

SIMULATION BEST PRACTICES WITH CHEMCAD

AND COMMON PITFALLS TO AVOID

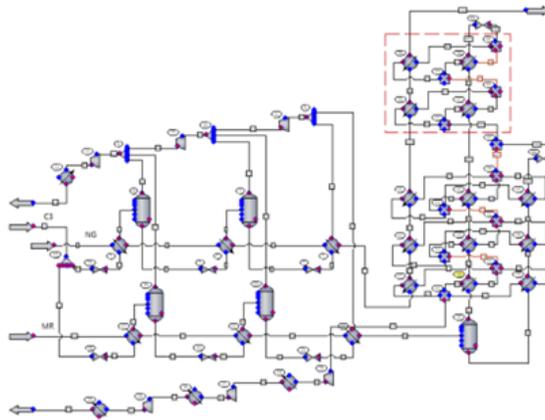
→ INTRODUCTION

The intent of this article is not to teach engineering principles or to limit how the software can or should be used. The guidelines listed here are assembled from decades of simulation experience within the Chemstations CHEMCAD support team, and are based on proven methods for effective process simulation.

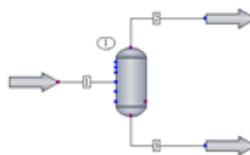
Combined with a solid background in chemical engineering, following these guidelines will enable you to work more efficiently and create a good foundation for your simulation projects.

→ START SIMPLE

Start by building a simulation in simple segments. If you already know all the unit operations that need to be added to the flowsheet, it may be tempting to build the entire process at the beginning. Consider the following example, though: if this flowsheet does not converge, where is the source of error?



It's more difficult to troubleshoot a large simulation. Instead, build and run unit operations one at a time, and check the results as you go.



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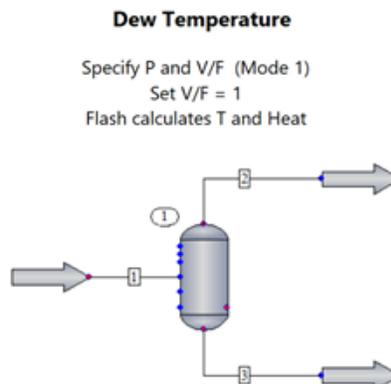
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This way, you can more easily identify what fails or what you've omitted as you build a flowsheet. A converged segment is a stronger starting point for the next segment.

If an operation or segment does not converge, check for error and warning messages. Even if the segment does converge, it's still a good idea to check the Messages pane in CHEMCAD for warnings. While you may choose to ignore warning messages initially, they might later serve as breadcrumbs, leading back to the source of an error that pops up down the road. As your simulation grows in complexity, keep in mind what is needed to solve each segment or operation, such as degrees of freedom.

→ PAUSE FOR A REALITY CHECK

A converged simulation does not mean the results are correct. You should already have a qualitative idea about the expected behavior of your fluid or the process before trying to simulate it. Investigate whether the simulation produces results that make sense. For example, a quick flash calculation to check the dew point of a fluid can determine whether it's an approximate match for the expected value.



Test the system response to possible variations in operating conditions. For example, it would be wise to model temperature variation for a heat exchanger in winter versus summer. Does the model predict a phase change at a higher temperature? Is it correct? The properties and phase behavior calculated during simulation depend on your selected thermodynamic model, so it's critical to examine the model and predicted properties before proceeding.

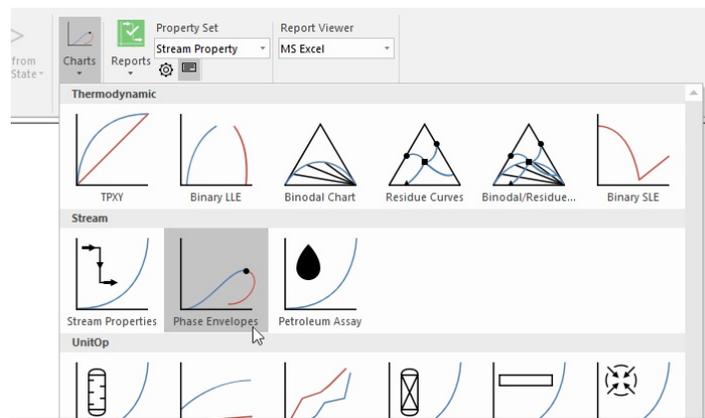


→ GET COMFORTABLE WITH PRACTICAL THERMODYNAMICS

Thermodynamic models determine the phase equilibrium (such as VLE and LLE) and various property predictions throughout the simulation. Different models will give different results at the same temperature and pressure. How do you know which model to choose?

There are several methods for checking the model prediction:

- Examine phase behavior for a single component or a mixture by plotting the phase envelope. Here you can check, for example, whether the model is predicting a reasonable dew point for a gas mixture.



- Plotting TPxy charts will help identify phase behavior between two components, a key to simulating accurate separations. CHEMCAD offers an option to plot charts from any combination of thermodynamic settings for comparison. Here you can check whether the model correctly predicts an azeotrope, for example, and compare one model's performance against another.
- Use a simple flash vessel to quickly test phase separation, or to check properties at various conditions.

When testing model predictions, be sure to test the behavior for the full range of expected operating conditions. Check for the system response to possible variations in temperatures and pressures, as well as increased concentrations of components. For example, consider whether a system with trace water concentration suddenly sees a larger concentration of water. Are the phase separation and concentration of the water components behaving as expected?

Unless you have high confidence in the reliability of your compositional or component data, the recommended approach is to focus on modeling the correct behavior and not looking for an exact match of the values.

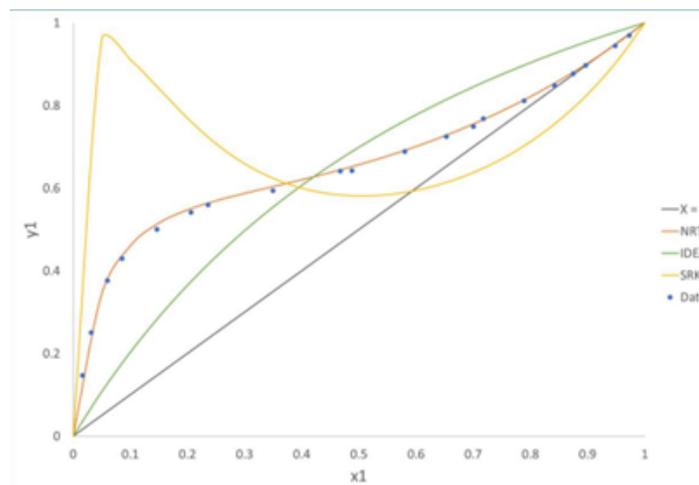


→ CHOOSING THE BEST THERMODYNAMIC MODEL

It used to be that thermodynamic simulation was primarily used by academics with advanced degrees and experts in the field. However, evolving technology and industry trends have shifted this responsibility to the general engineer with a license for process simulation. Even with all the technological advances made recently (yes, CHEMCAD will recommend thermodynamic settings based on selected components), the industry still requires engineers to check their results and make the best model selection decisions.

Knowledge about which thermodynamic settings will work best comes from study and experience. Start by checking articles and other literature to see what has worked for similar systems. There are many resources—including books, journals, and data companies such as DIPPR—that can provide real data. For more advice on where to gather reliable materials for study and data, reach out to CHEMCAD’s support team or check chemstations.com for knowledge articles on the subject.

Real systems are imperfect, clean reliable data can be hard to find, and science has yet to produce a perfect model that can match all components under all conditions. When it comes to choosing thermodynamic settings that will work best for your system, the key is accepting compromises. A model that works really well for certain mixtures at one set of operating conditions may not do well for other components in the system, or at other conditions. Determine what properties and behavior are most important to your project’s interests, and use these criteria as the basis for your model selection.

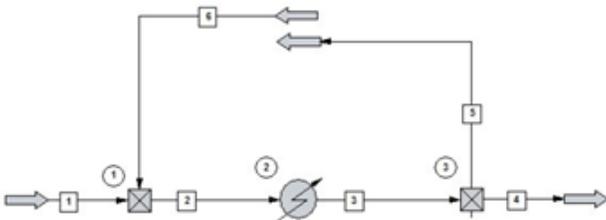
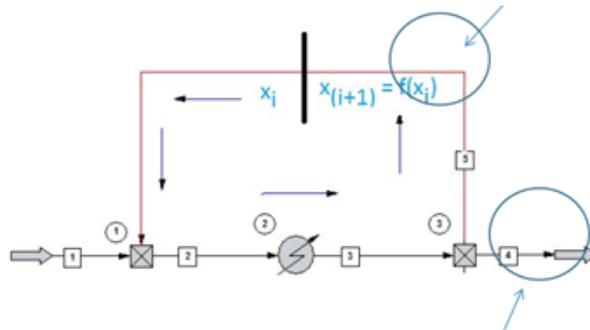


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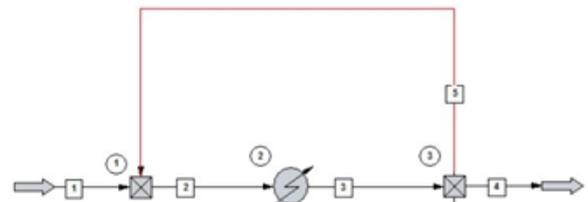
→ ADVICE FOR HANDLING RECYCLES

Once solid thermodynamics are established and the process simulation is built in small steps, it may be time to add more layers of complexity. One such challenge can be adding recycle streams. As noted earlier in this article, the best way to manage more complex processes is to start simple. In this case, that means making a good initial estimate for the recycle rate and letting CHEMCAD calculate the product stream.



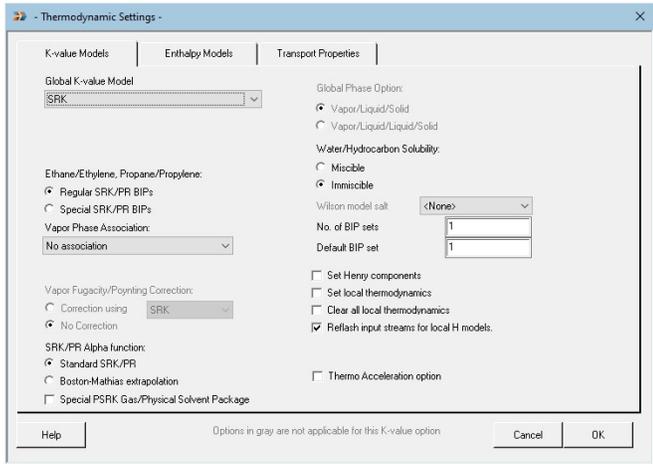
Start by splitting the recycle into separate inlet and outlet streams, as shown here.

Once the simulation has converged, the simulator has a better starting point for when the streams are reattached as one loop.



→ AVOID THE COMMON PITFALLS IN PROCESS SIMULATION

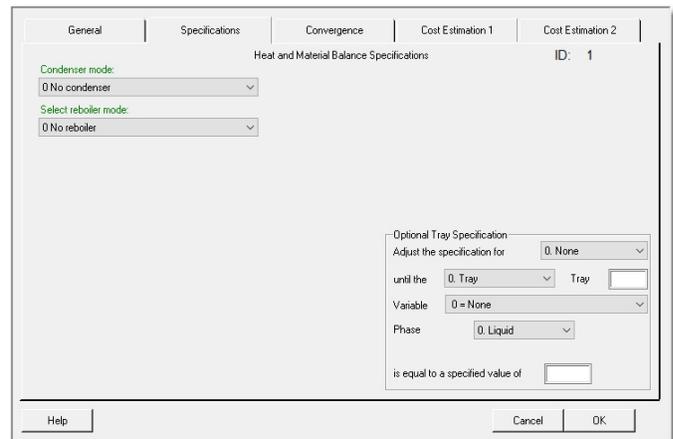
Default values are not necessarily the best starting point for your simulation.



These values or options are designated by the program, and are there to provide a general starting point. Use your best engineering judgement to determine whether the default values are appropriate for your system.

For example, you can browse through the Thermodynamic Settings dialog and consider whether some of the check boxes or radio buttons apply to your system.

Or, after specifying a unit operation such as a distillation column, browse through the other available tabs and menu options. Consider whether you've made the best selections in various drop-down menus, or whether the boxes are checked for appropriate options. If you have any doubts, use the CHEMCAD help system to look up the details of the models or settings you are considering.



Software can't determine on its own when results are not real.

Even after a successful run without error messages, your results could still be unrealistic. If a heat exchanger duty approaches the energy of the sun, for example, an engineer should notice that there's an issue, where a simulator cannot. Or if your thermodynamic model doesn't predict an azeotrope where one exists, a simulated separation may run without error—but it will never match the real column behavior. This is why it's so important to pause and check results as you build the flowsheet, to confirm that the simulated behavior lines up with reality.



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It isn't necessary to match a specific UnitOp symbol to each piece of real-world equipment to get real results.

The CHEMCAD palette provides a wide variety of unit operations, but you may need a piece of equipment that doesn't appear there. The underlying equations and principles behind the unit operations are what really matter, not the icon that appears on your flowsheet.

For example, a symbol representing a centrifugal compressor is available on the UnitOp palette, but if you need to model a more specialized Lysholm screw compressor, that isn't a built-in option. You can still model the Lysholm compressor, though, by adding a series of compressors and air coolers to the flowsheet to model the correct unit operation behavior. Simple icons like a flash vessel, a heat exchanger, or a pipe segment can also represent different equipment or operations to provide qualitative insights into a process, such as how a system reacts to pressure or temperature changes.

Focusing on an exact match between simulation and test data may be a fruitless effort.

Keep in mind the limitations of the model as well as the measured data. Consider the following when matching real and predicted data:

- How accurate are the measurements, and when were the devices last calibrated? If the data accuracy is unknown, the data can still be used to check qualitative overall trends rather than matching data to the decimal point.
- How much confidence is there that the measurements were taken at steady-state conditions?
- Were trace chemicals ignored? Does it matter?
- If the concentration of the contaminants is doubled or tripled, can the correct separation or reaction still be modeled?
- What is the basis of the thermodynamic VLE model? What are the known strengths and weaknesses of the selected model?
- Check to see if any important thermodynamic data is missing. It may be necessary to fill in or adjust BIPs.

→ THE BIGGEST MISTAKE OF ALL?

That would be having questions or doubts and **not** reaching out to Chemstations' support team. Our knowledgeable support staff have decades of experience in process simulations with CHEMCAD, and are available to provide you with guidance and support.

