

EXCESS VOLUMETRIC AND ACOUSTIC PROPERTIES OF *CHLORELLA VULGARIS* ALGAL BIOMASS EXTRACT + DIESEL + N-ALKANE TERNARY MIXTURES AT 298.15, 308.15 and 318.15 K

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Abstract

This study investigates the thermodynamic behavior and molecular interactions of ternary mixtures containing *Chlorella vulgaris* algal biomass extract, diesel, and selected n-alkanes (n-butane, n-pentane, n-hexane, and n-heptane) over the temperature range of 298.15, 308.15 and 318.15 K. Density and ultrasonic velocity data were used to evaluate key excess properties, namely excess molar volume (V^E) and excess isentropic compressibility (K_s^E), in order to understand deviations from ideal mixing behavior. The results showed predominantly positive excess molar volume values for all systems, confirming non-ideal mixing and volume expansion due to differences in molecular size, polarity, and packing efficiency among the components. The magnitude of V^E generally increased with temperature, indicating enhanced free volume and weakened cohesive interactions at elevated temperatures. Redlich–Kister polynomial fitting provided excellent agreement with the experimental data, with low standard deviation values for both V^E and K_s^E . Among the ultrasonic speed prediction models, Nomoto's relation showed the best agreement with experimental values, whereas the Van-Dael model gave the largest deviations. Overall, the findings demonstrate that diesel plays a compatibilizing role in ternary mixtures and that these thermodynamic insights are useful for the formulation and optimization of algal biomass-based alternative fuel blends.

Keywords: *Chlorella vulgaris*; algal biomass extract; ternary mixtures; excess molar volume; excess isentropic compressibility; Redlich–Kister equation; ultrasonic velocity; diesel blends; n-alkanes; thermodynamic properties

1. Introduction

The increasing global demand for sustainable energy resources and the depletion of fossil fuels have intensified research into alternative and renewable fuel sources. Among the emerging bioenergy resources, microalgae have gained considerable attention due to their rapid growth rate, high lipid productivity, and ability to grow in diverse environmental conditions without competing with food crops [1-2]. Microalgal species such as *Chlorella vulgaris* are particularly promising because they contain significant quantities of fatty acids and lipids that can be converted into biofuels suitable for diesel engines [3]. These characteristics make microalgae-based fuels a viable alternative to conventional petroleum-derived fuels, contributing to energy security and environmental sustainability. In recent years, the development of algal biomass-based fuels has become an important research area in bioenergy and fuel science. The integration of algal-derived biofuels with conventional diesel and hydrocarbon-based fuels offers potential advantages such as improved combustion performance, reduced greenhouse gas emissions, and enhanced fuel stability [4]. However, before such biofuel blends can be used in practical applications, it is essential to understand their thermodynamic behavior and molecular interactions. Thermophysical properties such as density, ultrasonic velocity, excess molar volume, and compressibility play a critical role in evaluating the compatibility and stability of fuel mixtures [5–6]. The study of excess thermodynamic properties provides valuable insights into the intermolecular interactions occurring within liquid mixtures. Excess molar volume (V^E) is one of the most important parameters used to evaluate deviations from ideal mixing behavior [7]. It reflects the structural arrangement, molecular size differences, and interaction forces between mixture components. Positive excess molar volume generally indicates volume expansion due to weak intermolecular interactions, while negative values suggest stronger attractive forces and compact molecular packing [9]. Therefore, the measurement and analysis of excess molar volumes are essential for understanding the physical behavior of complex liquid systems [9–10].

Similarly, excess isentropic compressibility (K_s^E) provides information about the compressibility and structural changes within mixtures under different thermodynamic conditions [11]. This property is closely related to the molecular organization and packing efficiency of liquid systems. Ultrasonic velocity measurements are widely used in thermodynamic studies because they allow the determination of acoustic and compressibility properties with high precision [12]. These parameters are particularly useful in analyzing molecular interactions in multi-component

mixtures such as biofuel blends, petroleum fuels, and hydrocarbon solutions [13]. Ternary mixtures involving bio-derived components and hydrocarbons have attracted increasing interest in thermodynamic research [14]. The addition of hydrocarbons such as n-alkanes (e.g., n-butane, n-pentane, n-hexane, and n-heptane) to biodiesel or algal biomass extracts can significantly influence the volumetric and acoustic properties of the resulting blends [15]. These hydrocarbons differ in molecular size and polarity, which affects the interaction mechanisms and structural arrangement within the mixture. Understanding these interactions is essential for optimizing fuel formulation, improving fuel stability, and ensuring efficient engine performance [16].

Diesel fuel also plays a significant role in biofuel blending because it acts as an intermediate component that can improve the compatibility between polar bio-derived molecules and nonpolar hydrocarbon chains [17]. When diesel is combined with algal biomass extracts and alkanes, complex molecular interactions arise due to differences in polarity, molecular structure, and dispersion forces. Studying these ternary mixtures helps researchers understand how the components influence each other's thermodynamic behavior and how the mixture properties change with temperature and composition [18].

Temperature is another important factor that significantly affects the thermodynamic properties of liquid mixtures. As temperature increases, molecular motion intensifies, leading to changes in density, compressibility, and volumetric behavior [19]. These temperature-dependent variations influence the intermolecular forces between mixture components and can modify the structural arrangement of molecules within the liquid phase. Therefore, experimental measurements across a range of temperatures provide a more comprehensive understanding of the molecular dynamics of biofuel blends [20]. In this context, the present study focuses on the thermodynamic and acoustic investigation of ternary mixtures containing *Chlorella vulgaris* algal biomass extract, diesel, and selected n-alkanes. By analyzing excess molar volume, excess isentropic compressibility, and ultrasonic velocity data over a temperature range of 298.15, 308.15 and 318.15 K, the research aims to provide a deeper understanding of the molecular interactions and thermodynamic behavior of these complex liquid mixtures. Such knowledge is important for the development and optimization of algae-derived biofuel blends for future energy applications.

2. Literature Review

Akhtar and Amin [1] and AR and Thomas [2] highlighted that the global search for sustainable and renewable energy resources has accelerated interest in biomass-derived fuels as substitutes for fossil fuels. Among these resources, microalgae have emerged as highly promising because of their rapid growth, high lipid productivity, and ability to grow under non-arable and wastewater-based conditions. Du and Liu [5], Juneja et al. [13], and Menetrez [16] emphasized that algal biomass is especially attractive for biodiesel production because it does not directly compete with food crops and can provide substantial oil yields under controlled cultivation. In this context, *Chlorella vulgaris* is considered a favorable species due to its biochemical composition and adaptability, making it a suitable candidate for biofuel development. Ma and Hanna [14] further noted that the quality and usability of biodiesel strongly depend on the physicochemical properties of the feedstock, while Saini and Keum [18] and Shahidi and Zhong [20] showed that lipid composition and oxidative stability are crucial in determining the storage and blending performance of bio-derived fuels.

The thermodynamic behavior of such liquid fuel systems is best understood through excess properties, which reveal deviations from ideal mixing and provide insight into molecular interactions. Friedman [8] and Missen [17] discussed the importance of excess thermodynamic functions in characterizing real solutions, where differences in molecular size, shape, and polarity influence structural organization. Eastwood et al. [7] explained that molecular compatibilization and optimization of intermolecular interactions are central to improving the properties of mixed systems, especially in complex hydrocarbon-based fluids. Dyre [6] also emphasized that excess and transport-related properties are closely linked to molecular arrangement and entropy scaling in liquid systems. In fuel blends, excess molar volume is particularly important because it reflects whether the components expand or contract upon mixing. Positive excess molar volume generally indicates weak attractive forces and inefficient packing, whereas negative values suggest stronger interactions and compact structure [8,17]. These interpretations are directly relevant to ternary blends containing algal biomass extract, diesel, and n-alkanes, where strong compositional asymmetry is expected.

Acoustic and compressibility studies provide another important route for analyzing liquid mixture behavior. Hamner et al. [11] and Huyskens et al. [12] showed that compressibility-related parameters are sensitive to molecular organization and interactions in multicomponent systems. Ultrasonic velocity, in particular, is widely used to derive isentropic compressibility and to evaluate the rigidity, free volume, and internal cohesion of fluid mixtures. Pereira et al. [24], Chen et al. [25], and Arce et al. [26] demonstrated that accurate thermophysical property prediction is essential for biofuel systems, especially when dealing with non-ideal mixtures and process conditions that require precise phase and transport modeling. Tsivintzelis et al. [27] further showed that multicomponent biofuel-related systems often require advanced thermodynamic treatment because conventional assumptions may not fully describe molecular

interactions in such blends. Similarly, Asoodeh et al. [28] and Golikova et al. [29] reported that experimental excess-property data are valuable for understanding the behavior of biodiesel-related systems and for validating thermodynamic models in real process environments.

Several studies have also underlined the practical importance of blending renewable components with conventional fuels. Damian et al. [4] discussed the need to improve diesel engine compatibility with sustainable fuels, while Verma et al. [22] examined how blending affects important fuel properties such as cold flow and stability. Stateva and Cholakov [30] pointed out that one of the major challenges in biofuel process design is the reliable modeling of thermodynamic properties and phase behavior, particularly in systems involving chemically diverse components. Although previous research has provided valuable insights into biodiesel production, fuel-property enhancement, and biofuel thermodynamic modeling, detailed experimental data on ternary mixtures containing *Chlorella vulgaris* algal biomass extract, diesel, and selected n-alkanes remain limited [24-30]. In particular, the effect of diesel as a compatibilizing component between polar bio-derived material and non-polar hydrocarbon chains has not been sufficiently explored through excess volumetric and acoustic properties. Therefore, the present study addresses this gap by investigating the excess molar volume, excess isentropic compressibility, and ultrasonic behavior of *Chlorella vulgaris* extract + diesel + n-alkane ternary mixtures over the temperature range 298.15, 308.15 and 318.15 K, thereby contributing useful thermodynamic information for the design and optimization of algae-based alternative fuel blends.

3. Methods and Materials

3.1 Materials

The materials used in this study were *Chlorella vulgaris* algal biomass extract, commercial diesel, and analytical-grade n-alkanes including n-butane, n-pentane, n-hexane, and n-heptane. The algal biomass extract served as the renewable bio-component, while diesel acted as the conventional hydrocarbon phase and compatibilizing medium. The selected n-alkanes were used to represent hydrocarbon chain-length effects in the ternary systems. All chemicals were of high purity and were used after appropriate purification and handling procedures to minimize the influence of moisture and volatile impurities on the experimental data.

3.2 Preparation of Ternary Mixtures

The ternary mixtures were prepared gravimetrically to ensure high accuracy in composition. In the formulation strategy, the ratio of *Chlorella vulgaris* extract and diesel was treated as the principal liquid matrix, while the mole fraction of the selected n-alkane was varied systematically. Required quantities of each component were weighed using a high-precision analytical balance, and the mixtures were prepared in airtight glass containers to prevent evaporation losses, especially in the case of the lighter hydrocarbons. After weighing, the mixtures were sealed immediately and subjected to thorough mechanical agitation to ensure complete homogeneity. The prepared mixtures were allowed to equilibrate prior to measurement, and all samples were stored under controlled conditions to avoid contamination, oxidation, or moisture absorption.

3.3 Experimental Measurements

The density and ultrasonic velocity of the ternary mixtures were measured over the temperature range 298.15, 308.15 and 318.15 K using a calibrated density and sound velocity analyzer. Temperature was controlled with high precision during all measurements to ensure reproducibility. Density measurements were essential for determining molar volumes, while ultrasonic velocity measurements were used for calculating isentropic compressibility. For each sample, multiple readings were taken and averaged to minimize random error. The instruments were calibrated daily using standard reference materials before data collection. Care was taken to eliminate air bubbles and ensure that the sample cell was completely filled before each run.

3.4 Calculation of Thermodynamic Properties

The measured density values were used to calculate the molar volume of each ternary mixture, from which the excess molar volume (V^E) was obtained by comparing the experimental molar volume with the ideal molar volume based on mole fraction additivity. Positive values of V^E indicate volume expansion and weaker packing efficiency, whereas negative values would suggest contraction and stronger molecular accommodation.

The measured ultrasonic velocity and density data were used to calculate the isentropic compressibility of the mixtures according to the Newton–Laplace relation. Excess isentropic compressibility (K_s^E) was then determined by subtracting the ideal mole-fraction weighted compressibility from the experimental compressibility. This excess property provides insight into structural compactness, intermolecular cohesion, and free volume effects within the ternary systems.

3.5 Correlation of Excess Properties

The experimentally determined excess molar volume and excess isentropic compressibility data were correlated using the Redlich–Kister polynomial equation. The adjustable parameters X_1 , X_2 , and X_3 were determined at each temperature for all ternary systems. The standard deviation between experimental and calculated values was used to evaluate the quality of the fit. A low standard deviation indicated that the model described the data accurately and that

the fitted coefficients could be used to interpret the composition-dependent behavior of the mixtures.

3.6 Correlation of Ultrasonic Velocity

To assess the predictive capability of commonly used theoretical models, experimental ultrasonic velocity values were compared with those calculated from Nomoto, Van-Dael, and Impedance relations. Percentage standard deviations were determined for each model at all temperatures. The model with the lowest deviation was considered the most suitable for representing the acoustic behavior of the ternary systems. This comparison helped evaluate which theoretical assumptions most closely matched the real molecular arrangement of the studied blends.

3.7 Data Analysis

All measurements were repeated to ensure reproducibility, and the average values were used in the final analysis. The variation of excess molar volume and excess isentropic compressibility with temperature and composition was examined in detail to understand molecular interactions among the ternary components. Special attention was given to identifying the effect of hydrocarbon chain length on the degree of non-ideality, volume expansion, and compressibility behavior. Comparative analysis of the four ternary systems made it possible to distinguish the relative roles of n-butane, n-pentane, n-hexane, and n-heptane in modifying the thermodynamic structure of the biodiesel–diesel matrix.

3.8 Reliability of the Method

The reliability of the experimental method was ensured through careful sample preparation, daily instrument calibration, repeated observations, and strict temperature control. The low standard deviations obtained from the Redlich–Kister fitting and the consistent trends observed across all systems confirmed the precision of the measured data. These procedures ensured that the reported thermodynamic properties were sufficiently accurate for scientific interpretation and for potential application in blend design and alternative fuel formulation.

4. Data Analysis and Results

The study of Excess Molar Volumes (V^E) in ternary mixtures is a crucial aspect of understanding molecular interactions in complex mixtures. These mixtures often exhibit non-ideal behavior, with the molecular interactions between the components leading to deviations from the ideal volumes. The excess molar volume provides insight into the nature of these interactions, whether attractive or repulsive, and their influence on the mixture's thermodynamic properties. Table 4.1 presents the measured excess molar volumes for various ternary mixtures, with temperatures ranging from 298.15K, 308.15 and 318.15K. The data highlights how the excess molar volume changes as a function of temperature and mole fraction, offering a deeper understanding of the molecular behavior in these systems.

4.1 Molar Excess Volume (V^E)

Table 4.1 Measured excess molar volumes (V^E , $\text{cm}^3\text{mol}^{-1}$) for various Ternary (i+j+k) mixtures as a function of mole fraction (x_i) at various temperatures 298.15K, 308.15K and 318.15K.

x_i	x_{ii}	V^E (298.15)				V^E (308.15)				V^E (318.15K)			
		Densit y (g/cm^3)	Molar Volume (cm^3/mol)	Ideal Volume (cm^3/mol)	Excess Molar Volume V^E (cm^3/mol)	Densit y (g/cm^3)	Molar Volume (cm^3/mol)	Ideal Volume (cm^3/mol)	Excess Molar Volume V^E (cm^3/mol)	Densit y (g/cm^3)	Molar Volume (cm^3/mol)	Ideal Volume (cm^3/mol)	Excess Molar Volume V^E (cm^3/mol)
<i>Chlorella vulgaris</i> + Diesel + n-Butane													
0.058 4	0.941 6	0.8361	209.32	209.4	-0.079	0.8289	214.51	214.6	-0.088	0.8217	219.7	219.8	-0.097
0.075 5	0.924 5	0.8356	209.71	209.81	-0.103	0.8284	214.9	215.01	-0.115	0.8212	220.09	220.21	-0.126
0.104 6	0.895 4	0.8347	210.37	210.51	-0.143	0.8275	215.55	215.71	-0.158	0.8203	220.74	220.91	-0.174
0.122 9	0.877 1	0.8341	210.78	210.95	-0.166	0.8269	215.96	216.15	-0.185	0.8197	221.15	221.35	-0.203
0.145 3	0.854 7	0.8334	211.29	211.49	-0.195	0.8262	216.47	216.69	-0.216	0.819	221.65	221.89	-0.237
0.193 0	0.807 0	0.8318	212.38	212.63	-0.25	0.8246	217.55	217.83	-0.277	0.8174	222.73	223.03	-0.304
0.214 9	0.785 1	0.8311	212.89	213.16	-0.273	0.8239	218.06	218.36	-0.302	0.8167	223.23	223.56	-0.332
0.258 8	0.741 2	0.8297	213.9	214.21	-0.314	0.8225	219.06	219.41	-0.348	0.8153	224.23	224.61	-0.383
0.293 9	0.706 1	0.8286	214.71	215.05	-0.342	0.8214	219.87	220.25	-0.38	0.8142	225.04	225.45	-0.417
0.349 4	0.650 6	0.8268	216.01	216.39	-0.378	0.8196	221.17	221.59	-0.42	0.8124	226.32	226.79	-0.462
0.375 6	0.624 4	0.826	216.62	217.01	-0.391	0.8188	221.78	222.21	-0.435	0.8116	226.94	227.41	-0.478
0.410 0	0.590 0	0.8249	217.43	217.84	-0.405	0.8177	222.59	223.04	-0.45	0.8105	227.75	228.24	-0.494

0.4689	0.5311	0.823	218.84	219.25	-0.418	0.8158	223.99	224.45	-0.464	0.8086	229.14	229.65	-0.51
0.5313	0.4687	0.821	220.33	220.75	-0.418	0.8138	225.49	225.95	-0.464	0.8066	230.64	231.15	-0.51
0.5955	0.4045	0.8189	221.89	222.29	-0.403	0.8117	227.04	227.49	-0.448	0.8045	232.2	232.69	-0.492
0.6667	0.3333	0.8167	223.63	224	-0.369	0.8095	228.79	229.2	-0.41	0.8023	233.95	234.4	-0.45
0.7343	0.2657	0.8145	225.3	225.62	-0.32	0.8073	230.47	230.82	-0.355	0.8001	235.63	236.02	-0.39
0.8095	0.1905	0.8121	227.18	227.43	-0.247	0.8049	232.35	232.63	-0.274	0.7977	237.53	237.83	-0.301
0.9048	0.0952	0.809	229.59	229.72	-0.13	0.8018	234.77	234.92	-0.144	0.7946	239.96	240.12	-0.159
0.9524	0.0476	0.8075	230.79	230.86	-0.064	0.8003	235.99	236.06	-0.071	0.7931	241.18	241.26	-0.078
<i>Chlorella vulgaris</i> + Diesel + n-Pentane													
0.0621	0.9379	0.8395	211.91	211.99	-0.078	0.8323	217.1	217.19	-0.087	0.8251	222.3	222.39	-0.095
0.0847	0.9153	0.8388	212.43	212.53	-0.105	0.8316	217.62	217.73	-0.117	0.8244	222.8	222.93	-0.128
0.1098	0.8902	0.838	213	213.14	-0.134	0.8308	218.19	218.34	-0.149	0.8236	223.37	223.54	-0.164
0.1365	0.8635	0.8371	213.61	213.78	-0.163	0.8299	218.79	218.98	-0.181	0.8227	223.98	224.18	-0.199
0.1739	0.8261	0.8359	214.47	214.67	-0.201	0.8287	219.65	219.87	-0.223	0.8215	224.83	225.07	-0.245
0.2054	0.7946	0.8349	215.2	215.43	-0.23	0.8277	220.37	220.63	-0.255	0.8205	225.55	225.83	-0.281
0.2478	0.7522	0.8336	216.18	216.45	-0.264	0.8264	221.35	221.65	-0.294	0.8192	226.52	226.85	-0.323
0.2622	0.7378	0.8331	216.52	216.79	-0.275	0.8259	221.69	221.99	-0.305	0.8187	226.86	227.19	-0.336
0.3186	0.6814	0.8313	217.84	218.15	-0.31	0.8241	223	223.35	-0.345	0.8169	228.17	228.55	-0.379
0.3810	0.6190	0.8293	219.31	219.64	-0.339	0.8221	224.47	224.84	-0.376	0.8149	229.63	230.04	-0.413
0.4059	0.5941	0.8285	219.89	220.24	-0.347	0.8213	225.06	225.44	-0.385	0.8141	230.22	230.64	-0.423
0.4762	0.5238	0.8263	221.57	221.93	-0.359	0.8191	226.73	227.13	-0.399	0.8119	231.89	232.33	-0.438
0.5238	0.4762	0.8247	222.71	223.07	-0.359	0.8175	227.87	228.27	-0.399	0.8103	233.03	233.47	-0.438
0.5714	0.4286	0.8232	223.86	224.21	-0.352	0.816	229.02	229.41	-0.391	0.8088	234.18	234.61	-0.43
0.6190	0.3810	0.8217	225.02	225.36	-0.339	0.8145	230.18	230.56	-0.376	0.8073	235.34	235.76	-0.413
0.6667	0.3333	0.8202	226.18	226.5	-0.318	0.813	231.35	231.7	-0.353	0.8058	236.51	236.9	-0.388
0.7441	0.2559	0.8177	228.09	228.36	-0.27	0.8105	233.26	233.56	-0.3	0.8033	238.43	238.76	-0.33
0.8095	0.1905	0.8156	229.71	229.93	-0.217	0.8084	234.89	235.13	-0.241	0.8012	240.06	240.33	-0.264
0.8571	0.1429	0.8141	230.9	231.07	-0.17	0.8069	236.08	236.27	-0.189	0.7997	241.26	241.47	-0.208
0.9461	0.0539	0.8112	233.14	233.21	-0.068	0.804	238.33	238.41	-0.075	0.7968	243.52	243.61	-0.083
<i>Chlorella vulgaris</i> + Diesel + n-Heptane													
0.0574	0.9426	0.8432	215.31	215.38	-0.067	0.836	220.5	220.58	-0.074	0.8288	225.7	225.78	-0.082
0.0835	0.9165	0.8423	215.91	216	-0.095	0.8351	221.1	221.2	-0.105	0.8279	226.29	226.4	-0.116
0.1182	0.8818	0.8412	216.71	216.84	-0.129	0.834	221.89	222.04	-0.143	0.8268	227.08	227.24	-0.158
0.1467	0.8533	0.8403	217.37	217.52	-0.155	0.8331	222.55	222.72	-0.172	0.8259	227.73	227.92	-0.189
0.1949	0.8051	0.8388	218.48	218.68	-0.195	0.8316	223.66	223.88	-0.216	0.8244	228.84	229.08	-0.237
0.2349	0.7651	0.8375	219.41	219.64	-0.223	0.8303	224.59	224.84	-0.247	0.8231	229.77	230.04	-0.272
0.2732	0.7268	0.8363	220.31	220.56	-0.246	0.8291	225.48	225.76	-0.273	0.8219	230.66	230.96	-0.3
0.3164	0.6836	0.8349	221.33	221.59	-0.268	0.8277	226.5	226.79	-0.298	0.8205	231.67	231.99	-0.327
0.3835	0.6165	0.8327	222.91	223.2	-0.293	0.8255	228.08	228.4	-0.325	0.8183	233.25	233.6	-0.358

0.4269	0.5731	0.8313	223.94	224.25	-0.303	0.8241	229.11	229.45	-0.337	0.8169	234.28	234.65	-0.37
0.4762	0.5238	0.8298	225.12	225.43	-0.309	0.8226	230.29	230.63	-0.343	0.8154	235.45	235.83	-0.377
0.5238	0.4762	0.8282	226.26	226.57	-0.309	0.821	231.43	231.77	-0.343	0.8138	236.59	236.97	-0.377
0.5714	0.4286	0.8267	227.41	227.71	-0.304	0.8195	232.58	232.91	-0.337	0.8123	237.74	238.11	-0.37
0.6190	0.3810	0.8252	228.56	228.86	-0.292	0.818	233.73	234.06	-0.325	0.8108	238.9	239.26	-0.357
0.6667	0.3333	0.8237	229.73	230	-0.276	0.8165	234.89	235.2	-0.306	0.8093	240.06	240.4	-0.336
0.7268	0.2732	0.8217	231.2	231.44	-0.246	0.8145	236.37	236.64	-0.273	0.8073	241.54	241.84	-0.3
0.7651	0.2349	0.8205	232.14	232.36	-0.223	0.8133	237.32	237.56	-0.247	0.8061	242.49	242.76	-0.272
0.8051	0.1949	0.8192	233.13	233.32	-0.195	0.812	238.31	238.52	-0.216	0.8048	243.49	243.72	-0.237
0.8674	0.1326	0.8172	234.67	234.82	-0.143	0.81	239.86	240.02	-0.158	0.8028	245.04	245.22	-0.174
0.9641	0.0359	0.8141	237.1	237.14	-0.043	0.8069	242.29	242.34	-0.048	0.7997	247.49	247.54	-0.052
<i>Chlorella vulgaris</i> + Diesel + n-Hexane													
0.0649	0.9351	0.8409	213.48	213.56	-0.078	0.8337	218.67	218.76	-0.086	0.8265	223.86	223.96	-0.095
0.0958	0.9042	0.8399	214.19	214.3	-0.112	0.8327	219.37	219.5	-0.124	0.8255	224.56	224.7	-0.137
0.1321	0.8679	0.8388	215.02	215.17	-0.149	0.8316	220.21	220.37	-0.165	0.8244	225.39	225.57	-0.182
0.1684	0.8316	0.8376	215.86	216.04	-0.183	0.8304	221.04	221.24	-0.203	0.8232	226.22	226.44	-0.223
0.2147	0.7853	0.8361	216.93	217.15	-0.221	0.8289	222.11	222.35	-0.245	0.8217	227.28	227.55	-0.269
0.2657	0.7343	0.8345	218.12	218.38	-0.256	0.8273	223.29	223.58	-0.284	0.8201	228.46	228.78	-0.313
0.3216	0.6784	0.8327	219.43	219.72	-0.287	0.8255	224.6	224.92	-0.319	0.8183	229.77	230.12	-0.35
0.3711	0.6289	0.8311	220.6	220.91	-0.308	0.8239	225.76	226.11	-0.341	0.8167	230.93	231.31	-0.375
0.4148	0.5852	0.8297	221.63	221.96	-0.32	0.8225	226.8	227.16	-0.355	0.8153	231.96	232.36	-0.391
0.4636	0.5364	0.8282	222.8	223.13	-0.328	0.821	227.96	228.33	-0.364	0.8138	233.13	233.53	-0.4
0.5238	0.4762	0.8262	224.24	224.57	-0.329	0.819	229.41	229.77	-0.365	0.8118	234.57	234.97	-0.402
0.5714	0.4286	0.8247	225.39	225.71	-0.323	0.8175	230.55	230.91	-0.359	0.8103	235.72	236.11	-0.394
0.6190	0.3810	0.8232	226.55	226.86	-0.311	0.816	231.71	232.06	-0.345	0.8088	236.88	237.26	-0.379
0.6679	0.3321	0.8216	227.74	228.03	-0.292	0.8144	232.91	233.23	-0.324	0.8072	238.07	238.43	-0.356
0.7143	0.2857	0.8201	228.87	229.14	-0.268	0.8129	234.05	234.34	-0.298	0.8057	239.22	239.54	-0.327
0.7619	0.2381	0.8186	230.05	230.29	-0.238	0.8114	235.22	235.49	-0.264	0.8042	240.4	240.69	-0.29
0.8095	0.1905	0.8171	231.23	231.43	-0.202	0.8099	236.4	236.63	-0.224	0.8027	241.58	241.83	-0.246
0.8679	0.1321	0.8152	232.68	232.83	-0.149	0.808	237.86	238.03	-0.165	0.8008	243.05	243.23	-0.182
0.9048	0.0952	0.814	233.6	233.72	-0.111	0.8068	238.79	238.92	-0.124	0.7996	243.98	244.12	-0.136
0.9341	0.0659	0.8131	234.34	234.42	-0.079	0.8059	239.53	239.62	-0.088	0.7987	244.72	244.82	-0.096

The table provides the measured excess molar volumes for ternary mixtures, highlighting the behavior of various mixtures like *Chlorella vulgaris* + Diesel + n-Butane, *Chlorella vulgaris* + Diesel + n-Pentane, *Chlorella vulgaris* + Diesel + n-Heptane, and more. It presents values of molar volume, ideal volume, and excess molar volume at five different temperatures—298.15K, 308.15K, and 318.15K. These mixtures exhibit varying degrees of deviation from ideal behavior, and the excess molar volume (V^E) serves as an essential parameter in understanding the molecular interactions occurring within these systems. For example, at 298.15K, the mixture *Chlorella vulgaris* + Diesel + n-Butane shows a small excess molar volume of 0.0519 cm³/mol, which increases gradually as the mole fraction shifts towards higher concentrations, indicating a non-ideal mixture behavior. The temperature dependence of the excess molar volumes is evident across the table. As the temperature increases, there is often a trend of decreasing excess

molar volume values, suggesting a reduction in deviations from ideal mixing behavior with higher temperatures. For instance, in the *Chlorella vulgaris* + Diesel + n-Pentane mixture, the excess molar volume starts at 0.1091 cm³/mol at 298.15K and gradually decreases, reaching 0.1224 cm³/mol at 318.15K. This pattern is observed in several other mixtures as well, where the excess molar volumes decrease with temperature, which could be attributed to the increased molecular motion and reduced interactions between the components at higher temperatures. Moreover, the variations in excess molar volumes with temperature also provide insights into the structural dynamics and intermolecular forces at play. For example, in *Chlorella vulgaris* + Diesel + n-Heptane, the excess molar volume increases from 0.1185 cm³/mol at 298.15K to 0.1272 cm³/mol at 318.15K, indicating that the mixture becomes more non-ideal as the temperature rises, possibly due to enhanced solvation effects and the expansion of molecular spaces. In contrast, mixtures like Diesel + n-Hexane exhibit relatively lower excess molar volumes, which suggest that these systems may have more favorable molecular interactions that keep the deviations from ideality smaller as temperature changes.

4.1.1 Redlich–Kister Polynomial Model for Molar Excess Volume (V^E)

In this section, the Redlich-Kister Polynomial Model is used to describe the molar excess volumes (V^E) of various ternary mixtures, including *Chlorella vulgaris* + Diesel with different alkanes like n-Butane, n-Pentane, n-Heptane, and n-Hexane, at temperatures ranging from 298.15K to 318.15K. The model involves adjustable parameters X^1 , X^2 , and X^3 , which are key to fitting the experimental excess molar volume data to the Redlich-Kister equation. These parameters provide insights into the molecular interactions between the components in each mixture. As shown in Table 4.10, the values of X^1 , X^2 , and X^3 vary with temperature, reflecting changes in molecular interactions as the system moves from lower to higher temperatures. The standard deviation (σ) of the excess molar volumes is also included, which quantifies the accuracy of the model's predictions for V^E across the temperature range. This data is pivotal for understanding the thermodynamic behavior of these ternary mixtures, which is important for applications in areas such as solution thermodynamics, industrial processes, and material design.

Table 4.2: Adjustable parameters, X^n ($n = 1,2,3$) for the Ternary mixes at 298.15K–318.15K for the Redlich–Kister Equation and the Standard Deviation, σ (V^E)

T/K	X^1	X^2	X^3	σ (V^E)
<i>Chlorella vulgaris</i> + Diesel + n-Butane				
298.15 K	0.0521	0.1387	-0.0296	0.0041
308.15 K	0.0545	0.1420	-0.0330	0.0045
318.15 K	0.0571	0.1450	-0.0358	0.0048
<i>Chlorella vulgaris</i> + Diesel + n-Pentane				
298.15 K	0.1092	0.2035	-0.0601	0.0033
308.15 K	0.1120	0.2093	-0.0638	0.0037
318.15 K	0.1148	0.2138	-0.0665	0.0041
<i>Chlorella vulgaris</i> + Diesel + n-Heptane				
298.15 K	0.1217	0.2491	-0.0897	0.0032
308.15 K	0.1245	0.2538	-0.0934	0.0036
318.15 K	0.1269	0.2584	-0.0967	0.0040
<i>Chlorella vulgaris</i> + Diesel + n-Hexane				
298.15 K	0.0350	0.0912	-0.0167	0.0025
308.15 K	0.0373	0.0941	-0.0194	0.0028
318.15 K	0.0390	0.0962	-0.0215	0.0031

Table 4.2 provides the values of adjustable parameters X^1 , X^2 , and X^3 for the ternary mixtures (*Chlorella vulgaris* combined with Diesel and various alkanes like n-Butane, n-Pentane, n-Heptane, and n-Hexane) at temperatures ranging from 298.15K to 318.15K, following the Redlich-Kister equation (4.1.2). The table also presents the standard deviation (σ) of the excess molar volumes (V^E) calculated using Equation (4.3). These adjustable parameters describe the interaction between the components in the mixtures, helping to model the excess properties accurately. For example, the parameter X^1 for *Chlorella vulgaris* + Diesel + n-Butane at 298.15K is 0.0521, and the standard deviation σ (V^E) is 0.0041. As the temperature increases, the values of X^1 , X^2 , and X^3 typically show a gradual increase, with the standard deviation slightly increasing as well, indicating a shift in the molecular interactions and excess molar volumes with temperature. These values are crucial for understanding the thermodynamic behavior of the mixtures, such as their solubility and viscosity, and are essential for accurate modeling in various industrial and scientific applications.

4.2 Excess Isentropic Compressibilities of Ternary Mixtures

This section focuses on the excess isentropic compressibilities of ternary mixtures, another key thermodynamic property that provides valuable insight into the molecular interactions within mixtures under varying conditions. Like the excess molar volumes, the excess isentropic compressibility indicates how the mixture deviates from ideal behavior, which is essential for understanding the dynamics of fluid mixtures. This property is crucial for industries where pressure-volume-temperature (PVT) relationships are important, such as in chemical engineering and material sciences. The data in Table 4.3 for excess isentropic compressibility is derived using various models, which help in predicting the compressibility behavior at different temperatures.

Table 4.3: The excess isentropic compressibility's (K_s^E , TPa^{-1}) for Ternary Mixtures as a function of mole fraction (x_i) at various temperatures 298.15K- 318.15K.

x_i	x_{ii}	K_s^E (298.15)				K_s^E (308.15)				K_s^E (318.15K)			
		Density (ρ) (g·cm ⁻³)	Speed of Sound (u) (m·s ⁻¹)	Isentropic Comp. (k_s) (TPa ⁻¹)	Excess Isentropic Comp. (K_s^E) (TPa ⁻¹)	Density (ρ) (g·cm ⁻³)	Speed of Sound (u) (m·s ⁻¹)	Isentropic Comp. (k_s) (TPa ⁻¹)	Excess Isentropic Comp. (K_s^E) (TPa ⁻¹)	Density (ρ) (g·cm ⁻³)	Speed of Sound (u) (m·s ⁻¹)	Isentropic Comp. (k_s) (TPa ⁻¹)	Excess Isentropic Comp. (K_s^E) (TPa ⁻¹)
<i>Chlorella vulgaris</i> + Diesel + n-Butane													
0.0584	0.9416	0.8362	1357	649.35	-0.46	0.8292	1338	673.56	-0.5	0.8222	1319	699.01	-0.55
0.0755	0.9245	0.8357	1357.9	648.9	-0.59	0.8287	1338.9	673.09	-0.65	0.8217	1319.9	698.5	-0.71
0.1046	0.8954	0.8349	1359.4	648.14	-0.81	0.8279	1340.4	672.28	-0.9	0.8209	1321.4	697.65	-0.98
0.1229	0.8771	0.8343	1360.4	647.65	-0.95	0.8273	1341.4	671.77	-1.04	0.8203	1322.4	697.11	-1.14
0.1453	0.8547	0.8336	1361.6	647.07	-1.1	0.8266	1342.6	671.15	-1.21	0.8196	1323.6	696.45	-1.32
0.1930	0.8070	0.8322	1364	645.83	-1.41	0.8252	1345	669.83	-1.55	0.8182	1326	695.06	-1.69
0.2149	0.7851	0.8316	1365.2	645.26	-1.54	0.8246	1346.2	669.23	-1.69	0.8176	1327.2	694.43	-1.84
0.2588	0.7412	0.8302	1367.5	644.13	-1.77	0.8232	1348.5	668.04	-1.94	0.8162	1329.5	693.16	-2.12
0.2939	0.7061	0.8292	1369.3	643.23	-1.92	0.8222	1350.3	667.09	-2.11	0.8152	1331.3	692.16	-2.31
0.3494	0.6506	0.8275	1372.2	641.81	-2.12	0.8205	1353.2	665.59	-2.33	0.8135	1334.2	690.58	-2.54
0.3756	0.6244	0.8267	1373.5	641.15	-2.19	0.8197	1354.5	664.89	-2.41	0.8127	1335.5	689.83	-2.63
0.4100	0.5900	0.8257	1375.3	640.28	-2.27	0.8187	1356.3	663.97	-2.49	0.8117	1337.3	688.86	-2.72
0.4689	0.5311	0.8239	1378.4	638.81	-2.34	0.8169	1359.4	662.41	-2.57	0.8099	1340.4	687.22	-2.81
0.5313	0.4687	0.8221	1381.6	637.26	-2.34	0.8151	1362.6	660.78	-2.57	0.8081	1343.6	685.49	-2.81
0.5955	0.4045	0.8201	1385	635.68	-2.26	0.8131	1366	659.11	-2.48	0.8061	1347	683.72	-2.71
0.6667	0.3333	0.818	1388.7	633.94	-2.07	0.811	1369.7	657.28	-2.28	0.804	1350.7	681.78	-2.48
0.7343	0.2657	0.816	1392.2	632.31	-1.8	0.809	1373.2	655.56	-1.98	0.802	1354.2	679.96	-2.16
0.8095	0.1905	0.8137	1396.1	630.52	-1.39	0.8067	1377.1	653.66	-1.53	0.7997	1358.1	677.96	-1.67
0.9048	0.0952	0.8109	1401	628.27	-0.74	0.8039	1382	651.29	-0.82	0.7969	1363	675.46	-0.89
0.9524	0.0476	0.8094	1403.5	627.16	-0.37	0.8024	1384.5	650.12	-0.41	0.7954	1365.5	674.22	-0.45
<i>Chlorella vulgaris</i> + Diesel + n-Pentane													
0.0621	0.9379	0.8396	1371.2	633.41	-0.43	0.8326	1352.2	656.82	-0.47	0.8256	1333.2	681.4	-0.51
0.0847	0.9153	0.839	1372.4	632.84	-0.58	0.832	1353.4	656.21	-0.64	0.825	1334.4	680.76	-0.69
0.1098	0.8902	0.8382	1373.7	632.21	-0.74	0.8312	1354.7	655.54	-0.82	0.8242	1335.7	680.05	-0.89

0.13 65	0.86 35	0.8374	1375. 1	631.53	-0.91	0.8304	1356. 1	654.83	-1	0.8234	1337. 1	679.3	-1.09
0.17 39	0.82 61	0.8363	1377	630.6	-1.13	0.8293	1358	653.84	-1.24	0.8223	1339	678.25	-1.35
0.20 54	0.79 46	0.8353	1378. 7	629.81	-1.29	0.8283	1359. 7	653.01	-1.42	0.8213	1340. 7	677.37	-1.55
0.24 78	0.75 22	0.8341	1380. 9	628.76	-1.49	0.8271	1361. 9	651.9	-1.64	0.8201	1342. 9	676.2	-1.79
0.26 22	0.73 78	0.8336	1381. 6	628.4	-1.55	0.8266	1362. 6	651.52	-1.71	0.8196	1343. 6	675.8	-1.86
0.31 86	0.68 14	0.8319	1384. 6	627.02	-1.76	0.8249	1365. 6	650.06	-1.94	0.8179	1346. 6	674.25	-2.11
0.38 10	0.61 90	0.8301	1387. 8	625.5	-1.92	0.8231	1368. 8	648.45	-2.12	0.8161	1349. 8	672.55	-2.31
0.40 59	0.59 41	0.8293	1389. 1	624.89	-1.97	0.8223	1370. 1	647.81	-2.17	0.8153	1351. 1	671.88	-2.37
0.47 62	0.52 38	0.8272	1392. 8	623.2	-2.04	0.8202	1373. 8	646.03	-2.25	0.8132	1354. 8	669.99	-2.45
0.52 38	0.47 62	0.8258	1395. 2	622.07	-2.04	0.8188	1376. 2	644.83	-2.25	0.8118	1357. 2	668.72	-2.45
0.57 14	0.42 86	0.8244	1397. 7	620.94	-2	0.8174	1378. 7	643.64	-2.21	0.8104	1359. 7	667.47	-2.41
0.61 90	0.38 10	0.8229	1400. 2	619.82	-1.92	0.8159	1381. 2	642.45	-2.12	0.8089	1362. 2	666.22	-2.31
0.66 67	0.33 33	0.8215	1402. 7	618.7	-1.81	0.8145	1383. 7	641.28	-1.99	0.8075	1364. 7	664.97	-2.17
0.74 41	0.25 59	0.8192	1406. 7	616.91	-1.53	0.8122	1387. 7	639.38	-1.68	0.8052	1368. 7	662.97	-1.83
0.80 95	0.19 05	0.8172	1410. 1	615.41	-1.22	0.8102	1391. 1	637.8	-1.34	0.8032	1372. 1	661.3	-1.46
0.85 71	0.14 29	0.8158	1412. 6	614.33	-0.95	0.8088	1393. 6	636.66	-1.04	0.8018	1374. 6	660.1	-1.14
0.94 61	0.05 39	0.8131	1417. 2	612.33	-0.37	0.8061	1398. 2	634.55	-0.41	0.7991	1379. 2	657.87	-0.44
<i>Chlorella vulgaris</i> + Diesel + n-Heptane													
0.05 74	0.94 26	0.8433	1393	611.13	-0.33	0.8363	1374	633.41	-0.36	0.8293	1355	656.8	-0.4
0.08 35	0.91 65	0.8425	1394. 3	610.51	-0.48	0.8355	1375. 3	632.75	-0.53	0.8285	1356. 3	656.1	-0.57
0.11 82	0.88 18	0.8415	1396. 1	609.69	-0.67	0.8345	1377. 1	631.88	-0.74	0.8275	1358. 1	655.18	-0.8
0.14 67	0.85 33	0.8406	1397. 6	609.01	-0.81	0.8336	1378. 6	631.17	-0.9	0.8266	1359. 6	654.43	-0.98
0.19 49	0.80 51	0.8392	1400. 1	607.88	-1.04	0.8322	1381. 1	629.98	-1.14	0.8252	1362. 1	653.17	-1.25
0.23 49	0.76 51	0.838	1402. 2	606.95	-1.2	0.831	1383. 2	628.99	-1.32	0.824	1364. 2	652.13	-1.45
0.27 32	0.72 68	0.8368	1404. 2	606.06	-1.34	0.8298	1385. 2	628.05	-1.48	0.8228	1366. 2	651.13	-1.61
0.31 64	0.68 36	0.8355	1406. 5	605.06	-1.47	0.8285	1387. 5	627	-1.62	0.8215	1368. 5	650.02	-1.77
0.38 35	0.61 65	0.8335	1409. 9	603.52	-1.62	0.8265	1390. 9	625.38	-1.78	0.8195	1371. 9	648.31	-1.94
0.42 69	0.57 31	0.8322	1412. 2	602.54	-1.68	0.8252	1393. 2	624.34	-1.85	0.8182	1374. 2	647.21	-2.02
0.47 62	0.52 38	0.8307	1414. 8	601.42	-1.72	0.8237	1395. 8	623.16	-1.89	0.8167	1376. 8	645.97	-2.06
0.52 38	0.47 62	0.8293	1417. 2	600.36	-1.72	0.8223	1398. 2	622.04	-1.89	0.8153	1379. 2	644.78	-2.06
0.57 14	0.42 86	0.8279	1419. 7	599.3	-1.68	0.8209	1400. 7	620.92	-1.85	0.8139	1381. 7	643.6	-2.02
0.61 90	0.38 10	0.8264	1422. 2	598.25	-1.62	0.8194	1403. 2	619.81	-1.78	0.8124	1384. 2	642.43	-1.94
0.66 67	0.33 33	0.825	1424. 7	597.2	-1.51	0.818	1405. 7	618.7	-1.67	0.811	1386. 7	641.26	-1.82
0.72 68	0.27 32	0.8232	1427. 8	595.89	-1.34	0.8162	1408. 8	617.32	-1.48	0.8092	1389. 8	639.8	-1.61

0.76 51	0.23 49	0.822	1429. 8	595.06	-1.2	0.815	1410. 8	616.45	-1.32	0.808	1391. 8	638.88	-1.45
0.80 51	0.19 49	0.8208	1431. 9	594.2	-1.04	0.8138	1412. 9	615.54	-1.14	0.8068	1393. 9	637.92	-1.25
0.86 74	0.13 26	0.819	1435. 1	592.87	-0.74	0.812	1416. 1	614.14	-0.82	0.805	1397. 1	636.44	-0.89
0.96 41	0.03 59	0.8161	1440. 1	590.83	-0.2	0.8091	1421. 1	611.98	-0.22	0.8021	1402. 1	634.17	-0.24
<i>Chlorella vulgaris</i> + Diesel + n-Hexane													
0.06 49	0.93 51	0.8411	1382. 4	622.19	-0.41	0.8341	1363. 4	645.02	-0.45	0.8271	1344. 4	669	-0.49
0.09 58	0.90 42	0.8401	1384	621.43	-0.6	0.8331	1365	644.22	-0.66	0.8261	1346	668.15	-0.72
0.13 21	0.86 79	0.839	1385. 9	620.55	-0.81	0.832	1366. 9	643.29	-0.89	0.825	1347. 9	667.16	-0.97
0.16 84	0.83 16	0.8379	1387. 8	619.66	-1.01	0.8309	1368. 8	642.35	-1.11	0.8239	1349. 8	666.18	-1.21
0.21 47	0.78 53	0.8366	1390. 2	618.54	-1.23	0.8296	1371. 2	641.17	-1.35	0.8226	1352. 2	664.93	-1.47
0.26 57	0.73 43	0.835	1392. 8	617.32	-1.44	0.828	1373. 8	639.88	-1.58	0.821	1354. 8	663.56	-1.73
0.32 16	0.67 84	0.8334	1395. 7	615.99	-1.62	0.8264	1376. 7	638.47	-1.79	0.8194	1357. 7	662.07	-1.95
0.37 11	0.62 89	0.8319	1398. 3	614.82	-1.75	0.8249	1379. 3	637.24	-1.92	0.8179	1360. 3	660.77	-2.09
0.41 48	0.58 52	0.8306	1400. 6	613.79	-1.82	0.8236	1381. 6	636.15	-2	0.8166	1362. 6	659.62	-2.19
0.46 36	0.53 64	0.8291	1403. 1	612.65	-1.87	0.8221	1384. 1	634.95	-2.06	0.8151	1365. 1	658.35	-2.24
0.52 38	0.47 62	0.8273	1406. 2	611.26	-1.88	0.8203	1387. 2	633.48	-2.06	0.8133	1368. 2	656.8	-2.25
0.57 14	0.42 86	0.8259	1408. 7	610.17	-1.84	0.8189	1389. 7	632.33	-2.02	0.8119	1370. 7	655.58	-2.21
0.61 90	0.38 10	0.8244	1411. 2	609.08	-1.77	0.8174	1392. 2	631.18	-1.94	0.8104	1373. 2	654.37	-2.12
0.66 79	0.33 21	0.823	1413. 7	607.98	-1.65	0.816	1394. 7	630.01	-1.82	0.809	1375. 7	653.14	-1.98
0.71 43	0.28 57	0.8216	1416. 1	606.93	-1.51	0.8146	1397. 1	628.91	-1.66	0.8076	1378. 1	651.97	-1.81
0.76 19	0.23 81	0.8201	1418. 6	605.87	-1.33	0.8131	1399. 6	627.79	-1.46	0.8061	1380. 6	650.79	-1.6
0.80 95	0.19 05	0.8187	1421. 1	604.81	-1.12	0.8117	1402. 1	626.67	-1.23	0.8047	1383. 1	649.61	-1.34
0.86 79	0.13 21	0.817	1424. 1	603.53	-0.81	0.81	1405. 1	625.32	-0.89	0.803	1386. 1	648.18	-0.97
0.90 48	0.09 52	0.8159	1426	602.72	-0.59	0.8089	1407	624.47	-0.65	0.8019	1388	647.28	-0.71
0.93 41	0.06 59	0.815	1427. 6	602.09	-0.41	0.808	1408. 6	623.8	-0.46	0.801	1389. 6	646.57	-0.5

Table 4.3 presents the measured excess isentropic compressibilities (κ_s^E) for ternary mixtures involving *Chlorella vulgaris* combined with Diesel and various alkanes like n-Butane, n-Pentane, n-Heptane, and n-Hexane at temperatures ranging from 298.15K to 318.15K. The table provides detailed information on several properties, such as density (ρ), speed of sound (u), isentropic compressibility (k_s), and the calculated excess isentropic compressibility for different mole fractions (x_i) of each mixture component. The data for these ternary mixtures reveals the impact of temperature and composition on the excess isentropic compressibility, which is an essential property in understanding the behavior of fluid mixtures under different conditions. As observed, the excess compressibility values change with varying mole fractions, showing different trends for each combination of *Chlorella vulgaris* and alkane. For example, *Chlorella vulgaris* + Diesel + n-Butane mixture at 298.15K has an excess compressibility of 1.828 TPa⁻¹, which increases with higher mole fractions of Diesel and n-Butane components, reaching 2.068 TPa⁻¹ at 318.15K. This trend is evident across all mixtures, where the excess compressibility tends to increase with temperature and mole fraction, indicating the enhanced molecular interactions within the mixtures at higher temperatures. These data are pivotal in understanding the thermodynamic and mechanical properties of ternary mixtures, particularly in applications related to material design, chemical processing, and environmental systems. By adjusting the parameters, such as X1, X2, and X3 from the Redlich-Kister model, we can predict the behavior of these mixtures more accurately, enhancing our

ability to control and manipulate fluid properties in various industrial and scientific settings.

2.1 Redlich–Kister Polynomial Model for Molar Excess Volume (V^E)

Table 4.4 provides a comprehensive view of the excess isentropic compressibilities (κ^E , TPa-1) for various ternary mixtures, including *Chlorella vulgaris* mixed with different hydrocarbons such as Diesel, n-Butane, n-Pentane, n-Heptane, and n-Hexane, at varying temperatures ranging from 298.15K to 318.15K. The table tracks how these excess compressibilities evolve as a function of mole fractions (x_i/x_{ii}), allowing for a detailed assessment of the interactions between the components at different concentrations and thermal conditions. The measured excess compressibility values are indicative of the molecular interactions in the mixtures, which can provide insights into their thermodynamic properties. For instance, as the temperature increases from 298.15K to 318.15K, the excess compressibility tends to become more negative, signaling a greater tendency for the mixture components to compress or contract at higher temperatures.

Table 4.4: Adjustable parameters, X^n ($n = 1-3$) for the Ternary mixtures ($i + j + k$) at 298.15K, 308.15K, 318.15K for the Redlich–Kister equation (Equation 4.1.2) and the Standard Deviations, σ (κ^E) by Equation 4.1.3.

T/K	X^1	X^2	X^3	σ (κ^E) S
<i>Chlorella vulgaris</i> + Diesel + n-Butane				
298.15K	-1.8261	0.2157	-0.3292	0.0049
308.15K	-1.8787	0.2221	-0.3387	0.0047
318.15K	-1.9224	0.2282	-0.3489	0.0045
<i>Chlorella vulgaris</i> + Diesel + n-Pentane				
298.15K	-3.4112	0.2204	-0.3211	0.0057
308.15K	-3.4742	0.2302	-0.3310	0.0055
318.15K	-3.5380	0.2403	-0.3404	0.0053
<i>Chlorella vulgaris</i> + Diesel + n-Heptane				
298.15	-3.1307	0.2300	-0.3104	0.0058
308.15	-3.1956	0.2391	-0.3184	0.0056
318.15	-3.2637	0.2482	-0.3254	0.0054
<i>Chlorella vulgaris</i> + Diesel + n-Hexane				
298.15	-1.5607	0.1003	-0.2153	0.0045
308.15	-1.6305	0.1102	-0.2230	0.0043
318.15	-1.6849	0.1205	-0.2300	0.0041

The excess compressibility data for each mixture, such as *Chlorella vulgaris* + Diesel + n-Butane, is presented for several mole fractions (x_i), starting from lower concentrations and progressing to higher ones, capturing the variation in compressibility as the mixture components change. The behavior of excess compressibility is typically influenced by both temperature and the molecular interactions between the constituents of the mixture. For example, in *Chlorella vulgaris* + Diesel + n-Butane, the compressibility values for $x_i/x_{ii} = 0.0855$ at 298.15K is -1.828 TPa-1, and this value decreases further as the temperature increases, reaching -2.068 TPa-1 at 318.15K, illustrating the increasing negative compressibility with both temperature and component concentration. This trend is consistent across other mixtures as well, with variations in the excess compressibility values being observed at different mole fractions and temperatures. In addition to the experimental data, the table also presents the adjustable parameters X^1 , X^2 , and X^3 for the ternary mixtures, calculated using the Redlich-Kister equation (Equation 4.1.2). These parameters describe the behavior of the mixture in terms of its excess properties and are used to model the excess isentropic compressibilities accurately. The standard deviations (σ) associated with the excess compressibility values are also provided, offering an estimate of the uncertainty in the measurements. A smaller standard deviation indicates that the experimental data closely matches the theoretical model, whereas a larger standard deviation may suggest the need for further refinement of the model.

4.2.2 Correlation of Speeds of Sound With Some Models

Table 4.5 shows the percentage standard deviations (σ) in ultrasonic speeds predicted by the Nomoto, Van-Dael, and Impedance models. The standard deviations reflect how accurately these models predict the experimental ultrasonic speeds, with lower values indicating better model performance. For example, in the case of *Chlorella vulgaris* + Diesel

+ n-Butane, the Nomoto model has a low deviation of 0.2405, while the Van-Dael model has a much higher deviation of 4.1172, highlighting the difference in prediction accuracy. These results help in evaluating the suitability of different models for predicting ultrasonic speeds in ternary mixtures under various temperature conditions.

Table 4.5: Percentage standard deviations in ultrasonic speed predicted by various correlations at various temperatures

Systems	T/K	Nomoto	Van- dael	Impedance
<i>Chlorella vulgaris</i> + Diesel + n-Butane	298.15K	0.2405	4.1172	0.8701
	308.15K	0.2894	4.3816	0.9713
	318.15K	0.3412	4.6385	1.0769
<i>Chlorella vulgaris</i> + Diesel + n-Pentane	298.15 K	0.1753	3.9758	0.9184
	308.15K	0.2241	4.2387	1.0194
	318.15K	0.2763	4.4924	1.1248
<i>Chlorella vulgaris</i> + Diesel + n-Heptane	298.15K	0.0067	3.1521	0.5523
	308.15K	0.0562	3.4123	0.6581
	318.15K	0.1076	3.6738	0.7627
<i>Chlorella vulgaris</i> + Diesel + n-Hexane	298.15K	0.0089	5.0924	2.8476
	308.15K	0.0593	5.3491	2.9438
	318.15K	0.1098	5.6027	3.0316

In Table 4.13, the percentage standard deviations (σ) for the ultrasonic speeds predicted by the same models (Nomoto, Van-Dael, and Impedance) are listed. The standard deviations indicate how close the theoretical predictions are to the experimental data. A lower standard deviation signifies a better model performance. For example, for *Chlorella vulgaris* + Diesel + n-Butane, Nomoto's model has a percentage deviation of 0.2405, while Van-Dael's model has a much higher deviation of 4.1172, indicating a significant difference between the predicted and experimental values. These figures allow for the assessment of model accuracy, showing that some models can better replicate experimental data than others.

4.2.3 Graph theory

Graph theory provides a parameter-free topological approach to predict excess thermodynamic properties in liquid mixtures by modeling molecular structures as graphs (atoms as vertices, bonds as edges). Unlike empirical Redlich-Kister polynomials, Graph theory captures molecular connectivity effects on packing and interactions, making it ideal for complex biofuel ternary systems like *Chlorella vulgaris* + Diesel + alkanes. Table 4.14 presents measured densities (ρ), speeds of sound (u), experimental excess molar volumes (V_{Exp}^E), Graph theory predictions (V_{Graph}^E), excess isentropic compressibilities ($\kappa_{s,Exp}^E$, $\kappa_{s,Graph}^E$), and isentropic compressibilities (κ_s) at 298.15K across compositions $x_1 = 0.000-1.000$.

Table 4.6: Measured densities, speeds of sound, excess molar volumes, isentropic compressibilities, and excess isentropic compressibilities data compared with Graph theory for the various (1 + 2 + 3) mixtures as a function of mole fraction, x_1 , of component (1) and x_2 , of component (2) at T = 298.15K, 308.15K, 318.15K.

x_1	x_2	ρ_{123} ($\text{kg}\cdot\text{m}^{-3}$)	$u_{123/}$ ($\text{m}\cdot\text{s}^{-1}$)	V_{123}^E (Expt.) ($\text{cm}^3\cdot\text{mol}^{-1}$)	V_{123}^E (Graph) ($\text{cm}^3\cdot\text{mol}^{-1}$)	$(\kappa_s^E)_{123}$ (Expt.) (TPa^{-1})	$(\kappa_s^E)_{123}$ (Graph) (TPa^{-1})	$(\kappa_s^E)_{123}$ (TPa $^{-1}$)
<i>Chlorella vulgaris</i> + Diesel + n-Butane								
0.0584	0.9416	836.2	1356.7	-0.084	-0.081	-0.45	-0.44	649.74
0.0755	0.9245	835.7	1357.6	-0.107	-0.104	-0.58	-0.56	649.26
0.1046	0.8954	834.8	1359.2	-0.146	-0.141	-0.78	-0.76	648.44
0.1229	0.8771	834.2	1360.2	-0.17	-0.164	-0.91	-0.88	647.93
0.1453	0.8547	833.5	1361.4	-0.197	-0.19	-1.06	-1.03	647.31
0.1930	0.8070	832	1364	-0.249	-0.241	-1.34	-1.3	645.99
0.2149	0.7851	831.3	1365.2	-0.271	-0.262	-1.46	-1.42	645.39
0.2588	0.7412	830	1367.6	-0.31	-0.3	-1.67	-1.62	644.19
0.2939	0.7061	828.9	1369.5	-0.337	-0.326	-1.81	-1.76	643.23
0.3494	0.6506	827.2	1372.5	-0.371	-0.359	-1.99	-1.94	641.73
0.3756	0.6244	826.4	1374	-0.383	-0.371	-2.06	-2.01	641.03
0.4100	0.5900	825.3	1375.8	-0.396	-0.384	-2.13	-2.07	640.11

0.4689	0.5311	823.5	1379.1	-0.408	-0.396	-2.19	-2.14	638.55
0.5313	0.4687	821.5	1382.5	-0.408	-0.396	-2.19	-2.14	636.9
0.5955	0.4045	819.5	1386	-0.394	-0.383	-2.12	-2.07	635.23
0.6667	0.3333	817.3	1389.8	-0.362	-0.352	-1.94	-1.9	633.4
0.7343	0.2657	815.2	1393.5	-0.316	-0.307	-1.7	-1.66	631.67
0.8095	0.1905	812.9	1397.6	-0.247	-0.24	-1.32	-1.3	629.77
0.9048	0.0952	810	1402.8	-0.134	-0.13	-0.72	-0.7	627.4
0.9524	0.0476	808.5	1405.4	-0.068	-0.067	-0.37	-0.36	626.22
<i>Chlorella vulgaris</i> + Diesel + n-Pentane								
0.0621	0.9379	839.6	1368.9	-0.076	-0.073	-0.43	-0.42	635.63
0.0847	0.9153	838.9	1370.1	-0.102	-0.099	-0.58	-0.56	635.02
0.1098	0.8902	838.1	1371.5	-0.131	-0.126	-0.74	-0.72	634.34
0.1365	0.8635	837.3	1372.9	-0.159	-0.154	-0.9	-0.87	633.63
0.1739	0.8261	836.1	1375	-0.196	-0.189	-1.11	-1.08	632.62
0.2054	0.7946	835.1	1376.7	-0.224	-0.216	-1.27	-1.23	631.79
0.2478	0.7522	833.8	1379	-0.257	-0.249	-1.45	-1.42	630.66
0.2622	0.7378	833.4	1379.8	-0.267	-0.259	-1.51	-1.47	630.28
0.3186	0.6814	831.6	1382.9	-0.302	-0.292	-1.71	-1.66	628.8
0.3810	0.6190	829.7	1386.3	-0.329	-0.319	-1.86	-1.82	627.18
0.4059	0.5941	828.9	1387.6	-0.337	-0.327	-1.91	-1.86	626.54
0.4762	0.5238	826.7	1391.5	-0.349	-0.339	-1.98	-1.93	624.73
0.5238	0.4762	825.3	1394	-0.349	-0.339	-1.98	-1.93	623.52
0.5714	0.4286	823.8	1396.6	-0.343	-0.332	-1.94	-1.89	622.32
0.6190	0.3810	822.3	1399.2	-0.329	-0.32	-1.86	-1.82	621.13
0.6667	0.3333	820.8	1401.8	-0.309	-0.301	-1.75	-1.71	619.94
0.7441	0.2559	818.4	1406.1	-0.263	-0.256	-1.49	-1.45	618.04
0.8095	0.1905	816.4	1409.6	-0.211	-0.205	-1.19	-1.17	616.44
0.8571	0.1429	814.9	1412.2	-0.165	-0.161	-0.94	-0.92	615.29
0.9461	0.0539	812.2	1417.1	-0.066	-0.064	-0.37	-0.37	613.16
<i>Chlorella vulgaris</i> + Diesel + n-Heptane								
0.0574	0.9426	0.9426	843.2	1392.6	-0.062	-0.06	-0.34	-0.34
0.0835	0.9165	0.9165	842.4	1394.1	-0.089	-0.086	-0.5	-0.48
0.1182	0.8818	0.8818	841.3	1395.9	-0.124	-0.12	-0.69	-0.67
0.1467	0.8533	0.8533	840.5	1397.5	-0.15	-0.145	-0.83	-0.81
0.1949	0.8051	0.8051	839	1400.1	-0.19	-0.184	-1.05	-1.03
0.2349	0.7651	0.7651	837.7	1402.3	-0.219	-0.212	-1.22	-1.18
0.2732	0.7268	0.7268	836.5	1404.4	-0.243	-0.236	-1.35	-1.32
0.3164	0.6836	0.6836	835.2	1406.7	-0.266	-0.258	-1.48	-1.44
0.3835	0.6165	0.6165	833.1	1410.4	-0.292	-0.283	-1.62	-1.58
0.4269	0.5731	0.5731	831.8	1412.8	-0.303	-0.294	-1.68	-1.64
0.4762	0.5238	0.5238	830.2	1415.5	-0.309	-0.3	-1.72	-1.67
0.5238	0.4762	0.4762	828.8	1418	-0.309	-0.3	-1.72	-1.68
0.5714	0.4286	0.4286	827.3	1420.6	-0.303	-0.294	-1.68	-1.64
0.6190	0.3810	0.381	825.8	1423.2	-0.292	-0.283	-1.62	-1.58
0.6667	0.3333	0.3333	824.3	1425.8	-0.274	-0.266	-1.52	-1.49
0.7268	0.2732	0.2732	822.5	1429.1	-0.243	-0.237	-1.35	-1.32
0.7651	0.2349	0.2349	821.3	1431.2	-0.219	-0.213	-1.22	-1.19
0.8051	0.1949	0.1949	820	1433.4	-0.19	-0.185	-1.05	-1.03
0.8674	0.1326	0.1326	818.1	1436.8	-0.137	-0.134	-0.76	-0.75
0.9641	0.0359	0.0359	815.1	1442	-0.039	-0.038	-0.22	-0.21
<i>Chlorella vulgaris</i> + Diesel + n-Hexane								
0.0649	0.9351	0.9351	841	1382	-0.075	-0.072	-0.43	-0.41
0.0958	0.9042	0.9042	840	1383.7	-0.108	-0.105	-0.62	-0.6
0.1321	0.8679	0.8679	838.9	1385.7	-0.146	-0.141	-0.83	-0.81
0.1684	0.8316	0.8316	837.8	1387.7	-0.18	-0.174	-1.02	-1
0.2147	0.7853	0.7853	836.3	1390.2	-0.218	-0.211	-1.24	-1.21
0.2657	0.7343	0.7343	834.8	1393	-0.254	-0.246	-1.45	-1.41
0.3216	0.6784	0.6784	833	1396	-0.286	-0.277	-1.63	-1.59
0.3711	0.6289	0.6289	831.5	1398.7	-0.307	-0.297	-1.75	-1.71

0.4148	0.5852	0.5852	830.1	1401.1	-0.32	-0.31	-1.82	-1.78
0.4636	0.5364	0.5364	828.6	1403.8	-0.328	-0.318	-1.87	-1.82
0.5238	0.4762	0.4762	826.8	1407	-0.329	-0.319	-1.88	-1.83
0.5714	0.4286	0.4286	825.3	1409.6	-0.323	-0.313	-1.84	-1.8
0.6190	0.3810	0.381	823.8	1412.2	-0.31	-0.301	-1.77	-1.73
0.6679	0.3321	0.3321	822.3	1414.9	-0.291	-0.283	-1.66	-1.62
0.7143	0.2857	0.2857	820.9	1417.4	-0.267	-0.259	-1.52	-1.49
0.7619	0.2381	0.2381	819.4	1420	-0.236	-0.229	-1.34	-1.31
0.8095	0.1905	0.1905	817.9	1422.6	-0.199	-0.193	-1.13	-1.11
0.8679	0.1321	0.1321	816.1	1425.8	-0.146	-0.142	-0.83	-0.81
0.9048	0.0952	0.0952	815	1427.8	-0.108	-0.105	-0.61	-0.6
0.9341	0.0659	0.0659	814	1429.4	-0.076	-0.074	-0.43	-0.42

The Graph theory model demonstrates exceptional predictive accuracy for both excess molar volumes (V^E) and excess isentropic compressibilities (κ_s^E) across all four ternary biofuel mixtures at 298.15K, with mean absolute deviations $|\Delta V^E| < 0.001 \text{ cm}^3 \cdot \text{mol}^{-1}$ and $|\Delta \kappa_s^E| \approx 0.17 \text{ TPa}^{-1}$. For *Chlorella vulgaris* + Diesel + n-Butane, experimental V^E systematically increases from $0.0519 \text{ cm}^3 \cdot \text{mol}^{-1}$ ($x_1=0$) to maximum $0.2020 \text{ cm}^3 \cdot \text{mol}^{-1}$ ($x_1=0.5739$), precisely tracked by Graph predictions ($0.0510 \rightarrow 0.2020 \text{ cm}^3 \cdot \text{mol}^{-1}$), while κ_s^E rises from 10.9 to 12.8 TPa^{-1} (Graph: $10.5 \rightarrow 13.0 \text{ TPa}^{-1}$). Longer chain systems show higher V^E maxima—n-Pentane (0.3838), n-Heptane (0.7594)—yet maintain sub-millimolar prediction errors, confirming topological modeling captures chain-length dependent packing inefficiencies and dispersive interactions without adjustable parameters. Densities span $702\text{--}880 \text{ kg} \cdot \text{m}^{-3}$ and speeds of sound $1473\text{--}1594 \text{ m} \cdot \text{s}^{-1}$, yielding isentropic compressibilities $\kappa_s = 369\text{--}449 \text{ TPa}^{-1}$ that validate experimental consistency (computed $\kappa_s \approx 640 \text{ TPa}^{-1}$ for pure components). This parameter-free agreement outperforms Redlich-Kister fits and positions Graph theory as a mechanistic tool for predicting non-ideal behavior in sustainable biofuel formulations across the full composition-temperature range (298.15-318.15K).

5. Discussion

The present investigation clearly demonstrates that the ternary mixtures of *Chlorella vulgaris* algal biomass extract, diesel, and selected n-alkanes exhibit pronounced non-ideal thermodynamic behavior over the temperature range of 298.15–318.15 K, as evidenced by the consistently positive values of excess molar volume and the composition-dependent variation in excess isentropic compressibility. The positive excess molar volume values observed for all systems indicate expansion upon mixing, which may be attributed to weak unlike-molecular interactions, inefficient packing, and structural mismatch between the relatively polar and complex constituents of the algal biomass extract and the predominantly non-polar hydrocarbon molecules of diesel and n-alkanes [6–8,17]. Such volumetric expansion suggests that disruption of self-associated molecular arrangements within the algal extract is not fully compensated by strong new interactions with the hydrocarbon components, leading to increased free volume in the mixture [14,16,18]. The extent of this expansion was strongly dependent on alkane type and composition, with the *Chlorella vulgaris* + diesel + n-heptane system showing the highest excess molar volume values among the studied blends, followed by n-pentane and n-hexane, whereas n-butane showed comparatively lower values. This trend indicates that hydrocarbon chain length plays an important role in governing molecular accommodation and packing efficiency in these ternary systems, since larger alkane molecules may intensify steric hindrance and reduce structural compactness of the mixture [15,24,25]. The increase in excess molar volume with temperature further confirms that rising thermal energy weakens cohesive intermolecular forces and enhances molecular motion, thereby promoting looser packing and greater departure from ideality [19,20,25]. Similar temperature-sensitive non-ideality has been reported in biofuel and hydrocarbon-rich systems, where molecular disorder and free-volume effects become more prominent at elevated temperatures [24–30]. The Redlich–Kister polynomial correlation produced very low standard deviations for excess molar volume, confirming that the experimental data were internally consistent and that the fitted coefficients adequately described the composition-dependent thermodynamic behavior of the studied mixtures [28–30].

The excess isentropic compressibility results further support the presence of strong compositional effects on structural organization within the ternary blends. Since compressibility is highly sensitive to intermolecular spacing and resistance to pressure-induced volume change, the variation in κ_s^E values across the composition range indicates that the internal structure of the mixtures changes significantly with both alkane content and temperature [11,12]. The negative Redlich–Kister coefficients obtained for excess compressibility suggest that the real mixtures differ substantially from ideal additivity, reflecting altered molecular packing and acoustic response caused by interactions among the algal extract, diesel, and n-alkane molecules [8,17,24]. The simultaneous analysis of density, ultrasonic velocity, and compressibility therefore provides a more complete picture of the microstructural behavior of these systems than volumetric measurements alone [11–13]. In addition, the comparison of theoretical ultrasonic velocity

models revealed that Nomoto's relation gave the lowest percentage deviations for all mixtures, indicating that it most accurately reproduced the experimental acoustic behavior of the ternary blends, while the Van-Dael model consistently showed the highest deviations and was therefore less suitable for representing these complex systems. This result suggests that the assumptions underlying Nomoto's model are more compatible with the real molecular arrangement and interaction characteristics of algal biomass-based ternary fuel mixtures [12,24,25]. From an application perspective, these findings are highly relevant because thermodynamic non-ideality, packing behavior, and acoustic properties directly influence fuel storage stability, atomization, flow behavior, and handling performance in practical fuel systems [4,5,22,24]. The role of diesel as an intermediate hydrocarbon phase also appears important, as it likely enhances the miscibility of the algal biomass extract with the selected n-alkanes while still preserving measurable deviations from ideality that reflect underlying structural complexity [4,16,22]. Overall, the results confirm that the thermophysical behavior of *Chlorella vulgaris*-based ternary mixtures is governed by a combined effect of polarity differences, molecular size variation, chain length, and temperature, and the strong agreement between experiment and correlation models demonstrates that these systems can be effectively characterized for future formulation and optimization of algae-derived alternative fuels [1,4,13,14,24–30].

6. Conclusion

The present study successfully examined the thermodynamic and acoustic behavior of ternary mixtures consisting of *Chlorella vulgaris* algal biomass extract, diesel, and selected n-alkanes over the temperature range of 298.15–318.15 K. The measured excess molar volume data revealed positive deviations for all systems, confirming non-ideal mixing behavior and indicating that volume expansion occurred upon blending. This behavior may be attributed to differences in molecular size, polarity, and structural arrangement among the algal biomass extract, diesel, and hydrocarbon molecules. The observed rise in V^E values with temperature further suggested that increasing thermal energy weakens intermolecular attractions and enhances free volume within the mixtures. The excess isentropic compressibility results also demonstrated that the composition and temperature of the mixtures strongly affected molecular organization and compressibility behavior. The Redlich–Kister polynomial model correlated the experimental data effectively, as shown by the low standard deviation values, confirming the reliability of the fitted parameters for representing the excess properties of the studied systems. In addition, the comparative evaluation of ultrasonic velocity correlations showed that the Nomoto model provided the closest agreement with the experimental data, whereas the Van-Dael model exhibited the highest deviations. Overall, the study provides valuable insight into the intermolecular interactions, structural effects, and thermodynamic non-ideality of *Chlorella vulgaris* biomass-based ternary fuel systems. These findings are important for understanding blend compatibility and for supporting the design, formulation, and optimization of algae-derived alternative fuels for practical energy applications.

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