1. Theory for Gas Viscosity

I) Polynomial equation for low pressure(HC_VSGEQN)

Polynomial equation is used for gas viscosity for low pressure.

$$VSG = \sum_{i=0}^{4} A_i T^i \tag{1}$$

where, T is Kelvin and VSG is cP.

II) Corresponding-States Method by Lucas for Low Pressure (HC_VSGLUCAS_LP)

Lucas proposed the following relation ;

$$\eta\xi = \left[0.807 T_r^{0.618} - 0.357\exp(-0.449 T_r) + 0.340\exp(-4.058 T_r) + 0.018\right] F_P^0 F_Q^0 \tag{2}$$

where, η is in mP, T_r is the reduced temperature, and F_P^0 and F_Q^0 are correction factors to account for polarity of quantum effects. ξ is reduced, inverse viscosity and defined by -

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

where, T_c is Kelvins, M is in g/mol, and P_c is in bars.

To obtain F_P^0, a reduced dipole moment is proposed by

$$\mu_r = 52.46\frac{\mu^2 P_c}{T_c^2} \tag{4}$$

where μ is in debyes. Then F_P^0 are defined as :

$$\begin{aligned} F_P^0 &= 1 && 0 \le \mu_r < 0.022 \\ F_P^0 &= 1 + 30.55(0.292 - Z_c)^{1.72} && 0.022 \le \mu_r < 0.075 \\ F_P^0 &= 1 + 30.55(0.292 - Z_c)^{1.72}\left|0.96 + 0.1(T_r - 0.7)\right| && 0.075 \le \mu_r \end{aligned} \tag{5}$$

F_Q^0 is used only for the quantum gases such as He, H_2, and D_2.

$$F_Q^0 = 1.22 Q^{0.15}\left\{1 + 0.00385\left[(T_r - 12)^2\right]^{1/M} sign(T_r - 12)\right\} \tag{6}$$

where Q = 1.38 for He, Q = 0.76 for H_2, and Q = 0.52 for D_2. Sign( ) indicates that one should use +1 or –1 depending on whether the value in parenthesis is greater than or less than zero.

Reference :

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

III) Chung et al. method for Low Pressure(HC_VSGCHUNG_LP)

Chung et al. method is expressed as :

$$\eta = 40.785 \frac{F_c (MT)^{1/2}}{V_c^{2/3} \Omega_v} \quad (7)$$

where,

η = viscosity, mP

M = molecular weight, g/mol

T = temperature, K

V_c = critical volume, cm^3/mol

Ω_v = viscosity collision integral from following equation (8) and $T^* = 1.2593 T_r$

$$\Omega_v = A(T^*)^{-B} + C\exp(-DT^*) + E\exp(-FT^*) \quad (8)$$

where, $A = 1.16145$, $B = 0.14874$, $C = 0.52487$, $D = 0.77320$, $E = 2.16178$, and $F = 2.43787$.

$$F_c = 1 - 0.2756\omega + 0.059035 m_r^4 + \kappa \quad (9)$$

In eq. (9), ω is the acentric factor and κ is a special correction for highly polar substances such as alcohols and acids and shown in following table.

Table 1. The association Factor κ in Eq. (9) (Chung et al., 1988)

Compound	κ	Compound	κ
Methanol	0.215	n-Propanol	0.122
Ethanol	0.175	n-Hexanol	0.114
n-Propanol	0.143	n-Heptanol	0.109
i-Propanol	0.143	Acetic Acid	0.0916
n-Butanol	0.132	Water	0.0716
i-Butanol	0.132		

For other alcohols not shown in Table 1, κ = 0.0682+4.704[(number of –OH groups)/molecular weight].

Dimensionless dipole moment, μ_r is expressed by

$$m_r = 131.3 m / (V_c T_c)^{1/2} \quad (10)$$

where, V_c is in $cm^3/mole$, T_c is in Kelvins, and m is in debyes.

References :

Chung, T.-H., M. Ajlan, L. L. Lee, and K.E. Starling, *Ind. Eng. Chem. Res*., **27**, 671, 1988

Chung, T.-H., L.L.Lee, and K.E. Starling, *Ind. Eng. Chem. Fundam.*, **23**, 8, 1984

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

IV) Corresponding-States Method by Lucas for High Pressure (HC_VSGLUCAS_HP)

For high pressure, Chung et al. used the following procedure.

$$Z_1 = \eta^0 \xi = \left[0.807 T_r^{0.618} - 0.357\exp(-0.449 T_r) + 0.340\exp(-4.058 T_r) + 0.018\right] F_P^0 F_Q^0 \quad (11)$$

where, η^0 is the low-pressure viscosity. Next calculate Z_2. If $T_r \le 1.0$ and $P_r < (P_{vp}/P_c)$, then

$$Z_2 = 0.600 + 0.760 P_r^a + (6.990 P_r^b - 0.6)(1 - T_r) \quad (12)$$

with $\alpha = 3.262 + 14.98 P_r^{5.508}$ and $\beta = 1.390 + 5.746 P_r$.

If ($1 < T_r < 40$) and ($0 < P_r \leq 100$), then

$$Z_2 = \eta^0 \xi \left[1 + \frac{a P_r^e}{b P_r^f + (1 + c P_r^d)^{-1}} \right] \tag{13}$$

where $\eta^0 \xi$ is calculated by eq. (11) and

$$a = \frac{a_1}{T_r} \exp(\alpha_2 T_r^g) \qquad b = a(b_1 T_r - b_2) \qquad c = \frac{c_1}{T_r} \exp(c_2 T_r^d)$$

$$d = \frac{d_1}{T_r} \exp(d_2 T_r^e) \qquad e = 1.3088 \qquad f = f_1 \exp(f_2 T_r^V)$$

and

$$a_1 = 1.245 \times 10^{-3} \qquad a_2 = 5.1726 \qquad g = -0.3286$$
$$b_1 = 1.6553 \qquad b_2 = 1.2723$$
$$c_1 = 0.4489 \qquad c_2 = 3.0578 \qquad \delta = -37.7332$$
$$d_1 = 1.7368 \qquad d_2 = 2.2310 \qquad \varepsilon = -7.6351$$
$$f_1 = 0.9425 \qquad f_2 = -0.1853 \qquad V = 0.4489$$

After calculating Z_1 and Z_2, we define

$$Y = Z_2 / Z_1 \tag{14}$$

and the correction factors F_P and F_Q,

$$F_P = \frac{1 + (F_P^0 - 1) Y^{-3}}{F_P^0} \tag{15}$$

$$F_Q = \frac{1 + (F_Q^0 - 1)[Y^{-1} - 0.007(\ln Y)^4]}{F_Q^0} \tag{16}$$

where F_P^0 and F_Q^0 are computed by eq. (5) and eq. (6), respectively. Finally, the gas viscosity for high pressure is calculated as

$$\eta = Z_2 F_P F_Q / \xi \tag{17}$$

and ξ is defined in Eq. (3).

Reference :

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

V) Chung et al. method for High Pressure(HC_VSGCHUNG_HP)

Chung et al. suggested the following expression for describing the fact that the fluid has a high density for high pressure.

$$\eta = \eta^* \frac{36.344 (M T_c)^{1/2}}{V_c^{2/3}} \tag{18}$$

where,

η = viscosity, mP

M = molecular weight, g/mol

T_c = critical temperature, K

V_c = critical volume, cm^3/mol

and

$$\eta^* = \frac{(T^*)^{1/2}}{\Omega_v}\left\{F_c\left[(G_2)^{-1} + E_6 y\right]\right\} + \eta^{**} \tag{18}$$

$T^* = 1.2593 T_r$ and Ω_v and F_c is defined as eqs. (8) and (9), respectively. With molar density, ρ in mol/cm^3,

$$y = \frac{\rho V_c}{6} \tag{19}$$

$$G_1 = \frac{1 - 0.5y}{(1-y)^3} \tag{20}$$

$$G_2 = \frac{E_1\{[1 - \exp(-E_4 y)]/y\} + E_2 G_1 \exp(E_5 y) + E_3 G_1}{E_1 E_4 + E_2 + E_3} \tag{21}$$

$$\eta^{**} = E_7 y^2 G_2 \exp\left[E_8 + E_9 (T^*)^{-1} + E_{10} (T^*)^{-2}\right] \tag{22}$$

and the parameters E_1 and E_{10} are shown in Table 2. μ_r is defined by eq. (10) and the association factor, κ is shown in Table 1.

Table 2. Chung et al. coefficients to calculate $E_i = a_i + b_i \omega + c_i \mu_r^4 + d_i \kappa$

i	a_i	b_i	c_i	d_i
1	3.324	50.412	-51.680	1189.0
2	1.210×10^{-3}	-1.154×10^{-3}	-6.257×10^{-3}	0.03728
3	5.283	254.209	-168.48	3898.0
4	6.623	38.096	-8.464	31.42
5	19.745	7.630	-14.354	31.53
6	-1.900	-12.537	4.985	-18.45
7	24.275	3.450	-11.291	69.35
8	0.7972	1.117	0.01235	-4.117
9	-0.2382	0.06770	-0.8163	4.025
10	0.06863	0.3479	0.5926	-0.727

References :

Chung, T.-H., M. Ajlan, L. L. Lee, and K.E. Starling, *Ind. Eng. Chem. Res*., **27**, 671, 1988

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

2. KDB Routines for Gas Viscosity Calculation

KDB gas viscosity calculation subroutines contain one KDB correlation equation and four estimation methods, which are Lucas method and Chung et al. method for low- and high-pressure.

Subroutine Name	Description	Required Common Blocks
HC_VSGEQN	KDB correlation equation for low pressure	HC_KVSG
HC_VSGLUCAS_LP	Lucas method for low pressure	HC_NAME, HC_PROP
HC_VSGCHUNG_LP	Chung et al. method for low pressure	HC_PROP
HC_VSGLUCAS_HP	Lucas method for high pressure	HC_NAME, HC_PROP, HC_KPVP
HC_VSGCHUNG_LP	Chung et al. method for high pressure	HC_NAME, HC_PROP

I) HC_VSGEQN

1. Usage : CALL HC_VSGEQN(ICN,T,VSG,IST)
2. Arguments

ICN : Component ID number (1-50) to calculate gas viscosity for low pressure (integer, input)

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

VSG : Gas viscosity in cP (real*8, output)

IST : Status of calculation (integer, output)

= 0 : Normal termination

= 501 : Gas viscosity coefficient not available

= 502 : Out of range for the application

II) HC_VSGLUCAS_LP

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

ICN : COMPONENT NUMBER (1-50) TO CALCULATE GAS VISCOSITY (INTEGER, INPUT)

T : TEMPERATURE IN KELVIN (REAL*8, INPUT)

VSG : GAS VISCOSITY IN MICRO POISE (REAL*8, OUTPUT)

IST : STATUS OF CALCULATION (INTEGER, OUTPUT)

= 0 : NORMAL TERMINATION

= 511 : CRITICAL TEMPERATURE DATA NOT AVAILABLE

= 512 : CRITICAL PRESSURE DATA NOT AVAILABLE

= 513 : CRITICAL COMPRESSIBILITY DATA NOT AVAILABLE

= 514 : DIPOLE MOMENT DATA NOT AVAILABLE

3. Required Properties

Critical temperature in K, critical pressure in kPa, accentric factor, and dipole moment in debye

III) HC_CHUNG_LP

1. Usage : CALL HC_CHUNG_LP(IDN,T,PVP,IST)

2. Arguments

IDN : COMPONENT NUMBER (1-50) TO CALCULATE GAS VISCOSITY
(INTEGER, INPUT)

T : TEMPERATURE IN KELVIN (REAL*8, INPUT)

VSG : GAS VISCOSITY IN MICRO POISE (REAL*8, OUTPUT)

IST : STATUS OF CALCULATION (INTEGER, OUTPUT)

= 0 : NORMAL TERMINATION

= 531 : CRITICAL TEMPERATURE DATA NOT AVAILABLE

= 532 : CRITICAL PRESSURE DATA NOT AVAILABLE

= 533 : CRITICAL VOLUME DATA NOT AVAILABLE

= 534 : ACCETRIC FACTOR DATA NOT AVAILABLE

= 535 : DIPOLE MOMENT DATA NOT AVAILABE

3. Required Properties

Critical temperature in K, critical pressure in kPa, critical volume in m^3/kg-mol, acentric factor, and dipole moment in debye

IV) HC_VSGLUCAS_HP

1. USAGE : CALL HC_VSGLUCAS_HP(ICN,T,P,VSG,IST)

2. ARGUMENTS

ICN : COMPONENT NUMBER (1-50) TO CALCULATE GAS VISCOSITY
(INTEGER, INPUT)

T : TEMPERATURE IN KELVIN (REAL*8, INPUT)

P : PRESSURE IN KPA (REAL*8, INPUT)

VSG : GAS VISCOSITY IN MICRO POISE (REAL*8, OUTPUT)

IST : STATUS OF CALCULATION (INTEGER, OUTPUT)

= 0 : NORMAL TERMINATION

= 521 : CRITICAL TEMPERATURE DATA NOT AVAILABLE

= 522 : CRITICAL PRESSURE DATA NOT AVAILABLE

= 523 : ACCETRIC FACTOR DATA NOT AVAILABLE

= 524 : CRITICAL COMPRESSIBILITY DATA NOT AVAILABLE

= 525 : OUT OF RANGE FOR THE APPLICATION

3. Required properties

Critical temperature in K, critical pressure in kPa, acentric factor, and dipole moment in debye

V) HC_VSGCHUNG_HP

1. USAGE : CALL HC_VSGCHUNG_HP(IDN,T,P,METH,IVOL,VSG,IST)

2. ARGUMENTS

IDN : COMPONENT NUMBER (1-50) TO CALCULATE GAS VISCOSITY
(INTEGER, INPUT)

T : TEMPERATURE IN KELVIN (REAL*8, INPUT)

P : PRESSURE IN KPA (REAL*8, INPUT)

METH : METHOD SELECTION FLAG(INTEGER)
= 1 -----> CHUNG et al. METHOD
= 2 -----> BRULE AND STARLING METHOD
IVOL : IF THERE IS EXPERIMENTAL VOLUME DATA, IVOL = 1
ELSE IF, IVOL = 2 AND CALCULATE VOLUME BY EOS(CB_SOL)
VOL : MOLAR VOLUME IN CM^3/MOL (REAL*8, INPUT IF IVOL=1)

VSG : GAS VISCOSITY IN MICRO POISE (REAL*8, OUTPUT)
IST : STATUS OF CALCULATION (INTEGER, OUTPUT)
= 0 : NORMAL TERMINATION
= 541 : CRITICAL TEMPERATURE DATA NOT AVAILABLE
= 542 : CRITICAL PRESSURE DATA NOT AVAILABLE
= 543 : CRITICAL VOLUME DATA NOT AVAILABLE
= 544 : DIPOLE MOMENT DATA NOT AVAILABLE
= 545 : ACCETRIC FACTOR DATA NOT AVAILABLE
= 1546 : NO CONVERGENCE IN CALCULATION OF DENSITY BY EOS(SRK)

4. Required properties

Critical temperature in K, critical pressure in kPa, critical volume in m^3/kg-mol, acentric factor, and dipole moment in debye

5. Comment

If there is experimental volume data at given temperature, specify IVOL as 1 and give experimental volume to VOL.