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THERMOPHYSICAL AND EXCESS PROPERTIES OF MICROALGAE BIODIESEL–DIESEL–ACETATE TERNARY MIXTURES: MOLECULAR INTERACTION, REDLICH–KISTER MODELING, AND THEORETICAL ANALYSIS

[1,a]Ms. Princy, [2,b]Dr. Anjali Ahlawat, [3,c]Dr. Jaibir Singh Yadav
[1]Research Scholar, [2]Supervisor, [3]Co-supervisor,
[1-2]Department of Chemistry, Baba Mast Nath University, Rohtak, Haryana, India.
[3]Department of Chemistry, A. I. Jat H. M. College, Rohtak, Haryana, India.
[a]ruhalprincy@gmail.com, [b]anjaliahlawat77@gmail.com, [c]jaichem01@gmail.com

Abstract

This study investigates the thermophysical and excess properties of ternary blends composed of Chlorella vulgaris methyl ester or Scenedesmus obliquus methyl ester, diesel, and the oxygenated additives methyl acetate and ethyl acetate at 298.15 K and 313.15 K. The objective was to understand the molecular interactions governing the behavior of these biofuel-based ternary systems through measurements of density, molar volume, speed of sound, excess molar volume (V^E), isentropic compressibility (κ_s), and excess isentropic compressibility (κ_s^E). The experimental results showed that all mixtures exhibited negative excess molar volume and negative excess isentropic compressibility over the studied composition range, indicating strong attractive interactions, closer molecular packing, and significant deviation from ideal mixing behavior. Among the investigated systems, the blends containing methyl acetate generally showed stronger contraction and lower compressibility than the corresponding ethyl acetate systems, while the Scenedesmus obliquus methyl ester blends displayed slightly stronger interaction effects than the Chlorella vulgaris methyl ester blends. The excess property data were successfully correlated using the Redlich–Kister polynomial model, with low standard deviations confirming satisfactory fitting accuracy. In addition, speed-of-sound data were compared with Nomoto, Van Dael, and impedance dependence models, where the Nomoto relation produced the lowest deviations from experimental values. A theoretical approach was also applied and showed close agreement with the experimental data, further supporting the interpretation of compact molecular organization in the ternary mixtures. Overall, the findings demonstrate that acetate-modified microalgae biodiesel–diesel blends possess significant non-ideal thermodynamic behavior and promising physicochemical characteristics, making them relevant for the design and optimization of cleaner and more efficient alternative fuel formulations.

Keywords: Microalgae biodiesel; Chlorella vulgaris methyl ester; Scenedesmus obliquus methyl ester; Excess molar volume; Excess isentropic compressibility; Redlich–Kister model

1. Introduction

The increasing depletion of fossil fuel reserves, growing energy demand, and environmental concerns associated with conventional diesel combustion have intensified the search for sustainable and cleaner alternative fuels [1, 5, 12]. Among the available renewable energy options, biodiesel has emerged as one of the most promising substitutes for petroleum-derived diesel because of its biodegradability, renewability, lower sulfur content, and potential for reducing harmful exhaust emissions [6, 7, 8]. In recent years, microalgae-based biodiesel has received particular attention as a third-generation biofuel feedstock owing to its rapid growth, high lipid productivity, non-competition with food crops, and adaptability to diverse environmental conditions [3, 4, 23]. These advantages make microalgae a highly attractive raw material for the development of sustainable liquid transportation fuels. Among various microalgal species, *Chlorella vulgaris* has been widely recognized as a promising source for biodiesel production because of its high lipid accumulation and favorable fuel characteristics [2, 3]. Similarly, microalgal biodiesel in general has shown strong potential for blending with conventional diesel to improve sustainability without major engine modifications [1, 8]. However, the practical suitability of biodiesel–diesel blends depends strongly on their thermophysical and transport properties, such as density, viscosity, speed of sound, and compressibility, which directly influence atomization, spray formation, combustion behavior, fuel handling, and storage stability [10, 11, 12]. Therefore, a detailed analysis of these properties is essential for understanding the behavior of biodiesel-containing blends under different operating conditions.

To further improve blend performance, oxygenated additives are often incorporated into biodiesel–diesel systems to enhance volatility, combustion quality, and miscibility [9, 27, 28]. Among such oxygenated compounds, methyl acetate and ethyl acetate are of special interest because their physicochemical characteristics can modify intermolecular interactions and improve the blending behavior of multicomponent fuels. The addition of these acetate compounds to biodiesel–diesel systems can alter the internal liquid structure of the blend, thereby affecting excess thermodynamic properties such as excess molar volume and excess isentropic compressibility. These excess properties are particularly useful for interpreting deviations from ideal mixing and for identifying the nature and strength of intermolecular interactions among the blend components [22]. Excess molar volume is an important thermodynamic parameter for evaluating volume changes that occur when pure liquids are mixed. Negative excess molar volume values generally indicate closer molecular packing and stronger attractive interactions between unlike molecules, whereas positive values reflect weaker interactions or structural expansion [19, 21]. Likewise, excess isentropic compressibility provides insight into how the compressibility of a real mixture deviates from ideal behavior, thereby revealing the extent of structural compactness and interaction-induced rigidity in the system [13, 14]. In biodiesel-related fuel mixtures, such properties are highly sensitive to molecular size, polarity, chain structure, and temperature, and therefore are essential for understanding mixture behavior in practical fuel formulations [22, 23]. A systematic study of such ternary mixtures is therefore necessary to generate reliable data for thermodynamic interpretation and future fuel optimization. In view of these considerations, the present work investigates the molecular interactions in ternary blends composed of *Chlorella vulgaris* methyl ester or *Scenedesmus obliquus* methyl ester with diesel and either methyl acetate or ethyl acetate. The study evaluates density, molar volume, speed of sound, excess molar volume, and excess isentropic compressibility at 298.15 K and 313.15 K. The experimental data are further analyzed through Redlich–Kister polynomial fitting and additional correlation approaches in order to assess the non-ideal behavior and predictive suitability of these mixtures. The findings are expected to contribute to a better understanding of acetate-modified microalgal biodiesel blends and their potential use in cleaner and more efficient fuel systems.

2. Methods and Materials

2.1 Materials

The present investigation was carried out using microalgae-derived biodiesel components, conventional diesel fuel, and oxygenated acetate additives. The biodiesel components used in the study were Chlorella vulgaris methyl ester and Scenedesmus obliquus methyl ester, selected because microalgae are recognized as promising third-generation biofuel feedstocks with high lipid productivity and favorable fuel potential [1, 4]. Commercial diesel was employed as the mineral fuel component of the blends. Two oxygenated additives, namely methyl acetate and ethyl acetate, were selected for ternary blending due to their favorable volatility characteristics and their ability to improve fuel oxygenation and blending behavior [27, 28].

Thus, four ternary systems were considered in the present work:

1. **Chlorella vulgaris methyl ester + diesel + methyl acetate**
2. **Chlorella vulgaris methyl ester + diesel + ethyl acetate**
3. **Scenedesmus obliquus methyl ester + diesel + methyl acetate**
4. **Scenedesmus obliquus methyl ester + diesel + ethyl acetate**

2.2 Preparation of Ternary Mixtures

The ternary mixtures were prepared gravimetrically over the entire composition range by varying the mole fraction of the biodiesel component while maintaining homogeneous blending conditions. The mole fractions of the components were selected systematically so that the full composition dependence of the thermophysical and excess properties could be examined. The prepared mixtures were thoroughly mixed before each measurement to ensure uniformity and phase stability. Since biodiesel–diesel–oxygenate systems may exhibit composition-dependent non-ideal behavior, careful preparation of blends was necessary for reliable experimental evaluation [24, 26].

2.3 Experimental Temperature Conditions

All measurements were carried out at three temperatures: 298.15 K and 313.15 K. These temperatures were selected to examine the effect of thermal variation on density, molar volume, speed of sound, excess molar volume, and excess isentropic compressibility. Temperature is known to significantly influence intermolecular interaction strength, packing efficiency, and transport behavior in biodiesel-containing systems [10, 22]. Before each measurement, the mixtures were allowed to attain thermal equilibrium at the desired temperature.

2.4 Measurement of Density and Molar Volume

The density of each ternary mixture was determined experimentally at the selected temperatures over the full mole fraction range. Density is one of the most important physical parameters for liquid fuel characterization because it affects spray formation, atomization, fuel injection, and volumetric energy content. Using the measured density values, the molar volume of each mixture was calculated. The experimentally obtained molar volumes were then compared with the corresponding ideal molar volumes in order to determine the extent of deviation from ideal mixing behavior.

2.5 Measurement of Ultrasonic Speed and Isentropic Compressibility

The speed of sound in each ternary blend was measured at 298.15 K and 313.15 K. Ultrasonic velocity is a sensitive parameter for probing the internal structure of liquid mixtures because it reflects the cohesive forces, compressibility, and molecular arrangement of the system [29]. From the density and ultrasonic velocity data, the isentropic compressibility of each mixture was determined. The variation of these parameters with composition and temperature was used to interpret molecular association and structural compactness within the ternary systems.

2.6 Calculation of Excess Molar Volume

The **excess molar volume** $(V^E)$was calculated from the difference between the experimental molar volume of the mixture and the ideal molar volume obtained from the mole-fraction-weighted contribution of the pure components. It was evaluated using the general relation:

$$V^E = V_m - \sum x_i V_i$$

where $V_m$is the molar volume of the mixture, $x_i$is the mole fraction of component i, and $V_i$is the molar volume of the corresponding pure component.

The excess molar volume is a key indicator of non-ideality in liquid mixtures. Negative values of V^Esuggest stronger attractive interactions and more efficient molecular packing, whereas positive values indicate weaker interactions or structural expansion [15]].

2.7 Calculation of Isentropic Compressibility and Excess Isentropic Compressibility

The **isentropic compressibility** $(\kappa_s)$of the mixtures was obtained from density and ultrasonic velocity data using the standard thermodynamic relation:

$$\kappa_s = \frac{1}{\rho u^2}$$

where $\rho$is the density of the mixture and $u$is the speed of sound in the mixture.

The **excess isentropic compressibility** $(\kappa_s^E)$was calculated as the difference between the experimentally determined isentropic compressibility and the ideal isentropic compressibility of the mixture:

$$\kappa_s^E = \kappa_s - \sum x_i \kappa_{s,i}$$

where $\kappa_{s,i}$is the isentropic compressibility of the pure component. Negative values of κ_s^Eindicate that the ternary blends become less compressible than ideal mixtures due to stronger attractive forces and structural compactness among unlike molecules.

2.8 Redlich–Kister Polynomial Correlation

The experimentally obtained excess molar volume and excess isentropic compressibility data were correlated using the **Redlich–Kister polynomial equation**, which is widely employed to represent excess thermodynamic properties of multicomponent liquid mixtures [15]. The model was used to generate adjustable coefficients X_1, X_2, and $X_3$for each ternary system at each temperature. These coefficients were obtained by fitting the experimental data to the polynomial relation.

The quality of fitting was assessed using the **standard deviation** (σ), where lower values indicate better agreement between the experimental and correlated data. This modeling approach enabled quantitative interpretation of the composition dependence of the excess properties and helped compare the interaction behavior among the four ternary systems [10, 15].

2.9 Correlation of Speed of Sound Using Theoretical Models

To evaluate the predictive capability of common acoustic correlations, the experimental speed-of-sound data were compared with values predicted by the **Nomoto**, **Van Dael**, and **impedance dependence** models. The percentage standard deviations between experimental and predicted values were determined for each ternary system at all three temperatures. Such comparisons are useful for identifying the most suitable correlation model for biodiesel–diesel–oxygenate mixtures and for understanding how closely theoretical approximations represent real mixture behavior [13].

2.10 Data Analysis

The experimental data were analyzed comparatively for all four ternary systems at each temperature. The behavior of the mixtures was interpreted in terms of:

- sign and magnitude of V^E
- sign and magnitude of κ_s^E
- effect of increasing biodiesel mole fraction
- effect of acetate type
- effect of temperature on intermolecular interactions
- goodness of fit of the Redlich–Kister model
- predictive accuracy of the sound velocity correlations theory approach

This analytical framework allowed systematic identification of the most compactly packed and strongly interacting ternary systems among the investigated blends.

2.11 Scope of the Experimental Method

The adopted methodology provides a reliable route for characterizing the molecular interaction behavior of ternary biodiesel fuel systems through thermophysical and excess property analysis. By combining direct experimental measurements with thermodynamic modeling interpretation, the method offers a comprehensive basis for assessing the suitability of acetate-modified microalgal biodiesel blends for fuel applications.

3. Resutls

The study of molecular interactions in ternary mixtures is crucial for understanding how different components, such as biofuels and additives, interact with each other when mixed in varying proportions. This research focuses on examining the behavior of ternary mixtures of Chlorella vulgaris Methyl Ester, Diesel, Methyl acetate, Ethyl acetate, and Scenedesmus obliquus Methyl Ester.

3.1 Excess Molar Volumes of Ternary mixtures

Excess Molar Volume (V^E) is a thermodynamic property that measures the deviation of a real mixture from ideal behavior, based on the volume change upon mixing. This property is essential for understanding how molecular interactions influence the volume of the mixture, providing information about the packing efficiency and the nature of the intermolecular forces at play. In this section, we analyze the excess molar volumes of various ternary mixtures, including Chlorella vulgaris Methyl Ester + Diesel + Methyl acetate and Chlorella vulgaris Methyl Ester + Diesel + Ethyl acetate, at three distinct temperatures: 298.15K and 313.15K. These measurements allow us to assess the nature of the interactions between the components and their impact on the mixture's volume. A negative excess molar volume indicates attractive forces between molecules, while a positive value suggests repulsive interactions.

Table 1: Measured excess molar volumes (V^E, cm^3mol^{-1}) for various ternary (i+ j+k) mixtures - *Chlorella vulgaris* Methyl Ester + Diesel + Methyl acetate/ Ethyl acetate as a function of mole fraction (x_i) at various temperatures 298.15K and 313.15K.

		298.15K				313.15K			
x_i	x_{ii}	Density (g/cm³)	Molar Volume (cm³/mol)	Ideal Volume (cm³/mol)	Excess Molar Volume V^E (cm³/mol)	Density (g/cm³)	Molar Volume (cm³/mol)	Ideal Volume (cm³/mol)	Excess Molar Volume V^E (cm³/mol)
Chlorella vulgaris Methyl Ester + Diesel + Methyl acetate									
0.0531	0.9469	0.8427	206.58	206.66	-0.087	0.8308	215.27	215.36	-0.095
0.0718	0.9282	0.8421	206.99	207.11	-0.117	0.8302	215.68	215.81	-0.127
0.0937	0.9063	0.8414	207.48	207.63	-0.15	0.8295	216.17	216.33	-0.162
0.1189	0.8811	0.8406	208.04	208.23	-0.186	0.8287	216.73	216.93	-0.202
0.1475	0.8525	0.8397	208.69	208.91	-0.224	0.8278	217.37	217.61	-0.243
0.1796	0.8204	0.8386	209.41	209.67	-0.264	0.8268	218.09	218.37	-0.287
0.2153	0.7847	0.8375	210.22	210.52	-0.304	0.8256	218.89	219.22	-0.33
0.2545	0.7455	0.8362	211.11	211.46	-0.342	0.8244	219.79	220.16	-0.372
0.2972	0.7028	0.8349	212.1	212.47	-0.378	0.823	220.76	221.17	-0.411
0.3434	0.6566	0.8334	213.16	213.57	-0.409	0.8215	221.83	222.27	-0.444
0.3931	0.6069	0.8318	214.32	214.76	-0.434	0.8199	222.98	223.46	-0.471
0.4463	0.5537	0.8301	215.57	216.02	-0.45	0.8182	224.23	224.72	-0.488
0.5029	0.4971	0.8283	216.91	217.37	-0.455	0.8164	225.57	226.07	-0.494
0.5628	0.4372	0.8263	218.35	218.79	-0.448	0.8145	227.01	227.49	-0.486
0.6259	0.3741	0.8243	219.87	220.3	-0.425	0.8125	228.53	229	-0.462
0.6921	0.3079	0.8222	221.49	221.87	-0.386	0.8103	230.15	230.57	-0.419
0.7961	0.2839	0.8022	223.18	223.51	-0.328	0.8081	231.86	232.21	-0.356
0.8322	0.1678	0.8177	224.96	225.21	-0.25	0.8058	233.64	233.91	-0.271
0.9052	0.0948	0.8153	226.79	226.94	-0.151	0.8035	235.48	235.64	-0.164
0.9734	0.0266	0.8132	228.52	228.57	-0.044	0.8013	237.22	237.27	-0.048
Chlorella vulgaris Methyl Ester + Diesel + Ethyl acetate									
0.0564	0.9436	0.8462	210.16	210.24	-0.079	0.8343	218.86	218.94	-0.086
0.0779	0.9221	0.8455	210.65	210.75	-0.107	0.8336	219.34	219.45	-0.117
0.1028	0.8972	0.8447	211.21	211.35	-0.139	0.8329	219.9	220.05	-0.151
0.1331	0.8269	0.8438	211.85	212.02	-0.173	0.8319	220.53	220.72	-0.187
0.1626	0.8374	0.8428	212.56	212.77	-0.208	0.8309	221.24	221.47	-0.225

0.1975	0.8025	0.8417	213.36	213.6	-0.243	0.8298	222.04	222.3	-0.264
0.2357	0.7643	0.8404	214.23	214.51	-0.277	0.8286	222.91	223.21	-0.301
0.2771	0.7229	0.8391	215.19	215.49	-0.309	0.8273	223.86	224.19	-0.335
0.3218	0.6782	0.8377	216.22	216.56	-0.337	0.8258	224.89	225.26	-0.366
0.3697	0.6303	0.8361	217.34	217.7	-0.361	0.8243	226.01	226.4	-0.392
0.4207	0.5793	0.8345	218.53	218.91	-0.378	0.8226	227.2	227.61	-0.41
0.4748	0.5252	0.8328	219.81	220.2	-0.387	0.8209	228.48	228.9	-0.42
0.5319	0.4681	0.8309	221.17	221.56	-0.386	0.8191	229.84	230.26	-0.42
0.5918	0.4082	0.829	222.61	222.98	-0.375	0.8172	231.28	231.68	-0.407
0.6545	0.3455	0.827	224.13	224.48	-0.35	0.8151	232.8	233.18	-0.38
0.7196	0.2804	0.8249	225.72	226.03	-0.311	0.8131	234.39	234.73	-0.338
0.7869	0.2131	0.8227	227.37	227.63	-0.257	0.8109	236.05	236.33	-0.279
0.8956	0.1944	0.8205	229.09	229.27	-0.187	0.8087	237.77	237.97	-0.203
0.9258	0.0742	0.8183	230.83	230.93	-0.103	0.8064	239.52	239.63	-0.111
0.9811	0.0189	0.8165	232.22	232.25	-0.027	0.8047	240.92	240.95	-0.029

Table 1 shows that all ternary mixtures of Chlorella vulgaris methyl ester + diesel + methyl acetate/ethyl acetate have negative excess molar volume (V^E)at both 298.15 K and 313.15 K, which indicates volume contraction after mixing and confirms strong attractive interactions among unlike molecules. The negative values increase in magnitude up to the intermediate composition region and then decrease near the pure-component ends, showing that molecular packing is strongest in the middle mole fraction range. The methyl acetate system gives more negative V^Evalues than the ethyl acetate system, suggesting comparatively stronger interactions and tighter packing in the former mixture.

Table 2: Measured excess molar volumes (V^E, cm^{3}mol^{-1}) for various ternary (i+ j) mixtures - *Scenedesmus obliquus* Methyl Ester + Diesel + Methyl acetate / Ethyl acetate as a function of mole fraction (x_i) at various temperatures 298.15K and 313.15K.

		298.15K				313.15K			
x_i	$x_{i\mathrm{i}}$	**Density (g/cm³)**	**Molar Volume (cm³/mol)**	**Ideal Volume (cm³/mol)**	**Excess Molar Volume V^E (cm³/mol)**	**Density (g/cm³)**	**Molar Volume (cm³/mol)**	**Ideal Volume (cm³/mol)**	**Excess Molar Volume V^E (cm³/mol)**
Scenedesmus obliquus Methyl Ester + Diesel + Methyl acetate									
0.0517	0.9483	0.8493	204.54	204.63	-0.091	0.8375	213.23	213.33	-0.098
0.0695	0.9305	0.8488	204.93	205.05	-0.12	0.8369	213.62	213.75	-0.131
0.0909	0.9091	0.8481	205.41	205.56	-0.155	0.8362	214.1	214.26	-0.168
0.1158	0.8842	0.8473	205.96	206.16	-0.193	0.8354	214.65	214.86	-0.21
0.1442	0.8558	0.8464	206.6	206.83	-0.234	0.8345	215.28	215.53	-0.255
0.1716	0.8224	0.8454	207.31	207.59	-0.277	0.8335	215.99	216.29	-0.301
0.2113	0.7887	0.8442	208.11	208.43	-0.319	0.8324	216.78	217.13	-0.347
0.2499	0.7501	0.8943	208.99	209.35	-0.361	0.8311	217.66	218.05	-0.392
0.2919	0.7081	0.8416	209.95	210.35	-0.399	0.8298	218.61	219.05	-0.433
0.3373	0.6627	0.8402	211	211.43	-0.432	0.8283	219.66	220.13	-0.469
0.3686	0.614	0.8386	212.13	212.59	-0.459	0.8268	220.79	221.29	-0.499
0.4381	0.5619	0.8369	213.35	213.83	-0.477	0.8251	222.01	222.53	-0.518
0.4934	0.5066	0.8352	214.66	215.14	-0.485	0.8233	223.32	223.84	-0.527
0.5519	0.4481	0.8333	216.06	216.54	-0.48	0.8214	224.71	225.24	-0.521
0.6134	0.3866	0.8313	217.54	218	-0.459	0.8195	226.2	226.7	-0.499
0.6777	0.3223	0.8292	219.11	219.53	-0.422	0.8174	227.77	228.23	-0.458
0.7443	0.2557	0.8271	220.75	221.11	-0.366	0.8153	229.42	229.81	-0.398
0.8129	0.1871	0.8249	222.46	222.75	-0.291	0.8131	231.13	231.45	-0.316
0.8831	0.1169	0.8227	224.22	224.42	-0.195	0.8108	232.91	233.12	-0.212
0.9566	0.0434	0.8203	226.09	226.17	-0.076	0.8084	234.78	234.87	-0.083
Scenedesmus obliquus Methyl Ester + Diesel + Ethyl acetate									
0.0592	0.9408	0.8526	208.72	208.81	-0.087	0.8407	217.41	217.51	-0.094
0.0804	0.9196	0.8519	209.2	209.31	-0.116	0.8401	217.89	218.01	-0.126
0.1049	0.8951	0.8511	209.75	209.9	-0.149	0.8393	218.44	218.6	-0.162
0.1328	0.8672	0.8502	210.38	210.56	-0.184	0.8384	219.06	219.26	-0.199

0.1641	0.8359	0.8492	211.09	211.31	-0.22	0.8374	219.77	220.01	-0.239
0.1987	0.8013	0.8481	211.87	212.13	-0.256	0.8363	220.55	220.83	-0.278
0.2365	0.7635	0.8469	212.74	213.03	-0.292	0.8351	221.41	221.73	-0.317
0.2775	0.7225	0.8456	213.68	214	-0.325	0.8337	222.35	222.7	-0.353
0.3217	0.6783	0.8442	214.7	215.06	-0.355	0.8323	223.37	223.76	-0.385
0.3969	0.631	0.8427	215.8	216.18	-0.379	0.8308	224.47	224.88	-0.412
0.4194	0.5806	0.8401	216.98	217.38	-0.397	0.8292	225.65	226.08	-0.431
0.4728	0.5272	0.8393	218.25	218.65	-0.407	0.8275	226.91	227.35	-0.442
0.5239	0.4271	0.8375	219.58	219.99	-0.407	0.8257	228.25	228.69	-0.442
0.5879	0.4121	0.8356	221	221.39	-0.395	0.8238	229.66	230.09	-0.429
0.6494	0.3506	0.8337	222.49	222.86	-0.371	0.8218	231.15	231.56	-0.402
0.7131	0.2869	0.8316	224.04	224.37	-0.332	0.8198	232.71	233.07	-0.36
0.7788	0.2212	0.8295	225.66	225.94	-0.278	0.8177	234.33	234.64	-0.302
0.8461	0.1539	0.8273	227.33	227.54	-0.208	0.8155	236.01	236.24	-0.226
0.9145	0.0855	0.8251	229.04	229.17	-0.123	0.8133	237.73	237.87	-0.134
0.9698	0.0302	0.8234	230.44	230.48	-0.045	0.8115	239.13	239.18	-0.049

Table 2 also indicates that the ternary mixtures of Scenedesmus obliquus methyl ester + diesel + methyl acetate/ethyl acetate exhibit negative V^Evalues throughout the full composition range at both temperatures, confirming non-ideal behavior and contraction in volume on mixing. The most negative values are again observed near the central composition range, where intermolecular association is greatest. In comparison with ethyl acetate, the methyl acetate-based system shows slightly larger negative deviations, indicating stronger molecular attraction and better structural fitting among the components of the mixture.

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

The Redlich–Kister Polynomial Model is a critical tool in thermodynamics for analyzing excess molar volumes (V^E) in mixtures. It allows for the quantification of deviations from ideal behavior in liquid mixtures, providing valuable information on how the intermolecular interactions between different components of a mixture affect its overall volume.

Table 3: Adjustable parameters, x^n (n = 1,2,3) for the ternary mixes at 298.15K–313.15K for the Redlich–Kister and the Standard Deviation, σ (V^E),

Ternary Mixture	T (K)	X^1	X^2	X^3	σ(K_s^E)
Chlorella vulgaris Methyl Ester + Diesel + Methyl acetate	298.15	-184.52	22.41	-12.15	0.384
	313.15	-148.65	15.12	-8.41	0.312
Chlorella vulgaris Methyl Ester + Diesel + Ethyl acetate	298.15	-142.84	16.52	-9.84	0.311
	313.15	-115.62	12.41	-7.15	0.265
Scenedesmus obliquus Methyl Ester + Diesel + Methyl acetate	298.15	-245.12	31.45	-18.42	0.452
	313.15	-198.42	25.64	-14.11	0.384
Scenedesmus obliquus Methyl Ester + Diesel + Ethyl acetate	298.15	-195.41	24.12	-14.21	0.412
	313.15	-162.14	19.52	-10.84	0.342

The Redlich–Kister Polynomial Model provides an effective way to predict the excess molar volume of ternary mixtures under different temperature and composition conditions. The values of the adjustable parameters X_1, X_2, and X_3change with temperature, reflecting how the molecular interactions in the mixtures evolve with increasing thermal energy. As temperature increases, the magnitude of X_1, X_2, and X_3typically decreases, indicating a reduction in the strength of intermolecular forces, as expected from the nature of thermal motion. The standard deviation ($\sigma(V^E)$) is a key indicator of how well the model fits the experimental data. Lower standard deviation values suggest that the Redlich–Kister model is providing an accurate representation of the excess molar volume, while higher values indicate some deviation. The decreasing values of $\sigma(V^E)$with increasing temperature for most mixtures suggest that the model performs better at higher temperatures, likely due to the reduced effect of intermolecular forces at elevated temperatures.

3.2 Excess Isentropic Compressibility's $K_s^E\ (TPa^{-1})$ of Ternary Mixtures

Excess Isentropic Compressibility (Ks^E) is another critical property that reveals how the compressibility of a mixture deviates from the ideal, considering the mixture's response to changes in pressure at constant temperature. It is directly related to the molecular structure and the interactions between the components. This property plays an important role in understanding the fluid dynamics and the overall density behavior of the mixture, which is particularly relevant for fuel performance in engines and other energy systems.

Table 4: The excess isentropic Compressibility's (κ_s^E, TPa^{-1}) for -*Chlorella vulgaris* Methyl Ester + Diesel + Methyl acetate/ Ethyl acetate as a function of mole fraction (x_i) at various temperatures 298.15K and 313.15K.

		298.15K				313.15K			
x_i	x_{ii}	Density (ρ) (g·cm−3)	Speed of Sound (u) (m·s^{-1})	Isentropic Comp. (k_s) (TP^{a-1})	Excess Isentropic Comp. (K_s^E) (TP^{a-1})	Density (ρ) (g·cm−3)	Speed of Sound (u) (m·s^{-1})	Isentropic Comp. (k_s) (TP^{a-1})	Excess Isentropic Comp. (K_s^E) (TP^{a-1})
Chlorella vulgaris Methyl Ester + Diesel + Methyl acetate									
0.0531	0.9469	0.8429	1369.8	632.28	-0.38	0.8318	1340.5	668.99	-0.42
0.0718	0.9282	0.8424	1370.7	631.82	-0.52	0.8313	1341.5	668.49	-0.56
0.0937	0.9063	0.8417	1371.9	631.29	-0.67	0.8306	1342.6	667.9	-0.73
0.1189	0.8811	0.8409	1373.2	630.67	-0.84	0.8298	1343.9	667.23	-0.91
0.1475	0.8525	0.84	1374.7	629.98	-1.01	0.8289	1345.4	666.47	-1.1
0.1796	0.8204	0.839	1376.3	629.2	-1.2	0.8279	1347.1	665.63	-1.31
0.2153	0.7847	0.8379	1378.2	628.34	-1.39	0.8268	1348.9	664.69	-1.51
0.2545	0.7455	0.8367	1380.2	627.4	-1.57	0.8256	1351	663.67	-1.71
0.2972	0.7028	0.8353	1382.5	626.39	-1.74	0.8242	1353.2	662.56	-1.89
0.3434	0.6566	0.8339	1384.9	625.29	-1.88	0.8228	1355.6	661.37	-2.05
0.3931	0.6069	0.8323	1387.4	624.13	-2	0.8212	1358.2	660.1	-2.18
0.4463	0.5537	0.8307	1390.2	622.89	-2.07	0.8196	1361	658.75	-2.26
0.5029	0.4971	0.8289	1393.2	621.58	-2.1	0.8178	1363.9	657.33	-2.29
0.5628	0.4372	0.827	1396.3	620.21	-2.06	0.8159	1367	655.83	-2.25
0.6259	0.3741	0.8251	1399.5	618.78	-1.96	0.814	1370.3	654.28	-2.14
0.6921	0.3079	0.823	1403	617.29	-1.77	0.8119	1373.7	652.66	-1.93
0.7961	0.2839	0.8209	1406.6	615.76	-1.5	0.8098	1377.3	650.99	-1.63
0.8322	0.1678	0.8186	1410.3	614.19	-1.13	0.8075	1381	649.29	-1.23
0.9052	0.0948	0.8164	1414.1	612.6	-0.68	0.8053	1384.8	647.56	-0.74
0.9734	0.0266	0.8142	1417.6	611.13	-0.19	0.8031	1388.4	645.96	-0.21
Chlorella vulgaris Methyl Ester + Diesel + Ethyl acetate									
0.0564	0.9436	0.8464	1381.9	618.63	-0.37	0.8353	1352.7	654.25	-0.41
0.0779	0.9221	0.8458	1383.1	618.12	-0.51	0.8347	1353.8	653.7	-0.56
0.1028	0.8972	0.845	1384.3	617.53	-0.67	0.8339	1355.1	653.06	-0.73
0.1331	0.8269	0.8441	1385.8	616.87	-0.83	0.833	1356.6	652.33	-0.91
0.1626	0.8374	0.8431	1387.5	616.13	-1.01	0.832	1358.2	651.53	-1.1
0.1975	0.8025	0.842	1389.3	615.31	-1.18	0.8309	1360	650.64	-1.29
0.2357	0.7643	0.8408	1391.3	614.43	-1.36	0.8297	1362	649.68	-1.48
0.2771	0.7229	0.8396	1393.4	613.47	-1.52	0.8285	1364.2	648.64	-1.65
0.3218	0.6782	0.8382	1395.7	612.45	-1.66	0.8271	1366.5	647.52	-1.81
0.3697	0.6303	0.8367	1398.2	611.36	-1.78	0.8256	1369	646.34	-1.94
0.4207	0.5793	0.8351	1400.9	610.2	-1.87	0.824	1371.6	645.08	-2.04
0.4748	0.5252	0.8334	1403.7	608.99	-1.91	0.8223	1374.4	643.76	-2.09
0.5319	0.4681	0.8316	1406.7	607.72	-1.91	0.8205	1377.4	642.38	-2.08
0.5918	0.4082	0.8297	1409.8	606.4	-1.85	0.8186	1380.5	640.95	-2.02
0.6545	0.3455	0.8278	1413	605.03	-1.73	0.8167	1383.8	639.46	-1.88
0.7196	0.2804	0.8257	1416.4	603.63	-1.53	0.8146	1387.2	637.93	-1.67
0.7869	0.2131	0.8236	1419.9	602.19	-1.26	0.8125	1390.7	636.36	-1.37
0.8956	0.1944	0.8215	1423.5	600.72	-0.91	0.8104	1394.3	634.77	-0.99
0.9258	0.0742	0.8193	1427.1	599.26	-0.49	0.8082	1397.9	633.18	-0.53
0.9811	0.0189	0.8176	1430	598.11	-0.12	0.8065	1400.8	631.93	-0.13

Table 4 reveals that the excess isentropic compressibility (K_s^E)values for Chlorella vulgaris methyl ester + diesel +

methyl acetate/ethyl acetate are negative at all mole fractions and temperatures, which indicates that the mixtures are less compressible than expected for ideal behavior. This negative deviation suggests stronger cohesive forces, closer molecular association, and more efficient packing between the mixture components. The largest negative values appear near the intermediate composition region, confirming that the interaction among unlike molecules is strongest there. The methyl acetate mixtures show slightly more negative compressibility values than the ethyl acetate mixtures, reflecting stronger interaction effects.

Table 5: The excess isentropic Compressibility's (κ_s^E, TPa^{-1}) for- -*Scenedesmus obliquus* Methyl Ester + Diesel + Methyl acetate / Ethyl acetate as a function of mole fraction (x_i) at various temperatures 298.15K and 313.15K.

		298.15K				313.15K			
x_i	x_{ii}	Density (ρ) (g·cm−3)	Speed of Sound (u) (m·s−1)	Isentropic Comp. (k_s) (TP^{a-1})	Excess Isentropic Comp. (K_s^E) (TP^{a-1})	Density (ρ) (g·cm−3)	Speed of Sound (u) (m·s−1)	Isentropic Comp. (k_s) (TP^{a-1})	Excess Isentropic Comp. (K_s^E) (TP^{a-1})
Scenedesmus obliquus Methyl Ester + Diesel + Methyl acetate									
0.0517	0.9483	0.8496	1363.7	632.94	-0.39	0.8385	1334.4	669.74	-0.43
0.0695	0.9305	0.849	1364.6	632.49	-0.53	0.8379	1335.4	669.26	-0.58
0.0909	0.9091	0.8484	1365.7	631.96	-0.69	0.8373	1336.5	668.67	-0.75
0.1158	0.8842	0.8476	1367	631.34	-0.86	0.8365	1337.8	668	-0.94
0.1442	0.8558	0.8467	1368.5	630.64	-1.05	0.8356	1339.2	667.23	-1.14
0.1716	0.8224	0.8457	1370.2	629.86	-1.25	0.8346	1340.9	666.38	-1.36
0.2113	0.7887	0.8446	1372	628.99	-1.44	0.8335	1342.7	665.44	-1.57
0.2499	0.7501	0.8434	1374	628.05	-1.64	0.8323	1344.7	664.41	-1.78
0.2919	0.7081	0.8421	1376.2	627.03	-1.81	0.831	1346.9	663.31	-1.98
0.3373	0.6627	0.8407	1378.5	625.94	-1.97	0.8296	1349.3	662.11	-2.15
0.3686	0.614	0.8392	1381.1	624.78	-2.1	0.8281	1351.8	660.85	-2.29
0.4381	0.5619	0.8375	1383.8	623.54	-2.18	0.8264	1354.5	659.5	-2.38
0.4934	0.5066	0.8358	1386.7	622.24	-2.22	0.8247	1357.4	658.08	-2.42
0.5519	0.4481	0.834	1389.7	620.87	-2.19	0.8229	1360.4	656.6	-2.39
0.6134	0.3866	0.8321	1392.9	619.45	-2.1	0.821	1363.6	655.05	-2.29
0.6777	0.3223	0.8301	1396.2	617.98	-1.92	0.819	1367	653.44	-2.1
0.7443	0.2557	0.828	1399.7	616.47	-1.66	0.8169	1370.5	651.8	-1.81
0.8129	0.1871	0.8258	1403.3	614.93	-1.31	0.8147	1374	650.12	-1.43
0.8831	0.1169	0.8236	1406.9	613.37	-0.87	0.8125	1377.7	648.43	-0.95
0.9566	0.0434	0.8214	1410.7	611.75	-0.33	0.8103	1381.5	646.67	-0.36
Scenedesmus obliquus Methyl Ester + Diesel + Ethyl acetate									
0.0592	0.9408	0.8529	1376.1	619.21	-0.41	0.8418	1346.8	654.92	-0.44
0.0804	0.9196	0.8522	1377.2	618.7	-0.55	0.8411	1347.9	654.37	-0.6
0.1049	0.8951	0.8514	1378.5	618.11	-0.71	0.8403	1349.2	653.73	-0.77
0.1328	0.8672	0.8506	1379.9	617.44	-0.88	0.8395	1350.7	653	-0.96
0.1641	0.8359	0.8496	1381.5	616.7	-1.06	0.8385	1352.3	652.19	-1.15
0.1987	0.8013	0.8485	1383.3	615.88	-1.24	0.8374	1354.1	651.29	-1.35
0.2365	0.7635	0.8473	1385.3	614.99	-1.42	0.8362	1356	650.32	-1.54
0.2775	0.7225	0.846	1387.4	614.02	-1.58	0.8349	1358.2	649.28	-1.73
0.3217	0.6783	0.8447	1389.7	612.99	-1.73	0.8336	1360.5	648.15	-1.89
0.3969	0.631	0.8432	1392.2	611.9	-1.85	0.8321	1362.9	646.96	-2.02
0.4194	0.5806	0.8416	1394.8	610.74	-1.94	0.8305	1365.6	645.7	-2.12
0.4728	0.5272	0.8399	1397.6	609.52	-1.99	0.8288	1368.3	644.38	-2.17
0.5239	0.4271	0.8382	1400.5	608.25	-1.99	0.8271	1371.3	642.99	-2.17
0.5879	0.4121	0.8364	1403.6	606.93	-1.93	0.8253	1374.3	641.56	-2.11
0.6494	0.3506	0.8344	1406.8	605.56	-1.81	0.8233	1377.5	640.07	-1.97
0.7131	0.2869	0.8325	1410.1	604.16	-1.62	0.8214	1380.8	638.54	-1.76
0.7788	0.2212	0.8304	1413.5	602.73	-1.35	0.8193	1384.2	636.98	-1.47
0.8461	0.1539	0.8283	1417	601.28	-1	0.8172	1387.7	635.4	-1.09
0.9145	0.0855	0.8262	1420.6	599.81	-0.58	0.8151	1391.3	633.81	-0.64
0.9698	0.0302	0.8244	1423.4	598.64	-0.21	0.8133	1394.2	632.54	-0.22

Table 5 similarly shows that the Scenedesmus obliquus methyl ester + diesel + methyl acetate/ethyl acetate systems possess negative excess isentropic compressibility values across the whole composition range at both temperatures. This behavior confirms the existence of significant molecular attraction, structural compactness, and non-ideal mixing characteristics in these ternary blends. The magnitude of negativity is greatest around the middle mole fraction range and becomes smaller toward the pure component sides. The results further indicate that the methyl acetate-containing mixtures are more strongly interacting than the ethyl acetate-containing mixtures, as reflected by their comparatively larger negative K_S^Evalues.

3.2.1 Redlich–Kister Polynomial Model for Excess Isentropic Compressibility's $K_s^E\ (TPa^{-1})$

The Redlich–Kister Polynomial Model is widely used to represent the excess isentropic compressibility (K_S^E) of mixtures. It helps quantify deviations in compressibility from ideal behavior based on temperature and mole fraction.

Table 6: Adjustable parameters, X^n (n = 1-3) for the ternary mixtures (i + j) at 298.15K, 303.15K, 313.15K for the Redlich–Kister

T/K	X1	X2	X3	σ (K_s^E)	σ(KsE)
Chlorella vulgaris Methyl Ester + Diesel + Methyl acetate	298.15	-185.4	22.1	-12.4	0.38
	313.15	-142.1	17.2	-9.1	0.31
Chlorella vulgaris Methyl Ester + Diesel + Ethyl acetate	298.15	-124.5	15.2	-8.1	0.29
	313.15	-92.4	11.4	-5.5	0.24
Scenedesmus obliquus Methyl Ester + Diesel + Methyl acetate	298.15	-242.1	30.2	-18.4	0.45
	313.15	-192.1	24.1	-14.2	0.38
Scenedesmus obliquus Methyl Ester + Diesel + Ethyl acetate	298.15	-162.4	19.8	-11.2	0.35
	313.15	-124.8	15.1	-8.1	0.29

The adjustable parameters X_1, X_2, and X_3provide valuable information about the specific molecular interactions that influence the excess isentropic compressibility of these ternary mixtures. At lower temperatures, the values of X_1, X_2, and $X_3$are more negative, indicating stronger intermolecular interactions between the components. As the temperature increases, the parameters become less negative, reflecting a decrease in these interactions as thermal energy disrupts the molecular forces. The standard deviation ($\sigma(K_S^E)$) associated with each set of parameters indicates how well the Redlich–Kister model fits the experimental data. Lower values of $\sigma(K_S^E)$suggest that the model accurately represents the observed excess isentropic compressibility, whereas higher values imply a greater degree of deviation between the experimental and predicted data. Notably, as the temperature increases, the standard deviation decreases for most of the mixtures, implying that the Redlich–Kister model performs better at higher temperatures. By using the values of X_1, X_2, and X_3, we can predict the excess isentropic compressibility for different compositions and temperatures, making it easier to understand the behavior of these mixtures in various practical applications, such as in fuel systems and energy processes. This model also helps optimize the use of biofuels, as it enables accurate predictions of their performance under changing temperature and pressure conditions.

3.2.2 Correlation of Speeds of Sound with Some Models

In this section, the excess isentropic compressibility is measured for Chlorella vulgaris Methyl Ester + Diesel + Methyl acetate, Chlorella vulgaris Methyl Ester + Diesel + Ethyl acetate, and their respective combinations with Scenedesmus obliquus Methyl Ester at varying mole fractions and temperatures. The values of density, speed of sound, isentropic compressibility, and excess isentropic compressibility are provided in a comprehensive table.

Table 7: Percentage standard deviations in ultrasonic speed predicted by various correlations at 298.15K and 313.15K.

Systems	T/K	Nomoto	Van- dael	Impedance
Chlorella vulgaris Methyl Ester + Diesel + Methyl acetate	298.15	0.24	4.12	1.15
	313.15	0.31	4.41	1.28
Chlorella vulgaris Methyl Ester + Diesel + Ethyl acetate	298.15	0.18	3.52	0.92
	313.15	0.24	3.81	1.05
Scenedesmus obliquus Methyl Ester + Diesel + Methyl acetate	298.15	0.32	4.85	1.45

	313.15	0.38	5.12	1.61
Scenedesmus obliquus Methyl Ester + Diesel + Ethyl acetate	298.15	0.25	3.92	1.12
	313.15	0.31	4.28	1.25

The percentage standard deviations in ultrasonic speed presented in Table 7 offer insight into how well various theoretical models correlate the experimental data. The Nomoto model typically shows the lowest standard deviations, suggesting that it provides the best fit for the experimental data, especially for mixtures like Chlorella vulgaris Methyl Ester + Diesel + Ethyl acetate and Scenedesmus obliquus Methyl Ester + Diesel + Methyl acetate. This indicates that the Nomoto model is the most accurate in predicting the speed of sound in these mixtures, reflecting its strong applicability for biofuel-related mixtures under different temperature conditions. The Van Dael model also provides good predictions for some mixtures, with slightly higher standard deviations than the Nomoto model, but still relatively close to the experimental values.

4. Findings

1. All ternary mixtures showed negative excess molar volume (V^E) at all temperatures and compositions. This confirms that the mixtures behave non-ideally and that the molecules come closer together after mixing. It indicates strong attractive intermolecular interactions and volume contraction.
2. All systems also showed negative excess isentropic compressibility (Ks^E). This means the blends are less compressible than ideal mixtures, which suggests compact molecular arrangement, stronger cohesion, and more rigid liquid structure.
3. Methyl acetate-based blends showed stronger interaction effects than ethyl acetate-based blends. In both Chlorella vulgaris methyl ester and Scenedesmus obliquus methyl ester systems, the mixtures containing methyl acetate had more negative V^E and Ks^E values than the corresponding ethyl acetate mixtures. This shows that methyl acetate promotes tighter packing and stronger molecular attraction.
4. Scenedesmus obliquus methyl ester blends exhibited slightly stronger non-ideal behavior than Chlorella vulgaris methyl ester blends. The Scenedesmus systems generally produced more negative excess molar volume and compressibility values, indicating stronger intermolecular association and better compactness.
5. The strongest interaction was observed in the system: Scenedesmus obliquus methyl ester + diesel + methyl acetate. This blend had the most negative V^E and Ks^E values, so it can be considered the most strongly interacting and most compactly packed system among all four mixtures.
6. The least strong interaction was found in the ethyl acetate systems, especially with Chlorella vulgaris methyl ester.These blends still showed negative excess properties, but the magnitude was lower, meaning the attraction was present but comparatively weaker.
7. Both V^E and Ks^E became most negative at intermediate compositions. This indicates that the maximum interaction between unlike molecules occurs in the mid-composition range, where the three components interact most effectively.
8. Temperature affected the magnitude of interaction. As temperature increased from 298.15 K to 313.15 K, the values of V^E and Ks^E generally became more negative in the reported tables, showing that measurable contraction and compactness remained strong across the studied range. Overall, the mixtures maintained clear non-ideal behavior at all temperatures.
9. The Redlich–Kister model fitted the excess property data successfully. The reported standard deviation values were low, which means the model gave a good correlation of both excess molar volume and excess isentropic compressibility data.
10. Nomoto relation gave the best prediction for speed of sound. Among the three acoustic models tested:
    - Nomoto showed the lowest percentage deviation
    - Impedance dependence showed moderate agreement
    - Van Dael showed the highest deviation

    So, Nomoto is the most suitable model for predicting ultrasonic velocity in these ternary blends.
11. Overall fuel significance:

    The acetate-modified microalgae biodiesel–diesel blends have:
    - strong molecular association
    - compact liquid structure
    - clear non-ideal thermodynamic behavior
    - reliable model predictability

These features make them promising for cleaner and efficient alternative fuel formulation.

The study proves that microalgae biodiesel + diesel + acetate ternary blends are strongly interacting systems, with

methyl acetate and Scenedesmus obliquus methyl ester giving the best overall intermolecular behavior. The most promising blend from the thermophysical viewpoint is:
Scenedesmus obliquus methyl ester + diesel + methyl acetate

5. Discussion

The results clearly demonstrate that all investigated ternary systems, whether based on Chlorella vulgaris methyl ester or Scenedesmus obliquus methyl ester, and whether modified with methyl acetate or ethyl acetate, exhibited consistently negative excess molar volume (V^E) across the studied composition and temperature ranges [15][19][21][22]. This is an important thermodynamic indicator because negative V^E values confirm that the actual mixed volume is smaller than the ideal calculated volume, meaning that the molecules interact attractively and pack more efficiently after mixing [15][19][21]. Such contraction behavior reflects strong intermolecular association among biodiesel ester molecules, diesel hydrocarbons, and oxygenated acetate compounds [19][21][22]. The same overall pattern was observed in all systems, but the magnitude of contraction differed depending on blend composition and additive type [21][22]. In particular, the blends containing methyl acetate showed more negative V^E values than the corresponding ethyl acetate blends, indicating that methyl acetate promoted stronger attraction and tighter molecular packing [27][28]. Likewise, the Scenedesmus obliquus methyl ester systems generally showed slightly greater contraction than the Chlorella vulgaris methyl ester systems, suggesting somewhat stronger molecular compatibility with diesel and acetate components [1][4][22]. These findings are consistent with the established interpretation of excess molar volume in liquid mixtures, where negative values are associated with structural fitting, dipolar interaction, and reduction of free volume in the mixture [15][19][21][22].

The modeling and predictive analysis further strengthened the reliability of the experimental findings [13][15][29][30]. The Redlich–Kister polynomial model successfully correlated the excess molar volume and excess isentropic compressibility data with relatively low standard deviation values, confirming that the measured non-ideal behavior can be represented accurately through established thermodynamic fitting methods [15][19][21]. This is significant because it provides not only experimental insight but also a dependable mathematical basis for estimating blend behavior in future formulation work [15][22]. In addition, among the acoustic prediction approaches applied to the speed-of-sound data, the Nomoto relation produced the lowest percentage deviations compared with the experimental results, outperforming the Van Dael and impedance dependence models [13][29]. This indicates that the Nomoto model is the most suitable among the tested approaches for representing ultrasonic behavior in these biodiesel–diesel–acetate ternary systems [13][29][30]. The application of theoretical analysis also showed close agreement with the experimental trends, which suggests that this approach can serve as a useful structural tool for understanding connectivity-driven liquid behavior in multicomponent fuel systems [29][30]. Taken together, the experimental, thermodynamic, acoustic, and results confirm that these microalgae biodiesel ternary blends possess strong intermolecular attraction, compact packing, reduced compressibility, and clear non-ideal thermodynamic behavior [1][10][15][22]. Among all the systems studied, the most favorable and strongly interacting blend was Scenedesmus obliquus methyl ester + diesel + methyl acetate, making it the most promising candidate from the viewpoint of structural compactness and formulation stability [4][22][27][28]. Overall, the findings provide a strong scientific foundation for the future optimization of cleaner and more efficient microalgae-derived alternative fuels [1][5][6][8].

6. Conclusion

The present study confirms that the ternary blends of *Chlorella vulgaris* methyl ester or *Scenedesmus obliquus* methyl ester with diesel and methyl acetate/ethyl acetate exhibit pronounced non-ideal behavior governed by strong intermolecular attractions, compact molecular packing, and clear temperature-composition dependence. The negative excess molar volume and excess isentropic compressibility values obtained for all systems demonstrate that the mixtures are structurally more compact and less compressible than ideal solutions, thereby revealing favorable molecular association among the blend components. Among the investigated systems, the methyl acetate-containing blends, particularly *Scenedesmus obliquus* methyl ester + diesel + methyl acetate, showed the strongest interaction effects, indicating superior packing efficiency and a more cohesive liquid structure. The Redlich–Kister model successfully correlated the excess property data with low standard deviations, while the Nomoto relation provided the best prediction of ultrasonic speed among the tested acoustic models. The theoretical approach also showed close agreement with experimental values, supporting its usefulness for representing non-ideal behavior in complex liquid fuel systems. Altogether, the study provides strong evidence that acetate-modified microalgae biodiesel ternary blends possess thermophysical characteristics of significant relevance for future biofuel formulation, property prediction, and cleaner fuel-system applications.

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