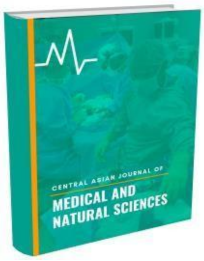

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Article

Thermodynamic and Interfacial Analysis of Polypropylene Glycol: Dependence of the Gradient Energy Coefficient on Molecular Weight Using Simha–Somcynsky and Cahn–Hilliard Theories

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Abstract: This study presents a theoretical analysis of the thermophysical and interfacial properties of polypropylene glycol with different molecular weights using a combined Simha–Somcynsky equation of state and Cahn–Hilliard diffuse-interface framework. Properties including gradient energy coefficient, surface tension, density, specific volume, hole fraction, and occupied volume fraction were evaluated over 313–473 K and 0.1–150 MPa. Results show that increasing molecular weight reduces specific volume and density but increases surface tension and gradient energy coefficient, while increasing temperature produces opposite trends. Numerical accuracy was assessed through volume deviation measures. The approach reliably captures molecular-weight-dependent interfacial behavior relevant to PPG material design applications.

Keywords: Polymer Thermodynamics, Interfacial Properties, Phase Separation, Modified Cell Theory, Thermal Expansion.

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1. Introduction

Polymers have become some of the most important materials of industry and science because of their structure diversity and tunable properties. Considered as long chain molecules consisting of repeating units called monomers, polymers possess various physical and chemical properties that can be modified by molecular structure, monomer type and molecular weight [1], [2]. They have uses ranging from the mundane to the cutting edge, in consumer products, aerospace technology, laser printers and medical devices. PPG is a versatile light end oligomer and tailor-made viscosity can be made use of to adjust for different systems, while at the same time being highly flexible in addition to its compatibility with various substrates. PPG is a popular ingredient for hydraulic fluids, adhesive formulations, cosmetics, insulating foams and pharmaceutical applications [3]. Molecular weight directly gives effect on the specific volume, density, surface tension and thermodynamics properties of PPG which are the most important parameter to characterize its behavior [4]. Molecular weight also clearly influences the temperature responsive property of PPG. For longer chains the packing efficiency, free volume and interface dynamics of polymer change with decreasing density. It is important to have these parameters and to utilize the response of the polymer to both heat and pressure, particularly within high performance industrial and medical applications

[5]. The gradient energy parameter (κ) is the key parameter to describe how much energy will be cost due to this spatial variation in polymer density in the model. It is also closely related to the surface energy, Surface tension and phase separation of these systems and hence important in the study of interface kinetics. To describe the way this behaviour takes place, it will be described that Cahn–Hilliard equation is a standard theoretical model on how phase composition evolves in time for multiphase systems within which the minimizing of an overall free energy occurs [6]. Herein, we used a single thermodynamic model consisting of the SS equation of state (EOS) and Cahn–Hilliard theory to study the thermo-physical properties for PPG with different molecular sizes. With respect to the method, we start with investigating studies of the gradient energy coefficient, the surface tension and so on as function of different temperatures for a better understanding how dependent on molecular structure of mesoscopic thermal phenomenon [7].

2. Materials and Methods

In the present work, a general thermodynamic approach is employed by directly combining Simha–Somcynsky (SS) equation of state with Cahn–Hilliard (CH) diffuse-interface theory to study the themophysical and interfacial properties for different molecular weights of PPG. The bulk thermodynamics of the polymer system is described using the SS theory and energetics due to spatial density variations are determined using CH formulation as well as interfacial properties like gradient energy coefficient and surface tension.This method has the advantage of providing a unified description of both bulk and interfacial properties, and it does not contain any adjustable parameters, which makes it suitable for investigating molecular weight dependent behavior in polymer systems.

2.1 Cahn- Hilliard Free Energy Formulation

The Cahn–Hilliard equation is well known as a multiphase modeling of composition evolution in material science. It is a conservation law, and it preserves the atomic density when spatial modulations are absent. This equation is relevant for modeling phase separation and interface growth in heterogenous media [8].The local free energy density $\alpha(\rho, \nabla\rho, \nabla^2\rho, \ldots)$ is expressed as:

$$f(\rho, \nabla\rho, \nabla^2\rho, \ldots) = f_0(\rho) + \frac{1}{2} k\, (\nabla\rho)^2 \tag{1}$$

where $f_0(\rho)$ represents the free energy density of the homogeneous bulk system, $\boldsymbol{\rho}$ is the mass density, and k is the gradient energy coefficient. The second term accounts for the energetic penalty associated with spatial variations in density and governs the formation and stability of interfaces. The total Helmholtz free energy of the system occupying a volume V is given by

$$F = \int_V \left[f_0(\rho) + \frac{1}{2} k (\nabla\rho)^2 \right] dV \tag{2}$$

The first contribution corresponds to the bulk thermodynamics, while the gradient term controls interfacial structure and thickness. [9].

2.2 Surface Tension within the CH Model

For a planar interface where the density varies along a single spatial coordinate, the equilibrium interfacial structure is obtained by minimizing the free energy functional with respect to density variations. Under these conditions, the surface tension σ, defined as the excess free energy per unit area, can be written as ,To get the surface tension, which is a crucial property of an interface, the previous energy equation is divided by the interfacial area and integrated across the interface in one dimension:

$$\sigma = \int_{\rho_\alpha}^{\rho_\beta} \sqrt{2k\left[f_0(\rho) - {f_0}^{eq}\right]}\, d\rho \tag{3}$$

where ϱ_𝛼 and ϱ_β are the densities of the two coexisting phases (e.g., polymer-rich and polymer-poor phases), and 〖f_0〗^eq is the equilibrium free energy determined from the common tangent construction. This formulation explicitly demonstrates the direct link between the gradient energy coefficient and the interfacial properties of the polymer system

2.3 Simha-Somcynsky Equation of State

The bulk free energy density f_0 (ϱ) and all related thermodynamic quantities required in the CH formulation are obtained from the Simha–Somcynsky equation of state, also known as the Modified Cell Theory. This theory provides a molecular-based description of amorphous and molten polymers by assuming that polymer segments occupy cells separated by voids, leading to the concept of free volume. The SS equation of state describes the relationship between pressure, temperature, and specific volume through reduced variables T^*, P^*, and V^*, s of these, and renormalize them to scale with characteristic molecular parameters associated with cohesive and repulsive interactions. Use of the scaled variables allows direct comparison between different polymerization runs (with different number average molecular weights) and results in a significant numerical convergence acceleration.

2.4 Numerical Implementation

The Simha–Somcynsky equations are solved numerically by the Newton–Raphson iteration method. Initial values for density and free volume were selected from reasonable physical parameters of polymer melts. Iterations were performed until convergence was obtained, which was defined by the relative change in density and hole fraction between successive iterations being less than. After the SS model converged, it delivered the macroscopic thermodynamic properties such as density, specific volume hole fraction, and bulk free energy. These quantities were then employed as input values for the direct evaluation of and, using the Cahn–Hilliard expression, for the gradient energy coefficient and surface tension calculations σ. All the calculations were conducted in a temperature range of 313–473 K and under pressures from 0.1 to 150 MPa. This approach of number-inducing harmonization enables internal consistency of bulk thermodynamics and interfacial properties, and meets the demand for methodological transparency necessary for achieving reproducibility. Here, Δ𝛼 represents the free energy difference between two coexisting phases (e.g., liquid and vapor). The resulting expression gives the Helmholtz free energy per unit area across the interface, with density gradients driving the structure [10]. To model equilibrium, Euler's equation is applied to the energy functional I :

$$I - \left(\frac{d\rho}{dx}\right)\left[\frac{\partial I}{\partial(d\rho/dx)}\right] = 0 \qquad (4)$$

2.5 Scope and Validity of the Model

It is important to stress that in the present approach, PPG is modelled as an homogeneous polymer melt and the focus is made on equilibrium interfacial properties. The SS–CH combined approach is well adapted for studying MW effects on free volume, surface tension, and gradient energy. Extensions of the present model to pressure-dependent behavior, multicomponent systems, or non-equilibrium dynamics can be addressed in future work.

Continuation of Cahn–Hilliard Theory: Surface Tension Derivation

Starting from the earlier equation:

$$\Delta\alpha - k\left(\frac{d\rho}{dx}\right)^2 = 0 \qquad (5)$$

This equation can be rearranged to:

$$\Delta\alpha = k\left(\frac{d\rho}{dx}\right)^2 \qquad (6)$$

Solving for dx, we isolate the differential:

$$dx = \left(\frac{\Delta\alpha(\rho)}{k}\right)^{-1/2} d\rho \qquad (7)$$

This expression shows the spatial increment dx in terms of the density function and energy. Substituting $\Delta\alpha(\rho)$ as a function of ρ, we obtain:

$$dx = k^{-1/2}\Delta\alpha(\rho)^{-1/2}d\rho \qquad (8)$$

Now, inserting equation (13) into the surface tension expression:

$$\gamma = \int_{-\infty}^{\infty} 2\,\Delta\alpha(\rho)dx \qquad (9)$$

we get the surface tension in terms of a density integral:

$$\gamma = 2\int_{-\infty}^{\infty}[k\Delta\alpha(\rho)]^{1/2}\,dx \qquad (10)$$

This result allows us to compute the surface tension based on the local free energy difference across a density gradient [10].Let Ω denote the domain over which the Cahn–Hilliard equation is solved, with $\partial\Omega$ representing its boundary. In this section, we first address the binary system before introducing the multicomponent model and the stress-enhanced diffusion case [11]. Take the information from my article that published in kirkuk university will supply yioou to complete the derivatives. In the binary case, the Cahn–Hilliard equation is interpreted as a diffuse interface model. Here, c is the mass fraction of one component in a two-component system. The total free energy of the system, based on Ginzburg–Landau formalism, is given by:

$$F(c) = \int_{\Omega}\left[f(c) + \frac{K}{2}\mid\nabla c\mid^2\right]dV \qquad (11)$$

This equation describes the system's energy as a combination of a bulk free energy density $f(c)$ and a gradient energy term representing interface effects [12][13]. The Simha–Somcynsky theory, abbreviated as Modified Cell Theory (MCT), is one of the most prominent theoretical models used to describe the thermodynamic behavior of polymers in their amorphous or molten states. This theory is the compartmentalization concept, which proposes that every structural unit in a polymer chain exists in cells of defined volume and separation (some free spaces or voids) between them, leading to observable exterior properties and internal energy. It should be noted that the molecules are not occupying entirely the volume of the material but a void fraction is actually present where: h = volumetric % pore (void) space For example, in cases as softening bitumen's surface tension and density depend on temperature and pressure vary with compressibility. The theory further assumes that the forces between the molecules can be broken down into cohesive and repulsive parts so as to form a semi-realistic equation-of-state which is valid for thermal states [14].

The equation of state in this model is expressed as follows:

$$P = \frac{C\cdot T}{V - V^{1/3}(V^{1/3}-\delta)} + \frac{2T}{V^2}\left(B - \frac{A}{V^2}\right) \qquad (12)$$

Where: P is the pressure, T is the absolute temperature, V is the specific volume, C is a parameter related to the molecular degrees of freedom (chain structure), δ is a structural correction factor, and A, B are constants associated with the cohesive and repulsive energy between molecules [15], [16].

3. Results anad Discussion

Based on the Modified Cell Theory (MCT) and using the Cahn–Hilliard (CH) formulation a systematic theoretical study was performed of four systems of polypropylene glycol (PPG) with variable molecular weights: PPG400, PPG1025, PPG2000 and PPG4000. We are interested in how the temperature and molecular weight affect bulk thermodynamics, interfacial properties, and gradient energy for these mixtures.

3.1 Thermophysical Properties and Molar Mass Influence

Reduced thermophysical properties calculated by Simha–Somcynsky equation of state are presented in Table 1.

Table 1. Theoretical Thermophysical Properties of PPG Polymers Calculated Using Modified Cell Theory.

Polymers	T*(K)	V*(cc/gm)	P*(MPa)	ε*(k.K)	K*(erg·cm/gr²)	*V10⁶	C	S	maxErr	MinErr
PPG400	8559.12	0.000954	802.267	350.516	0.00010317	37.03	4.3	10.3	0.49746	1.19E-05
PPG1025	8710.19	0.000963	762.958	340.549	0.00031244	37.391	10.4	26.4	0.48549	0.000963
PPG2000	9373.64	0.00098	715.663	326.355	0.00093541	38.061	18	51.5	0.32922	0.00041
PPG4000	9362.5	0.000983	710.596	325.692	6.6651E-05	38.18	35.9	103	0.31409	0.002031

Table 2. Normalized Interfacial and Surface Properties of PPG Polymers at Various Temperatures.

Polymer	T (K)	Density ϱ (kg/m³)	$(\tilde{\gamma})\gamma/\gamma^*$	$(\tilde{K})\kappa/\kappa^*$
PPG400	313.2	992.02	0.4656	0.0838
PPG1025	313.2	985.22	0.9147	0.1235
PPG2000	313.2	979.29	1.5092	0.1578
PPG4000	313.2	976.10	2.3045	0.1839

Table 3. Normalized Interfacial and Surface Properties of PPG Polymers at 473 K.

Polymer	T (K)	Density ϱ (kg/m³)	γ^*/γ	κ/κ^*
PPG400	473	866.11	2.0875	0.2043
PPG1025	473	863.93	1.8086	0.1992
PPG2000	473	866.37	1.5066	0.1846
PPG4000	473	863.77	1.5066	0.1845

The results exhibit clean and regular trends with molecular weight. Higher molecular weight PPGs hence have less specific volume and density, which is consistent with a denser packing of the chains and higher intermolecular cohesion resulting from longer chain length and greater entanglement. However, lower molecular weight PPGs exhibit higher specific volumes and free volume contents due to fewer chain entanglement restrictions. The numerical sensitivity of the SS-based computations was checked, using the reported maximum and minimum deviation criteria. The low deviation values, in particular for PPG4000, demonstrate the accuracy and stability of the numerical approach that justifies a priori application of MCT throughout molecular weights..

3.2 Temperature Dependence of Specific Volume and Density

The effect of temperature on specific volume at constant pressure (0.1 MPa) is plotted in Fig. 1. One common feature for all PPG systems is that the temperature-dependent variation of specific volume increases more or less linearly over 20-100°C, as observed for amorphous polymer melts, attributed to thermal expansion due to enhanced segmental mobility. At the same temperature, PPG400 has the highest specific volume and PPG4000 the lowest one, indicating that molecular weight mainly define packing efficiency.

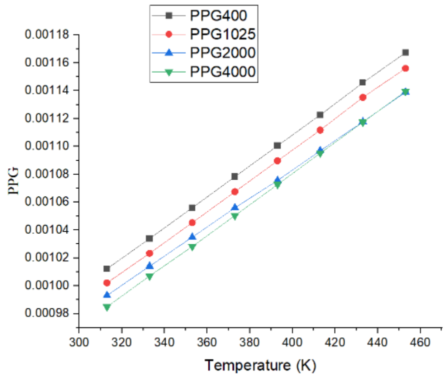

Figure 1. Specific volume as a function of temperature for different PPG polymers (PPG400, PPG1025, PPG2000, PPG4000) at constant pressure of 0.1 MPa.

The corresponding density–temperature relation (Figure 2) exhibits an opposite behavior of the monotonic decrease of density with increasing temperature for all molecular weights. PPGs with lower molecular weights, i.e., 400 MWt and below reveal a slope increase in the density drop which is more indicative of their susceptibility to thermal agitation as a result of their less compacted molecular structure. Under lower molecular weight, thermal expansion of the systems was less inhibited due to weaker chain entanglement and cohesive interaction. These trends are in perfect agreement with free volume theory and polymer thermodynamics.

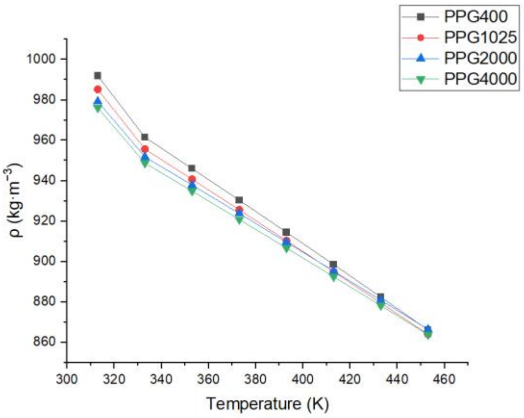

Figure 2. Density as a function of temperature for PPG polymers (PPG400, PPG1025, PPG2000, PPG4000) at a pressure of 0.1 MPa.

3.3 Hole Fraction and Occupied Volume Fraction

The hole fraction, as the fraction of unoccupied volume of the system is hereafter referred direct evidence for free volume characteristics of polymer systems. As presented in Table 4 and Figure 3, the hole fraction reduces with increasing temperature for all PPGs.

Thermal motion typically favors expand. 31 but they can also in principle trap excitations within them from escaping to the system again, this decrease in h exhibiting only thermally induced chain rearrangement and enhanced packing efficiency at constant pressure in the context of the Modified Cell Theory.

Table 4. Hole Fraction (h = 1 − y) Values for PPG Polymers at Different Temperatures.

PPG4000	PPG2000	PPG1025	PPG400	Temperature (K)
0.19188	0.19126	0.18037	0.07641	313
0.17737	0.17855	0.15707	0.07523	333
0.1627	0.16545	0.13457	0.07061	353
0.14797	0.15216	0.11296	0.06376	373
0.13291	0.13843	0.09189	0.05515	393
0.11718	0.12395	0.07096	0.04495	413
0.10049	0.10847	0.04984	0.03322	473

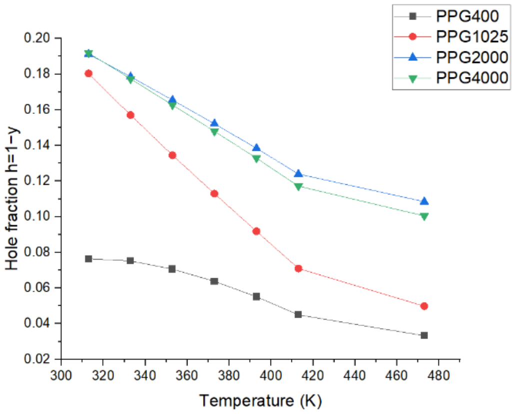

Figure 3. Hole fraction h=1−y as a function of temperature for PPG polymers (PPG400, PPG1025, PPG2000, PPG4000) at constant pressure of 0.1 MPa.

In the case of lower MW PPGs, a less pronounced hole fraction is observed at all temperatures, suggesting denser local packing and diminished internal void space. Larger molecular weight polymers have in the first place a higher proportion of holes, because the increased entanglement and conformational disorder can only be lost through partial relaxation h.

The occupied volume fraction $y = 1 - h$ thus increases with temperature for all molecular weights (Table 5, Figure 4). This behavior may look counterintuitive, however, it can be interpreted as a polymeric entropic rearrangement process where molecular chains are able to explore new preferred packing conformations at high temperatures. Chains are able to overcome local constraints and reorganize at small scales due to available thermal energy, under the constant load these chains densify mesoscopically despite increased molecular mobility. Analogously, in theoretical investigations of cell-like models for polymer melts such behavior has been also observed.

Table 5. Values of the Occupied Volume Fraction y for PPG Polymers from 313 K to 453 K.

T (K)	PPG400	PPG1025	PPG2000	PPG4000
313	0.957665	0.957302	0.955678	0.955714
333	0.958820	0.958469	0.956738	0.956784
353	0.959421	0.959075	0.957280	0.957331
373	0.960046	0.959703	0.957838	0.957894
393	0.960697	0.960355	0.958415	0.958476
413	0.961379	0.961037	0.959014	0.959080
433	0.962093	0.961750	0.959639	0.959710
453	0.962845	0.962497	0.960291	0.960369

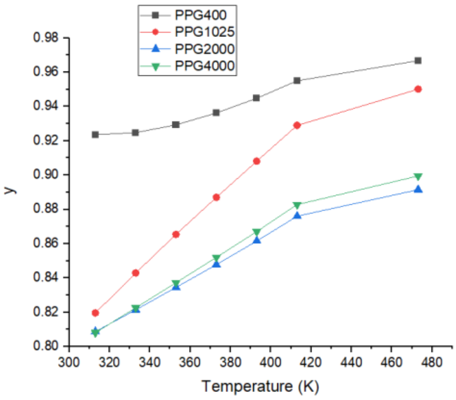

Figure 4. Occupied site fraction y as a function of temperature for PPG polymers (PPG400, PPG1025, PPG2000, PPG4000) at a pressure of 0.1 MPa.

3.4 Surface Tension Behavior

The surface tension dependence on temperature behaviour of the studied PPG systems is shown in Figure 5. In all cases, surface tension decreases almost linearly with temperature as the stronger cohesive forces between molecules decrease with increased thermal vibration of the particles in the interface. PPG400 exhibits the largest decrease, which is in accordance with its shorter chain and more segmental mobility. Higher molecular weight PPGs (PPG4000 in particular) exhibit high surface tension values in the entire temperature range. This is ascribed to a higher degree of intermolecular attraction and the greater entanglement of chains which stabilise interface against thermal disruption. These results are consistent with mean-field models of polymeric interfaces, and have direct implications on wetting, coating stability, and interfacial adhesion applications.

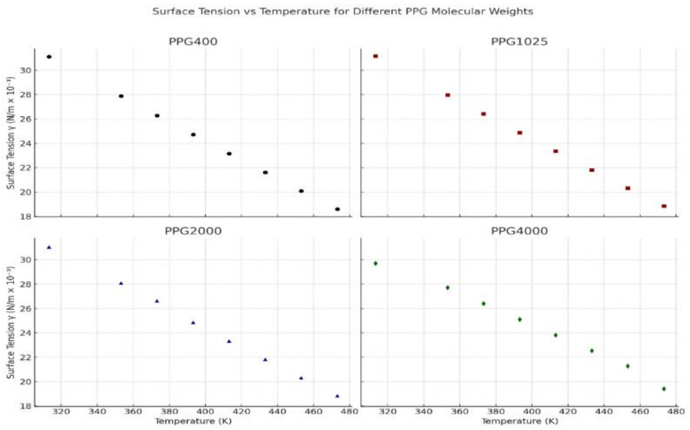

Figure 5. Shows the relationship between temperature and surface tension for polypropylene glycol (PPG) samples with varying molecular weights (PPG400, PPG1025, PPG2000, PPG4000).

3.5 Gradient Energy Coefficient and Interfacial Stability

The temperature dependence of the reduced gradient energy coefficient $\tilde{k}$ is shown in Figure 6. For all PPG systems, k decreases monotonically with increasing temperature, indicating a reduced energetic penalty for spatial density variations at elevated thermal conditions. This behavior originated from the higher segmental mobility and the better homogeneity of the polymer matrix, which lead to decreasing "resistance" toward interfacial gradients. At a given temperature, the gradient energy coefficients of higher molecular weight PPGs are much greater than those of lower molecular weight ones. Especially PPG4000 indicates the largest values, indicating high structural resistance for density fluctuation from long-range entanglement and cohesive interaction. In contrast, PPG400 exhibits the smallest S based on its less complex molecular structure and lower interfacial rigidity. This molecular-weight-dependent curve again demonstrates that the gradient energy coefficient is a sensitive indicator of interfacial stability and structural resistance in polymers, and can be justified as an input into the Cahn–Hilliard model to predict polymer interfaces.

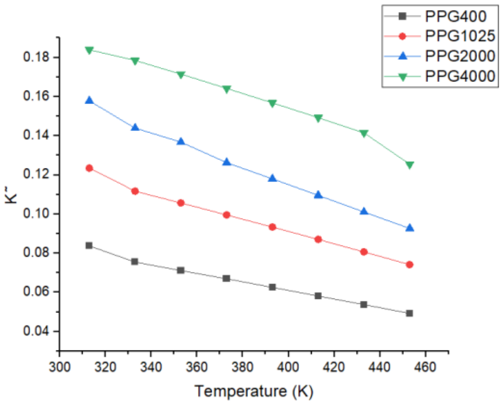

Figure 6. Reduced gradient energy coefficient K˜as a function of temperature for PPG polymers (PPG400, PPG1025, PPG2000, PPG4000) at a pressure of 0.1 MPa.

3.6 Reduced Surface Tension Analysis

The dependence of the reduced surface tension and normalized surface tension ratios as a function of temperature is indicated in Figure 7. Decreased reduced surface tension with increasing temperature is additional evidence that entropic effects are more important than enthalpic contributions at elevated temperatures. Smaller PPGs reduce at a faster pace resulting from their greater mobility whereas larger molecular weights offer bigger normalized surface tension values pointing to a stronger intermolecular attraction. Such a temperature dependence observed for the intermediate molecular weight (e.g., PPG2000) indicates that there may exist an equilibrium between two factors upon interfacial energy, that is, entropy and enthalpy. Such a balance may be characteristic of transition interfacial behavior, of being particular importance for applications in which the surface properties will remain stable over a wide range of temperature isnan .

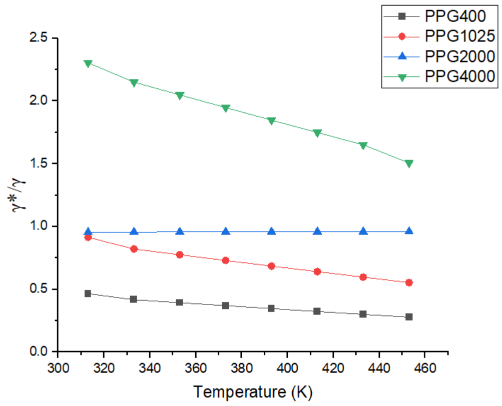

Figure 7. Reduced surface tension γ^*/γ as a function of temperature for PPG polymers (PPG400, PPG1025, PPG2000, PPG4000) at a pressure of 0.1 MPa.

3.7 Implications and Physical Significance

In general, the data imply that MW and temperature cooperate to influence thermophysical and interfacial properties of PPG systems. Higher molecular weight leads to greater interfacial stiffness and resistance against density gradients, while larger temperature induces a reduction in the surface tension and gradient energy penalty by supporting molecular mobility. The SS–CH framework incorporates both these trends and physically interprets the interplay of free volume, chain entanglement and interfacial energetics in polymer melts.

4. Conclusion

A unified theoretical framework comprising the Simha–Somcynsky equation of state and Cahn–Hilliard diffuse-interface theory was utilized in order to study thermophysical and interfacial characteristics of PPG with different molecular weights. It is found that the specific volume and density decrease, while the surface tension (ST) and gradient energy coefficients H also increase, with increasing molecular weight (MW), which indicates higher intermolecular cohesion and chain entanglement between a polymer's chains. The temperature rises result in an increase of specific volume and decrease in density, surface tension and free energy gradient that manifest themselves by reduction of the cohesive interactions and the enhanced segmental mobility. Entropic chain re-arrangement and packing optimization give rise to activity dependent hole and occupied volume fraction. The SS–CH model can serve as a predictive, physics-based method for the prediction of molecular-weight-dependent interfacial phenomena in polymer melts.

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