Getting the Most Value from CHEMCAD

When you've just purchased a new smartphone, do you keep all the factory default settings and jump straight into making phone calls? That would mean missing out on so many features of the technology. While CHEMCAD NXT can be used straight "out of the box" to build and simulate process flow diagrams, to get more value from the technology, consider exploring all the features that can support the daily needs of chemical engineers.

Which model can accurately predict all physical properties for any system under all conditions?

Unfortunately, one does not exist. Predicting thermophysical properties often requires a patchwork of equations and settings. CHEMCAD NXT's Thermodynamic Suggestions tool can recommend settings based on selected components. However, getting accurate physical properties is one of the most critical and universal functions for a process simulator, so there are other tools in CHEMCAD NXT meant to help validate thermophysical properties.

For instance, you can compare several combinations of thermodynamic settings simultaneously using the TPxy diagrams. Also, use TPxy diagrams to visualize the relative amounts of components and phase transitions through the range of process conditions. If experimental data are available, validate the results by plotting experimental data with the simulated data. Not every K-value method can predict an azeotrope. So, if the process involves LLE, use TPxy charts to check whether an azeotrope is predicted and under what conditions. For example, the Txy diagram in Figure 1 can be generated using CHEMCAD to compare the predicted phase behavior from K-value models NRTL and WILS (Wilson) for an ethanol and water mixture.
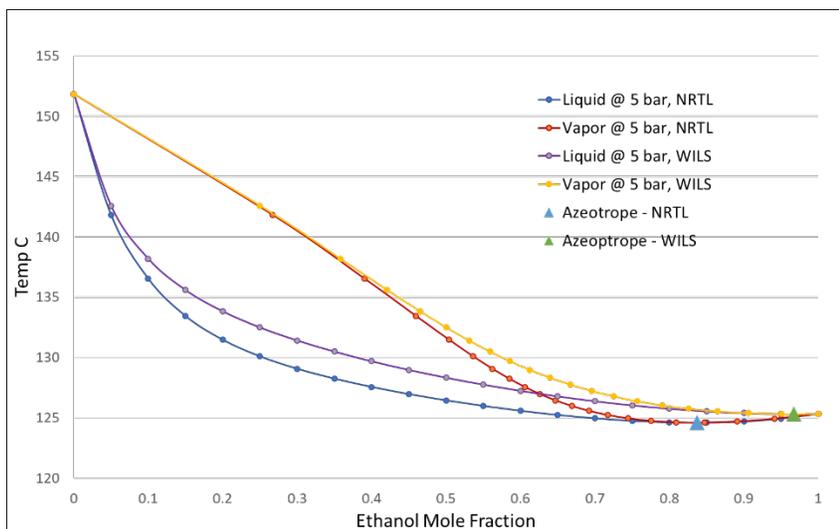

Figure 1 - Txy Chart for Ethanol / Water mixture at 5 bar

While the economic benefits of thermophysical modeling are not easy to quantify, there is a clear advantage to anticipating the phase behavior through a range of process conditions and having the confidence that your model is producing accurate results.

Walking a tightrope in process design? Use CHEMCAD NXT's analysis tools.

Chemical engineering can be a tough balancing act: minimizing capital costs, operating within optimal use of material and energy, keeping within safety and environmental guidelines. CHEMCAD NXT offers a flexible approach to engineering challenges with an array of features designed to navigate complex simulation and optimization.

Engineers can run sensitivity analyses to test system vulnerabilities or to design a piece of equipment. For example, the sensitivity analysis tool can be used to explore operating parameters like how a change in feed composition can affect the product streams. It can also be used for design situations like finding the optimal feed tray location in a distillation column.
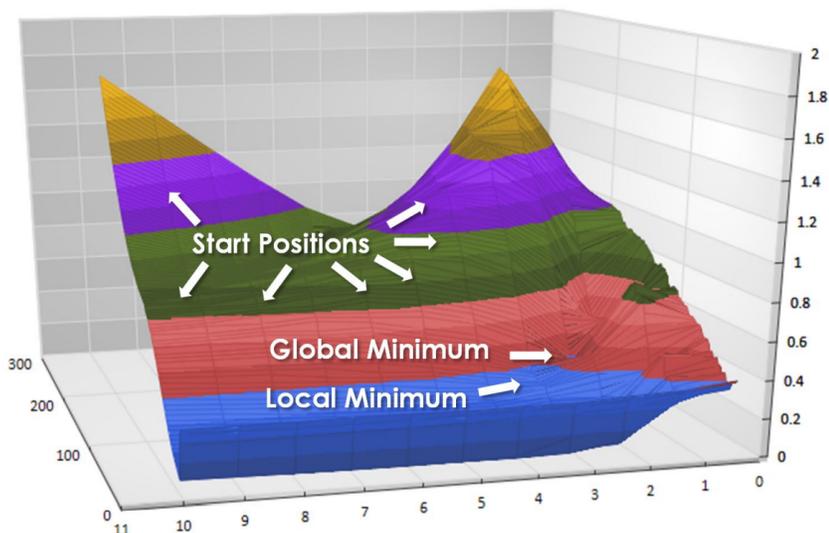

Figure 2 - Optimizing to a global minimum

Can the process be further optimized? CHEMCAD NXT's optimization tool can help to search for the optimal variable settings in your simulation--for example, to minimize operating costs or maximize product quality. Figure 2 illustrates the potential for an optimization calculation to get stuck at a local minimum. However, because CHEMCAD NXT can run multiple starting positions in parallel within a short time, you can quickly find the global minimum for the objective function and feel confident about the results.

Powerful enough to create a digital twin of your process

Use the CHEMCAD NXT data reconciliation technology to match a simulation to real process data. When coupled with CHEMCAD NXT's data interface capabilities (i.e., COM or OPC), it is possible to produce a live link where the model is updated in real time to create a digital copy of the real process.

Flexibility to handle everyday tasks

CHEMCAD NXT supports many everyday tasks that users may not be aware of. Have you used the built-in unit converter? Press F6 and select a property from the list to instantly view that property in different units. Just looking for a quick fluid property? Consult the extensive component database included with CHEMCAD NXT and use a dummy stream to calculate a single property. Try using a flash vessel to represent pipes, separators, or something more abstract, such as multiple unit operations. In fact, many unit operations have multiple calculation options built in that can accomplish a desired task without adding all the equipment in the field to the model itself. So, whether you mean to check a pressure drop using a single pipe or build a detailed piping network, let the flexibility of CHEMCAD NXT work for you.

→ Engineering advanced

Like much of today's technology, CHEMCAD NXT continues to evolve into a more powerful tool designed to be flexible, customizable, and robust. To get the most value from CHEMCAD, be sure to take full advantage of the features that tackle everyday tasks as well as the complex challenges chemical engineers face.

One more thing to take advantage of: Chemstations' world-class technical support team, standing by to ensure that users experience all that CHEMCAD NXT has to offer: **www.chemstations.com/Support**.

➜ *Engineering advanced*