

# Study the Physical Properties PVT of Polyethylene Glycol using the Simha-Somcynsky Theory

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## Abstract

In this study, the structure of polyethylene glycol polymer with different molecular weights was investigated, and the physical properties were studied in terms of pressure, volume and temperature using a theory called Simha-Somcynsky (SS). which shows irregular lattice structure in terms of the hole fraction depending on which thermodynamic quantities are expressed in the statistical thermodynamics of polymers. Therefore, it is necessary to determine the hole fraction and occupied site fraction  $y$ . Thermodynamic properties and hole fraction were investigated in the range of temperature between 283 - 450 K, and at a pressure up to 150 MP. Average error and maximum error in specific volume were determined as 0.036% and 0.28%, respectively, as the highest error in peg302. The other important determination was that the polyethylene glycol had glass transition temperatures ranging from 55 to 60 K.

## 1. Introduction:

Polymer materials exhibit different physical and thermodynamic behavior due to microscopic defects in their structure. These defects play a significant role in material characterization, particularly in their durability, resistance, transparency and brittleness. Polyethylene glycol is used in industries such as medicine and pharmaceuticals, chemical applications, biological studies, personal care products, toothpastes, soap industry, and ceramic production.

This study aims to examine the structure and physical properties (pressure, volume and temperature) of polyethylene glycol polymer and establish the thermodynamic relationship, such as phase transportations and glass transition temperature of polyethyleneglycol at different molecular weights.

## 2. Theory:

The monomers or segments are the smallest part of polymer molecules. The repetition of these segments creates the polymer molecule and their placement one by one in the lattice structure creates the polymers statistics. Simha - Somcynsky (SS) [1], [2] theory consists of filled and empty cells in the same lattice [3]. The polymer segments make up the full cell and the empty cell is in the same lattice, adding a new understanding to the cell theory.

The cell theory has been applied to short-chain and long-chain polymer structures [4] and their mixtures [5], [6], [7] and very good results have been obtained. The volume fraction ratio [8] of the filled and empty cells in the polymer lattice structure is given below,

$$y = \frac{N_s}{N_h + N_s} = 1 - h \quad (1)$$

The configuration of the combinatorial factor [9], which expression of the partition function [10] of occupied and



empty cells, is given by,

$$Z_{conf} = g(N, y) \left[ v_f(\tilde{V}, y) \right]^{cN} \exp \left[ \frac{E_0(\tilde{V}, \tilde{T}, y)}{kT} \right] \quad (2)$$

$$g(N, y) = y^{-N} (1-y)^{-sN \left( \frac{1-y}{y} \right)} \quad (3)$$

The total energy of the polymer lattice structure is  $E_0$

$$E_0 = \frac{1}{2} y N q_z \epsilon^* \left[ A \left( \frac{v^*}{\omega} \right)^4 - 2B \left( \frac{v^*}{\omega} \right)^2 \right] \quad (4)$$

Here  $\omega = yV/sN$  is represent the occupied site fraction value. The unoccupied site or hole fraction [11] value in the lattice is given by,

$$v_f = v^* \left\{ y \left[ (y\tilde{V})^{1/3} - 2^{-1/6} \right] + (1-y)(y\tilde{V})^{1/3} \right\}^3 \quad (5)$$

Here, in the free volume, the first part denotes the void in the occupied cell, and the second part denotes the unoccupied cells in the lattice. The Helmholtz free energy [12] of the polymer lattice structure was obtained.

$$\begin{aligned} F_{conf} &= -kT \ln Z_{conf} \\ &= NkT \ln y + kT sN \left( \frac{1-y}{y} \right) \ln(1-y) \\ &= -3kT cN \left\{ \ln \left[ (y\tilde{V})^{1/3} - 2^{-1/6} y \right] + \frac{1}{3} \ln(v^*) \right\} + \frac{1}{2} \\ &\quad y N q_z v^* (y\tilde{V})^{-2} \\ &\quad + \frac{1}{2} y N q_z v^* (y\tilde{V})^{-2} \left[ 1.011 (y\tilde{V})^{-2} - 2.049 \right] \end{aligned} \quad (6)$$

The occupancy rate of the system remains constant only in case of equilibrium state. Thus, the derivative of the Helmholtz free energy with respect to  $y$  must be zero.

$$\begin{aligned} \left( \frac{\partial F}{\partial y} \right)_{V, T, c/s} &= \frac{s}{3c} \left[ \frac{s-1}{s} + \frac{\ln(1-y)}{y} \right] - \frac{\eta - \frac{1}{3}}{1-\eta} - \frac{y}{6\tilde{T}} \\ &\quad \left( y\tilde{V} \right)^{-2} \left[ 2.409 - 3.033 \left( y\tilde{V} \right)^{-2} \right] = 0 \end{aligned} \quad (7)$$

Here  $\eta = 2^{-1/6} y (y\tilde{V})^{-1/3}$ . Derivative of the Helmholtz energy with respect to  $V$ , the second equation of state [13] is obtained.

$$P = - \left( \frac{\partial F}{\partial V} \right)_T = P[\tilde{V}, \tilde{T}] = P \left[ \tilde{V}, \tilde{T}; y \left( \tilde{V}, \tilde{V} \right) \right] \quad (8)$$

$$\frac{\tilde{P}\tilde{V}}{\tilde{T}} = \frac{1}{1-\eta} + \frac{2y}{\tilde{T}} (y\tilde{V})^{-2} \left[ (1.011(y\tilde{V})^{-2}) - 1.2045 \right] \quad (9)$$

The relationship between the theoretical and experimental PVT values and the explicit expression of the reduced parameters [14]. are given below.

$$\tilde{P} = \frac{P}{P^*}, \quad \tilde{V} = \frac{V}{V^*}, \quad \tilde{T} = \frac{T}{T^*}, \quad (10)$$

where,

$$P^* = \frac{cT^*R^*}{mV}, \quad V^* = \frac{v^*s}{m}, \quad T^* = \frac{q_z \epsilon^*}{c} \quad (11)$$

$$\left( \frac{P^*}{T^*} \right) M_o = \left( \frac{c}{s} \right) R \quad (12)$$

$M_o$  represents the mass of the segment and  $R$  is the gas constant.

### 3. Results and Discussions:

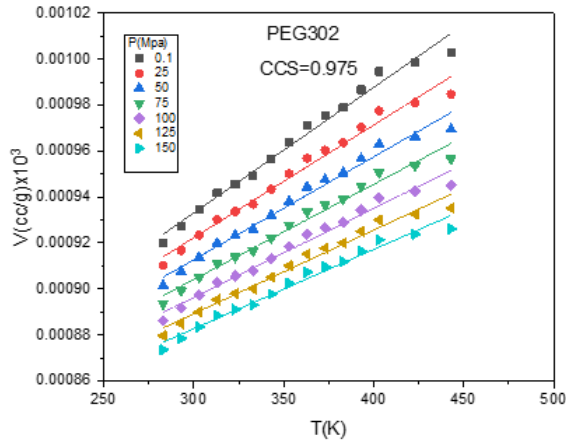
The scaling parameters  $P^*$ ,  $V^*$  and  $T^*$ , in addition to the structural flexibility parameter of the polymers (with  $3c = s + 3$  and  $3c/s$ ) were calculated from equations 7 and 9 [15], [16] overlaying the experimental PVT data of polyethyleneglycol of different molecular weight onto the theoretical surface. Here,  $c$  was assumed as an adjustable parameter. On the other hand, expanding pressure and temperature values to the first power in  $V^*$  and  $T^*$ , would lead to  $N$  equations obtained from  $N$  Matrix experimental PVT data and solved for two unknowns  $V^*$  and  $T^*$  using Pseudo Inverse Matrix Technique (PIMT) [17]. We used the minimum absolute deviation method to calculate the relative percent error in a specific volume using Eq.13.

$$\Delta V(\%) = \frac{100}{N} \sum_i \frac{|V_i^{exp} - V_i^{calc}|}{V_i^{exp}} \quad (13)$$

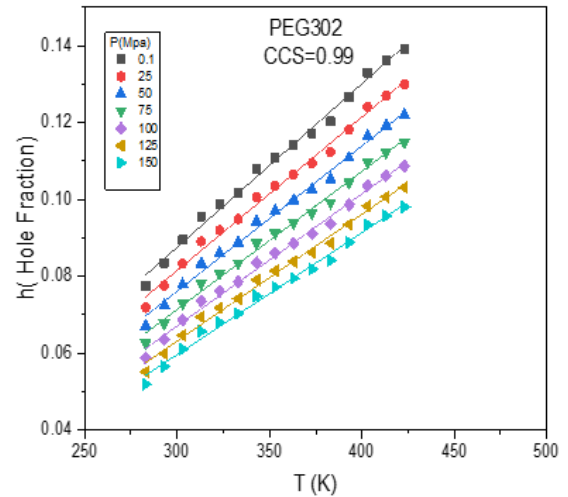
$\Delta V(max) = \max(\Delta V_i)$  We selected and evaluated the best  $c$  values with the scaling parameters  $P^*$ ,  $V^*$  and  $T^*$  at the point where the error was minimum. The parameters acquired with the mean and maximum percent error in a specific volume are reported in Table 1 for the specified polymers.

The mean percentage deviation is 0.03%, 0.0% and 0.04% for PEG302, PEG692 and PEG18500, respectively, and the maximum percentage errors are 0.28%, 0.16% and 0.12%, respectively. These parameters can be easily used to calculate the hole fraction and their derivative models. The results are illustrated in Figure1, Figure2 and Figure3.

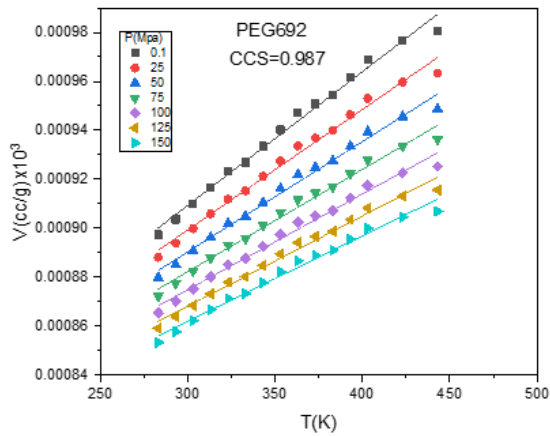
The vibration of atoms and the mobility of the molecular caused an increase in the hole fraction. However, as the



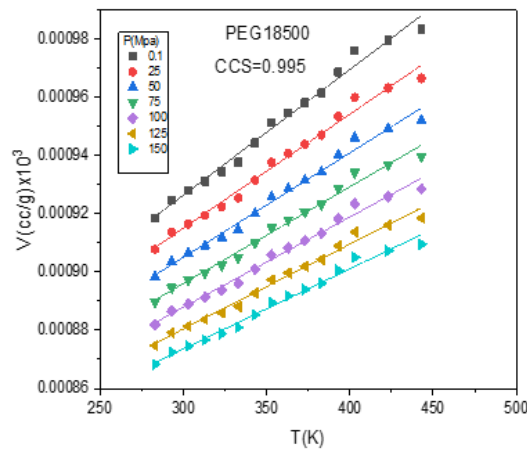
**Figure 1.** The hole fraction as a function of temperatures for PEG302 at different pressure.



**Figure 4.** The specific volume as a function of temperatures for PEG302 at different pressure.



**Figure 2.** The hole fraction as a function of temperatures for PEG302 at different pressure.



**Figure 3.** The hole fraction as a function of temperatures for PEG302 at different pressure.

pressure increases, it causes a contraction in the polymer structure and thus a decrease in the hole ratio occurs. As the molecular weight increases, the viscosity of the polymers increases, but has a smaller hole fraction. Thus, differences in hole fraction can be attributed to molecular weight as well as structural disorder due to differences in molecular weigh.

The calculation of specific volume and hole fraction was investigated at 283–443 K and up to pressure ranges (0.1,25, 50, 75, 100, 125 and 150) MPa. The specific volume and Simha somcynsky hole fraction were calculated by adapting the equations (7) and (9) (SS theory).  $N$  experimental data number,  $V_i$  experiment and  $V_{i\text{theory}}$  the mean and the maximum percentage deviation in the specific volume, were obtained from the equations 13.  $h_{ss}$  Represent the hole fraction value that calculated by simha somcynsky theory.

In Figure 4, Figure5 and Figure 6, of PEG302, PEG692 and PEG18500 respectively, the variation of the specific volume with temperatures from 283 K to 443K, is plotted adiabatically for pressure values of 0.1, 25, 50, 75, 100, 125 and 150 MPa. The pressure values increase as you go down, and each curve gives us isobars curves. It is seen that the specific volume increases as the temperature increases for each isotherm. In these regions, the mobility of the polymer molecules increases and causes an increase in the specific volume.

The nonlinear behavior at low temperatures is due to the non-equilibrium of the polymer structure at temperatures below the glass transition temperature. It behaves linearly at temperatures above the glass transition temperatures. The variation of the specific volume exhibits parabolic behavior at low pressures and linear behavior at very high pressures.

Figure 7 The specific volume was plotted with the inverse

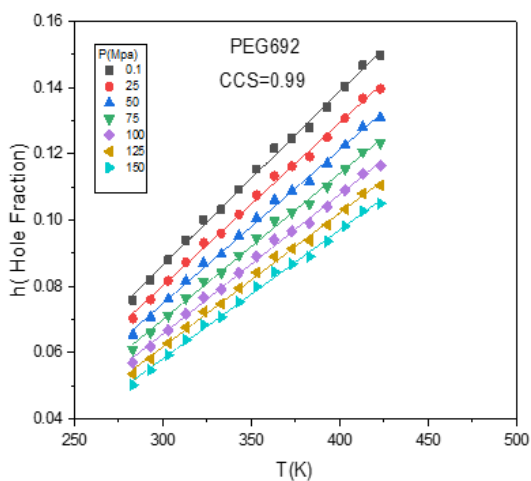


Figure 5. The specific volume as a function of temperatures for PEG692 at different pressure.

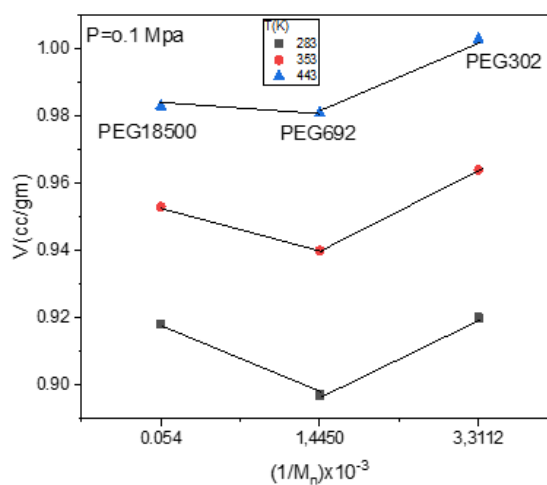


Figure 7. The hole fraction as a function of temperatures for PEG302 at different pressure.

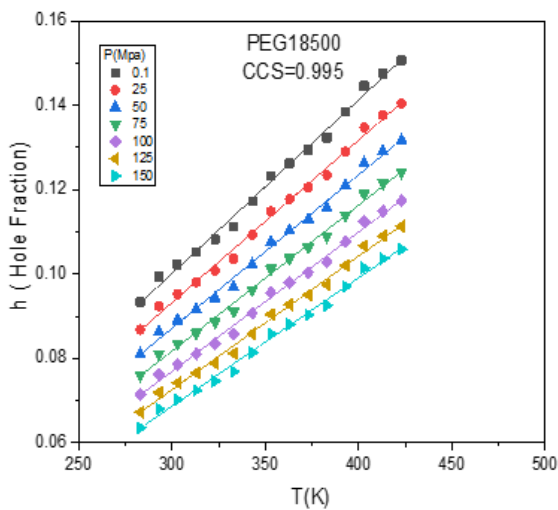


Figure 6. The specific volume as a function of temperatures for PEG18500 at different pressure.

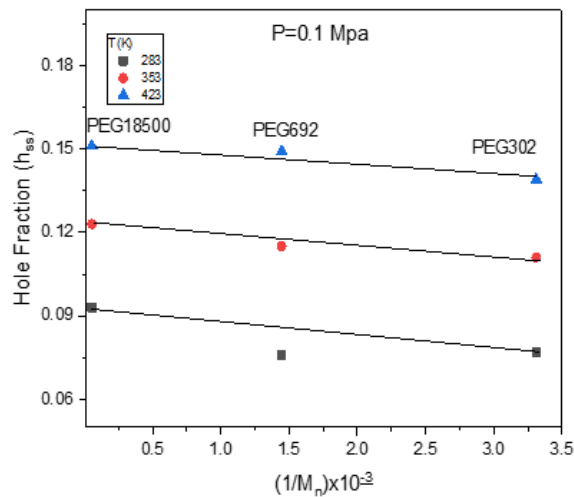


Figure 8. The hole fraction as a function of temperatures for PEG302 at different pressure.

of the molecular weight at three different temperatures. As the degree of polymerization increased, a relative decrease in the specific volume was detected, the physical reason is that the chain structure has formed cross-links and thus the pressure inside the system has increased. Figure 8 The hole fraction is plotted with molecular weight inverse at three different temperatures. As the degree of polymerization increased, a relative increase was found in the hole fraction, the physical reason being the polymer chain structure has flexibility.

#### 4. Conclusion:

It is very important industrially to learn about the structure and thermodynamic properties of polymers. Experimental measurement of thermodynamic properties, especially at high pressure, high density and temperatures, is a very difficult and challenging task. Guiding experimental data gains importance in theoretical studies.

The SS theory, which provides the thermodynamic parameters, was used for this purpose. This theory is applicable in homogeneous and in homogeneous polymer systems, and its quantitative success encourages to extract the characteristic properties of other polymer structures. The fact that the number of polymers is very low in nature, polymer synthesis processes are now inevitable for the scientific world.

These synthesized polymers can be in the form of oligomers or macromolecules Finding the thermodynamic properties and physical characteristic parameters of new polymers using SS theory has been the reason for this study. It will not be difficult to determine from the graphs of the specific volume-temperature relationship that the polyethylene glycol glassy transition temperature is between (55 - 60) K.

**Table 1.** Shows the characteristic parameters of polyethylene glycol at different molecular weights. The characteristic parameters  $P^*$ ,  $V$  and  $T^*$  are experimental data [12] at equilibrium state.

Polimerler	$\langle c \rangle$	$P^*(\text{Mpa})$	$V^*(\text{cm}^3/\text{gr}) 10^{-3}$	$T^*(\text{K})$	$\varepsilon^*(\text{K})$	s	$m_o(\text{kg})$	$\% \Delta V$	$\% \Delta V_{max}$
PEG302	3.6	1080.720	0.85	9274	389.4	8	0.03606	0.03	0.28
PEG692	8.2	1038.530	0.86	9138	386.3	19	0.03604	0.03	0.16
PEG18500	216	1035.500	0.86	9268	389.9	513	0.0360	0.04	0.12

**Table 2.** The specific volume values corresponding temperatures at different pressure for PEG302.

T(K)	283	293	303	313	323	333	343	353	363	373	383	393	403	423	443
The specific volume for PEG302	0.92	0.927	0.934	0.942	0.946	0.949	0.956	0.964	0.971	0.975	0.979	0.987	0.995	0.999	1.003
	0.91	0.917	0.923	0.93	0.934	0.937	0.943	0.95	0.957	0.96	0.964	0.97	0.977	0.981	0.985
	0.901	0.908	0.914	0.92	0.923	0.926	0.932	0.938	0.944	0.948	0.95	0.957	0.963	0.966	0.97
	0.894	0.899	0.905	0.911	0.914	0.917	0.922	0.928	0.934	0.936	0.939	0.945	0.951	0.954	0.957
	0.886	0.892	0.897	0.903	0.906	0.908	0.913	0.919	0.924	0.927	0.929	0.934	0.94	0.942	0.945
	0.88	0.885	0.89	0.895	0.898	0.9	0.905	0.91	0.915	0.918	0.92	0.925	0.93	0.933	0.935
	0.874	0.878	0.883	0.888	0.891	0.893	0.898	0.903	0.907	0.91	0.912	0.917	0.921	0.924	0.926

**Table 3.** The specific volume values corresponding temperatures at different pressure for PEG692.

T(K)	283	293	303	313	323	333	343	353	363	373	383	393	403	423	443
The specific volume for PEG692	0.897	0.904	0.91	0.917	0.923	0.927	0.934	0.94	0.947	0.951	0.954	0.962	0.969	0.977	0.9813
	0.888	0.894	0.9	0.906	0.912	0.915	0.921	0.927	0.934	0.937	0.94	0.946	0.953	0.96	0.963
	0.88	0.885	0.891	0.896	0.902	0.905	0.911	0.916	0.922	0.925	0.928	0.934	0.939	0.946	0.949
	0.872	0.877	0.883	0.888	0.893	0.896	0.901	0.906	0.912	0.914	0.917	0.922	0.928	0.933	0.936
	0.865	0.87	0.875	0.88	0.885	0.888	0.893	0.897	0.902	0.905	0.907	0.912	0.917	0.923	0.925
	0.859	0.864	0.868	0.873	0.878	0.88	0.885	0.889	0.894	0.897	0.899	0.904	0.908	0.913	0.916
	0.853	0.858	0.862	0.867	0.871	0.873	0.878	0.882	0.887	0.889	0.891	0.895	0.9	0.905	0.907

**Table 4.** The specific volume values corresponding temperatures at different pressures for PEG18500.

T(K)	283	293	303	313	323	333	343	353	363	373	383	393	403	423	443
The specific volume for PEG18500	0.918	0.925	0.928	0.931	0.934	0.938	0.944	0.951	0.955	0.958	0.962	0.969	0.976	0.98	0.983
	0.908	0.914	0.916	0.919	0.922	0.925	0.931	0.938	0.941	0.944	0.947	0.953	0.96	0.963	0.967
	0.898	0.904	0.906	0.909	0.912	0.915	0.92	0.926	0.929	0.931	0.934	0.94	0.946	0.949	0.952
	0.89	0.895	0.897	0.9	0.902	0.905	0.91	0.915	0.918	0.921	0.923	0.929	0.934	0.937	0.94
	0.882	0.887	0.889	0.891	0.894	0.896	0.901	0.906	0.908	0.911	0.913	0.918	0.923	0.926	0.929
	0.875	0.879	0.881	0.884	0.886	0.888	0.893	0.897	0.9	0.902	0.904	0.909	0.914	0.916	0.919
	0.868	0.872	0.875	0.877	0.879	0.881	0.885	0.89	0.892	0.894	0.896	0.901	0.905	0.907	0.91

**Table 5.** The hole fraction ( $h_{ss} = 1 - y$ ) values corresponding temperatures at different pressures for PEG302.

T(K)	283	293	303	313	323	333	343	353	363	373	383	393	403	423	443
The specific volume for PEG302	0.077	0.083	0.089	0.096	0.099	0.101	0.108	0.111	0.114	0.117	0.120	0.127	0.133	0.136	0.139
	0.072	0.078	0.083	0.089	0.092	0.095	0.101	0.103	0.106	0.109	0.112	0.118	0.124	0.12	0.130
	0.067	0.072	0.078	0.083	0.086	0.089	0.094	0.097	0.099	0.103	0.105	0.111	0.116	0.119	0.122
	0.063	0.068	0.073	0.078	0.081	0.083	0.089	0.091	0.094	0.097	0.099	0.104	0.109	0.112	0.115
	0.059	0.064	0.069	0.074	0.076	0.079	0.084	0.086	0.089	0.091	0.094	0.099	0.104	0.106	0.109
	0.055	0.060	0.065	0.069	0.072	0.074	0.079	0.081	0.084	0.086	0.089	0.093	0.098	0.101	0.103
	0.052	0.057	0.061	0.066	0.068	0.070	0.075	0.077	0.079	0.082	0.084	0.089	0.093	0.096	0.098

**Table 6.** The hole fraction ( $h_{ss} = 1 - y$ ) values corresponding temperatures at different pressures for PEG692.

T(K)	283	293	303	313	323	333	343	353	363	373	383	393	403	423	443
The specific volume for PEG692	0.076	0.082	0.088	0.094	0.100	0.103	0.109	0.115	0.12	0.125	0.128	0.134	0.140	0.146	0.149
	0.070	0.076	0.082	0.087	0.093	0.096	0.102	0.107	0.113	0.116	0.119	0.125	0.130	0.136	0.139
	0.065	0.071	0.076	0.082	0.087	0.090	0.095	0.100	0.106	0.109	0.111	0.117	0.122	0.128	0.130
	0.061	0.066	0.071	0.076	0.082	0.084	0.089	0.094	0.099	0.102	0.105	0.110	0.115	0.120	0.123
	0.057	0.062	0.067	0.072	0.077	0.079	0.084	0.089	0.094	0.097	0.099	0.104	0.109	0.114	0.116
	0.053	0.058	0.063	0.067	0.072	0.074	0.079	0.084	0.089	0.091	0.094	0.098	0.103	0.108	0.110
	0.050	0.055	0.059	0.064	0.068	0.071	0.075	0.079	0.084	0.087	0.089	0.093	0.098	0.102	0.105

**Table 7.** The hole fraction ( $h_{ss} = 1 - y$ ) values corresponding temperatures at different pressures for PEG18500.

T(K)	283	293	303	313	323	333	343	353	363	373	383	393	403	423	443
The specific volume for PEG18500	0.093	0.099	0.102	0.105	0.108	0.111	0.117	0.123	0.126	0.129	0.132	0.138	0.145	0.147	0.151
	0.086	0.092	0.095	0.098	0.101	0.104	0.109	0.115	0.117	0.121	0.123	0.129	0.135	0.138	0.140
	0.081	0.086	0.089	0.092	0.094	0.097	0.102	0.108	0.110	0.113	0.116	0.121	0.126	0.129	0.132
	0.076	0.080	0.084	0.086	0.088	0.091	0.096	0.101	0.104	0.106	0.109	0.114	0.119	0.122	0.124
	0.071	0.076	0.079	0.081	0.083	0.086	0.091	0.096	0.098	0.100	0.103	0.108	0.112	0.115	0.117
	0.067	0.072	0.074	0.077	0.079	0.081	0.086	0.090	0.092	0.095	0.097	0.102	0.107	0.109	0.111
	0.064	0.068	0.070	0.072	0.075	0.077	0.081	0.086	0.088	0.090	0.093	0.097	0.101	0.104	0.106

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**Data Availability Statement:** All of the data supporting the findings of the presented study are available from corresponding author on request.

**Declarations:**

**Conflict of interest:** The authors declare that they have no conflict of interest.

**Ethical approval:** The manuscript has not been published or submitted to another journal, nor is it under review.

## References

- [1] S. M. Nuri. Extracting the density gradient profile of polyethylene glycol from bulk to surface. *Kirkuk University Journal-Scientific Studies*, 12(4): 338–351, 2017, doi:10.32894/kujss.2017.132379.
- [2] I. Bodurov, T. Yovcheva, Sainov, and S. PMMA. films refractive index modulation via tio2 nanoparticle inclusions and corona poling. *Colloid and Polymer Science*, 292(11): 3045–3048, 2014, doi:10.1007/s00396-014-3373-y.
- [3] Park HE, Lim ST, Laun HM, and Dealy JM. Measurement of pressure coefficient of melt viscosity: drag flow versus capillary flow. *Rheologica Acta*, 47: 1023–1038, 2008, doi:10.1007/s00397-008-0296-x.
- [4] John Wiley and Sons. *Handbook of Introduction to Physical Polymer Science*. Inc., Hoboken ,New Jersey in Canada, 4<sup>th</sup> edition, 2006, 10.24237/djps.1402.403B.
- [5] R. Cardinaels, Van Puyvelde, and P. Moldenaers. Evaluation and comparison of routes to obtain pressure coefficients from high-pressure capillary rheometry data. *Rheologica Acta*, 46(4): 507–520, 2007, doi:10.1007/s00397-006-0148-5.
- [6] F. Sahin, C. Tav, and Yahsi. Linking the viscous and vacancy behavior of mixtures of high-molecular-weight hydrocarbons. *International Journal of Thermophysics*, 27(5): 1501–1514, 2006, doi:10.1007/s10765-006-0099-1.
- [7] D. Buta and K. F. Freed. Lattice polymers with structured monomers: A monte carlo study of thermodynamic properties of melts and solutions. *Journal of Chemical Physics*, 116(24): 10959–10966, 2002, doi:10.1063/1.1478766.
- [8] A. Sorrentino and R. Pantani. Pressure-dependent viscosity and free volume of atactic and syndiotactic polystyrene. *Rheologica Acta*, 48(4): 467–478, 2009, doi:10.1007/s00397-009-0348-x.
- [9] G. Akdeniz, U. Yahsi, and C. Tav. Viscous behavior of ps, pp, and abs in terms of temperature and pressure-dependent hole fraction. *Journal of Applied Polymer Science*, 117(1): 110–113, 2010, doi:10.1002/app.31565.
- [10] U. Yahsi and F. Sahin. Linking the viscous and vacancy behavior of high molecular weight hydrocarbons. *Rheologica Acta*, 43(2): 159–167, 2004, doi:10.1007/s00397-003-0330-y.
- [11] T. Sedlacek, R. Cermak, B. Hausnerova, M. Zatloukal, A. Boldizar, and P. Saha. On pvt and rheological measurements of polymer melts - correction of the hole fraction - viscosity relationship. *International Polymer Processing*, 20(3): 286–295, 2005, doi:10.3139/217.1890.
- [12] S. Küzeci. Simha-somcynsky ve cahn hilliard kuramlarını kullanarak polimerlerin yüzey serbest hacim derinlik profilinin Çıkarılması. *Doktora Tezi, Marmara Üniversitesi Fen Bilimleri Enstitüsü*, pages 3–5, 2011.
- [13] M. Aslan. *Statistical Thermodynamics of Branched And Dendrimer Macromolecular Structures*. PhD thesis, Marmara University ,Istanbul, 2009.
- [14] H. Kahl and S. Enders. Calculation of surface properties of pure fluids using density gradient theory and soft-eos. *Fluid Phase Equilibria*, 172: 27–42, 2000, doi:10.1016/S0378-3812(00)00361-7.
- [15] L. A. Utracki and R. Simha. Analytical representation of solutions to lattice-hole theory. *Macromolecular Theory and Simulations*, 10(1): 17–24, 2001.
- [16] S. Walfram. *Mathematica. Addison-Wesley Publishing Company*. Inc, Redwood City California, 2<sup>ed</sup> edition, 1991, doi:10.25130/tjps.25.2020.092.
- [17] S. C. Chapra and R. P. Canale. *Numerical Method for Engineers*. McGraw Hill, USA, 6<sup>th</sup> edition, 2010.



دراسة الخواص الفيزيائية (الضغط، الحجم ودرجة الحرارة) لبولي اثيلين كلايكول باستخدام نظرية سمها - سومسينيسكي

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### الخلاصة

في هذه الدراسة تم فحص بنية بوليمر البولي اثيلين كلايكول بأوزان جزيئية مختلفة و دراسة الخصائص الفيزيائية من حيث المتغيرات (الضغط والحجم ودرجة الحرارة) باستخدام نظرية سمها سومسينيسكي التي اظهرت التوزيع اللانظامي وذلك بوجود خلايا فراغية والجزء الفراغي في المواقع المشغولة في الشبكة والتي تؤثر على الديناميكية الحرارية الاحصائية للبوليمرات. وقد تم فحص الخصائص الترموديناميكية بتحديد النسبة الفراغية في الشبكة، و قياس المتغيرات في نطاق درجة حرارة 283-450 كلفن وضغط 150 ميجا باسكال، و كذلك تحديد متوسط الخطأ والحد الأقصى للخطأ في حجم 0.036 % و 0.28 % على التوالي، كأعلى خطأ في بولي اثيلين كلايكول 302 . و قد اثبت أن بولي اثيلين كلايكول يحتوي على درجات حرارة انتقال زجاجي تتراوح بين 55-60 كلفن.

**الكلمات الدالة:** النسبة الفراغية؛ نظرية سمها سومسينيسكي؛ نظرية الشبكة؛ القابلية الحركية الفراغية؛ بولي اثيلين كلايكول؛ الطول المقطعي.

**التمويل:** لا يوجد.

**بيان توفر البيانات:** جميع البيانات الداعمة لنتائج الدراسة المقدمة يمكن طلبها من المؤلف المسؤول.

**اقرارات:**

**تضارب المصالح:** يقر المؤلفون أنه ليس لديهم تضارب في المصالح.

**الموافقة الأخلاقية:** لم يتم نشر المخطوطة أو تقديمها لمجلة أخرى، كما أنها ليست قيد المراجعة.