

Predict

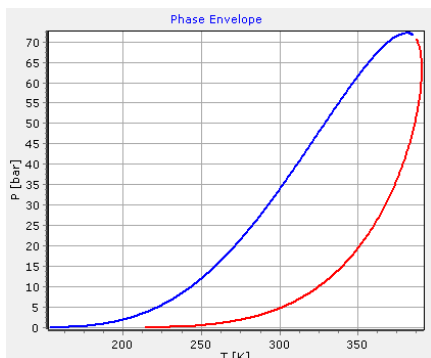
Calculation of Vapor-Liquid Equilibria, Solubilities, Activities and Excess Properties with the Models PSRK, VTPR, UNIFAC, Mod. UNIFAC, NIST-mod. UNIFAC(Do), mod. UNIFAC(Ly) and a Variety of EOS Mixing Rules.

Description

The stand-alone package Predict 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 and the group contribution methods UNIFAC, Mod. UNIFAC(Do), NIST-mod. UNIFAC and Mod. UNIFAC (Ly). Calculations with EOS mixing rules are also possible. The supported calculations are:

1. Vapor-liquid equilibria (VLE)
 - a. 2/3 Flash
 - b. VLE
 - c. Henry
 - d. Phase Envelope
2. Solubility
 - a. Solubility in supercritical fluids (SCF)
 - b. Solid-Liquid Equilibrium (SLE)
 - c. Liquid-Liquid Equilibrium (LLE)
3. Activity
 - a. Activity coefficients (ACT)
 - b. Activity coefficients at infinite dilution
 - c. Activity coefficient of given components with a list of solvents at infinite dilution
4. Excess Properties
 - a. Excess enthalpy (HE)
 - b. Excess volume (VE)
 - c. Excess heat capacity (CPE)

Results are displayed in tables and diagrams and can be copied to the Windows clipboard, saved to file or printed.



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

x [11]	x [31]
0.00	1.00
0.01	0.99
0.02	0.98
0.03	0.97
0.04	0.96
0.05	0.95
0.06	0.94
0.07	0.93
0.08	0.92
0.09	0.91
0.10	0.90

Main Menu

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 all the estimation methods PSRK, VTPR, UNIFAC, Mod. UNIFAC(Do), NIST-mod. UNIFAC and Mod. UNIFAC (Ly).
- structural group lists for all possible components

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

Changes and errors are possible regarding all information.