

# 1 (Equation of State – I)

가 . lattice lattice fluid .  
 . off-lattice .  
 가 .

## Statistical Association Fluid Theory (SAFT)

Chapman (1988,1990) Perturbation Theory, TPT) . Wertheim SAFT . SAFT . (Thermodynamic Huang Radoz (1990) hard sphere , Helmhotz 가

$$\frac{A}{NkT} = \frac{A^{ideal}}{NkT} + \frac{A^{seg}}{NkT} + \frac{A^{chain}}{NkT} + \frac{A^{assoc}}{NkT}$$

A  $A^{ideal}$  Helmhotz  
 Helmhotz . Helmhotz , hard sphere

$$\frac{A^{seg}}{NkT} = m \left( \frac{A^{hs}}{NkT} + \frac{A^{disp}}{NkT} \right)$$

Hard sphere Carnahan Starling(1969)

$$\frac{A^{hs}}{NkT} = \frac{4\eta - 3\eta^2}{(1-\eta)^2}$$

Huang Radoz (1990) square well ( Alder et al, 1972) . (D<sub>ij</sub>)  
 Alder Chen Kreglewski (1977)  
 PVT data 2

$$\frac{a_0^{disp}}{RT} = \sum_i \sum_j D_{ij} \left[ \frac{u}{kT} \right]^i \left[ \frac{\eta}{\tau} \right]^j$$

$$\frac{A^{chain}}{NkT} = -(m-1) \ln \frac{1-\eta/2}{(1-\eta)^3}$$

$A^{assoc}$

$$\frac{A^{assoc}}{NkT} = \sum_A \left[ \ln X^A - \frac{X^A}{2} \right] + \frac{1}{2} M$$

Helmhotz

Huang	Radoz (1990,1991)	100	60
			hard sphere,
			가
	Yu	Chen (1994)	41
	8	-	Economou
Tsonopoulos (1997)	/		
Fu	Sandler (1995)	Lee (Lee et al, 1985)	square well
	SAFT		simplified SAFT
			SAFT

### Hard Sphere Statistical Associating Fluid Theory (HS-SAFT)

HS-SAFT (Chapman et al., 1988) SAFT  
 van der Waals 가 hard sphere HS-  
 SAFT Helmholtz

$$\frac{A}{NkT} = \frac{A^{ideal}}{NkT} + \frac{A^{hs}}{NkT} + \frac{A^{mf}}{NkT} + \frac{A^{chain}}{NkT} + \frac{A^{assoc}}{NkT}$$

$A^{hs}$   $A^{mf}$  hard sphere long range meanfield  
 , (  $A^{mono}$  )

$$\frac{A^{mono}}{NkT} = \frac{A^{hs}}{NkT} + \frac{A^{mf}}{NkT}$$

Galindo (1996,1997) Garcia-Lisbona (1998) HS-SAFT hard  
 sphere Boublik (1970)

$$\frac{A^{hs}}{NkT} = \frac{6}{\pi\rho} \left[ \left( \frac{\zeta_s^3}{\zeta_3^2} - \zeta_0 \right) \ln(1-\zeta_3) + \frac{3\zeta_1\zeta_2}{(1-\zeta_3)} + \frac{\zeta_2^3}{\zeta_3(1-\zeta_3)^2} \right]$$

( $\zeta_l$ )

$$\zeta_l = \frac{\pi\rho}{6} \sum_{i=1}^n x_i m_i \sigma_i^l$$

Galindo / Garcia-Lisbona / alkyl polyoxyethylene

### Lennard Jones Statistical Associationg Fluid Theory (LJ-SAFT)

Banaszak (1994) Lennard Jones  
8-mer, 16-mer, 32-mer  
Kraska Gubbins (1996)

LJ-SAFT

LJ  
dipole-dipole

가

LJ-SAFT Helmholtz

$$\frac{A}{NkT} = \frac{A^{ideal}}{NkT} + \frac{A^{seg}}{NkT} + \frac{A^{chain}}{NkT} + \frac{A^{assoc}}{NkT} + \frac{A^{dipole}}{NkT}$$

LJ Kolafa Nezbeda (1994), dipole-dipole Twu  
Gubbins (1978) Hard sphere  
dipole-dipole

$$\frac{A^{hs}}{NkT} = \frac{5}{3} \ln(1-\eta) + \frac{\eta(34-33\eta+4\eta^2)}{6(1-\eta)^2}$$

$$\frac{A^{seg}}{NkT} = \frac{m}{NkT} (A^{hs} + \exp(-\gamma\rho^{*2}))\rho T \Delta B_{2,hBH} + \sum_{ij} (C_{ij} T^{1/2} \rho^{*j})$$

$$\frac{A^{dipole}}{NkT} = \frac{A_2}{T} \left( \frac{1}{1-(A_3/A_2)} \right)$$

Kraska Gubbins  
SAFT  
(1998) LJ-SAFT Chen

### Square Well Statistical Associationg Fluid Theory (SW-SAFT)

1993 Banaszak SW-SAFT

$$Z^{swc} = mZ_{ref}^{sws} + (1-m) \left( 1 + \eta \frac{\partial \ln g^{sws}(\sigma, \eta)}{\partial \eta} \right)$$

$g^{sws}$   $Z_{ref}^{sws}$  square well sphere site-site

Barker-Henderson . 1995

Tavares TPTD

Adidharma Radosz (1998)

. 1997 Gil-Villegas

VR-SAFT

Helmholtz

$$\frac{A^{mono}}{NkT} = m \frac{A^m}{NkT} = m \left( \frac{A^{hs}}{NkT} + \beta A_1 + \beta^2 A_2 \right)$$

$$1.1 \leq \lambda \leq 1.8 \quad A_1, A_2$$

$$A_1 = A_1^{vdW} g^{hs} (1 : \eta_{eff})$$

$$A_2 = \frac{1}{2} \epsilon K^{hs} \eta \frac{\partial A_1^{sw}}{\partial \eta}$$

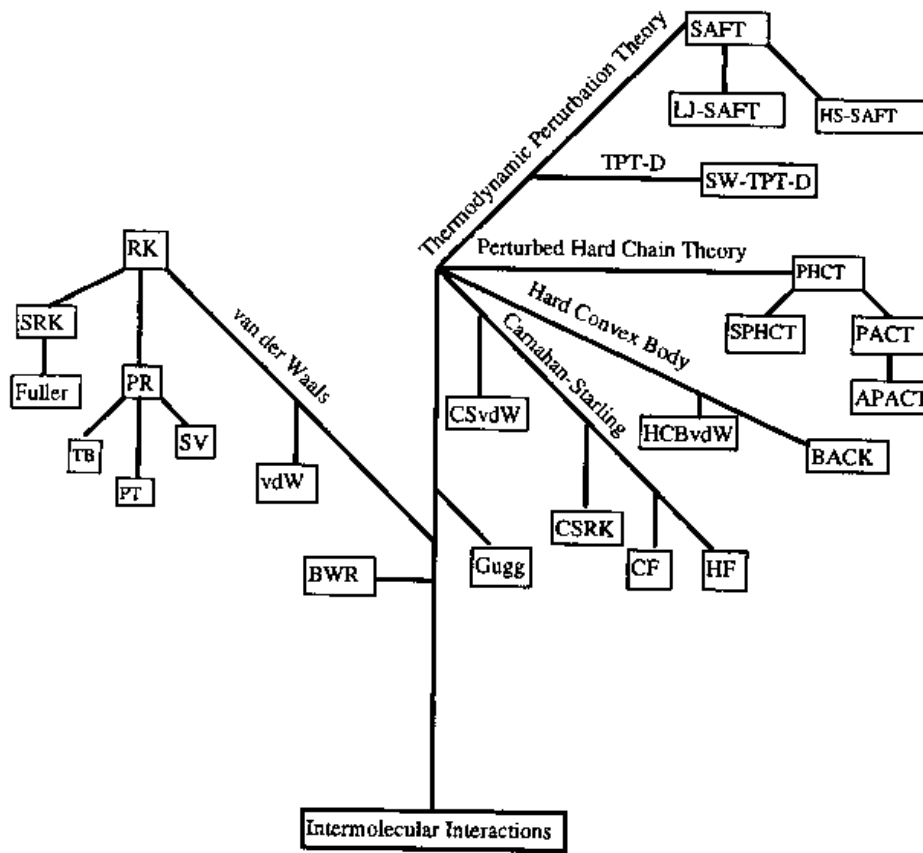
perfluoroalkanes

. McCabe (1998)

. Tavares (1997) square well

$$1 \leq \lambda \leq 2$$

square well



Equation-of-state tree showing the interrelationship between various equations of state.