1. Theory for Vapor Pressure Estimation

I) Quasipolynomial equation (HC_PVPEQN)

Simple but useful correlation equation of vapor pressure is :

$$\ln P_{vp} = \sum A_i T^i + A_{\ln} \ln T \tag{1}$$

Normally, *i* range from −1 to 6. KDB vapor pressure equation uses four-parameter correlation.

$$\ln P_{vp} = A_1 \ln T + A_2 / T + A_2 + A_3 T^2 \tag{2}$$

where, the units in eq. (2) are Kelvin and kPa.

II) Ambrose-Walton Corresponding-States Method (HC_PVPAW)

The Pitzer expansion is used.

$$\ln P_{vp} = f^{(0)}(T_r) + \omega f^{(1)}(T_r) + \omega^2 f^{(2)}(T_r) \tag{3}$$

We uses the following method developed by Ambrose and Walton.

$$f^{(0)} = \frac{-5.97616\tau + 1.29874\tau^{1.5} - 0.60394\tau^{2.5} - 1.06841\tau^5}{T_r} \tag{4}$$

$$f^{(1)} = \frac{-5.03365\tau + 1.11505\tau^{1.5} - 5.41217\tau^{2.5} - 7.46628\tau^5}{T_r} \tag{5}$$

$$f^{(2)} = \frac{-0.64771\tau + 2.41539\tau^{1.5} - 4.26979\tau^{2.5} + 3.25259\tau^5}{T_r} \tag{6}$$

In eqs. (4) to (6), $\tau = (1 - T_r)$.

Referece

D. Ambrose and J.Walton, *Pure & Appl.Chem.*, **61**, 1395 (1989)

Poling et al., "Properties of Gases and Liquids", 5th ed. McGraw-Hill, New York

III) Riedel Corresponding-States Method (HC_PVPRD)

Riedel corresponding states method uses the following expression for vapor pressure.

$$\ln P_{vp} = A + B/T + C \ln T + DT^6 \tag{7}$$

From a study of experimental vapor pressure data, Riedel found that

$$\ln P_{vp} / P_c = A^+ - B^+ / T_r + C^+ \ln T_r + D^+ T_r^6 \tag{8}$$

where

$$A^+ = -35Q \qquad B^+ = -36Q \qquad C^+ = 42Q + \alpha_c$$

$$D^+ = -Q \qquad Q = K(3.758 - \alpha_c)$$

K has a value of 0.0838 except for alcohols and acids. **For acids and alcohols**,

$$K = -0.120 + 0.025h \quad \text{for acids} \qquad (9)$$

and $$K = 0.373 - 0.030h \quad \text{for alcohols.} \qquad (10)$$

The parameter in these equations, *h*, is defined by following equation.

$$h = T_{br}\frac{\ln(P_c/101.325)}{1-T_{br}} \qquad (11)$$

where, P_c is in kPa, T_{br} is normal boiling point in Kelvin.

Next, α_c is obtained by following equation.

$$\alpha_c = \frac{3.758K\gamma_b + \ln(P_c/101.325)}{K\gamma_b - \ln T_{br}} \qquad (12)$$

$$\gamma_b = -35 + 36/T_{br} + 42\ln T_{br} - T_{br}^6 \qquad (13)$$

Referece :

L.Riedel, *Chem. Engtech*., **26**, 679 (1954)

A.Vetere, *Ind. Eng. Chem. Res.*, **30**, 2487 (1991)

Poling et al., "Properties of Gases and Liquids", 5th ed. McGraw-Hill, New York

2. KDB Routines for Vapor Pressure Calculation

KDB vapor pressure calculation subroutines contain KDB correlation equation and two estimation methods, which are Ambrose et al. and Riedel corresponding-states method.

Subroutine Name	Description	Required Common Blocks
HC_PVPEQN	KDB correlation equation	HC_KPVP
HC_PVPAW	Ambrose-Walton method	HC_PROP
HC_PVPRD	Riedel method	HC_PROP, HC_NAME

I) HC_PVPEQN

1. Usage : CALL HC_PVPEQN(ICN,T,PVP,IST)
2. Arguments

ICN : Component ID number (1-50) to calculate vapor pressure (integer, input)

T : Temperature in Kelvin (real*8, input)

PVP : Vapor pressure in kPa (real*8, output)

IST : Status of calculation (integer, output)

= 0 : Normal termination

= 101 : Vapor pressure coefficient not available

= 102 : Out of range for the application

II) HC_PVPAW

1. Usage : CALL HC_PVPAW(ICN,T,PVP,IST)
2. Arguments

ICN : Component ID number (1-50) to calculate vapor pressure
(integer, input)

T : Temperature in Kelvin (real*8, input)

PVP : Vapor pressure in kPa (real*8, output)

IST : Status of calculation (integer, output)

= 0 : Normal termination

= 111 : Critical temperature data not available

= 112 : Critical prssure data not available

= 113 : Accentric factor data not available

= 114 : Given T exceeds critical temperature

3. Required Properties

Critical temperature in K, critical pressure in kPa, and accentric factor

III) HC_PVPRD

1. Usage : CALL HC_PVPRD(ICN,T,PVP,IST)
2. Arguments

ICN : Component ID number (1-50) to calculate vapor pressure
(integer, input)

T : Temperature in Kelvin (real*8, input)

PVP : Vapor pressure in kPa (real*8, output)

IST : Status of calculation (integer, output)

= 0 : Normal termination

= 121 : Critical temperature data not available

= 122 : Critical prssure data not available

= 123 : Boiling point data not available

= 124 : Given T exceeds critical temperature

3. Required Properties

Critical temperature in K, critical pressure in kPa, and boiling point in K

4. Comments

For acids , ICLASS(ICN) have values of range from 15 to 19, and For alcohols, from 11 to 14.(See Description of common block in KDBROUTINE.PDF)