DDBST
Dortmund Data Bank
Software & Separation
Technology

Predictive EOS

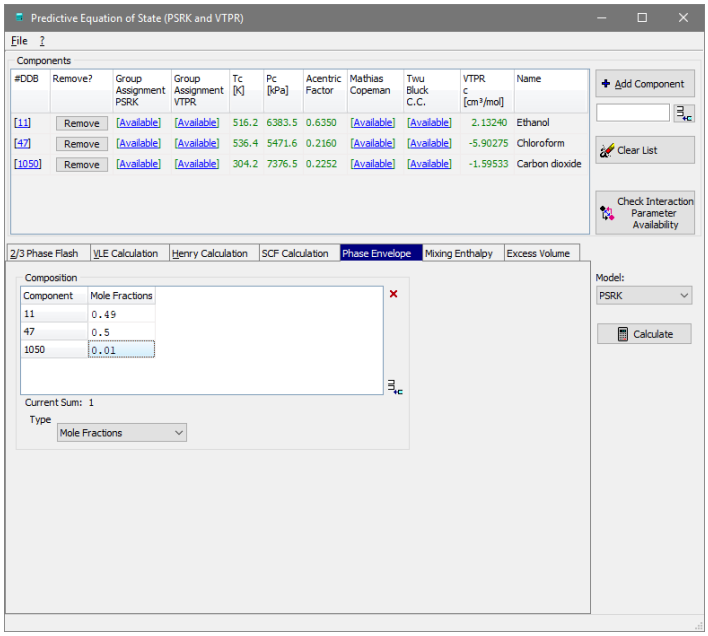
Calculation of Vapor-Liquid Equilibria, Two- and Three-Phase Flashes, Henry Coefficient Calculation, Solubility in Supercritical Fluids, Phase Envelopes, and Mixing Enthalpies with
The group contribution equations of state models PSRK and VTPR.

Description

The stand-alone package Predictive EOS allows a multitude of multicomponent mixture calculations using the thermodynamic models Predictive Soave-Redlich-Kwong (PSRK) and Volume-Translated-Peng-Robinson (VTPR) equations of state. These include:

1. Vapor-liquid equilibria (VLE)
2. Vapor-liquid-liquid equilibria (VLLE)
3. Gas solubilities (GLE, Henry coefficients)
4. Supercritical fluid extraction (SCF)
5. Phase envelopes (P/T - curves)
6. Mixing enthalpies
7. Excess volumes

The program handles bubble point, dew point and flash calculations. Results are displayed in tables and diagrams and can be copied to the Windows clipboard, saved to file or printed. The full set of DDB basic data is included in the Predictive EOS license.



Applications

The methods and calculations are used in a large variety of applications also including risk assessment to calculate the maximum pressure in a vessel after overheating of a reaction system.

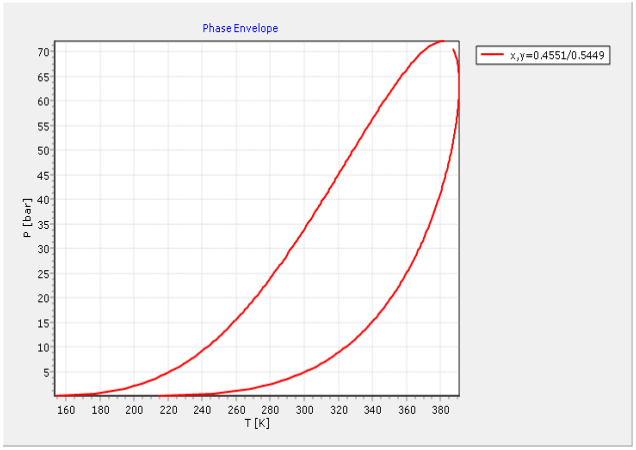
Scope of Supply

The software comes with

- the latest published parameter matrices for both the estimation methods PSRK and VTPR.
- structural group lists for more than 17,000 components

Members of the UNIFAC-Consortium (www.unifac.org) have access to the latest PSRK and VTPR parameters.

Changes and errors are possible regarding all information and prices.



Phase Envelope Calculation with VTPR; Carbon dioxide and *n*-Butane