

Extractor Design with Sensitivity Analysis (EXTR)

DESCRIPTION:

The ChemCAD's EXTR model can calculate liquid-liquid extraction (LLE) process provided that coefficients of the NRTL or UNIQUAC K-value equation are known. ChemCAD III utilizes DECHEMA library of Binary Interaction parameters, and many popular industrial systems are already covered. You also have the option to regress missing coefficients from literature or experimental data. The Binodal Plot feature allows user to prepare Jänecke triangle chart of LLE equilibria. We have performed a sophisticated Parameter Sensitivity Analysis (SA) supported by a Feed Forward Controller to see how much the number of separation stages and the flowrate of the water stream would influence the recovery of acetone from a benzene/acetone mixture.

NOTES:

1. The following K-value equations can predict presence of two liquid phases: NRTL, UNIQUAC, UNIFAC, UNIFAC LLE, and PSRK. NRTL and UNIQUAC equations require Binary Interaction Parameters (BIPs). All three: UNIFAC, UNIFAC LLE and PSRK use theoretical BIPs based on molecular structure of compounds (or UNIFAC groups). Using NRTL or UNIQUAC equation is recommended for EXTRactor model.
2. This example is rather qualitative than quantitative in nature. At the time of writing, ChemCAD's database was providing BIP's for the acetone/water pair only. So, the BIPs for acetone/benzene and water/benzene had to be regressed. (We have selected Regression from UNIFAC LLE.) The regression is launched with Util/BIP Regression feature. (The correct K-Value model, as e.g., NRTL must be set in the Thermo menu first.) After selecting 'Regress from UNIFAC LLE', the component selection list appears. With two components selected, the 'Regress NRTL Parameters' window appears, and it can usually be skipped with the ESC key. Also, the subsequent 'Regress Parameters' window can be skipped. Regression starts, and if the K-Value model is appropriate for the data, it usually converges. After

closing the regression report window, the 'Bip Set' screen appears. If the results are satisfactory, then you specify the BIP set number to store the data. (ChemCAD can handle up to 10 different BIP sets. These can be selected in the Thermo/K-Value window.) Typical BIP set number is 1. If you are not satisfied with the regression results, enter 0 /zero/ as the BIP set number, so the results will be ignored.

Please display the Plot/Binodal Plot to see the extractive equilibria diagram according to existing and regressed data.

3. The databases provided with ChemCAD are public knowledge, so you should verify the equilibrium data if you approach a critical project. It is especially valid for extraction, as that sort of data is scarce. We recommend acquiring literature or experimental txx LLE (extractive equilibria) data for your system, and performing regression for a three component system. The results you'd obtain can be plotted together with the experimental data as the Binodal Plot. The regressed BIPs should be written to the BIP set, say, #2, to avoid confusion with original VLE data used in distillation.
4. Please launch the Run/Sensitivity/Run Old Analysis option and review the Parameter Data. Then display the Parameter Plot of Water Flowrate against Acetone Extracted amount. Our Analysis varies the number of separation stages and the flowrate of extracting water, and it records the flowrate of acetone in the extract. Varying the number of stages creates a logical problem: the second feed stage of extractor **MUST** be located at the last stage. To overcome this, we set up a Feed Forward controller at the first feed stream. See how it works:

When SA starts, it firstly sets the Number of Stages in EXTR to some value, say, two. Then the CONTroller is run. It is told to read the Number of Stages value from the EXTR, and to write that number into the 2nd Feed Stage field of the EXTR. When the EXTR is executed, the second feed location is already equal to the number of stages.

This concept is useful in all staged separation processes (e.g., absorption), where a specific feed must be entered onto the last stage of a column.

