TJPS

TIKRIT JOURNAL OF PURE SCIENCE

Journal Homepage: http://main.tu-jo.com/ojs/index.php/TJPS/index

Reseaching the PVT properties and gradient energy coefficient with different parameters of Polystyrene (PS910)

S. M. Nuri[1], S.Y.Darweesh[2]
[1] Physics Depts College of Education For Pure Science , /Kirkuk University , Kirkuk , Iraq
[2] Physical Department , College of Education TuzKormato , Tikrit University , Tikrit , Iraq

DOI: http://dx.doi.org/10.25130/tjps.23.2018.056

Abstract

The Gradient energy coefficient (κ) in polymers and oligomers are playing an important role in polymer 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 chemical potential equation as well 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. Both Simha-Somcynsky (SS) and Cahn-Hilliard (CH) models are employed together to calculate the thermodynamic properties of polystyren.,These studies are written in a code program (Mathematica). At first pressure-volume-temperature (PVT) data for the SS theory, are calculated from the modified cell model (MCL) starting atmospheric pressure to 150 Mpa and temperature range from 313 to 473 K, as well. The PVT characteristic parameters of the SS theory are calculated using the data, with the average and maximum value of percentage deviation of specific volume are reported below 0.117 and 0.415 respectively.

1. Introduction

The Cahn-Hilliard(CH) theory that includes the free energy profile during the phase separation in a inhomogeneous mixture density for a homogeneous system and κ 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. The lattice fluid (LF) theory [1] 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[2] to extract the surface tension and surface density profile of polymers in broad range of temperature. Poser and Sanchez, Kahl and Enders [3], 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[4].
theory in conjunction with the Flory, Orwoll, and Vrij (FOV) [5] and Sanchez and Lacombe [6] (SL) equation of state theories. B. Sauer and T. Dee they has worked to obtained the surface tension and the gradient energy coefficient (κ) for linear, branched *n*-alkanes. The surface tension increase and surface entropy decrease with increasing molecular weight .The results of this study of various molecular weight of polyethylene glycol confirms the correlation between molecular weight and surface entropy.
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) [7] examined the relation between surface tension and hole fraction of the bulk properties by means of SS lattice-hole theory.

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 polymersand mix of molecular weight of different polymer, with significant quantitative achievement[8-10],

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 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 %0.415 maximum deviation in volume.

2. Theories

2.1 The Cahn-Hilliard Theory

The Cahn - Hilliard theory [11] correlates the thermodynamic characteristics of a system with an interface between two non-condensing phase. 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, α, of a system with an interface can be obtained by expanding the Helmholtz free energy in Taylor series around the equilibrium state:

$$\alpha(\rho, \nabla\rho, \nabla^2\rho, ...) = \alpha_0(\rho) + \kappa_1 \nabla^2\rho + \kappa_2 (\nabla\rho)^2 + \cdots \quad (1)$$

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

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

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

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

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

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

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 ρ and two phase equilibrium mixtures with liquid and gas states.

where μ_{l0} and μ_{v0} are the equilibrium chemical potentials of liquid and vapor,

The appropriate form of the Euler equation says:

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

where I represents the integrand of Cahn-Hillard equation . If we apply the integrand of Eq. (5) in Eq. (4) [12], 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

$$\Delta\alpha(\rho) - \kappa\left(\frac{d\rho}{dx}\right)^2 = const \quad ...(6)$$

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:

$$\Delta\alpha(\rho) = \kappa\left(\frac{d\rho}{dx}\right)^2 \quad ..(7)$$

Then we get the surface tension is

$$\gamma = 2\int_{\rho_v}^{\rho_l} [\kappa\Delta\alpha(\rho)]^{\frac{1}{2}} d\rho \quad ...(8)$$

The Simha-Somcynsky (SS)-EOS Theory

Simha-Somcynsky (SS) developed an equation of state (EOS) based on the lattice-hole model[13] 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:

$$y = 1 - h = \frac{sN}{sN + N_h} \quad ....(9)$$

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.:

$$\tilde{V} = V/V^*; \quad \tilde{T} = T/T^*; \quad \tilde{P} = P/P^* \quad (10)$$

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

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

where E_0 is the total lattice energy of the system employed Lennard-Johns potential energy, υ_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

$$\Delta S_m = k \ln g(N, y) \quad \dots(12)$$

Hence the combinatorial factor is expressed as

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

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

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

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, $\partial F/\partial y\big|_{\tilde{V},\tilde{T},c/s} = 0$

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

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 [14]).

From temperature dependence of the hole fraction law we have the relation:

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

$K(\tilde{T})$ is quite slowly varying function. Therefore the hole faction h or occupied site fraction y satisfies

$$y\tilde{V} = C = \text{constant} \quad \dots(17)$$

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

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

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

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

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

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

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

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

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

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

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

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

For polystyrene (PS910) the length of segment is $s = 24.3$ the equation (23) reduce to

$$\tilde{\gamma} = \frac{2(\tilde{\kappa}kT)^{1/2}}{\sqrt{C}}\int_{1-y}^{y}\left[23.3(y_b - y_s)\ln\left(\frac{y_b}{y_s}\right)\right]^{\frac{1}{2}}dy \quad \dots(24)$$

where the reduced variables are

$$\Delta\tilde{\alpha} = \Delta\alpha/P^*, \quad \tilde{\gamma} = \gamma/\gamma^*, \quad \tilde{\kappa} = \kappa/\kappa^* \quad \dots(25)$$

and the scaling parameters are

$$\gamma^* = \frac{kq_z}{s}\left(V^*m_0/N_v\right)^{-2/3}\varepsilon^*(N/m),$$

$$\kappa^* = \frac{q_z\left(V^*m_0\right)^{5/3}\varepsilon^*N_v^{-2/3}}{sm_0^2}\times 10^{11}\left(erg.cm^5/gr^2\right) \quad \dots(26)$$

The polystyrene (PS910) 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 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

$$\%\Delta V = \frac{100}{N}\sum\frac{V_{theory} - V_{exp}}{V_{exp}} \quad \dots(27)$$

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.

3. Results and Discussion
Some important thermodynamic parameters of polystyrene used in this work are shown in Table (1)

Table(1): The critical value of surface tension , temperature and characteristic parameters of PS910

γ_o (mN/m)	T_c (K)	$p^{\cdot}(Mpa)$	v^* (cc/gr)	$T^*(K)$
63.1 REF[7]	1121 REF[7]	1049.23	1.0697	19195
s	$q_z = s(z-2)+2$	m_o (gr/mol)	c	$10^6 v^*$
24.3	242	37.44	6.4	40.061
Our study				

The relationship between the parameters are   shown in Table 2.
extratced based on theoritically caluculations are

Table 2. Reduced surface tension and gradient energy coefficient of $Ps910$ $\kappa^* = 2.41 \times 10^{-4}$ $erg.cm^5/gr^2$,
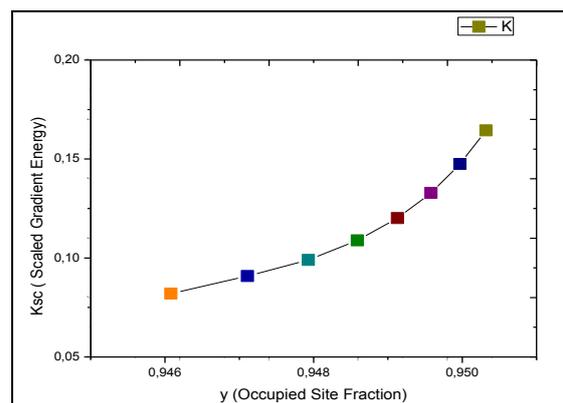
$\gamma^* = 0.0506$ erg/cm^2 , $\varepsilon^* = 501.43$ K

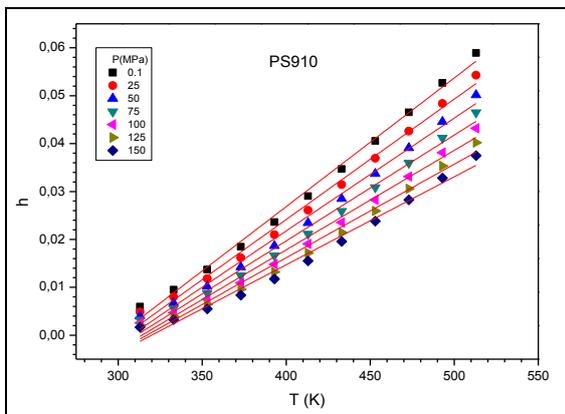| T(K)	YV	$\gamma_{s=24}^{exp}$ N/m	$\tilde{\gamma}_{s=24}$	$\tilde{\kappa}_{s=24}$	$h=1-y$	$\rho(kg/m^3)$
313	0.9460	0.0422	0.834	0.164	0.0059	982.172
353	0.9471	0.0409	0.809	0.147	0.0095	977.624
373	0.9479	0.0397	0.784	0.132	0.0137	972.620
393	0.9485	0.0384	0.759	0.120	0.0184	967.272
413	0.9491	0.0371	0.734	0.109	0.0236	961.662
433	0.9495	0.0359	0.710	0.098	0.0290	955.852
453	0.9499	0.0346	0.685	0.090	0.0347	949.883
473	0.9503	0.0334	0.661	0.082	0.0405	943.785

$\Delta Vmean = 0.117$, $\Delta V \max = 0.415$, $\langle yV \rangle = 0.9486 \pm 0.0025$
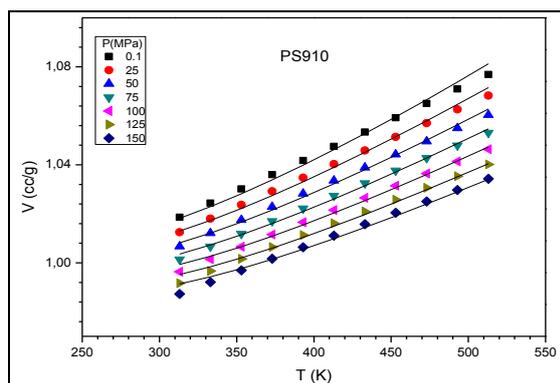
Fig(1) Plot of specific volume as a function of temperature of (PS910)

Fig(2) Plot of hole fraction as a function of temperature of (PS910)

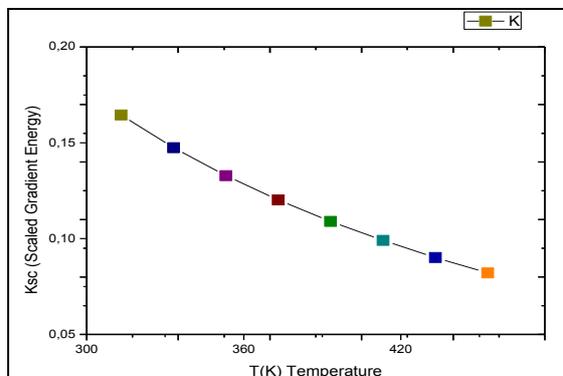$\kappa = 41.8951 - 87.837\,y + 46.1287\,y^2$ (fitting.equation1)

Fig(3) Plot of reduced gradient energycoefficient as a function of occupied site fraction of (PS910).

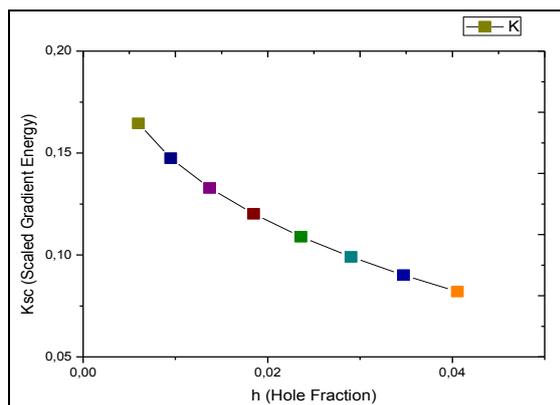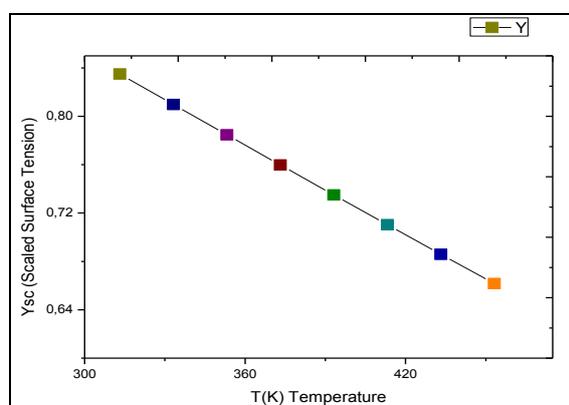$\kappa = 0.604498 - 0.00197706\,T + 1.8212 \times 10^{-6}\,T^2$ (fitting. equation2)

Fig(4) Plot of reduced gradient energy coefficient as a function of temperature of (PS910).

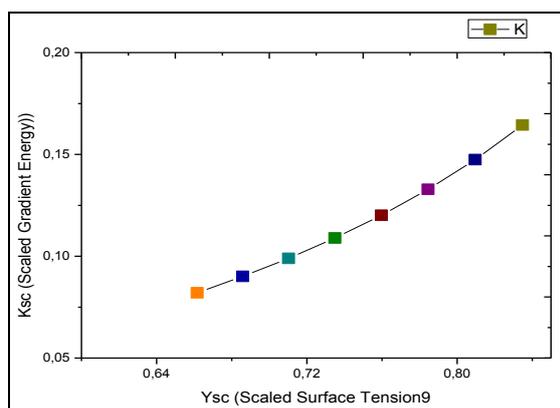$\kappa = 0.18687 - 4.42049\,h + 46.1287\,h^2$ (fitting.equation3)

Fig(5) Plot of reduced gradient energy coefficient as a function of hole fraction of (PS910).

$\gamma_{sc} = 1.24905 - 0.00138072T + 1.86567 \times 10^{-7}T^{2}$ (fitting. equation4)

Fig(6) Plot of reduced surface tension as a function of temperature of (PS910).

$\kappa sc = 0.397 - 1.225\gamma sc + 1.333(\gamma sc)^{2}$ (fitting. equation5)

Fig(7) Plot of reduced gradient energy coefficient as a function of reduced surface tension of (PS910)

Discussion

The pressure –volume –temperature (PVT) properties of polystyrene (PS910) as a function of molecular weight. Which were the aim of this studying. Figure (1) shows the temperature dependence of the specific volume of polysterene which is isobar curves at (0.1-150) Mpa Mpa. The dots reffer the experimental data and the line is calculated theoretically from SS theory. It is seen that as the temperature increases for

each identical pressure curve as well the specific volume increases. Because the mobility of polymer molecules in this region increases, thus causing an increase in specific volume. However the specific volume decreasing with increasing the pressure as it is expected.The specific volume shows the linear behavior when the pressure is high. But parabolic behavior when the pressure is decreasing. Figure(2) appear the temperature dependence on the hole fraction of polystrene (PS910) is isobar curves at (0.1-150) Mpa. The points represent the experimental data. The line at Fig (2) is calculated theoretically from SS theory. The hole fraction in Fig(2) shows upper regions the pressure decreasing and at high temperature locations. Thus causing the increasing in hole fraction of polystrene, this is indicated to flaws in polymer materials.

The Cahn-Hiliarid gradient energy coefficient for the binary system liquid polystyrene has been used to investigate its properties and to extract the correlation between occupied site fraction, scaled temperature, density and scaled surface tension with scaled gradient energy coefficients. 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 condition of Helmholtz equation (15). and another list of occupied site fraction using minimization 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 gradient energy coefficient with occupied site fraction profile as in figure (3). It shaws that increasing in occupied site fraction leads to an increase in gradient energy coefficient. The relationship between gradiet energy coeffficient with temperatue and hole frction is shown in figure (4) and (5) respectively. They show how the increasing values of temperature and hole fraction lead to decreasing in gradient energy coefficient because leads to decreasing in interaction between the molecules of polystyrene. The increasing in temperature follows increasing in hole fraction. The scaled surface tension is plotted against scaled temperature, figure (6), 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 (7), that shows the pattern of increaasing surface tension with increasing gradient energy coefficient.

The PVT data for SS theory, are calculated from the modified cell model (MCL) at various conditions, starting at atmospheric pressure up to 150 Mpa and at the temperature range from (313 - 473) K. Our average and maximum values of percentage deviation of specific volume for polystyrene are calculated as(0.117% - 0.415%) respectively.

References

[1] Freed, K.F.; Dudowicz, J.: "Pragmatic analysis for the range of validity of the lattice cluster theory", *Journal of Chemical Physics*, 100(2), 1307, 12, (1994).

[2] Poser, C,I., and Sanchez ,I. C., *J. Colliod interface Sci.* 69,539 (1989).

[3] Poser and Sanchez, 1981; Harrison et al., Kahl and Enders (1999).

[4] Sauer BB, Dee GT ,.. Phys., 95, 6749, Miqueu C, Mendiboure B, Graciaa C, Lachaise J, J. Modeling of the surface (1991).

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

[6] Carri, G. A., and Simha, R., J. Colloid Interface Sci. 178,483-494(1996).

[7] Utraki, L.A; Simha, R. Macromol. Chem. Phys., Mol.Theory Simol, 10, 17, (2001).

[8] Aslan, M.,Ph.D. thesis.; Yahsi, U.: Dallanmış ve Deformasyonlu Makromoleküler Yapılarının İstatistiki Termodinamiği in Fizik. Marmara Üniversitesi: İstanbul. P.17-27.(2009).

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

[10] Cahn,J. W., and Hilliard, J. E., *J. Chem. Phys*. 28, 258-267 (1958).

[11] Sauer, B. B., and Dee, G. T., *Macromolecules* 24 2124 (1991).

[12] Utraki, L.A; Simha, R. Macromol. Chem. Phys., Mol.Theory Simol**,** 10, 17.(2001)

[13] Jain, R. K., and Simha, R., J. Colloid and İnterface Sci. 216, 424-428 (1999).

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

بحث الخواص الثرمودينا ميكية (ضغط، حجم، درجة الحرارة ومعامل انحدار الطاقة) مع المتغيرات المختلفة للبولي ستايرين (PS910)

صايغن محمد نوري[1] ، صالح يونس درويش[2]

[1]قسم الفيزياء ، كلية التربية للعلوم الصرفة ، جامعة كركوك ، كركوك ، العراق

[2]قسم الفيزياء ، كلية التربية طوزخورماتو ، جامعة تكريت ، تكريت ، العراق

الملخص

معامل انحدار الطاقة (K) يلعب دورا مهما في بوليمرات او لليكومرات، بالاضافة الى فهم العديد من العمليات وخاصة في الكشف عن بوليمرات جديدة وفي تصنيف المواد، ولذا اصبح هدف هذه الدراسة هو كيفية تغير معامل انحدار الطاقة من العمق الى سطح البوليمر واستخراج لمحة معامل انحدار الطاقة مع نسبة المواقع المحتلة في الشبيكة والفجوات وفق نظرية سمها سومسينيسكي، ودرجة الحرارة والشد السطحي وفق نظرية كاهن هيليارد. وقد استخدمت النظريتين معا لدراسة هذه الخواص لمادة البولي ستايرين وقد توصلنا الى معادلة جديدة في ايجاد العلاقة بين المتغيرات المذكورة وقمنا بكتابة برنامج في (Mathematics) لحل انموذج الخلية الشبيكة البلورية المعدّلة (المعدّل) (MCL) (Modified Cell Modell) بدأ من الضغط الجوي الى 150 Mpa ومدى درجة الحرارة من K (313– 473)، وكان معدل نسبة الخطأ والقيمة العظمى في انحراف الحجم النوعي هي0.117 و0.415 على التوالي.

الكلمات المفتاحية: سمها سومسينيسكي، كاهن هيليارد، معامل انحدار الطاقة ، ضغط – حجم – درجة الحرارة ، الكثافة السطحية.