1. Theory for Pure-liquid Surface Tension

I) Brock and Bird Method (HC_SRFBROCK)

Brock and Bird proposed the following relation for nonpolar liquids.

$$\frac{\sigma}{P_c^{2/3}T_c^{1/3}} = (0.132\alpha_c - 0.279)(1-T_r)^{11/9} \tag{1}$$

Using the relation by Miller Eq. (1) is derived as ;

$$\sigma = P_c^{2/3}T_c^{1/3}Q(1-T_r)^{11/9} \tag{2}$$

$$Q = 0.1196\left[1+\frac{T_{br}\ln(P_c/1.01325)}{1-T_{br}}\right]-0.279 \tag{3}$$

where surface tension, σ is in dyne/cm, and temperature and pressure are in Kelvins and bars, respectively.

References :

Brock, J. R., and R. B. Bird, *AIChE J.*, **1**, 174, 1955

Miller, D. G., *Ind. Eng. Chem. Fundam.*, **2**, 78, 1963

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

II) Zuo and Stenby Method (HC_SRFZUO)

Zuo and Stenby proposed the two-reference fluid corresponding-state approach such as the following relation.

$$\sigma_r = \ln\left(1+\frac{\sigma}{T_c^{1/3}P_c^{2/3}}\right) \tag{4}$$

The units in Eq. (4) are bar, kelvins, and dyn/cm. In this method, σ_r for the fluid of interest is related to σ_r for two reference fluid which are methane (1) and n-octane (2) and related by the following expression.

$$\sigma_r = \sigma_r^{(1)} + \frac{\omega-\omega^{(1)}}{\omega^{(2)}-\omega^{(1)}}(\sigma_r^{(2)}-\sigma_r^{(1)}) \tag{5}$$

For methane,

$$\sigma^{(1)} = 40.520(1-T_r)^{1.287} \tag{6}$$

and for n-octane

$$\sigma^{(2)} = 52.095(1-T_r)^{1.21548} \tag{7}$$

References :

Zuo, Y.-X., and E. H. Stenby, *Can. J. Chem. Eng.*, **75**, 1130,

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

Notice : Method (I) and (II) are not satisfactory for polar fluid. For polar fluids, the following method is recommended.

III) Sastri and Rao Method (HC_SRFSR)

Sastri and Rao proposed the following equation to treat the components with strong hydrogen-bonding.

$$\sigma = KP_c^x T_b^y T_c^z \left[\frac{1-T_r}{1-T_{br}}\right]^m \qquad (8)$$

The units in Eq. (8) are kelvins and bars. Parameters for Eq. (8) are show in Table 1 for each class of components.

Table 1.Values of Constants for Sastri-Rao Method, Eq. (8)

	K	*x*	*y*	*z*	*m*
Alcohols	2.28	0.25	0.175	0	0.8
Acids	0.125	0.50	-1.5	1.85	11/9
All others	0.158	0.50	-1.5	1.85	11/9

References :

Sastri, S. R. S., and K. K. Rao, *Chem. Eng. J*., **59**, 181, 1995

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

2. KDB Routines for Pure-liquid Surface Tension Calculation

KDB pure-liquid surface tension calculation subroutines contain three estimation methods, which Brock-Bird method, Zuo-Stenby method, and Sastri-Rao method.

Subroutine Name	Description	Required Common Blocks
HC_SRFBROCK	Brock-Bird method	HC_PROP
HC_SRFZUO	Zuo-Stenby method	HC_PROP
HC_SRFSR	Sastri-Rao method for polar liquid	HC_NAME, HC_PROP

I) HC_SRFBROCK

1. USAGE : CALL HC_SRFBROCK(ICN,T,SRF,IST)

2. ARGUMENTS

ICN : COMPONENT NUMBER (1-50) TO CALCULATE SURFACE TENSION
(INTEGER, INPUT)

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

SRF : SURFACE TENSION IN dyn/cm (REAL*8, OUTPUT)

IST : STATUS OF CALCULATION (INTEGER, OUTPUT)

= 0 : NORMAL TERMINATION

= 911 : CRITICAL TEMPERATURE DATA NOT AVAILABLE

= 912 : CRITICAL PRESSURE DATA NOT AVAILABLE

= 913 : NORMAL BOILING POINT DATA NOT AVAILABLE

= 914 : GIVEN T EXCEEDS CRITICAL TEMPERATURE

3. Required properties

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

II) HC_SRFZUO

1. USAGE : CALL HC_SRFZUO(ICN,T,SRF,IST)

2. ARGUMENTS

ICN : COMPONENT NUMBER (1-50) TO CALCULATE SURFACE TENSION (INTEGER, INPUT)

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

SRF : SURFACE TENSION IN dyn/cm (REAL*8, OUTPUT)

IST : STATUS OF CALCULATION (INTEGER, OUTPUT)

= 0 : NORMAL TERMINATION

= 921 : CRITICAL TEMPERATURE DATA NOT AVAILABLE

= 922 : CRITICAL PRESSURE DATA NOT AVAILABLE

= 923 : ACENTRIC FACTOR DATA NOT AVAILABLE

= 924 : GIVEN T EXCEEDS CRITICAL TEMPERATURE

3. Required Properties

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

III) HC_SRFSR

1. USAGE : HC_SRFSR(ICN,T,SRF,IST)

2. ARGUMENTS

ICN : COMPONENT NUMBER (1-50) TO CALCULATE SURFACE TENSION (INTEGER, INPUT)

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

SRF : SURFACE TENSION IN dyn/cm (REAL*8, OUTPUT)

IST : STATUS OF CALCULATION (INTEGER, OUTPUT)

= 0 : NORMAL TERMINATION

= 931 : CRITICAL TEMPERATURE DATA NOT AVAILABLE

= 932 : CRITICAL PRESSURE DATA NOT AVAILABLE

= 933 : NORMAL BOILING POINT DATA NOT AVAILABLE

= 934 : GIVEN T EXCEEDS CRITICAL TEMPERATURE

3. Required Properties

Critical temperature in K, critical pressure in kPa, and normal boiling point in K ICLASS(ICN) must be specified according to Table 1 for each component.