergence Tolerances

In any simulation, there can be several levels of iterative calculations that take place when the simulator is running. Modern thermodynamic models are almost always iterative and their execution is at the bottom of all other computations. At the next level of possible iteration are equipment models (e.g., absorbers, flash tanks, Sulfur converters) because they may also be iterative in themselves, quite apart from the thermodynamic models they may use. There may also be several nested iterative procedures within a single equipment model. At yet a higher level, a series of equipment items may be strung together in a recycle loop; indeed, there may be loops within loops. An example is a Sulfur plant with upstream and downstream gas treating units such as an upstream AGRU and a downstream TGTU recycling acid gas back to the start of the Claus unit. At issue then is how to set convergence tolerances so that each iterative process is capable of converging without interference from the iterated results of inner loops.

Figure 1 shows a simple absorber and regenerator in the amine circuit of a conventional gas treating plant (AGRU). The recycle loop is the amine circuit. The functionality of the Recycle block (circled in Figure 1) was the subject of the January 2019 issue of ProTips and will not be repeated here. Suffice it to say that it is an iterative computational block whose convergence tolerance (Figure 2) must be set to a larger value (i.e., looser) than the tolerance for any other block embedded within the recycle loop, i.e., for the columns and flash tanks, and for the thermodynamic calculations. It ensures the recycle loop converges.

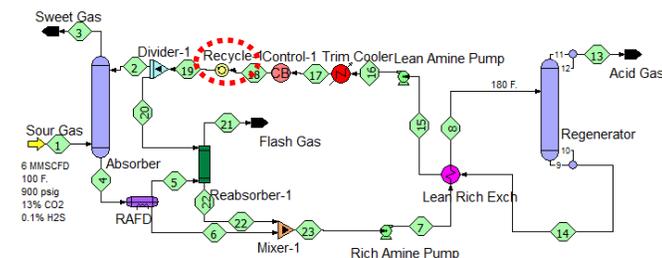


Figure 1. Example Recycle in Amine Circuit

The Recycle block might have its tolerance set at 0.002 (0.2%), for example. In that case the column blocks must have their tolerances set to smaller values than that, e.g., perhaps 0.001 (0.1% relative error), otherwise the Recycle block is being asked to solve to a tighter

tolerance than the random variability in its input data.

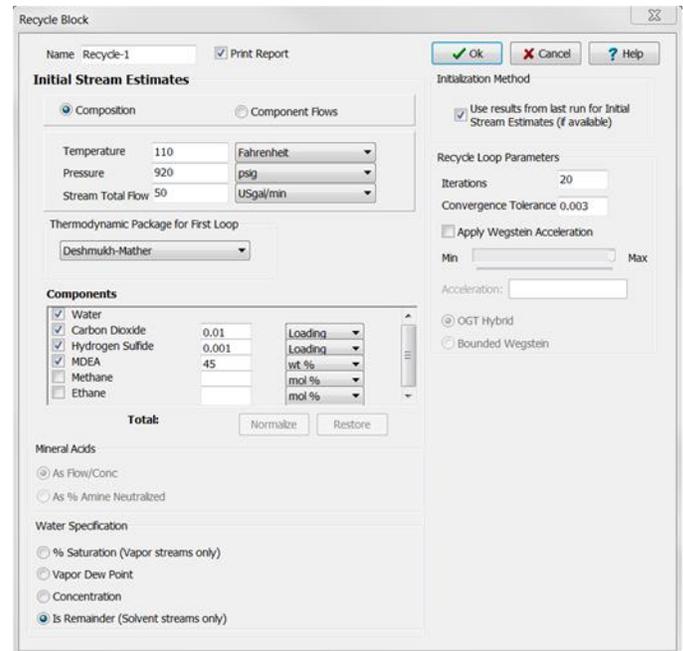


Figure 2. Recycle Block Data Input Dialog

ProTreat and SulphurPro automatically set the tolerance for internally nested loops (e.g., thermodynamics and iterative submodels) within a unit operation to smaller values than for the unit operation itself. Of course, at the very bottom of the chain is the allowable error in the thermodynamic calculations. By default this is set to 0.0001 (0.01%), although you can enter any other value you like (although advisably not larger).

PROTIP: When there are several levels of nested iterative computational processes (loops) in a flowsheet, the innermost loop must be converged the most tightly and the outermost least tightly. Other loops between these extremes should be converged to levels of tightness that progress from most to least as the loops range from innermost to outermost. Be careful to observe this rule with nested flowsheet recycles.

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