
ADVANCES IN CHEMICAL ENGINEERING

Edited by **Zeeshan Nawaz** and **Shahid Naveed**

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Advances in Chemical Engineering

Edited by Zeeshan Nawaz and Shahid Naveed

Published by InTech

Janeza Trdine 9, 51000 Rijeka, Croatia

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Publishing Process Manager Bojan Rafaj

Technical Editor Teodora Smiljanic

Cover Designer InTech Design Team

First published March, 2012

Printed in Croatia

A free online edition of this book is available at www.intechopen.com

Additional hard copies can be obtained from orders@intechopen.com

Advances in Chemical Engineering, Edited by Zeeshan Nawaz and Shahid Naveed

p. cm.

ISBN 978-953-51-0392-9

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Contents

Preface IX

Part 1 Fundamentals 1

- Chapter 1 **Application of Chebyshev Polynomials to Calculate Density and Fugacity Using SAFT Equation of State to Predict Asphaltene Precipitation Conditions** 3
Seyyed Alireza Tabatabaei-Nejad and Elnaz Khodapanah
- Chapter 2 **Based on Common Inverted Microscope to Measure UV-VIS Spectra of Single Oil-Gas Inclusions and Colour Analysis** 43
Ailing Yang
- Chapter 3 **Challenging Evaluation of the Hybrid Technique of Chemical Engineering – Proton NMR Technique for Food Engineering** 69
Yasuyuki Konishi and Masayoshi Kobayashi
- Chapter 4 **Modelling Approach for Redesign of Technical Processes** 93
Ivan Lopez-Arevalo, Victor Sosa-Sosa and Saul Lopez-Arevalo
- Chapter 5 **Application Potential of Food Protein Modification** 135
Harmen H.J. de Jongh and Kerensa Broersen

Part 2 Catalysis and Reaction Engineering 183

- Chapter 6 **Rational Asymmetric Catalyst Design, Intensification and Modeling** 185
Zeeshan Nawaz, Faisal Baksh, Ramzan Naveed and Abdullah Alqahtani
- Chapter 7 **Preparation, Catalytic Properties and Recycling Capabilities Jacobsen's Catalyst** 203
Jairo Cubillos

- Chapter 8 **Carbohydrate-Based Surfactants: Structure-Activity Relationships** 215
Hary Razafindralambo, Christophe Blecker and Michel Paquot
- Chapter 9 **CO₂ Biomitigation and Biofuel Production Using Microalgae: Photobioreactors Developments and Future Directions** 229
Hussein Znad, Gita Naderi, H.M. Ang and M.O. Tade
- Chapter 10 **Production of Biodiesel from Microalgae** 245
Marc Veillette, Mostafa Chamoumi, Josiane Nikiema, Nathalie Faucheux and Michèle Heitz
- Chapter 11 **Sulfonation/Sulfation Processing Technology for Anionic Surfactant Manufacture** 269
Jesús Alfonso Torres Ortega
- Chapter 12 **Pollutant Formation in Combustion Processes** 295
Grzegorz Wielgosiński
- Part 3 Process Engineering** 325
- Chapter 13 **Systematic Framework for Multiobjective Optimization in Chemical Process Plant Design** 327
Ramzan Naveed, Zeeshan Nawaz, Werner Witt and Shahid Naveed
- Chapter 14 **CFD Modelling of Fluidized Bed with Immersed Tubes** 357
A.M.S. Costa, F.C. Colman, P.R. Paraiso and L.M.M. Jorge
- Chapter 15 **Optimal Synthesis of Multi-Effect Evaporation Systems of Solutions with a High Boiling Point Rise** 379
Jaime Alfonzo Irahola
- Chapter 16 **Optimization of Spouted Bed Scale-Up by Square-Based Multiple Unit Design** 405
Giorgio Rovero, Massimo Curti and Giuliano Cavaglià
- Chapter 17 **Techno-Economic Evaluation of Large Scale 2,5-Dimethylfuran Production from Fructose** 435
Fábio de Ávila Rodrigues and Reginaldo Guirardello
- Chapter 18 **Inland Desalination: Potentials and Challenges** 449
Khaled Elsaid, Nasr Bensalah and Ahmed Abdel-Wahab

- Part 4 Separation Technology 481**
- Chapter 19 **Phase Diagrams in Chemical Engineering:
Application to Distillation and Solvent Extraction 483**
Christophe Coquelet and Deresh Ramjugernath
- Chapter 20 **Organic/Inorganic Nanocomposite
Membranes Development for Low
Temperature Fuel Cell Applications 505**
Touhami Mokrani
- Chapter 21 **Membrane Operations for Industrial Applications 543**
Maria Giovanna Buonomenna,
Giovanni Golemme and Enrico Perrotta
- Chapter 22 **Thermal Study on Phase Transitions of
Block Copolymers by Mesoscopic Simulation 563**
César Soto-Figueroa, Luis Vicente
and María del Rosario Rodríguez-Hidalgo

Preface

This book addresses the evolutionary stage of Chemical Engineering and provides an overview to the state of the art and technological advancements. Chemical Engineering applications have always been challenging. Optimization of plausible solutions to problems in economic manner through technology is worth. The script has been designed to enable the reader to access the desired knowledge on fundamentals and advancements in Chemical Engineering in a single text. The molecular perspective of Chemical Engineering is increasingly becoming important in the refinement of kinetic and thermodynamic modeling. As a result many of the theories, subject matters and approaches are being revisited and improved. The approach to industrial problems has been reviewed with modern trend in technology.

The subject of primary interest in this text is to highlight recent advances in chemical engineering knowledge. Therefore, the book is divided into four sections: fundamentals, catalysis & reaction engineering, process engineering and separation technology. Fundamentals covers, application of Chebyshev polynomials to analyze soft equation of state, UV-VIS Spectra analysis, proton NMR technique applications, and modeling approach for process redesign. Catalysis and reaction engineering discusses; asymmetric catalyst design, intensification, modeling, preparation, characterization and recycling, carbohydrate-based surfactants, bio-fuel production from micro-algae, biodiesel using triglycerides, and pollutant formation during combustion. Third section of process engineering focused on systematic multiobjective process optimization, CFD modeling of fluidized bed, optimization of evaporation system, spouted bed scale-up, desalination, and economic evaluation of macro scale production processes. Last section of the book has emphasized on separation technology includes phase diagram analysis, membranes developments and applications, and phase transitions study. Molecular chemistry, reaction engineering and modeling have been demonstrated to be interrelated and of value for practical applications. A rational and robust industrial design can be conceived with this understanding. The book can be of interest for undergraduate, graduate and professionals for a number of reasons besides the incorporation of innovation in the text.

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Part 1

Fundamentals

Application of Chebyshev Polynomials to Calculate Density and Fugacity Using SAFT Equation of State to Predict Asphaltene Precipitation Conditions

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1. Introduction

Equations of state are the essential tools to model physical and chemical processes in which fluids are involved. The majority of PVT calculations carried out for oil and gas mixtures are based on a cubic equation of state (EoS). This type of equations dates back more than a century to the famous Van der Waals equation (Van der Waals, 1873). The cubic equations of state most commonly used in the petroleum industry today are very similar to the Van der Waals equation, but it took almost a century for the petroleum industry to accept this type of equation as a valuable engineering tool. The Redlich and Kwong EoS (Redlich & Kwong, 1949) was modified from the VdW with a different attractive term, the repulsive term being the same. Since 1949 when Redlich and Kwong (RK) formulated their two-parameter cubic EoS, many investigators have introduced various modifications to improve ability of RK-EoS. Two other well-known cubic equations are Soave-Redlich-Kwong (SRK), (Soave, 1972) and Peng-Robinson (PR) (Peng & Robinson, 1976) equations which have different formulation of the attractive term and are popular in the oil industry in the thermodynamic modeling of hydrocarbon fluids.

There are thousands of cubic equations of states, and many noncubic equations. The noncubic equations such as the Benedict-Webb-Rubin equation (Benedict et al., 1942), and its modification by Starling (Starling, 1973) have a large number of constants; they describe accurately the volumetric behavior of pure substances. But for hydrocarbon mixtures and crude oils, because of mixing rule complexities, they may not be suitable (Katz & Firoozabadi, 1978). Cubic equations with more than two constants also may not improve the volumetric behavior prediction of complex reservoir fluids. In fact, most of the cubic equations have the same accuracy for phase behavior prediction of complex hydrocarbon systems; the simpler often do better (Firoozabadi, 1999).

Hydrocarbons and other non-polar fluid vapor-liquid equilibrium properties can be satisfactorily modeled using a symmetric approach to model both, the vapor and the liquid phase fugacity with the use of a Van der Waals type equation model (Segura et al., 2008), the Soave-Redlich-Kwong or Peng-Robinson equations being the most popular ones. When

polar fluids are involved at moderate pressures, activity coefficient models are more suitable for modeling the liquid phase. When a higher pressure range is also a concern, a symmetric EoS approach with complex mixing rules including an excess Gibbs energy term from an activity coefficient model can provide good results. Unfortunately, even those approaches show limitations for complex fluids and can drastically fail near the critical region, unless a specific treatment is included (Llovel et al., 2004, 2008).

Since the early 1980's, there has been increased interest in developing an EoS for pure fluids and mixtures of large polyatomic molecules that does not rely on a lattice description of molecular configurations. A rigorous statistical-mechanical theory for large polyatomic molecules in continuous space is difficult because of their asymmetric structure, large number of internal degrees of freedom, and strong coupling between intra- and intermolecular interactions. Nevertheless, a relatively simple model represents chain-like as freely joined tangent hard spheres (Chapman et al., 1984; Song et al., 1994; Wertheim, 1984). A hard-sphere-chain (HSC) EoS can be used as the reference system in place of the hard-sphere reference used in most existing equations of state for simple fluids. Despite their simplicity, hard-sphere-chain models take into account some significant features of real fluids containing chain-like molecules including excluded volume effects and chain connectivity. To describe the properties of fluids consisting of large polyatomic molecules, it is necessary to introduce attractive forces by adding a perturbation to a HSC EoS. Assuming that the influence of attractive forces on fluid structure is weak, a Van der Waals type or other mean-field term (e.g. square-well fluids) is usually used to add attractive forces to the reference hard-sphere-chain EoS (Prausnitz & Tavares, 2004).

Molecular-based equations of state, also rooted in statistical mechanics, retain their interest in chemical engineering calculations as they apply to a wide spectrum of thermodynamic conditions and compounds, being computationally much less demanding than molecular simulations. Among them, the Statistical Associating Fluid Theory (SAFT) EoS has become very popular because of its capability of predicting thermodynamic properties of several complex fluids, including chain, aromatic and chlorinated hydrocarbons, esters alkanols, carboxylic acids, etc. (Huang & Radosz, 1990). SAFT was envisioned as an application of Wertheim's theory of association (Wertheim, 1984, 1986) through the use of a first-order thermodynamic perturbation theory (TPT) to formulate a physically based EoS (Chapman et al., 1990; Huang & Radosz, 1991). The ambition of making SAFT an accurate equation for engineering purposes has promoted the development of different versions that tried to overcome the limitations of the original one (Economou, 2002; Muller & Gubbins, 1995).

SAFT has a similar form to group contribution theories in that the fluid of interest is initially considered to be a mixture of unconnected groups or segments. SAFT includes a chain connectivity term to account for the bonding of various groups to form polymers and an explicit intermolecular hydrogen bonding term. A theory based in statistical mechanics offers several advantages. The first advantage is that each of the approximations made in the development of SAFT has been tested versus molecular simulation results. In this way, the range of applicability of each term in the EoS has been determined. The second advantage is that the EoS can be systematically refined. Since any weak approximations in SAFT can be identified, improvement is made upon the EoS by making better approximations or by extending the theory. Like most thermodynamic models, SAFT approaches require the evaluation of several parameters relating the model to the

experimental system. A third advantage of SAFT-type equations versus other approaches is that, as they are based on statistical mechanics, parameters have a clear physical meaning; when carefully fitted they can be used with predictive power to explore other regions of the phase diagram far from the data and operating conditions used in the parameter regression, performing better than other models for interacting compounds like activity coefficient models (Prausnitz et al., 1999). In SAFT a chain molecule is characterized by the diameter or volume of a segment, the number of segments in the chain, and the segment-segment dispersion energy. For an associating or hydrogen bonding molecule, two more physical parameters are necessary: the association energy related to the change in enthalpy of association and the bond volume related to the change in entropy on association. The SAFT equation has found some impressive engineering applications on those fluids with chain bonding and hydrogen bonding (Chapman et al., 2004).

Asphaltenes are operationally defined as the portion of crude oil insoluble in light normal alkanes (e.g., n-heptane or n-pentane), but soluble in aromatic solvents (e.g., benzene or toluene). This solubility class definition of asphaltenes suggests a broad distribution of asphaltene molecular structures that vary greatly among crude sources. In general, asphaltenes possess fused ring aromaticity, small aliphatic side chains, and polar heteroatom-containing functional groups capable of donating or accepting protons inter- and intra-molecularly. Although asphaltene fractions can be complex molecular species mixtures, they convey, as a whole, an obvious chemical similarity, irrespective of crude geographic origin (Ting, 2003). Asphaltene stability depends on a number of factors including pressure, temperature, and compositions of the fluid; the latter incorporates the addition of light gases, solvents and other oils commingled operation or charges due to contamination. During pressure depletion at constant temperature, asphaltene aggregate formation is observed within a range above and below the bubble point. As pressure drops during production from the reservoir pressure, asphaltene precipitate can appear due to changes in the solubility of asphaltene in crude oil. The maximum asphaltene precipitation occurs at or around the bubble point pressure. Below the bubble point light gases come out of the solution increasing the asphaltene solubility again (Ting, 2003). Temperature changes also affect asphaltene precipitation, For hydrocarbons deposited in shallow structure, the wellhead flowing temperatures are typically not excessive, 110-140 °F. However, sea bottom temperature in deep water is cold, often near or below 40 °F, even in equatorial waters. Cooling of flow streams during transportation can lead to asphaltene precipitation (Huang & Radosz, 1991). Increases in temperature at constant pressure normally stabilize the asphaltene in crude oil. Depending on the composition of the oil, it is possible to find cases where precipitation first decreases and then increases with increasing temperature (Verdier et al., 2006). Also, depending on the temperature level, significant temperature effects can be observed (Buenrostro-Gonzales & Lira-Galeana, 2004). Changes in composition occur during gas injection processes employed in Enhanced Oil Recovery (EOR). Gas injection includes processes such as miscible flooding with CO₂, N₂ or natural gas or artificial gas lifting. The dissolved gas decreases asphaltene solubility and the asphaltene becomes more unstable (Verdier et al., 2006).

The tendency of petroleum asphaltenes to associate in solution and adsorb at interfaces can cause significant problems during the production, recovery, pipeline transportation, and refining of crude oil. Therefore, it is necessary to predict the conditions where precipitation

occurs and the amount of precipitate. The approach we have taken here to model is to use the SAFT EoS, as it explicitly builds on the association interaction and the chain connectivity term to account for the bonding of various groups. Therefore, the equation is able to provide insights on the asphaltene precipitation behavior. By some algebraic manipulations on this equation, we derive a simplified form of the compressibility factor or pressure as a function of density. Due to pressure explicit form of the SAFT EoS, an approximation technique based on Chebyshev polynomials to calculate density and hence fugacity requisite to perform phase equilibrium calculations is applied. To demonstrate the ability of SAFT EoS a binary system composed of ethanol and toluene is tested. Applying Chebyshev polynomial approximation, density is calculated for the above system at different temperatures in a range of 283.15 K to 353.15 K and for pressures up to 45 MPa. Evaluating fugacity is a necessary step in phase equilibrium calculations. Hence, fugacity is derived using SAFT EoS. Then the model is used to predict phase behavior of oil-asphaltene systems.

2. Formulation of the problem

2.1 SAFT equation of state

The statistical association fluid theory (SAFT) (Chapman et al., 1990) is based on the first order perturbation theory of Wertheim (Wertheim, 1987). The essence of this theory is that the residual Helmholtz energy is given by a sum of expressions to account not only for the effects of short-range repulsions and long-range dispersion forces but also for two other effects : chemically bonded aggregation (e.g. formation of chemically stable chains) and association and/or solvation (e.g. hydrogen bonding) between different molecules (or chains). For a pure component a three step process for formation of stable aggregates (e.g. chains) and subsequent association of these aggregates is shown in figure 1. Initially, a fluid consists of equal-sized, single hard spheres. Intermolecular attractive forces are added

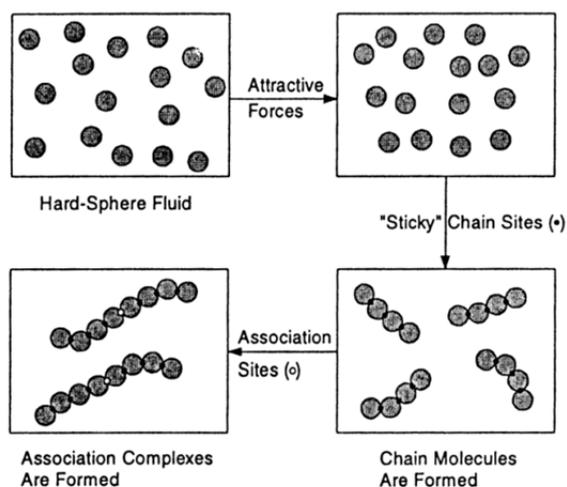


Fig. 1. Three steps to form chain molecules and association complexes from hard spheres in the SAFT model (Prausnitz et al., 1999).

which are described by an appropriate potential function, such as the square-well potential. Next, each sphere is given one, two or more "sticky spots", such that the spheres can stick together (covalent bonding) to form dimmers, trimers and higher stable aggregates as chains. Finally, specific interaction sites are introduced at some position in the chain to form association complex through some attractive interaction (e.g. hydrogen bonding). Each step provides a contribution to the Helmholtz energy.

Using SAFT EoS, the residual molar Helmholtz energy A^R contributes from formation of hard spheres, chains, dispersion (attraction), and association which would be in the form of:

$$A^R = A_{hs} + A_{ch} + A_{disp} + A_{assoc} \quad (1)$$

Here the sum of the first two terms is the hard-sphere-chain reference system accounting for molecular repulsion and chain connectivity (chemical bonding); the sum of the last two terms is the perturbation accounting for molecular attraction and for association due to specific interactions like hydrogen bonding. Application of the relation between molar Helmholtz energy, A , and the equation of state, gives the SAFT EoS for pure fluids (Prausnitz et al., 1999). We can write for compressibility factor of a real fluid:

$$Z = \frac{P}{\rho RT} = Z^{id} + Z_{hs} + Z_{ch} + Z_{disp} + Z_{Assoc} \quad (2)$$

with $Z^{id} = 1.0$ and for mixtures,

$$Z_{hs} = \frac{6}{\pi N_A \rho} \left[\frac{\xi_0 \xi_3}{1 - \xi_3} + \frac{3 \xi_1 \xi_2}{(1 - \xi_3)^2} + \frac{(3 - \xi_3) \xi_2^3}{(1 - \xi_3)^2} \right] \quad (3)$$

With

$$\xi_k = \frac{\pi N_A \rho}{6} \sum_{i=1}^{N_c} z_i r_i (d_i)^k \quad k = 0, 1, 2, 3 \quad (4)$$

$$d_i = \sigma_i [1 - 0.12 \exp(-3\varepsilon_i/kT)] \quad (5)$$

$$Z_{hs} = \frac{hs_1 \rho + hs_2 \rho^2 + hs_3 \rho^3}{1 + hs_4 \rho + hs_5 \rho^2 + hs_6 \rho^3} \quad (6)$$

here ρ is the total molar density, z_i is the mole fraction of component i , r_i is the number of segments per molecule i , and d_i is the temperature dependent segment diameter. The parameters T , N_A , k , ε_i and σ_i are temperature, Avogadro's and Boltzmann's constants, segment energy and diameter, respectively. By simple algebraic manipulation on Eq. (3), we arrive at the following simplified form of the hard sphere term:

where,

$$hs_1 = (\bar{r}S_3 + 3S_1S_2)P_{na} \quad (7)$$

$$hs_2 = (-2\bar{r}S_3^2 - 3S_1S_2S_3 + 3S_2^3)P_{na}^2 \quad (8)$$

$$hs_3 = (\bar{r}S_3^3 - S_2^3S_3)P_{na}^3 \quad (9)$$

$$hs_4 = -3S_3P_{na} \quad (10)$$

$$hs_5 = 3S_3^2P_{na}^2 \quad (11)$$

$$hs_6 = -S_3^3P_{na}^3 \quad (12)$$

The parameters used in Eqs. (7) - (12) are defined as the following:

$$\bar{r} = \sum_{i=1}^{N_c} z_i r_i \quad (13)$$

$$S_1 = \sum_{i=1}^{N_c} z_i r_i d_i \quad (14)$$

$$S_2 = \sum_{i=1}^{N_c} z_i r_i d_i^2 \quad (15)$$

$$S_3 = \sum_{i=1}^{N_c} z_i r_i d_i^3 \quad (16)$$

$$P_{na} = \frac{\pi N_A}{6} \quad (17)$$

The contribution accounting for the formation of chain molecules of the various components in the mixture is

$$Z_{ch} = \sum_{i=1}^{N_c} z_i (1 - r_i) L(d_i) \quad (18)$$

$$L(d_i) = \frac{2\xi_3 + 3d_i\xi_2 - 4\xi_3^2 + 2d_i^2\xi_2^2 + 2\xi_3^3 + d_i^2\xi_2^2\xi_3 - 3d_i\xi_2\xi_3^2}{(1 - \xi_3)(2 - 4\xi_3 + 3d_i\xi_2 + 2\xi_3^2 + d_i^2\xi_2^2 - 3d_i\xi_2\xi_3)} \quad (19)$$

where ξ_k ($k = 2, 3$) is given by Eq. (4). It is remarkable that no mixing rules are necessary in Eq. (3) and (18). After some arithmetic operations on Eq. (18), the following simplified density dependent equation for the chain term of SAFT EoS is presented as:

$$Z_{ch} = \sum_{i=1}^{N_c} z_i (1 - r_i) \frac{ch_1(d_i)\rho + ch_2(d_i)\rho^2 + ch_3(d_i)\rho^3}{2 + ch_4(d_i)\rho + ch_5(d_i)\rho^2 + ch_6(d_i)\rho^3 + ch_7(d_i)\rho^4} \quad (20)$$

where,

$$ch_1(d_i) = [2S_3 + 3d_i S_2] P_{na} \quad (21)$$

$$ch_2(d_i) = [-4S_3^2 + 2d_i^2 S_2^2] P_{na}^2 \quad (22)$$

$$ch_3(d_i) = [d_i^2 S_2^2 S_3 + 2S_3^3 - 3d_i S_2 S_3^2] P_{na}^3 \quad (23)$$

$$ch_4(d_i) = [-6S_3 + 3d_i S_2] P_{na} \quad (24)$$

$$ch_5(d_i) = [6S_3^2 + d_i^2 S_2^2 - 9d_i S_2 S_3] P_{na}^2 \quad (25)$$

$$ch_6(d_i) = [9d_i S_2 S_3^2 - 2S_3^3 - d_i^2 S_2^2 S_3] P_{na}^3 \quad (26)$$

$$ch_7(d_i) = [-3d_i S_2 S_3^3] P_{na}^3 \quad (27)$$

SAFT uses the following expression for the dispersion contribution to the compressibility factor (Pedersen & Christensen, 2007):

$$Z_{disp} = -2\pi\rho \frac{\partial(\xi_3 I_1)}{\partial(\xi_3)} \overline{r^2 \varepsilon \sigma^3} - \pi\rho\bar{r} \left[C_1 \frac{\partial(\xi_3 I_2)}{\partial(\xi_3)} + C_2 \xi_3 I_2 \right] \overline{r^2 \varepsilon^2 \sigma^3} \quad (28)$$

where

$$C_1 = 1 + \bar{r} \frac{8\xi_3 - 2\xi_3^2}{(1 - \xi_3)^4} + (1 - \bar{r}) \frac{20\xi_3 - 27\xi_3^2 + 12\xi_3^3 - 2\xi_3^4}{[(1 - \xi_3)(2 - \xi_3)]^2} \quad (29)$$

$$C_2 = -C_1^2 \left[\bar{r} \frac{-4\xi_3^2 + 20\xi_3 + 8}{(1 - \xi_3)^5} + (1 - \bar{r}) \frac{2\xi_3^3 + 12\xi_3^2 - 48\xi_3 + 40}{[(1 - \xi_3)(2 - \xi_3)]^3} \right] \quad (30)$$

$$\overline{r^2 \varepsilon \sigma^3} = \sum_{i=1}^{N_c} \sum_{j=1}^{N_c} z_i z_j r_i r_j \left(\frac{\varepsilon_{ij}}{kT} \right) \sigma_{ij}^3 \quad (31)$$

$$\overline{r^2 \varepsilon^2 \sigma^3} = \sum_{i=1}^{N_c} \sum_{j=1}^{N_c} z_i z_j r_i r_j \left(\frac{\varepsilon_{ij}}{kT} \right)^2 \sigma_{ij}^3 \quad (32)$$

$$I_1 = \sum_{j=0}^6 a_j(\bar{r}) \xi_3^j \quad (33)$$

$$I_2 = \sum_{j=0}^6 b_j(\bar{r}) \xi_3^j \quad (34)$$

In equations (31) and (32):

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j} (1 - k_{ij}) \quad (35)$$

$$\sigma_{ij} = \frac{1}{2} (\sigma_i + \sigma_j) \quad (36)$$

where k_{ij} is a binary interaction parameter similar to that in the mixing rule for the a -parameter of a cubic EoS (Pedersen & Christensen, 2007). In equation (33) and (34):

$$a_j(\bar{r}) = a_{0j} + \frac{\bar{r}-1}{\bar{r}} a_{1j} + \frac{\bar{r}-1}{\bar{r}} \cdot \frac{\bar{r}-2}{\bar{r}} a_{2j}, \quad j = 0, 1, \dots, 6 \quad (37)$$

$$b_j(\bar{r}) = b_{0j} + \frac{\bar{r}-1}{\bar{r}} b_{1j} + \frac{\bar{r}-1}{\bar{r}} \cdot \frac{\bar{r}-2}{\bar{r}} b_{2j}, \quad j = 0, 1, \dots, 6 \quad (38)$$

The universal constants for a_{0j} , a_{1j} , a_{2j} , b_{0j} , b_{1j} and b_{2j} are given in Table 1.

J	a_{0j}	a_{1j}	a_{2j}	b_{0j}	b_{1j}	b_{2j}
0	0.9105631	-0.3084017	-0.0906148	0.7240947	0.5755498	0.0976883
1	0.6361281	0.1860531	0.4527843	2.2382792	0.6995095	-0.2557575
2	2.6861348	-2.5030047	0.5962701	-4.0025849	3.8925674	-9.1558561
3	-26.547362	21.419793	-1.7241829	-21.003577	-17.215472	20.642076
4	97.759209	-65.255885	-4.1302112	26.855641	192.67226	-38.804430
5	-159.59154	83.318680	13.776632	206.55134	-161.82646	93.626774
6	91.297774	-33.746923	-8.6728470	-355.60235	-165.20769	-29.666905

Table 1. The universal constants for a_{0j} , a_{1j} , a_{2j} , b_{0j} , b_{1j} and b_{2j} parameters used in SAFT EoS (Pedersen & Christensen, 2007).

Again, simplification of Eq. (28), would yield the following density dependent form of the dispersion term in SAFT EoS: