1. Theory for Vapor Pressure Estimation

I ) Quasipolynomial equation (HC_PVPEQN)

Simple but useful correlation equation of vapor pressure is:

$$\ln P_v = \sum A_i T^{i-1} + A_n \ln T$$

(1)

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

$$\ln P_v = A_1 \ln T + A_2 / T + A_3 + A_4 T^2$$

(2)

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

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

The Pitzer expansion is used.

$$\ln P_v = f^{(0)} (T_r) + \alpha f^{(1)} (T_r) + \alpha^2 f^{(2)} (T_r)$$

(3)

We uses the following method developed by Ambrose and Walton.

$$f^{(0)} = \frac{-5.97616 \tau + 1.29874 \tau^{1.5} - 0.60394 \tau^{2.5} - 1.0684 \tau^5}{T_r}$$

(4)

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

(5)

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

(6)

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

Reference


III ) Riedel Corresponding-States Method (HC_PVPRD)

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

$$\ln P_v = A + B / T + C \ln T + DT^6$$

(7)

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

$$\ln P_v / P_c = A^* - B^* / T_r + C^* \ln T_r + D^* T_r^6$$

(8)

where
\[ A^* = -35Q \quad \quad B^* = -36Q \quad \quad C^* = 42Q + \alpha_c \]
\[ D^* = -Q \quad \quad \quad \quad Q = K(3.758 - \alpha_c) \]

\( K \) has a value of 0.0838 except for alcohols and acids. **For acids and alcohols**, \( K = -0.120 + 0.025h \) for acids
\[ \text{and} \quad K = 0.373 - 0.030h \quad \text{for alcohols.} \]

The parameter in these equations, \( h \), is defined by following equation.
\[ h = T_{br} \frac{\ln(P_c/101.325)}{1 - T_{br}} \]

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

Next, \( \alpha_c \) is obtained by following equation.
\[ \alpha_c = \frac{3.758K\psi_b + \ln(P_c/101.325)}{K\psi_b - \ln T_{br}} \]
\[ \psi_b = -35 + 36/T_{br} + 42\ln T_{br} - T_{br}^6 \]

Reference:


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.

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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 pressure 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 pressure 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)