ICE Module I - Batch Process Development Memo 5

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SUBJECT: Instructions for using ABACUSS II on MIT server

The attached document explains how to access ABACUSS II (Advanced Batch And Continuous Unsteady State Simulator). ABACUSS II will be used to simulate the distillation tasks and the first reaction task during the design of the Lucretex monomer process. You will be using ABACUSS II's dynamic simulation features. Dynamic simulation is the use of mathematical models to predict the time dependent or dynamic behavior of a chemical process (as opposed to steady-state simulation, which is only concerned with predicting the steady-state of a process).

In addition, you may find the following points helpful:

- Save your work frequently; the editor has been observed to crash during some delete/cut operations.
- Error messages from the compiler can be accurate without being revealing. You may have to change your assumption about what might be wrong to interpret the message correctly. For example, a coding error in line n-1 can cause a reported error in line n; line n may be entirely correct, of itself, but the compiler interprets it in the context of line n-1.
- Most ABACUSS statements reside inside the BLOCKS. However, INCLUDE statements are an exception.
- BLOCKS require END statements. Many of the sections within blocks do not require END statements, but some do. Among others, the WITHIN structure, and the RESET and REINITIAL sections in the SIMULATION block, require END statements.
- Remember to distinguish = and :=.
- Distinguish among different types of names:
 - file names used by the computer operating system to open and save files. A single file such as PhysicalProperties.ABACUSS contains many MODELs.
 - model names identify general MODELs that contain the parameters, variables, and equations to describe some operation or relationship. MODEL IdealGasEOS contains the ideal gas equation.
 - unit names a UNIT is a particular instance of a MODEL, so that the same MODEL may be used for multiple purposes in a simulation. The pathnames by which variables are identified comprise these UNIT names, <u>not</u> the MODEL names.
 - simulation names the results of a SIMULATION are written in output files that bear the name given to that particular simulation.
- When you have run a simulation and wish to modify your file for a different case, execute "remove from translation" to avoid name conflicts with the previous run.
- Desirable as it might seem, no new quantities may be introduced in a SIMULATION block. This means that you may not, for example, compute the ratio of two reaction products from your results. Any such quantity to be calculated must be written into a MODEL and then DISPLAYed in the SIMULATION.