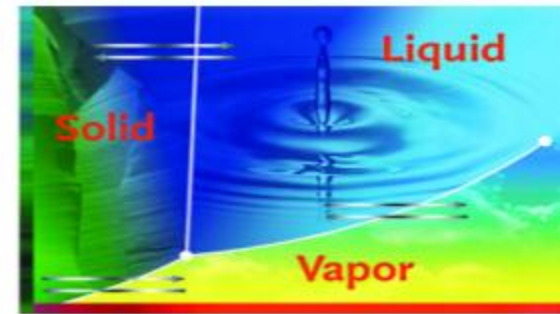


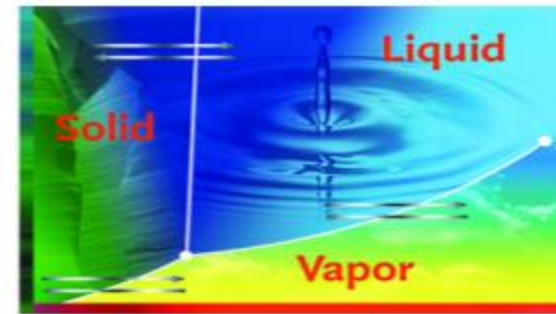
Chemical Thermodynamics for Process Simulation



P02.21

Required Input Parameters for the
Calculation of Saturated Vapor
Enthalpy

Chemical Thermodynamics for Process Simulation



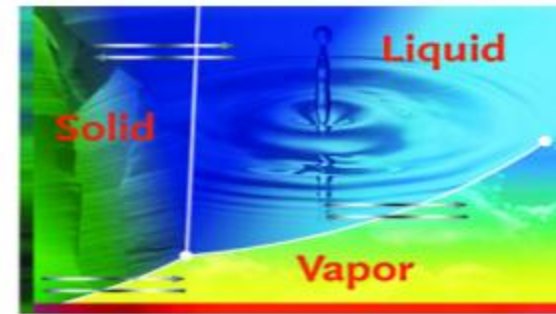
P02.21

Make a list of all the input parameters necessary for the calculation of the enthalpy of the saturated vapor of a pure substance if

- a) the Peng-Robinson equation of state
- b) the vapor pressure equation in combination with the Peng-Robinson equation of state
- c) the VTPR equation of state

is used. The vapor pressure itself shall not be an input parameter.

Chemical Thermodynamics for Process Simulation



P02.21 – Solution

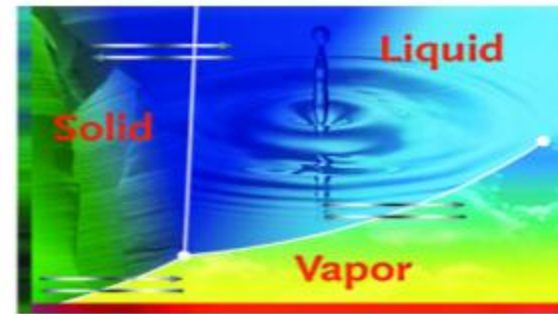
Depending on the reference state, the enthalpy of formation from the elements may be required. (reference state either elements at 25°C in their most stable state or component at 25°C, 1 atm in the ideal gas state).

The ideal gas heat capacity is required to calculate the enthalpy change of the component in the pressure zero limit.

In addition:

- a) the Peng-Robinson equation of state requires critical temperature, pressure and acentric factor.

Chemical Thermodynamics for Process Simulation



P02.21 – Solution

- b) the vapor pressure equation in combination with the Peng-Robinson equation of state requires critical pressure and temperature and allows to calculate the correct value of the α -function at any temperature from the vapor pressure.
- c) the VTPR equation of state requires critical temperature and pressure as well as the Twu α -function parameters.