1. Theory for Liquid Viscosity

I) Polynomial equation (HC_VSLEQN)

Polynomial equation is used for liquid viscosity.

$$\ln VSL = A + B/T + CT + DT^2 \tag{1}$$

where, T is Kelvin and VSL is cP.

II) Przezdziecki and Sridhar Method for low temperature (HC_VSLPS)

The authors propose the following equation ;

$$\boldsymbol{h}_{L} = \frac{V_{0}}{E(V - V_{0})} \tag{2}$$

where

 $\mathbf{h}_{L} =$ liquid viscosity, cP

V =liquid molar volume, cm³/mol

and

$$E = -1.12 + \frac{V_c}{12.94 + 0.10M - 0.23P_c + 0.0424T_{fP} - 11.58T_{fP}/T_c}$$
(3)

$$V_0 = 0.0085 \, \mathbf{w} T_c - 2.02 + \frac{V_m}{0.342 T_{fP} / T_c + 0.894} \tag{4}$$

where

 T_c = critical temperature, K P_c = critical pressure, bar V_c = critical volume, cm³/mol M = molecular weight, g/mol T_{fP} = freezing point, K W = acentric factor V_m = liquid molar volume at T_{fP} , cm³/mol

In this technique, V_m and V are estimated by the Gunn-Yamada method. They define liquid molar volume at system temperature and freezing point as following expression. Given molar volume, V^{R} at T^{R} , then at any other temperature T,

$$V(T) = \frac{f(T)}{f(T^R)} V^R$$
(5)

where

$$f(T) = H_1(1 - \mathbf{W}H_2) \tag{6}$$

$$H_1 = 0.33593 - 0.33953T_r + 1.51941T_r^2 - 2.02512T_r^3 + 1.11422T_r^4$$
(7)

$$H_2 = 0.29607 - 0.09045T_r - 0.04842T_r^2 \tag{8}$$

The reference volume for each compound was obtained from the liquid density data (VOLP) at 298.15K in KDB home page (http://thermo.korea.ac.kr). If not so, it is estimated by Rackett equation occupied in fortran subroutine

(RACETT.FOR). This method should not be used for alcohols. Also, The range of reduced temperature applicable is between 0.55 and 0.77.

References :

Prezdziecki et al., AIChE J., 31, 333 (1985)

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

III) Letsou and Stiel Method for high temperature (HC_VSLLETSOU)

Letsou and Stiel proposed the following relation at high temperature for $0.76 < T_r < 0.98$.

 $h\mathbf{x} = (h\mathbf{x})^{(0)} + \mathbf{w}(h\mathbf{x})^{(1)}$ (9)

and

$$(\mathbf{h}\mathbf{x})^{(0)} = 10^{-3} (2.648 - 3.725T_r + 1.309T_r^2)$$
(10)

$$(hx)^{(1)} = 10^{-3} (7.425 - 13.39T_r + 5.933T_r^2)$$
⁽¹¹⁾

$$\mathbf{x} = 0.176 \left(\frac{T_c}{M^3 P_c^4}\right)^{1/6}$$
(12)

References :

Letsou et al., AIChE J., 19, 409 (1973)

Reid et al., "Properties of Gases and Liquids", 4th ed. McGraw-Hill, New York

2. KDB Routines for Liquid Viscosity Calculation

KDB gas viscosity calculation subroutines contain one KDB correlation equation and two estimation methods, which are Przezdziecki and Sridhar Method for low temperature and Letsou and Stiel method for high temperature.

Subroutine Name	Description	Required Common Blocks
HC_VSLEQN	KDB correlation equation	HC_KVSL
HC_VSLPS	Przezdziecki and Sridhar Method for low temperature	HC_NAME, HC_PROP
HC_VSLLETSOU	Letsou and Stiel method for high temperature	HC_PROP

I) HC_VSLEQN

1. USAGE : CALL HC_VSLEQN(ICN,T,VSL,IST)

2. A RGUMENTS

ICN	: COMPONENT NUMBER (1-50) TO CALCULATE LIQUID VISCOSITY (INTEGER, INPUT)
Т	: TEMPERATURE IN KELVIN (REAL*8, INPUT)
VSG	: LIQUID VISCOSITY IN cP (REAL*8, OUTPUT)
IST	: STATUS OF CALCULATION (INTEGER, OUTPUT)

- = 0 : NORMAL TERMINATION
- = 601 : LIQUID VISCOSITY COEFFICIENT NOT AVAILABLE
- = 602 : OUT OF RANGE FOR THE APPLICATION

II) HC_VSLPS

1. USAGE : CALL HC_VSLPS(IDN,T,VISC,IST)

2. ARGUMENTS

IDN	: COMPONENT NUMBER (1-50) TO CALCULATE LIQUID VISCOSITY (INTEGER, INPUT)		
Т	: TEMPI	ERATURE IN KELVIN (REAL*8, INPUT)	
VISC	: LIQUI	D VISCOSITY IN CENTI POISE (REAL*8, OUTPUT)	
IST	: STATUS OF CALCULATION (INTEGER, OUTPUT)		
	= 0	: NORMAL OUTPUT OBTAINED	
	= 611	: CRITICAL TEMPERATURE DATA NOT AVAILABLE	
	= 612	: CRITICAL PRESSURE DATA NOT AVAILABLE	
	= 613	: ACENTRIC FACTOR DATA NOT AVAILABLE	
	= 614	: CRITICAL VOLUME DATA NOT AVAILABLE	
	= 615	: FREEZING POINT DATA NOT AVAILABLE	
	= 616	: MOLECULAR WEIGHT DATA NOT AVAILABLE	
	= 617	: ALCOHOLS CANNOT BE APPLIED TO PRZSRH METHOD	
	= 618	: NOT APPLICABLE TEMPERATURE RANGE	

3. Required properties

Critical temperature in K, critical pressure in kPa, acentric factor, critical volume in m³/kg-mol, freezing point in K, and molecular weight in g/mol

III) HC_VSLLETSOU

1. USAGE :CALL HC_VSLLET(IDN,T,VISC,IST)

2. ARGUMENTS

IDN	: COMPONENT NUMBER (1-50) TO CALCULATE LIQUID VISCOSITY (INTEGER, INPUT)
Т	: TEMPERATURE IN KELVIN (REAL*8, INPUT)

VISC : LIQUID VISCOSITY IN CENTI POISE (REAL*8, OUTPUT)

IST : STATUS OF CALCULATION (INTEGER, OUTPUT)

- = 0 : NORMAL OUTPUT OBTAINED
- = 621 : CRITICAL TEMPERATURE DATA NOT AVAILABLE
- = 622 : CRITICAL PRESSURE DATA NOT AVAILABLE
- = 623 : ACENTRIC FACTOR DATA NOT AVAILABLE
- = 624 : MOLECULAR WEIGHT DATA NOT AVAILABLE

= 625 : NOT APPLICABLE TEMPERATURE RANGE

3. Required properties

Critical temperature in K, critical pressure in kPa, acentric factor, and molecular weight in g/mol