

1. Theory for Gas Thermal Conductivity

I) Polynomial equation for low pressure(HC_THGEQN)

Polynomial equation is used for gas viscosity for low pressure.

$$THG = \sum_{i=0}^3 A_i T^i \quad (1)$$

where, T is Kelvin and THG is $W/(m \cdot K)$.

II) Chung et al. Method for Low Pressure (HC_THGCHUNG)

For low-pressure Chung et al. proposed the following relation ;

$$\frac{IM'}{hC_v} = \frac{3.75\Psi}{C_v / R} \quad (2)$$

where

$$\begin{aligned} I &= \text{thermal conductivity, } W/(m \cdot K) \\ M' &= \text{molecular weight, kg/mol} \\ h &= \text{low-pressure gas viscosity, } N \cdot s/m^2 \\ C_v &= \text{heat capacity at constant volume, } J/(mol \cdot K) \\ R &= \text{gas constant, } 8.314 \text{ J}/(mol \cdot K) \\ \Psi &= 1 + a[0.215 + 0.28288a - 1.061b + 0.26665Z] / [0.6366 + bZ + 1.061ab] \\ a &= C_v / R - 3/2 \\ b &= 0.7862 - 0.7109w + 1.3168w^2 \\ Z &= 2.0 + 10.5T_r^2 \end{aligned}$$

Reference :

- 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

III) Chung et al. method for High Pressure(HC_THGCHUNG_HP)

Chung et al. method was modified to apply for high pressure :

$$I = \frac{31.2h^0\Psi}{M'}(G_2^{-1} + B_6y) + qB_7y^2T_r^{1/2}G_2 \quad (3)$$

where

$$\begin{aligned} I &= \text{thermal conductivity, } W/(m \cdot K) \\ h &= \text{low-pressure gas viscosity, } N \cdot s/m^2 \\ M' &= \text{molecular weight, kg/mol} \\ \Psi &= 1 + a[0.215 + 0.28288a - 1.061b + 0.26665Z] / [0.6366 + bZ + 1.061ab] \\ a &= C_v / R - 3/2 \\ b &= 0.7862 - 0.7109w + 1.3168w^2 \end{aligned}$$

$$Z = 2.0 + 10.5T_r^2$$

$C_v =$ heat capacity at constant volume, J/(mol K)

$R =$ gas constant, 8.314 J/(mol K)

$$q = 3.586 \times 10^{-3} (T_c / M')^{1/2} / V_c^{2/3}$$

$T =$ temperature, K

$T_c =$ critical temperature, K

$$T_r = T / T_c$$

$V_c =$ critical volume, cm³/mol

$$y = \frac{V_c}{6V} \quad (4)$$

$$G_1 = \frac{1 - 0.5y}{(1 - y)^3} \quad (5)$$

$$G_2 = \frac{(B_1 / y)[1 - \exp(-B_4 y)] + B_2 G_1 \exp(B_5 y) + B_3 G_1}{B_1 B_4 + B_2 + B_3} \quad (6)$$

The coefficients B_1 to B_7 are defined by eq. (7) and shown in Table 1. The association factor κ is shown in Table 2.

$$B_i = a_i + b_i w + c_i m_r^4 + d_i k \quad (7)$$

Table 1. Values of B_i in Eq. (7)

i	a_i	b_i	c_i	d_i
1	2.4166E+0	7.4824E-1	-9.1858E-1	1.2172E+2
2	-5.0924E-1	-1.5094E+0	-4.9991E+1	6.9983E+1
3	6.6107E+0	5.6207E+0	6.4760E+1	2.7039E+1
4	1.4543E+1	-8.9139E+0	-5.6379E+0	7.4344E+1
5	7.9274E-1	8.2019E-1	-6.9369E-1	6.3173E+0
6	-5.8634E+0	1.2801E+1	9.5893E+0	6.5529E+1
7	9.1089E+1	1.2811E+2	-5.4217E+1	5.2381E+2

The reduced dipole moment is defined by the following equation.

$$m_r = 131.3m / (V_c T_c)^{1/2} \quad (8)$$

The association factor κ is shown in Table 2.

Table 2. The association Factor κ in Eq. (7) (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		

References :

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2. KDB Routines for Gas Thermal Conductivity 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_THGEQN	KDB correlation equation for low pressure	HC_KVSG
HC_THGCHUNG	Chung et al. method for low pressure	HC_NAME, HC_PROP
HC_THGCHUNG_HP	Chung et al. method for high pressure	HC_PROP

I) HC_THGEQN

1. USAGE :CALL HC_THGEQN(ICN,T,THL,IST)

2. ARGUMENTS

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

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

THG : GAS THERMAL CONDUCTIVITY IN W/m.K (REAL*8, OUTPUT)

IST : STATUS OF CALCULATION (INTEGER, OUTPUT)

= 0 : NORMAL TERMINATION

= 701 : GAS THERMAL CONDUCTIVITY COEFFICIENT NOT AVAILABLE

= 702 : OUT OF RANGE FOR THE APPLICATION

II) HC_THGCHUNG

1. USAGE : CALL HC_THGCHUNG(ICN,T,THG,IST)

2. ARGUMENTS

ICN : COMPONENT NUMBER (1-50) TO CALCULATE VAPOR PRESSURE (INTEGER, INPUT)

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

THG : THERMAL CONDUCTIVITY IN Watt/(m.K) (REAL*8, OUTPUT)

IST : STATUS OF CALCULATION (INTEGER, OUTPUT)

= 0 : NORMAL TERMINATION

= 711 : CRITICAL TEMPERATURE DATA NOT AVAILABLE

= 712 : ACCENTRIC FACTOR DATA NOT AVAILABLE

= 713 : MOLECULAR WEIGHT DATA NOT AVAILABLE

= 714 : NOT OBTAINED LOW PRESSURE GAS VISCOSITY

= 715 : NOT OBTAINED GAS HEAT CAPACITY

3. Required Properties

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

If there are not gas viscosity coefficient in KDB databank and you want to use HC_VSGLUCAS_LP, specify the pure properties such as critical pressure in kPa, critical volume in m³/kg-mol and dipole moment in debye.

Specify the ideal heat capacity coefficients for HC_CPGEQN.

III) HC_THGCHUNG_HP

1. USAGE : CALL HC_THGCHUNG_HP(ICN,T,P,THG,IST)

2. ARGUMENTS

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

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

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

RHO : EXPERIMENTAL DENSITY IN MOL/CM³(REAL*8, INPUT)

IEXP : CALCULATION OPTION FOR DENSITY

= 0 : IF NOT DENSITY DATA

= NOT ZERO : IF THERE IS DENSITY DATA

THG : THERMAL CONDUCTIVITY IN Watt/(m.K) (REAL*8, OUTPUT)

IST : STATUS OF CALCULATION (INTEGER, OUTPUT)

= 0 : NORMAL TERMINATION

= 721 : CRITICAL TEMPERATURE DATA NOT AVAILABLE

= 722 : CRITICAL VOLUME DATA NOT AVAILABLE

= 723 : ACCENTRIC FACTOR DATA NOT AVAILABLE

= 724 : DIPOLE MOMENT DATA NOT AVAILABLE

= 725 : MOLECULAR WEIGHT DATA NOT AVAILABLE

= 726 : NOT OBTAINED LOW PRESSURE GAS VISCOSITY

= 727 : NOT OBTAINED GAS HEAT CAPACITY

= 1728 : NO CONVERGENCE IN CALCULATION OF DENSITY BY EOS(SRK)

3. Required Properties

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

If there are not gas viscosity coefficient in KDB databank, you should use the program for calculating low-pressure gas thermal conductivity such as HC_VSGLUCAS_LP.

Specify the ideal heat capacity coefficients for HC_CPGEQN.

If you don't have a density data at given temperature, for calculating the density, use the subroutine CB_SRK. In this case, specify IEXP as 0 and P as given pressure.