# DIYALA JOURNAL FOR PURE SCIENCES

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

# Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane

**Saygın Muhamad Nuri [1] and Shanay Rajab Hasan [2]**

[1]Department of Physics – College of Education for Pure Science – Kirkuk University
[2]Health of Community Department – North Technical University - KIRKUK

[1]Saygin.kuzeci@yahoo.com
[2]Shnay.rajab@yahoo.com

## Abstract

The Gradient energy coefficient ($\kappa$) in polymers and oligomers (a few segments) play an important role in polymer blending, wetting, coating, adhesion process, foaming and a comprehensive role in the description as well as understanding of many processes especially in innovation of new polymer with classification of materials. As a result, the main reason in this study appear which has how the gradient energy coefficient changes from bulk to surface, has been establishing the new equation that helped us to extract the correlation between gradient energy coefficient and different parameters. The gradient energy coefficient has been related with hole fractions, temperature and density. The relationships between the above-mentioned parameters are then drawn according to our model. Both Simha-Somcynsky (SS) and Cahn-Hilliard (CH) models are employed together to calculate the thermodynamic properties of cyclohexane, namely, the hole fraction in temperature range at 313-473 K various presures up to 150 Mpa. Our values for the average and maximum percentage deviation of the specific volume of cyclohexane are calculated as 0.0196% and 0.0678% respectively

**Keywords:** lattice hole theory, Chan-Hilliard, gradien energy coefficient, Simha-Somcynsky, and surface tension.

## Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane

### Saygın Muhamad Nuri and Shanay Rajab Hasan

دراسة العلاقة بين معامل انحدار الطاقة مع النسبة المملوة في الشبيكة، الحرارة، الكثافة، والشد السطحي لبوليمر سايكلوهكسان السائل

**صايغن محمد نوري لطيف¹ و شناي رحب حسن²**

¹قسم الفيزياء – كلية التربية للعلوم الصرفة – جامعة كركوك
² قسم صحة المجتمع – المعهد التقني كركوك – الجامعة التقنية الشمالية

## الخلاصة

معامــل انحــدار الطاقـة فــي البـوليمرات و أولبكوميريلعــب دورا مهمــا فــي كثيــر مــن العمليــات منهــا المــزج، الرطوبــة، الطــلاء و اللواصــقا، عمليــة التصــاق، ارغــاء البـوليمرات بالاضــافة الــى فهــم العديــد مــن العمليــات وخصوصــا فــي الكشــف عــن البـوليمرات الجديــدة وفــي عمليــات تصــنيف المــواد. السـبب الرئيســي مــن هـذه الدراسـة هـو كيفيـة تغيـر معامـل انحـدار الطاقـة مـن العمـق الـى السـطح للبـوليمر.وفي هـذه الدراسـة تــم ايجـاد معادلــة جديــدة قـد تسـاعدنا فــي اسـتخراج العلاقـة بـين معامـل انحـدار الطاقـة، الجـزء المملـوء، درجـة الحـرارة، الكثافـة والشـد السـطحي لبـوليمر سايكلوهكسـان السـائل. باسـتخدام النظـريتين (سـيمها سومسينيسـكي وكـاهن هـيلارد) معـا فــي حسـاب الخـواص الثرمودينـاميكيـة للبـوليمر المذكور حصـلنا علـى قيم معامـل انحـدار الطاقـة والمتغيـرات المـذكورة و قمنـا برسـم المنحنيـات و مـن خلالهـا وجـدنا العلاقـة بـين معامـل انحـدار الطاقـة والمتغيـرات اعـلاه. ولقـد تـم الحصـول علـى هـذه القـيم تحـت مـدى درجـات الحـرارة مـن 313 الـى 473 كلفـن وتحـت الضـغوط مـن الضـغط الجـوي الـى 150 ميكـا باسـكال وكانـت نسـب الانحـراف فــي متوسـطة الحجـم النـوعي والقيمـة العظمـى هـي 0.0196 و0.0678 على التوالي.

**كلمات المفتاحية**: نظرية الشبيكة الفراغية، كاهن هيلارد، معامل انحدار الطاقة، سيمها سومسينسكي والشد السطحي.

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

## Introduction

The Cahn-Hilliard (CH) theory that includes the free energy profile during the phase separation in an inhomogeneous mixture density for a homogeneous system and $\kappa$ is a positive materials constant called the gradient energy coefficient or interaction coefficient for the component and the second part from same equation is the composition gradient contribution to the free energy [1]. The lattice fluid (LF) theory [2] is able to describe the thermodynamic properties of both low and high molecular weight. The LF model in conjunction with the Cahn-Hilliard theory (CH) is employed to develop a method for calculating the surface tension of nonpolar and slightly polar liquids of arbitrary molecular weight has worked by Poser and Sanchez [3] to extract the surface tension and surface density profile of polymers in broad range of temperature. Poser and Sanchez, Kahl and Enders [4], Dee-Sauer and C.Miqueu and co-workers they has worked extensively on the surface tension and surface density profile of polymers for broad ranges of temperatures and molecular weights using the Cahn-Hillard density gradient [5].theory in conjunction with the Flory, Orwoll, and Vrij (FOV) [6] and Sanchez and Lacombe [7] (SL) equation of state theories. B. Sauer and T. Dee they has worked to obtained the surface tension and the gradient energy coefficient ($\kappa$) for linear, branched *n*-alkanes. The surface tension increase and surface entropy [8] decrease with increasing molecular weight.

The surface thermodynamics properties of polymers are strongly correlated with the bulk properties, the bulk properties are inherently hole fraction dependent so we could constitute the correlate between surface tension and surface density profile with hole fraction or free volume of the bulk, Carri and Simha (CS) examined the relation between surface tension and hole fraction of the bulk properties by means of SS lattice-hole theory [9]. The Simha and Somsynsky (SS) come up with an arrangement in the model increasing the disorder by employed hole fractions in the underlying quasi lattice model. An established equation of state (e.o.s) was intensively applied to low and high molar mass of liquid polymers [10 and 11] and mix of molecular weight of different polymer, with significant quantitative achievement [12], The quantitative success of hole theory (SS) encouraged us to employ in conjunction with the Cahn-Hillard density gradient theory to inspection how the hole fraction changes from the bulk to surface and effectives on surface tension and its correlation with the surface density profile

# DIYALA JOURNAL FOR PURE SCIENCES

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

of binary polymers system. We are employed properties of SS theory as a nested with CH in the range of about 473 K temperature and up to about 1500 bar pressure. We have obtained %0.0196 maximum deviation in volume.

# Theories

## 1. The Cahn-Hilliard Theory

The Cahn-Hilliard theory [13] correlates the thermodynamic characteristics of a system with an interface between two non-condensing phases. In the interface between the liquid and the gas phase of a pure polymer in equilibrium condition, the density of the composition discontinues or behaves as gradient, consider a binary alloy in a two-phase equilibrium state. For the free energy of inhomogeneous systems, the density gradients varies from the bulk or liquid density to the surface or the vapor density continuously. This means that the Helmholtz free energy density, $\alpha$, of a system with an interface can be obtained by expanding the Helmholtz free energy in Taylor series around the equilibrium state:

$$\alpha(\rho, \nabla\rho, \nabla^2\rho, ...) = \alpha_0(\rho) + \kappa_1 \nabla^2\rho + \kappa_2 (\nabla\rho)^2 \tag{1}$$

where $\alpha_0(\rho)$ is the local free energy density of homogeneous polymer system and the coefficients of Laplacian and gradient density terms are

$$\kappa_1 = \left(\frac{\partial\alpha}{\nabla^2\rho}\right)_0 ; \quad \kappa_2 = \frac{1}{2}\left(\frac{\partial^2\alpha}{\partial(\nabla\rho)^2}\right)_0. \tag{2}$$

The subscript 0 in Eq. (2) indicates that the derivatives are to be evaluated in the limit of $\nabla\rho$ and $\nabla^2\rho$ going to zero. Here the density variation is assumed comparatively small to the reciprocal of the intermolecular distance. The Helmholtz free energy, $A$, of a system of volume $V$ is given by

$$A = \int_V [\alpha_0(\rho) + \kappa(\nabla\rho)^2] dV \tag{3}$$

where $\kappa$ is the gradient energy coefficient for the system. It is composed of two terms: the first

# DIYALA JOURNAL FOR PURE SCIENCES

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

is the local free energy of homogeneous system and the second is composition gradient contribution to the free energy.

We could write Eq. (3) in finally shape of surface tension for a planar interface tension is given

$$\gamma = \int_{-\infty}^{+\infty} [\Delta\alpha + \kappa(\frac{d\rho}{dx})^2]dx \qquad (4)$$

where $\Delta\alpha = \alpha_0(\rho) - (\rho_l \mu_{l0} + \rho_v \mu_{v0})$ is the difference between the Helmholtz free energy density of a homogeneous fluid of density $\rho$ and two-phase equilibrium mixtures with liquid and gas states.

where $\mu_{l0}$ and $\mu_{v0}$ are the equilibrium chemical potentials of liquid and vapor,

The appropriate form of the Euler equation says:

$$I - \left(\frac{d\rho}{dx}\right)\left[\frac{\partial I}{\partial(d\rho/dx)}\right] = 0 \qquad (5)$$

where $I$ represents the integrand of Cahn-Hillard equation. If we apply the integrand of Eq. (5) in Eq. (4) [14], we obtain a differential equation whose solution is the composition profile corresponding to invariance value (maximum, minimum or saddle points) of the integral. The

condition for invariance value is $\qquad \Delta\alpha(\rho) - \kappa\left(\frac{d\rho}{dx}\right)^2 = const \qquad (6)$

In this equation the constant value must be zero, and also both $\Delta\alpha(\rho)$ and $\frac{d\rho}{dx}$ tend to zero

when $x \to \pm\infty$. Hence a minimum value can be expressed as: $\quad \Delta\alpha(\rho) = \kappa\left(\frac{d\rho}{dx}\right)^2 \qquad (7)$

Then we get the surface tension I s $\gamma = 2\int_{\rho v}^{\rho l} [\kappa\Delta\alpha(\rho)]^{\frac{1}{2}} d\rho \qquad (8)$

## 2. The Simha-Somcynsky (SS)-EOS Theory

Simha-Somcynsky (SS) developed an equation of state (EOS) based on the lattice-hole model [15] introducing the temperature and volume dependent occupied site fraction, $y(V,T)$. The occupied site fraction, $y(V,T)$, and the complementary hole fraction, $h(V,T)$, are given by the following equation:

$$y = 1 - h = \frac{sN}{sN + N_h} \tag{9}$$

where $s$ is the number of segments in a molecule, and $N$ and $N_h$ are the number of molecules and holes respectively. The SS theory is formulated in terms of scaled volume, scaled temperature and scaled pressure, viz.:

$$\widetilde{V} = V/V^*; \quad \widetilde{T} = T/T^*; \quad \widetilde{P} = P/P^* \tag{10}$$

where the scaling parameters are as follows: $V^*$ is defined by molar volume $s\upsilon^*$ of the molecule, $T^*$ by $q_z \varepsilon^*/ck$ as a balance between attraction and thermal energy

contributed by the external degrees of freedom (where $k$ is the Boltzmann's constant), and $P^*$ is then assigned by the ratio between chain attraction energy $q_z \varepsilon^*$ and volume $s\upsilon^*$. Here $3c$ that appears explicitly in the equilibrium condition is the total degrees of freedom of molecule. In this article, we have considered the ideal chain flexibility employing $3c = s + 3$.

The configurational partition function for the ensemble can be written as

$$Z_{conf} = g(N, y)\left[\upsilon_f(y,V)\right]^{3c} \exp\left(-E_0(y,V)/kT\right) \tag{11}$$

where $E_0$ is the total lattice energy of the system employed Lennard-Johns potential energy, $\upsilon_f$ is the free volume, and $g(N, y)$ is the combinatorial factor that is the total number of distinguishable degenerate arrangements of the holes and molecules by Boltzmann's equation. It can be calculated from the mixing entropy of an assembly of molecules and holes as

$$\Delta S_m = k \ln g(N, y) \tag{12}$$

Hence the combinatorial factor is expressed as

$$g(N, y) \propto y^{-N} (1-y)^{-sN\left(\frac{1-y}{y}\right)}. \tag{13}$$

# DIYALA JOURNAL FOR PURE SCIENCES

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

The SS-EOS equation, derived from the configurational Helmholtz energy, is

$$\frac{\tilde{P}\tilde{V}}{\tilde{T}} = \frac{1}{1-\zeta} + \frac{2y}{\tilde{T}}Q(1.011Q-1.2045) \tag{14}$$

where $Q = \left(y\tilde{V}\right)^{-2}$ and $\zeta = 2^{-1/6}y\left(y\tilde{V}\right)^{-1/3}$. The occupied site fraction can be obtained from the minimization of the Helmholtz energy of an ensemble, $\left.\partial F/\partial y\right|_{\tilde{V},\tilde{T},c/s} = 0$

$$\frac{s}{3c}\left(\frac{s-1}{s} + \frac{\ln(1-y)}{y}\right) = \frac{\zeta - \frac{1}{3}}{1-\zeta} + \frac{y}{6\tilde{T}}Q(2.409 - 3.303Q). \tag{15}$$

Using the coupled Eqs. (14) - (15), we can determine the scaling parameters, $P^*, V^*, T^*$, and the structural parameter *3c/s*, which can be obtained by superimposing experimental *P-V-T* data on the theoretical $\tilde{P}, \tilde{V}, \tilde{T}$ surface. Having these parameters at hand, we can compute the hole fraction, *h(V,T)=1-y*, of the lattice model (as a measure of the free volume [16]). From temperature dependence of the hole fraction law we have the relation:

$$h = 1 - K(\tilde{T})/\tilde{V} \tag{16}$$

$K(\tilde{T})$ is quite slowly varying function. Therefore, the hole faction $h$ or occupied site fraction $y$ satisfies $y\tilde{V} = C = \text{constant}$ \tag{17}

For a binary system (occupied and unoppupied), Gibbs free energy of mixing $\Delta G_m$ for the athermal condition (leading to enthalpy of mixing $\Delta H_m = 0$) is defined as

$$\Delta G_m = -T\Delta S_m \propto kTN[\ln y + \frac{s(1-y)}{y}\ln(1-y)] \tag{18}$$

where the right hand side is obtained by substituting Eq(12) with Eq(13). The chemical potential of the system is given by

$$\mu = \frac{\partial \Delta G_m}{\partial N} = \left.\frac{\partial \Delta G_m}{\partial y}\right|_N \frac{\partial y}{\partial N} + \left.\frac{\partial \Delta G_m}{\partial N}\right|_y = kT\left(-(1-y)(s-1) + \ln y\right). \tag{19}$$

# DIYALA JOURNAL FOR PURE SCIENCES

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

We can then write the chemical potential difference between the surfaces:

$$\Delta\mu = \mu_b - \mu_s = kT\left[(y_b - y_s)(s-1) + \ln\left(\frac{y_b}{y_s}\right)\right] \qquad (20)$$

where the indices $b$ and $s$ refer to bulk and surface. On the other hand the scaled $\Delta\tilde{\alpha}$ is expressed in terms of chemical potential difference as

$$\Delta\tilde{\alpha} = \tilde{\rho}\Delta\tilde{\mu} = C^{-1}y\Delta\tilde{\mu} \qquad (21)$$

where the right hand side of Eq(21).is obtained by substituting Eq(17). Substituting Eqs(21) into Eq(8)., the scaled surface tension can be written as

$$\tilde{\gamma} = \frac{2}{\sqrt{C}}\int_{1-y}^{y}\left(\tilde{\kappa}\Delta\tilde{\mu}\right)^{\frac{1}{2}}dy \qquad (22)$$

After substituting the scaled value of chemical potential in equation (22) we get the final value

of surfac etension is
$$\tilde{\gamma} = \frac{2(\tilde{\kappa}kT)^{1/2}}{\sqrt{C}}\int_{1-y}^{y}\left[(y_b - y_s)(s-1) + \ln\left(\frac{y_b}{y_s}\right)\right]^{\frac{1}{2}}dy \qquad (23)$$

For Cyclohexane the length of segment is $s=1$ then the equation (23) reduce to

$$\tilde{\gamma} = \frac{2(\tilde{\kappa}kT)^{1/2}}{\sqrt{C}}\int_{1-y}^{y}\left[\ln\left(\frac{y_b}{y_s}\right)\right]^{\frac{1}{2}}dy \qquad (24)$$

where the reduced variables are $\Delta\tilde{\alpha} = \Delta\alpha / P^*$, $\tilde{\gamma} = \gamma / \gamma^*$, $\tilde{\kappa} = \kappa / \kappa^*$ (25)

and the scaling parameters are

$$\gamma^* = \frac{kq_z}{s}\left(V^*m_0 / N_v\right)^{-2/3}\varepsilon^*\left(N/m\right), \qquad \kappa^* = \frac{q_z\left(V^*m_0\right)^{5/3}\varepsilon^*N_v^{-2/3}}{sm_0^2}\times10^{11}\left(erg.cm^5 / gr^2\right) \qquad (26)$$

The cyclohexane material studied in this article in unique weight which was fitted for temperature range of (313-473) K and pressure range of 0.1-150MPa as written above. The SS

# DIYALA JOURNAL FOR PURE SCIENCES

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

theory employs these calculated specific density data to obtain the characteristic parameters viz. the scaling pressure, scaling temperature and scaling volume. These parameters are simultaneity fitting of the density data with the theory using the coupled Eqs. (13)-(14). Table1 shows these computed parameters with the average and maximum relative percentage error in

volume given by

$$\%\Delta V = \frac{100}{N} \sum \frac{V_{theory} - V_{exp}}{V_{exp}} \tag{27}$$

*Where $V_{theory}$* is the specific density calculated from the SS theory and *$V_{exp}$* is the one calculated from the Tait equation, and *N* is the number of data.

## Working Tools

Has been employed the Cahn-Hilliard (CH) theory in conjunction with Simha-Somcynsky (SS) theory, has been derived manually the new equation that helped us to extract the correlation between gradient energy coefficient with hole fractions, temperature, density and another parameters. These studies are written in a mathematica code program. At first, PVT data for the SS theory, are calculated from the modified cell model(MCL) starting  atmospheric pressure to 150Mpa and for the temperature range from  *313-473 K,*  then the relationships between the parameters are  then drawn by using the origin program and Math Type program to write the equations.

**Table 1:** The critical value of surface tension, temperature and characteristic parameters of $C_6H_{12}$

| $\gamma_o$ ( $mN/m$ ) | $T_c$ (K) | $P^*(Mpa)$ | $V^*$ ( $cc/gr$ ) | $T^*(K)$ |
|---|---|---|---|---|
| 63.91 REF [7] | 550.60 REF [7] | 962.042 | 1.2377 | 8413.18 |
| $s$ | $q_z = s(z-2)+2$ | $m_o$ ( $gr/mol$ ) | $c$ | $10^6 \upsilon^*$ |
| 1 | 12 | 84 | 1.43 | 103.971 |
| Our study | | | | |

Some important thermodynamic parameters of cyclohexane used in this work are shawn in Table 1

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

# Results and Discussion

The relationship between the parameters are extratcted based on theoritically caluculations are shawn in Table 2
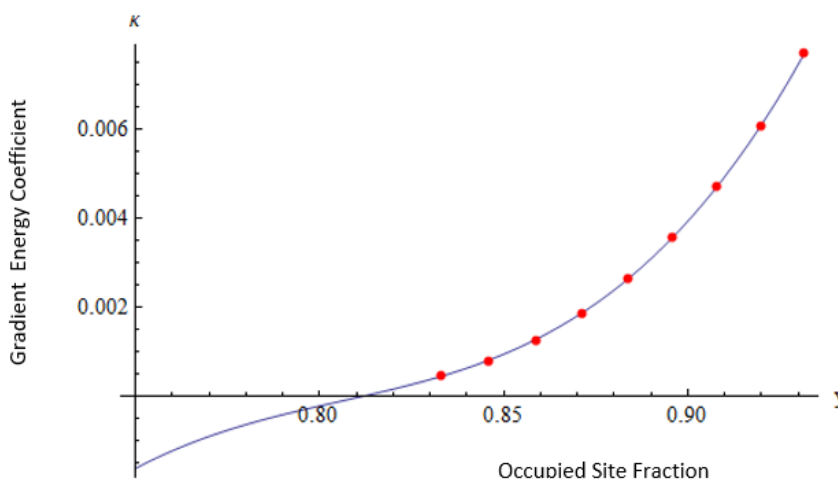
**Table 2:** Reduced surface tension and gradient energy coefficient for $C_6H_{12}$

| T(K) | $yV$ | $\gamma_{s=1}^{\exp}$ N/m | $\tilde{\gamma}_{s=1}$ | $\tilde{\kappa}_{s=1}$ | $h = 1 - y$ | $\rho(kg/m^3)$ |
|------|--------|--------|--------|---------|--------|----------|
| 313 | 0.9637 | 0.0228 | 0.042 | 0.00770 | 0.0683 | 780.941 |
| 353 | 0.9648 | 0.0182 | 0.034 | 0.00470 | 0.0921 | 760.199 |
| 373 | 0.9654 | 0.0160 | 0.029 | 0.00356 | 0.1041 | 749.651 |
| 393 | 0.9660 | 0.0138 | 0.025 | 0.00263 | 0.1164 | 738.981 |
| 413 | 0.9666 | 0.0117 | 0.021 | 0.00187 | 0.1287 | 728.187 |
| 433 | 0.9672 | 0.0096 | 0.018 | 0.00127 | 0.1413 | 717.262 |
| 453 | 0.9678 | 0.0076 | 0.014 | 0.00080 | 0.1540 | 706.202 |
| 473 | 0.9685 | 0.0058 | 0.010 | 0.00046 | 0.1668 | 694.998 |

$$\kappa^* = 5.497 \times 10^{-6} \, erg.cm^5/gr^2, \; \gamma^* = 0.535 \; N/m, \; \varepsilon^* = 1002.560 \; K$$

$$\Delta Vmean = 0.0167, \qquad \Delta V \max = 0.0196, \qquad \langle yV \rangle = 0.9660 \pm 0.0025$$

$$\kappa = -1.45476 + 5.37837\, y - 6.65127\, y^2 + 2.75129\, y^3 \qquad \text{(fitting.equation1)}$$



**Figure 1:** Plot of reduced gradient energy coefficient as a function of occupied site fraction for C₆H₁₂.

# DIYALA JOURNAL FOR PURE SCIENCES

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

$$\kappa = -1.245 + 0.005\,\rho - 8.216 \times 10^{-6}\,\rho^2 + 4.085 \times 10^{-9}\,\rho^3 \qquad \text{(fitting.equation2)}$$
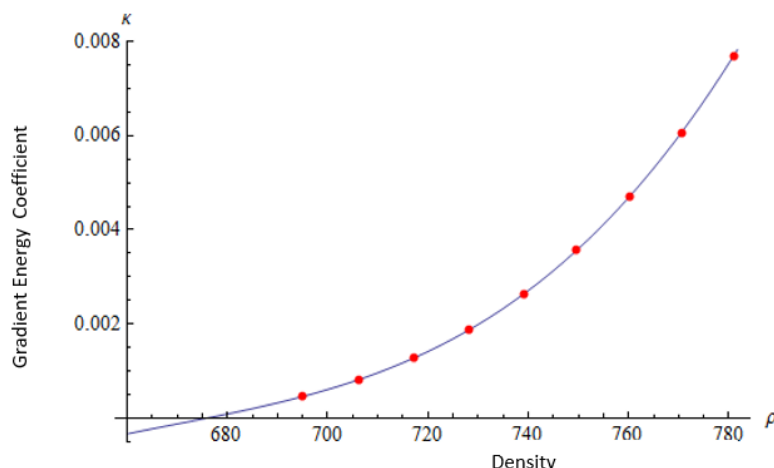


**Figure 2:** Plot of reduced gradient energy coefficient as a function of density for $C_6H_{12}$.

$$\kappa = 0.0551108 - 0.000222516\,T + 2.26458 \times 10^{-7}\,T^2 \qquad \text{(fitting.equation3)}$$
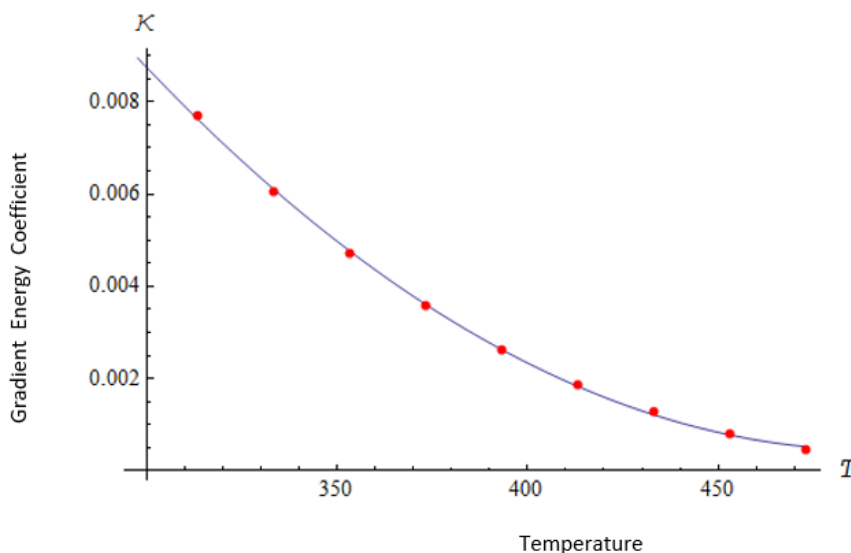


**Figure 3:** Plot of reduced gradient energy coefficient as a function of temperature for $C_6H_{12}$.

# DIYALA JOURNAL FOR PURE SCIENCES

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

$$\kappa = 0.019733 - 0.220483h + 0.63203h^2 \qquad \text{(fitting.equation4)}$$
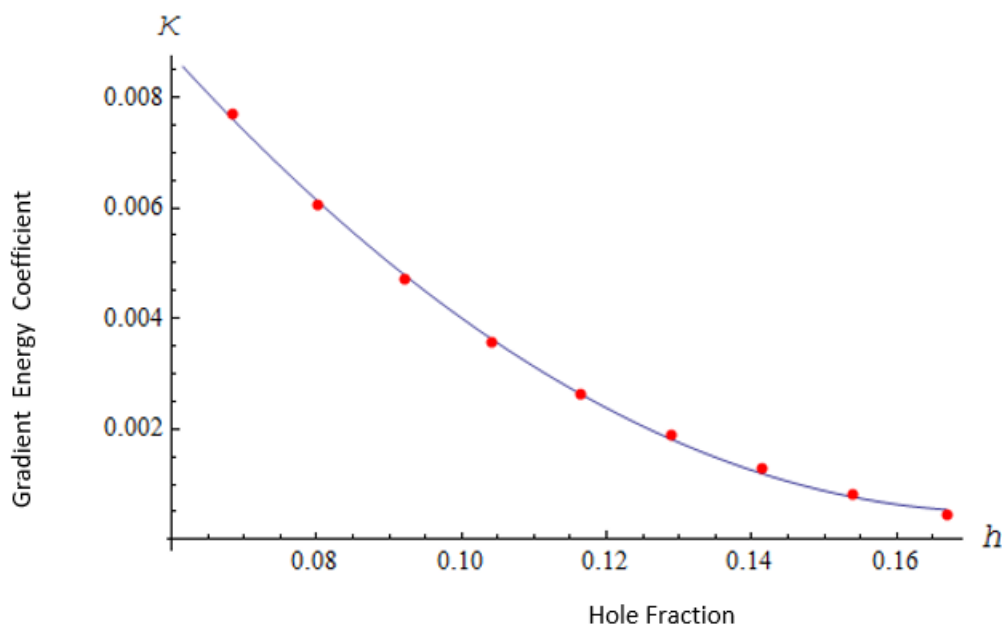


**Figure 4:** Plot of reduced gradient energy coefficient as a function of hole fraction for $C_6H_{12}$.

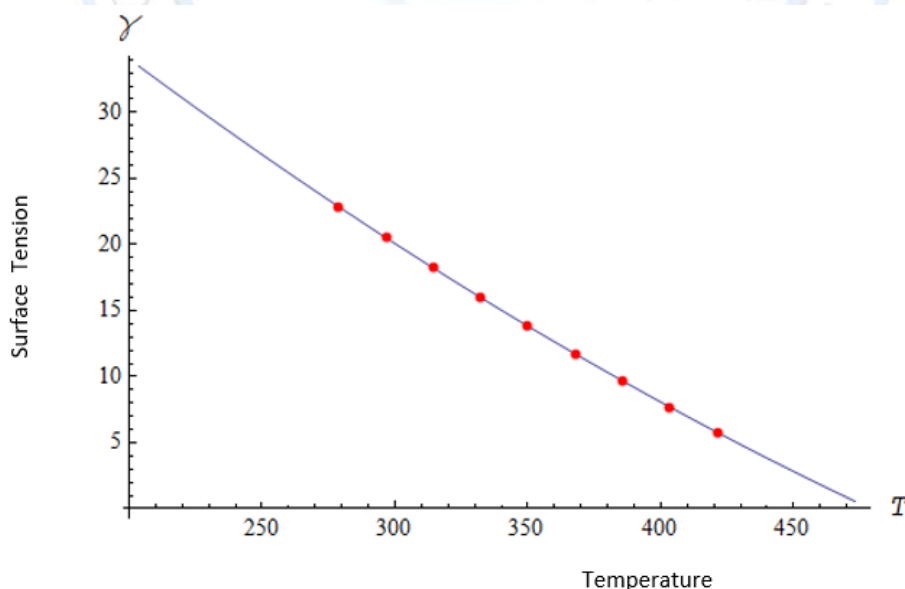$$\gamma = 67.9383 - 0.189217T + 0.000098913T^2 \qquad \text{(fitting.equation5)}$$



**Figure 5:** Plot of reduced surface tension as a function of temperature for $C_6H_{12}$ .

$$\kappa = (33.171 - 7.179\gamma + 1.717\gamma^2) \times 10^{-5} \qquad \text{(fitting.equation6)}$$

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**
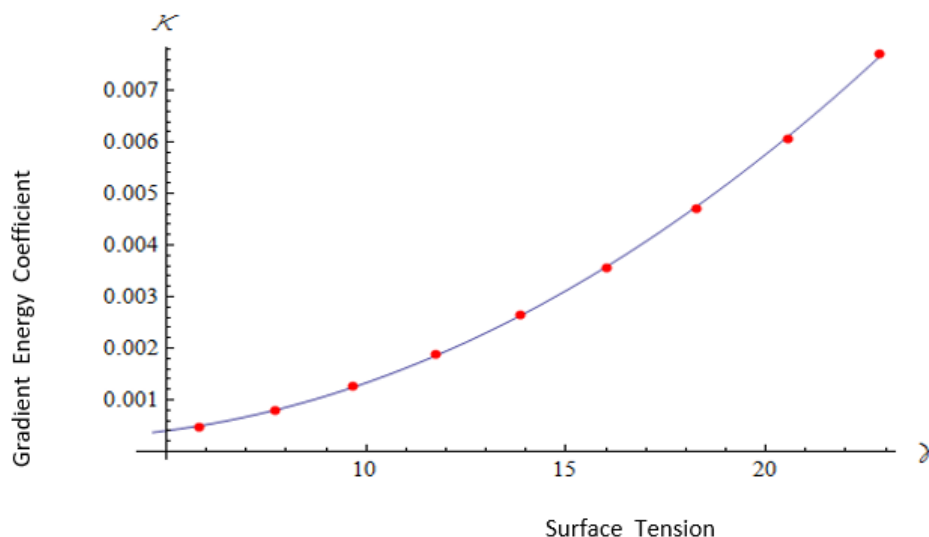
**Figure 6:** Plot of reduced gradient energy coefficient as a function of reduced surface tension for $C_6H_{12}$

$$\gamma(T) = \gamma_o(1 - T/T_c)^{11/9} \qquad (28)$$

## Discussion

The Cahn-Hiliarid gradient energy coefficient for the binary system liquid cyclohexane has been used to investigate its properties and to extract the correlation betwween occupied site fraction, scaled temperature, density and scaled surface tension with scaled gradient energy coefficient. in our model has been used To extract the pattern of dependance of gradient enegy coefficient on changes of studied parameters, the Hole Theory (SS) in conjunction with Chan-Hiliard theory were used. In this model, the surface energy and chemical potential as a function of occupied site fraction (y) are successfully derived based on the Hole Theory (SS) and Flory –Huggins Mean Field Theory(FHMF). On the other hand, the occupied site fraction profile that has been theoritically calculated is compared with the occupied surface depth profile. This study presents a list of surface tension data at different temperature from Guggenheim's equation (28) and another list of occupied sit fraction using minimization condition of Helmholtz equation(15).

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

Using the hole or occupied site fraction, the scaled surface tension and the $\tilde{\kappa}$ parameters as a function of temperature are calculated based on the surface tension data and the chemical potential expression that have been derived for surface studies. The scaled gradient energy coefficient parameters. Have, therefore been correlated with molecular weight by means of segmental length or number of segment (s), density, temperature and hole fraction. This is followed by drawing a correlation between energy gradient coefficient with occupied site fraction profile as in figure (1). It shaws that increasing occupied site fraction leads to an increase in gradient energy coefficient. Plotting $\tilde{\kappa}$ values against density, figure (2), indicated the similar pattern obtained in figure (1), as density increases with increasing occupied site fraction. The relationship between gradiet energy coeffficient with temperatue and hole frction is shown in figure (3) and (4) respectively. They show how the increasing values of temperature and hole fraction lead to decreasing in gradient energy coefficient because the increasing in temperature follows increasing in hole fraction. The scaled surface tension is plotted against scaled temperature, figure (5), to show how the increasing in temperature is leading to decreasing in gradient energy coefficient. The correlation between scaled energy gradient coefficient and scaled surface tension is plotted as in figure (6), that shows the pattern of increaasing surface tension with increasing gradient energy coefficient.

Initially, PVT data for SS theory, are calculated from the modified cell model (MCL) at various conditions, starting at atmospheric pressure upto 150 Mpa and at the temperature range from 313 to 473 K. Our average and maximum values of percentage deviation of specific volume for cyclohexane are calculated as 0.0196% and 0.0678% respectively.

## Conclusion

1. Has been certified that the hole fraction increase from bulk to surface or interface.

2. Only a very small fraction of the cyclohexane chains are close enough to a surface in order for their physical state and behavior are different.

3. When increasing the molecular weight of the polymer that refer to increasing in the length of segments that leads to increasing in the surface intensity (equation 23) and decreasing the interface thickness.

# DIYALA JOURNAL FOR PURE SCIENCES

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

4. The most of the polymers component is immiscible to blending, So main reason belong to multiphase, our the best conclusion from this study the high degree of polymerization, İt will help us to innovation the new polymers. Because the high degree of polymerization reducing (eliminating) the different phases.

5. Our model can be applied to all polymers.

## References

1. Freed, K.F. and Bawendi, (**1999**), M.G., Lattice Theories of Polymeric Fluids. *J. Chem. Phys*, **93**(6): p. 2194-2203.

2. Freed, K.F.; Dudowicz, J.: (1999). "Pragmatic analysis for the range of validity of the lattice cluster theory", J. Chem. Phys, 110(2) ; p .1307-1312

3. Poser, C,I., and  Sanchez ;(**1989**).. *Colliod interface Sci*. *J. Chem. Phys* 69,p.539

4. Poser  and Sanchez, Harrison et al., Kahl and Enders(1999).Phase Transformations and Spinoda Decomposition *J. Chem. Phys,204;1381.*

5. Sauer BB, Dee GT , Miqueu C,  Mendiboure  B, Graciaa C, Lachaise J, J. (**1991**), Modeling of the surface *J. Chem. Phys*, 95,  p.6749.

6. John Wiley & Sons, Inc.,Hoboken, New Jersey in Canada, (**2006**).  "Handbook of Introduction to Physical Polymer Science" L.H.Sperling .-4th ed  QD381.S635 USA , p .614-645.

7. Carri, G. A., and Simha, R., J. (**1996**). Colloid Interface Sci. *J. Chem. Phys* .178,  p 483-494.

8. Buta, D; Freed, K.F.: (**2002**). "Lattice polymers with structured monomers: A Monte Carlo study of thermodynamic properties of melts and solutions", *J. Chem. Phys*, 116(24) 10959-10966).

9. Utraki, L.A; Simha, R. Macromol. (**2001**).  *J. Chem. Phys*., Mol.Theory Simol, 10, p.17 .

10. Aslan, M.,Ph.D. thesis.; Yahsi, U.(**2009**)..: Dallanmış ve Dendrimer Makromoleküler Yapıların İstatistiki Termodinamiği in Fizik.Marmara Üniversitesi:İstanbul. P.17-27

**Studying the Relationship between Gradient Energy Coefficient with Occupied Site
Fraction, Temperature, Density and Surface Tension for Liquid Cyclohexane**

**Saygın Muhamad Nuri and Shanay Rajab Hasan**

11. John Wiley & Sons, (**2006**), "Handbook of Introduction to Physical Polymer Science" Inc.,Hoboken, New Jersey in Canada, L.H.S perling .-4th ed QD381.S635 USA , p .77-129

12. Cahn,J. W., and Hilliard, J. E. (**1958**).Molecular weight and temperatur dependence of polymer surface tesion,. 28, p.258-267

13. Sauer, B. B., and Dee, G. T., (**1991**). *Macromolecules, J. Chem. Phys,* 24,p.2124 .

14. Utraki, L.A; Simha, R. .( **2001**) Macromol. j. Chem. Phys., Mol.Theory Simol**,** 10, p.17.

15. Jain, R. K., and Simha, R., J. (**1999**). Colloid and İnterface Sci. j. Chem. Phys., 216,p. 424-428.

16. Algers J, Sperr P, Egger W, Ko¨ gel G, Maurer FHJ. (**2003**)**.**Physical Review**;** B 67(12)125404.