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Original article

Semi-empirical algorithm for estimation of calorimetric properties in binary liquid mixtures from acoustic and volumetric data

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ABSTRACT

In the present work, a semi-empirical algorithm is proposed for estimating the adiabatic coefficient (γ), the isothermal compressibility (κ_τ), the heat capacity at constant pressure (c_p), and constant volume (c_v), for liquid mixtures of organic compounds as a function of temperature and concentration. The algorithm was applied to the binary systems: 1,6-Dichlorohexene (x) + Dodecane (1-x) and 1,5-Dichloropentane (x) + Dodecane (1-x) reported in literature. The obtaining values for γ, c_p, c_v and κ_τ are reported at all concentrations and temperatures. The implementation of the algorithm required experimental data of the adiabatic coefficients of the pure components (γ_i^0) to 298.15 K, acoustic and volumetric data of the binary mixture in the entire concentration and temperature range between (278.15–328.15) K every 5 K. The results obtained are in excellent agreement with the experimental results.

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1. Introduction

The study of thermophysical properties of mixtures containing organic compounds is a fundamental topic at the industrial and scientific level (Chiu et al., 1999; Tkachenko et al., 2011). The analysis of their magnitudes and trends allows obtaining microscopic and macroscopic information on the behavior of different molecules in the liquid mixtures(González-Salgado et al., 2004). In this context, the adiabatic coefficient, heat capacities, and isothermal compressibilities are important quantities to achieve this goal (Chen et al., 2001; Paulechka et al., 2010). However, its obtaining and calculation in many cases is not easy or requires the use of specialized equipment that has a high monetary cost(Pandey et al., 2003; Srinivasa Reddy et al., 2016). One of the problems consists in obtaining the adiabatic coefficient, or also the heat capacity at constant volume ($\boldsymbol{c_v}$), perhaps due to the high sensitivity to changes in pressure and temperature compared to the heat capacity at constant pressure ($\boldsymbol{c_p}$). The reported values of the isobaric heat capacities of liquids are normally obtained by direct calorimetric determination, the relatively scarce values of isochoric heat capacities are for the most part obtained indirectly by the use of the acoustic method (Perkins and Magee, 2009; Wilhelm, 2010, 1955; Zorębski, 2014; Zorębski et al., 2017).

In the literature have been proposed different theoretical approach for estimating the heat capacities based primordially on the use of group contribution methods (Ceriani et al., 2009; Kolská et al., 2005; Marrero and Gani, 2001) or molecular volumes(Naef, 2019). Where some of them involve multiple steps and are quite tedious to follow. However, based on the importance of this topic in order to contribute to the solution of the previously mentioned difficulties regarding the accessibility of experimental data, in this work a semiempirical algorithm was developed to evaluate the adiabatic coefficient, supported by the abundance of densitometric and acoustic data. So , the access to the acoustic and densitometric data guarantee the evaluation of the adiabatic compressibility using Laplace's equation(González-Salgado et al., 2004), isothermal compressibility and heat capacities using Mayer's Relationship(Güémez et al., 1995). This indirect method is attractive because calorimetric determination of isochoric heat capacities of liquids is still difficult. In this context, Pandey and coworkers (Md Nayeem et al., 2014; Pandey et al., 2003) used

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the equation of the state for hard sphere to calculated the isothermal compressibility for six binary liquid mixtures: n-heptane + toluene (I); n-heptane + n-hexane (II); toluene + n-hexane (III); cyclohexane + n-heptane (IV); cyclohexane + n-hexane (V), and n-decane + n-hexane (VI) at 298.15 K, using density and speed of sound data. However, a deeply examination of the obtained results, showed that only one equation of the eight illustrated is close to the experimental results, showing anomalies if the system changes. So, the developed algorithm does not have this problem. Additionally, the proposed model provides an easy and low-cost protocol to complement the results obtained from volumetric and acoustic data of different organic liquid mixtures.

2. Methodology

2.1. Variable evaluation

To validate the proposed model, density and sound velocity data of 1,6-Dichlorohexene (x) + Dodecane (1-x) and 1,5-Dichloropentane (x) + Dodecane (1-x) obtained from Gómez-Díaz (González-Salgado et al., 2004) and coworkers were used (see Table 1).These data allow us to evaluate the adiabatic compressibility (κ_s), the molar volumes (V), the coefficient of thermal expansion (α), and the derivative of the density with respect to the temperature $\left(\frac{\partial\rho}{\partial T}\right)_p$. The adiabatic compressibility (κ_s), was evaluated using the Newton-Laplace equation:

$$\kappa_s = \frac{1}{C^2\rho} \tag{1}$$

where C is the speed of sound and ρ is the density.

Molar volumes V was evaluated using the following equation:

$$V = \frac{M_{effective}}{\rho} = \frac{x_1M_1 + x_2M_2}{\rho} \tag{2}$$

where $M_{effective} = x_1M_1 + x_2M_2$, is the molar mass of the mixture, x_i is the molar fraction of the component number 1 and 2 in the mixture.

The coefficient of thermal expansion α, at the temperature T can be calculated using the expression

$$\alpha = -\frac{1}{\rho}\left(\frac{\partial\rho}{\partial T}\right)_P \tag{3}$$

The slope $\left(\frac{\partial\rho}{\partial T}\right)_p$, it was obtained for all concentrations by deriving the equation resulting from the adjustment of the density data as a function of temperature using a third degree polynomial. This adjustment was necessary to achieve good slope behavior with temperature.

3. Method implementation

Z_1° was evaluated for $x_2 = 0.0000$, and z_2° for $x_2 = 1.0000$, using the Eq. (16), as input data of the 1,6-Dichlorohexene (x) + Dodecane (1-x) system: γ_1 = 1.2089 and γ_2 = 1.2649 and for the 1,5-Dichloropentane (x) + Dodecane (1-x) system: γ_1 = 1.2089 and γ_2 = 1.2855 for the pure components at the temperature of 298.15 K. The rest of the experimental measures ($\alpha_i, V_i, T_i, \kappa_{si}$) were reported by González-Salgado and coworkers(González-Salgado et al., 2004). In the Eqs. (13) to (15), $\bar{z}_i$, Q_i, and $\bar{J}$ were evaluated for each solution of Eq 17 was solved to obtain γ_i values for all temperatures and concentrations. Finally, we evaluated c_p, c_v and κ_τ using the γ_i values previously obtained.

Table 1
CAS registry number, suppliers, and purity.*

Component	CAS	Suppliers	Mol fraction
1,6-Dichlorohexene	2163-00-0	Sigma Aldrich	0.995
Dodecane	112-40-3	Sigma Aldrich	0.990
1,5-Dichloropentane	628-76-2	Sigma Aldrich	0.991

*The related information about chemical reagents were taken from the literature (González-Salgado et al., 2004).

4. Results and discussion

The semiempirical algorithm is based on the solid and well-grounded thermodynamic arguments. Based on this, it is possible to show that the heat capacity at constant pressure can be obtained by:

$$c_p = \lambda V\alpha \tag{4}$$

where λ, ***V*** and ***α*** are the caloric coefficient that measures the rate of change, of the caloric content with respect to the volume at constant pressure, the molar volume of the system and the coefficient of thermal expansibility.

Based on Eq. (1) and by analogy with Laplace's equation for adiabatic compressibility (κ_s), it is possible to express the isothermal compressibility (κ_τ), the heat capacity at constant pressure (c_p) and constant volume (c_v), using the following equations:

$$\kappa_{\tau i} = \frac{1}{\rho_i^{\xi_i}C_i^2} \tag{5}$$

$$c_{p_i} = z_i\alpha_i \tag{6}$$

$$c_{vi} = z_i^{y_i}\alpha_i \tag{7}$$

where ρ and c are the density and the speed of sound of the pure components or in the liquid mixture; the subscript i indicates that the variable is taken for each temperature. Here, ξ_i, z_i, y_i, and J are auxiliary functions defined using the adiabatic coefficient (γ) as follows:

$$\xi_i = 1 - \frac{ln\gamma_i}{ln\rho_i} \tag{8}$$

$$z_i = \gamma_i^{\frac{1}{1-y_i}} \tag{9}$$

$$y_i = \left(\frac{1}{\gamma_i}\right)^J \tag{10}$$

These (x, y, z, J) functions, are slightly temperature dependent at fixed concentration. J is characteristic of both, pure and mixed components, it is given by the expression:

$$J = -\frac{1}{Ln\gamma_i}Ln\left\{1 - \frac{Ln\gamma_i}{Ln\frac{\alpha_iV_iT_i}{(\gamma_i-1)\kappa_{si}}}\right\} \tag{11}$$

The Eq. (11) is in full agreement with the generalized Mayer equation(Güémez et al., 1995) for the isothermic compressibility.

On the other hand, empirical observations allowed us to infer that the J parameter, for a fixed concentration is approximately constant, this fact validates the use of the average ($\bar{J}$) instead of a specific J values. So, the determination of this parameter constitutes a key factor on which the development of this article is based. Therefore, we proposed to empirically evaluate this parameter from the following equation:

$$\bar{J} = -\frac{1}{Ln\left[1 + \frac{\alpha_iV_iT_i}{k_{si}Q_i}\right]}Ln\left\{1 - \frac{Ln\left[1 + \frac{\alpha_iV_iT_i}{k_{si}Q_i}\right]}{LnQ_i}\right\} \tag{12}$$

Table 2
Adiabatic coefficient (γ) estimated with Eq. (13), heat capacity at constant pressure (c_p), heat capacity at constant volume (c_v), and isothermal compressibility (κ_τ) of 1,6-Dichlorohexene system (x) + Dodecane (1-x) at different temperatures and concentrations.

T/K	γ^{exp}	γ^{est}	%error	C_p^{est}	%error	C_V^{est}	%error	κ_τ^{est}	%error
x_2 = 0.00000									
278.15	1.2129	1.2138	0.07	365.07	0.42	300.77	0.49	8.676E-10	0.07
283.15	1.2122	1.2127	0.05	367.52	0.26	303.06	0.30	8.970E-10	0.05
288.15	1.2113	1.2116	0.02	370.00	0.13	305.39	0.15	9.276E-10	0.02
293.15	1.2102	1.2103	0.01	372.51	0.06	307.79	0.07	9.594E-10	0.01
298.15	1.2089	1.2089	0.00	375.04	0.00	310.23	0.00	9.925E-10	0.00
303.15	1.2076	1.2075	0.01	377.60	0.05	312.72	0.05	1.027E-09	0.01
308.15	1.2060	1.2059	0.01	380.20	0.05	315.28	0.05	1.063E-09	0.01
313.15	1.2043	1.2043	0.00	382.82	0.02	317.88	0.03	1.100E-09	0.00
318.15	1.2026	1.2026	0.00	385.47	0.00	320.53	0.00	1.139E-09	0.00
323.15	1.2008	1.2008	0.01	388.15	0.04	323.23	0.04	1.179E-09	0.01
328.15	1.1987	1.1990	0.03	390.86	0.16	325.98	0.19	1.221E-09	0.03
x_2 = 0.04980									
278.15	1.2154	1.2156	0.02	358.89	0.09	295.25	0.10	8.601E-10	0.02
283.15	1.2145	1.2145	0.00	361.22	0.01	297.42	0.01	8.889E-10	0.00
288.15	1.2135	1.2133	0.02	363.57	0.09	299.65	0.10	9.192E-10	0.02
293.15	1.2122	1.2120	0.02	365.93	0.12	301.93	0.14	9.506E-10	0.02
298.15	1.2109	1.2106	0.03	368.33	0.16	304.26	0.19	9.833E-10	0.03
303.15	1.2094	1.2091	0.03	370.75	0.16	306.64	0.18	1.017E-09	0.03
308.15	1.2077	1.2075	0.02	373.21	0.13	309.09	0.15	1.053E-09	0.02
313.15	1.2060	1.2058	0.02	375.69	0.09	311.57	0.10	1.089E-09	0.02
318.15	1.2042	1.2041	0.01	378.19	0.03	314.09	0.04	1.128E-09	0.01
323.15	1.2022	1.2023	0.01	380.73	0.03	316.67	0.04	1.167E-09	0.01
328.15	1.2003	1.2004	0.01	383.29	0.08	319.30	0.09	1.209E-09	0.01
x_2 = 0.10030									
278.15	1.2164	1.2168	0.03	351.56	0.18	288.91	0.21	8.513E-10	0.03
283.15	1.2156	1.2158	0.02	353.81	0.11	291.00	0.13	8.798E-10	0.02
288.15	1.2145	1.2146	0.01	356.07	0.04	293.16	0.04	9.096E-10	0.01
293.15	1.2133	1.2133	0.00	358.37	0.00	295.37	0.00	9.406E-10	0.00
298.15	1.2119	1.2119	0.00	360.68	0.01	297.63	0.01	9.728E-10	0.00
303.15	1.2103	1.2103	0.00	363.02	0.01	299.93	0.02	1.006E-09	0.00
308.15	1.2087	1.2088	0.01	365.39	0.04	302.28	0.05	1.041E-09	0.01
313.15	1.2069	1.2071	0.02	367.79	0.09	304.69	0.11	1.077E-09	0.02
318.15	1.2051	1.2054	0.02	370.20	0.13	307.13	0.15	1.115E-09	0.02
323.15	1.2031	1.2035	0.03	372.66	0.19	309.63	0.22	1.154E-09	0.03
328.15	1.2011	1.2017	0.04	375.13	0.26	312.18	0.30	1.195E-09	0.04
x_2 = 0.14973									
278.15	1.2198	1.2193	0.04	346.17	0.22	283.91	0.26	8.428E-10	0.04
283.15	1.2189	1.2183	0.05	348.36	0.28	285.95	0.33	8.708E-10	0.05
288.15	1.2178	1.2170	0.06	350.57	0.35	288.05	0.41	9.003E-10	0.06
293.15	1.2165	1.2157	0.06	352.80	0.35	290.20	0.41	9.308E-10	0.06
298.15	1.2151	1.2143	0.07	355.06	0.37	292.40	0.44	9.627E-10	0.07
303.15	1.2135	1.2128	0.06	357.34	0.36	294.64	0.42	9.958E-10	0.06
308.15	1.2119	1.2112	0.05	359.65	0.32	296.94	0.37	1.030E-09	0.05
313.15	1.2101	1.2095	0.05	361.99	0.27	299.28	0.32	1.066E-09	0.05
318.15	1.2082	1.2078	0.03	364.35	0.20	301.66	0.24	1.103E-09	0.03
323.15	1.2062	1.2060	0.02	366.73	0.12	304.10	0.14	1.142E-09	0.02
328.15	1.2042	1.2041	0.01	369.14	0.04	306.57	0.04	1.182E-09	0.01
x_2 = 0.25271									
278.15	1.2243	1.2234	0.07	332.92	0.40	272.12	0.47	8.224E-10	0.07
283.15	1.2234	1.2224	0.08	334.97	0.42	274.02	0.50	8.495E-10	0.08
288.15	1.2222	1.2212	0.08	337.03	0.45	275.99	0.53	8.780E-10	0.08
293.15	1.2208	1.2199	0.08	339.12	0.44	277.99	0.52	9.075E-10	0.08
298.15	1.2194	1.2184	0.08	341.23	0.44	280.05	0.52	9.383E-10	0.08
303.15	1.2178	1.2169	0.07	343.36	0.42	282.15	0.49	9.703E-10	0.07
308.15	1.2161	1.2153	0.06	345.52	0.36	284.31	0.43	1.004E-09	0.06
313.15	1.2143	1.2137	0.05	347.70	0.31	286.49	0.36	1.038E-09	0.05
318.15	1.2124	1.2119	0.04	349.90	0.22	288.72	0.26	1.074E-09	0.04
323.15	1.2104	1.2101	0.03	352.13	0.15	291.00	0.17	1.111E-09	0.03
328.15	1.2082	1.2081	0.00	354.38	0.02	293.33	0.03	1.150E-09	0.00
x_2 = 0.40173									
278.15	1.2314	1.2303	0.10	313.91	0.51	255.2	0.61	7.889E-10	0.10
283.15	1.2303	1.2292	0.09	315.70	0.49	256.8	0.58	8.147E-10	0.09
288.15	1.2291	1.2279	0.09	317.51	0.50	258.6	0.60	8.416E-10	0.09
293.15	1.2276	1.2266	0.08	319.35	0.46	260.4	0.54	8.694E-10	0.08
298.15	1.2261	1.2251	0.08	321.20	0.44	262.2	0.52	8.985E-10	0.08
303.15	1.2244	1.2236	0.07	323.08	0.38	264.0	0.45	9.286E-10	0.07
308.15	1.2226	1.2219	0.06	324.97	0.32	266.0	0.37	9.599E-10	0.06
313.15	1.2207	1.2202	0.04	326.89	0.22	267.9	0.26	9.923E-10	0.04
318.15	1.2187	1.2184	0.02	328.82	0.13	269.9	0.15	1.026E-09	0.02

(continued on next page)

Table 2 (*continued*)

T/K	γ^{exp}	γ^{est}	%error	C_p^{est}	%error	C_V^{est}	%error	κ_τ^{est}	%error
323.15	1.2166	1.2165	0.00	330.78	0.02	271.9	0.02	1.061E-09	0.00
328.15	1.2143	1.2146	0.02	332.74	0.11	274.0	0.13	1.097E-09	0.02
x_2 = 0.50199									
278.15	1.2361	1.2350	0.09	300.73	0.48	243.5	0.57	7.639E-10	0.09
283.15	1.2350	1.2340	0.08	302.42	0.43	245.1	0.51	7.884E-10	0.08
288.15	1.2338	1.2328	0.08	304.12	0.43	246.7	0.51	8.141E-10	0.08
293.15	1.2324	1.2315	0.08	305.85	0.41	248.4	0.48	8.407E-10	0.08
298.15	1.2309	1.2301	0.07	307.59	0.37	250.1	0.44	8.684E-10	0.07
303.15	1.2292	1.2285	0.06	309.35	0.31	251.8	0.37	8.972E-10	0.06
308.15	1.2275	1.2269	0.04	311.13	0.24	253.6	0.29	9.271E-10	0.04
313.15	1.2256	1.2252	0.03	312.93	0.16	255.4	0.19	9.581E-10	0.03
318.15	1.2236	1.2235	0.01	314.74	0.06	257.3	0.07	9.902E-10	0.01
323.15	1.2215	1.2216	0.01	316.58	0.04	259.2	0.05	1.024E-09	0.01
328.15	1.2194	1.2196	0.02	318.42	0.12	261.1	0.14	1.058E-09	0.02
x_2 = 0.59998									
278.15	1.2421	1.2407	0.11	288.48	0.58	232.5	0.70	7.374E-10	0.11
283.15	1.2410	1.2397	0.11	289.98	0.57	233.9	0.68	7.607E-10	0.11
288.15	1.2397	1.2384	0.10	291.50	0.54	235.4	0.65	7.852E-10	0.10
293.15	1.2382	1.2371	0.09	293.03	0.48	236.9	0.58	8.104E-10	0.09
298.15	1.2366	1.2356	0.08	294.58	0.41	238.4	0.49	8.368E-10	0.08
303.15	1.2348	1.2341	0.06	296.15	0.32	240.0	0.39	8.641E-10	0.06
308.15	1.2329	1.2324	0.04	297.73	0.22	241.6	0.26	8.924E-10	0.04
313.15	1.2309	1.2307	0.02	299.33	0.11	243.2	0.13	9.218E-10	0.02
318.15	1.2288	1.2289	0.00	300.94	0.01	244.9	0.01	9.522E-10	0.00
323.15	1.2266	1.2270	0.03	302.57	0.14	246.6	0.17	9.839E-10	0.03
328.15	1.2242	1.2250	0.06	304.21	0.32	248.3	0.38	1.017E-09	0.06
x_2 = 0.70111									
278.15	1.2482	1.2467	0.11	275.29	0.58	220.8	0.70	7.078E-10	0.11
283.15	1.2472	1.2458	0.11	276.67	0.58	222.1	0.70	7.298E-10	0.11
288.15	1.2459	1.2446	0.10	278.06	0.53	223.4	0.63	7.529E-10	0.10
293.15	1.2443	1.2432	0.09	279.47	0.45	224.8	0.54	7.768E-10	0.09
298.15	1.2427	1.2418	0.07	280.89	0.37	226.2	0.44	8.016E-10	0.07
303.15	1.2409	1.2402	0.05	282.33	0.28	227.6	0.33	8.274E-10	0.05
308.15	1.2390	1.2386	0.03	283.78	0.15	229.1	0.18	8.542E-10	0.03
313.15	1.2370	1.2369	0.01	285.24	0.03	230.6	0.04	8.818E-10	0.01
318.15	1.2349	1.2351	0.02	286.72	0.10	232.1	0.12	9.104E-10	0.02
323.15	1.2326	1.2332	0.04	288.22	0.23	233.7	0.28	9.403E-10	0.04
328.15	1.2303	1.2312	0.07	289.71	0.37	235.3	0.44	9.711E-10	0.07
x_2 = 0.79862									
278.15	1.2561	1.2539	0.18	263.25	0.87	209.9	1.05	6.777E-10	0.18
283.15	1.2549	1.2529	0.16	264.43	0.79	211.1	0.95	6.984E-10	0.16
288.15	1.2533	1.2516	0.14	265.64	0.68	212.2	0.82	7.202E-10	0.14
293.15	1.2516	1.2503	0.11	266.85	0.55	213.4	0.66	7.426E-10	0.11
298.15	1.2499	1.2488	0.09	268.07	0.44	214.7	0.53	7.659E-10	0.09
303.15	1.2479	1.2472	0.06	269.31	0.30	215.9	0.36	7.901E-10	0.06
308.15	1.2458	1.2455	0.03	270.56	0.15	217.2	0.18	8.151E-10	0.03
313.15	1.2437	1.2437	0.00	271.82	0.02	218.6	0.02	8.410E-10	0.00
318.15	1.2414	1.2418	0.04	273.09	0.19	219.9	0.22	8.678E-10	0.04
323.15	1.2390	1.2399	0.07	274.38	0.36	221.3	0.43	8.957E-10	0.07
328.15	1.2365	1.2378	0.11	275.66	0.55	222.7	0.66	9.244E-10	0.11
x_2 = 0.89982									
278.15	1.2637	1.2615	0.17	250.00	0.84	198.2	1.02	6.441E-10	0.17
283.15	1.2621	1.2604	0.13	250.97	0.64	199.1	0.78	6.634E-10	0.13
288.15	1.2603	1.2591	0.10	251.95	0.48	200.1	0.57	6.837E-10	0.10
293.15	1.2584	1.2576	0.06	252.94	0.28	201.1	0.34	7.045E-10	0.06
298.15	1.2563	1.2561	0.02	253.93	0.10	202.2	0.12	7.262E-10	0.02
303.15	1.2542	1.2544	0.01	254.94	0.07	203.2	0.08	7.485E-10	0.01
308.15	1.2519	1.2526	0.05	255.95	0.26	204.3	0.32	7.718E-10	0.05
313.15	1.2496	1.2507	0.09	256.98	0.46	205.5	0.56	7.958E-10	0.09
318.15	1.2471	1.2488	0.14	258.00	0.68	206.6	0.81	8.205E-10	0.14
323.15	1.2445	1.2468	0.18	259.05	0.91	207.8	1.08	8.462E-10	0.18
328.15	1.2419	1.2446	0.22	260.09	1.12	209.0	1.34	8.728E-10	0.22
x_2 = 0.94934									
278.15	1.2683	1.2659	0.19	243.83	0.90	192.6	1.09	6.272E-10	0.19
283.15	1.2669	1.2649	0.16	244.73	0.77	193.5	0.93	6.458E-10	0.16
288.15	1.2650	1.2635	0.12	245.65	0.58	194.4	0.70	6.652E-10	0.12
293.15	1.2630	1.2621	0.08	246.57	0.37	195.4	0.44	6.854E-10	0.08
298.15	1.2609	1.2605	0.03	247.51	0.17	196.4	0.20	7.062E-10	0.03
303.15	1.2588	1.2589	0.01	248.45	0.03	197.4	0.03	7.277E-10	0.01
308.15	1.2565	1.2571	0.05	249.39	0.24	198.4	0.29	7.500E-10	0.05
313.15	1.2541	1.2552	0.09	250.35	0.46	199.4	0.55	7.730E-10	0.09
318.15	1.2516	1.2533	0.14	251.31	0.68	200.5	0.81	7.968E-10	0.14

Table 2 (*continued*)

T/K	γ^{exp}	γ^{est}	%error	C_p^{est}	%error	C_V^{est}	%error	κ_τ^{est}	%error
323.15	1.2490	1.2513	0.18	252.29	0.90	201.6	1.07	8.215E-10	0.18
328.15	1.2463	1.2491	0.23	253.26	1.14	202.7	1.36	8.470E-10	0.23
x_2 = 0.96911									
278.15	1.2702	1.2677	0.20	241.36	0.93	190.4	1.13	6.204E-10	0.20
283.15	1.2688	1.2667	0.17	242.28	0.79	191.3	0.95	6.387E-10	0.17
288.15	1.2670	1.2654	0.13	243.22	0.61	192.2	0.74	6.579E-10	0.13
293.15	1.2652	1.2641	0.09	244.16	0.42	193.2	0.51	6.777E-10	0.09
298.15	1.2632	1.2625	0.05	245.11	0.24	194.1	0.29	6.982E-10	0.05
303.15	1.2611	1.2609	0.01	246.08	0.07	195.2	0.09	7.195E-10	0.01
308.15	1.2589	1.2592	0.03	247.05	0.13	196.2	0.16	7.414E-10	0.03
313.15	1.2565	1.2574	0.07	248.03	0.33	197.3	0.40	7.641E-10	0.07
318.15	1.2541	1.2555	0.11	249.01	0.54	198.3	0.65	7.876E-10	0.11
323.15	1.2516	1.2535	0.15	250.01	0.75	199.4	0.90	8.119E-10	0.15
328.15	1.2490	1.2514	0.20	251.00	0.98	200.6	1.17	8.370E-10	0.20
x_2 = 1.00000									
278.15	1.2723	1.2701	0.17	237.00	0.82	186.6	0.99	6.094E-10	0.17
283.15	1.2705	1.2691	0.12	237.89	0.55	187.5	0.66	6.272E-10	0.12
288.15	1.2688	1.2678	0.08	238.78	0.37	188.3	0.45	6.460E-10	0.08
293.15	1.2669	1.2664	0.04	239.69	0.18	189.3	0.22	6.653E-10	0.04
298.15	1.2649	1.2649	0.00	240.60	0.00	190.2	0.00	6.853E-10	0.00
303.15	1.2629	1.2633	0.04	241.52	0.17	191.2	0.21	7.059E-10	0.04
308.15	1.2606	1.2616	0.08	242.45	0.38	192.2	0.46	7.273E-10	0.08
313.15	1.2583	1.2598	0.12	243.39	0.58	193.2	0.70	7.494E-10	0.12
318.15	1.2559	1.2579	0.16	244.33	0.79	194.2	0.95	7.722E-10	0.16
323.15	1.2534	1.2560	0.20	245.29	1.00	195.3	1.20	7.959E-10	0.20
328.15	1.2510	1.2539	0.23	246.23	1.12	196.4	1.35	8.202E-10	0.23

*The measurement used in this work were determined under pressure of 0.1 MPa. The standard uncertainties u are u(p) = 0.04 MPa for pressure, u(T) = 4.07 K for temperature , u(x) = 0.5946 for molar fraction (0.68 level of confidence).

Here $\bar{J}$ indicates that the average at fixed concentration of the mixture, where Q is is given by:

$$Q_i = \frac{\bar{z}_i\alpha_i + 2x_1x_2 ln\left(z_1^0\alpha_1^0/z_2^0\alpha_2^0\right) ln\left(z_1^0\alpha_1^0 z_2^0\alpha_2^0\right)}{\alpha_i} \quad (13)$$

$$\bar{z}_i = z_1^0 e^{x_2 Ln\left(\frac{z_2^0}{z_1^0}\right)} \ \text{with} z_2^0 < z_1^0 \quad (14)$$

where x_i is the mole fraction of the i-th component and z_i^0 is an input parameter, characteristic of the pure components, which is defined by Eq. (15) and is evaluated from the experimental data: $\alpha_i, V_i, T_i, \kappa_{si}$ and γ_i, which were taken from pure components at a specific temperature of the studied interval, more exactly approximately an average temperature of the studied interval. In this work, the temperature interval is between (278.15–328.15) K, with an increase of 5 K. The used of the previously mentioned value at a temperature of 298.15 K for both pure components give:

$$z_i^0 = \frac{\alpha_i^0 V_i^0 T}{(\gamma_i^0 - 1)k_{si}^0} \quad (15)$$

The prediction of the adiabatic coefficient (γ_i) at any temperature can then be reached by solving the Eq. (16).

$$f(\gamma_i) = \bar{J} + \frac{1}{Ln\gamma_i} Ln\left\{1 - \frac{Ln\gamma_i}{Ln\frac{\alpha_i V_i T_i}{(\gamma_i - 1)\kappa_{si}}}\right\} = 0 \quad (16)$$

Which results from equating Eqs. (12) and (13). Eq. (17) can be applied to both components, pure and mixed components. In this context, the problem is reduced to finding the value of γ_i that is a solution of Eq. (17) at all temperatures and concentrations of the different binary liquid mixtures. The resolution of Eq. (17) was solved by numerical manipulation. The results obtained are reported in Tables 2 and 3, for the pure liquids and their mixtures

The results obtained are in excellent agreement with the experimental results, obtaining for: γ, c_p, c_v, and κ_τ a percentage of absolute error with respect to the 1,6-Dichlorohexene (x) + Dodecane (1-x) system is practically below 1 at all concentrations. While with respect to the 1,5-Dichloropentane (x) + Dodecane (1-x) system, this was also practically below unity at all concentrations except for c_v, where the percentage of error in some concentrations was around two units.

5. Conclusion

A semiempirical algorithm was developed to evaluate the adiabatic coefficient, heat capacities and isothermal compressibility of binary liquid mixtures from acoustic and volumetric data. Mathematical developments were obtained using Laplace's equation and Mayer's Relationship. The new method was implemented with the systems (1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane in the entire concentration range and temperatures between (278.15–328.15) K. This algorithm is an easy protocol to implement, and represents an alternative to complement the results obtained from volumetric and acoustic data. The proposed model is not universal. However, it works well for mixtures and pure compounds whose product of density and the nth root of adiabatic compressibility is highly independent of temperature; In addition, it can be applied throughout a wide concentration and temperature range, and give information about 4 parameters (γ^{est}, C_p^{est}, C_V^{est}, κ_τ^{est}). Information that other models do not provide

Table 3
Adiabatic coefficient (γ) estimated with Eq. (13), heat capacity at constant pressure (c_p), heat capacity at constant volume (c_v), and isothermal compressibility (κ_τ) of 1,5-Dichloropentane(x) + Dodecane(1-x) at different temperatures and concentrations.

T/K	γ^{exp}	γ^{est}	%error	C_p^{est}	%error	C_V^{est}	%error	$\kappa_\tau{}^{est}$	%error
x_2 = 0.00000									
278.15	1.2129	1.2138	0.07	365.07	0.42	300.77	0.49	8.676E-10	0.07
283.15	1.2122	1.2127	0.05	367.52	0.26	303.05	0.30	8.970E-10	0.05
288.15	1.2113	1.2116	0.02	370.00	0.13	305.39	0.15	9.276E-10	0.02
293.15	1.2102	1.2103	0.01	372.51	0.06	307.78	0.07	9.594E-10	0.01
298.15	1.2089	1.2089	0.00	375.04	0.00	310.22	0.00	9.925E-10	0.00
303.15	1.2076	1.2075	0.01	377.60	0.05	312.72	0.05	1.027E-09	0.01
308.15	1.2060	1.2059	0.01	380.20	0.05	315.27	0.05	1.063E-09	0.01
313.15	1.2044	1.2043	0.00	382.82	0.02	317.88	0.03	1.100E-09	0.00
318.15	1.2026	1.2026	0.00	385.47	0.00	320.53	0.00	1.139E-09	0.00
323.15	1.2008	1.2009	0.01	388.15	0.04	323.23	0.04	1.179E-09	0.01
328.15	1.1987	1.1990	0.03	390.86	0.16	325.98	0.19	1.221E-09	0.03
x_2 = 0.05237									
278.15	1.2147	1.2159	0.10	355.55	0.57	291.89	0.85	8.616E-10	0.10
283.15	1.2138	1.2148	0.08	357.81	0.47	294.02	0.73	8.907E-10	0.08
288.15	1.2128	1.2136	0.07	360.10	0.38	296.20	0.62	9.209E-10	0.07
293.15	1.2115	1.2122	0.06	362.41	0.33	298.44	0.56	9.524E-10	0.06
298.15	1.2101	1.2108	0.05	364.75	0.31	300.72	0.54	9.852E-10	0.05
303.15	1.2086	1.2093	0.06	367.10	0.32	303.05	0.55	1.019E-09	0.06
308.15	1.2069	1.2076	0.06	369.49	0.35	305.44	0.58	1.055E-09	0.06
313.15	1.2051	1.2059	0.07	371.90	0.40	307.87	0.64	1.092E-09	0.07
318.15	1.2032	1.2042	0.08	374.34	0.46	310.35	0.70	1.130E-09	0.08
323.15	1.2013	1.2023	0.09	376.81	0.53	312.87	0.79	1.170E-09	0.09
328.15	1.1991	1.2005	0.11	379.32	0.65	315.45	0.92	1.211E-09	0.11
x_2 = 0.10136									
278.15	1.2172	1.2183	0.09	347.21	0.51	284.04	0.94	8.553E-10	0.09
283.15	1.2162	1.2172	0.09	349.43	0.48	286.12	0.90	8.840E-10	0.09
288.15	1.2151	1.2160	0.07	351.68	0.42	288.25	0.82	9.140E-10	0.07
293.15	1.2139	1.2147	0.07	353.96	0.38	290.44	0.78	9.452E-10	0.07
298.15	1.2125	1.2132	0.06	356.24	0.36	292.67	0.75	9.777E-10	0.06
303.15	1.2110	1.2117	0.06	358.56	0.35	294.95	0.73	1.011E-09	0.06
308.15	1.2093	1.2101	0.07	360.91	0.38	297.28	0.77	1.047E-09	0.07
313.15	1.2075	1.2084	0.07	363.28	0.43	299.67	0.82	1.083E-09	0.07
318.15	1.2056	1.2066	0.08	365.68	0.49	302.09	0.89	1.121E-09	0.08
323.15	1.2037	1.2048	0.09	368.10	0.56	304.56	0.96	1.161E-09	0.09
328.15	1.2015	1.2029	0.11	370.56	0.68	307.08	1.11	1.202E-09	0.11
x_2 = 0.20075									
278.15	1.2220	1.2238	0.14	331.04	0.77	268.84	1.52	8.405E-10	0.14
283.15	1.2215	1.2227	0.09	333.14	0.51	270.80	1.21	8.686E-10	0.09
288.15	1.2205	1.2215	0.08	335.27	0.45	272.81	1.14	8.980E-10	0.08
293.15	1.2192	1.2201	0.07	337.42	0.41	274.86	1.09	9.285E-10	0.07
298.15	1.2178	1.2187	0.07	339.58	0.40	276.96	1.07	9.602E-10	0.07
303.15	1.2163	1.2171	0.07	341.78	0.38	279.12	1.04	9.932E-10	0.07
308.15	1.2146	1.2155	0.08	344.00	0.43	281.32	1.09	1.028E-09	0.08
313.15	1.2128	1.2138	0.08	346.24	0.47	283.57	1.14	1.063E-09	0.08
318.15	1.2109	1.2120	0.09	348.51	0.52	285.86	1.20	1.100E-09	0.09
323.15	1.2083	1.2101	0.15	350.80	0.87	288.19	1.60	1.139E-09	0.15
328.15	1.2063	1.2082	0.16	353.12	0.92	290.57	1.65	1.179E-09	0.16
x_2 = 0.30395									
278.15	1.2277	1.2296	0.15	314.17	0.80	253.31	1.80	8.219E-10	0.15
283.15	1.2267	1.2284	0.14	316.08	0.75	255.10	1.74	8.493E-10	0.14
288.15	1.2256	1.2272	0.13	318.01	0.72	256.93	1.70	8.777E-10	0.13
293.15	1.2243	1.2258	0.13	319.96	0.69	258.81	1.65	9.073E-10	0.13
298.15	1.2228	1.2243	0.13	321.93	0.69	260.74	1.65	9.381E-10	0.13
303.15	1.2212	1.2227	0.13	323.92	0.69	262.70	1.64	9.701E-10	0.13
308.15	1.2194	1.2211	0.13	325.94	0.74	264.72	1.70	1.003E-09	0.13
313.15	1.2175	1.2193	0.14	327.97	0.80	266.77	1.76	1.038E-09	0.14
318.15	1.2155	1.2174	0.16	330.03	0.87	268.87	1.84	1.074E-09	0.16
323.15	1.2135	1.2155	0.17	332.12	0.94	271.01	1.91	1.111E-09	0.17
328.15	1.2114	1.2135	0.18	334.22	1.00	273.18	1.97	1.150E-09	0.18
x_2 = 0.3945									
278.15	1.2337	1.2356	0.15	300.38	0.80	240.64	1.96	8.037E-10	0.15
283.15	1.2328	1.2345	0.13	302.18	0.70	242.31	1.84	8.302E-10	0.13
288.15	1.2317	1.2332	0.12	304.01	0.65	244.04	1.76	8.578E-10	0.12
293.15	1.2303	1.2319	0.12	305.84	0.65	245.80	1.76	8.866E-10	0.12
298.15	1.2290	1.2304	0.11	307.71	0.61	247.61	1.71	9.164E-10	0.11
303.15	1.2274	1.2288	0.12	309.58	0.62	249.46	1.72	9.475E-10	0.12
308.15	1.2256	1.2271	0.12	311.49	0.66	251.36	1.75	9.798E-10	0.12
313.15	1.2237	1.2253	0.13	313.41	0.72	253.29	1.82	1.013E-09	0.13
318.15	1.2217	1.2234	0.14	315.35	0.79	255.27	1.89	1.048E-09	0.14

Table 3 (*continued*)

T/K	γ^{exp}	γ^{est}	%error	C_p^{est}	%error	C_V^{est}	%error	$\kappa_\tau{}^{est}$	%error
323.15	1.2196	1.2215	0.16	317.32	0.86	257.28	1.97	1.085E-09	0.16
328.15	1.2173	1.2195	0.18	319.30	0.99	259.33	2.12	1.122E-09	0.18
x_2 = 0.49832									
278.15	1.2406	1.2426	0.16	284.24	0.80	226.18	2.06	7.795E-10	0.16
283.15	1.2395	1.2414	0.15	285.86	0.79	227.69	2.05	8.049E-10	0.15
288.15	1.2384	1.2401	0.14	287.50	0.74	229.25	1.98	8.314E-10	0.14
293.15	1.2369	1.2387	0.15	289.15	0.75	230.85	1.99	8.590E-10	0.15
298.15	1.2354	1.2372	0.14	290.82	0.75	232.48	1.98	8.876E-10	0.14
303.15	1.2337	1.2355	0.15	292.50	0.77	234.16	2.00	9.174E-10	0.15
308.15	1.2318	1.2338	0.16	294.21	0.83	235.87	2.07	9.484E-10	0.16
313.15	1.2299	1.2319	0.17	295.93	0.89	237.63	2.12	9.806E-10	0.17
318.15	1.2279	1.2300	0.17	297.68	0.90	239.41	2.13	1.014E-09	0.17
323.15	1.2256	1.2280	0.19	299.45	1.04	241.24	2.28	1.049E-09	0.19
328.15	1.2236	1.2259	0.19	301.21	1.05	243.09	2.28	1.085E-09	0.19
x_2 = 0.60144									
278.15	1.2485	1.2502	0.14	268.52	0.68	212.33	1.94	7.519E-10	0.14
283.15	1.2476	1.2491	0.13	270.02	0.63	213.72	1.88	7.762E-10	0.13
288.15	1.2464	1.2479	0.12	271.55	0.60	215.16	1.84	8.014E-10	0.12
293.15	1.2450	1.2465	0.12	273.09	0.62	216.63	1.85	8.277E-10	0.12
298.15	1.2435	1.2450	0.12	274.66	0.61	218.15	1.84	8.550E-10	0.12
303.15	1.2418	1.2433	0.12	276.23	0.63	219.70	1.85	8.834E-10	0.12
308.15	1.2400	1.2416	0.13	277.82	0.68	221.29	1.90	9.129E-10	0.13
313.15	1.2380	1.2398	0.14	279.43	0.73	222.92	1.96	9.435E-10	0.14
318.15	1.2359	1.2378	0.15	281.06	0.80	224.58	2.03	9.753E-10	0.15
323.15	1.2338	1.2358	0.17	282.70	0.87	226.27	2.10	1.008E-09	0.17
328.15	1.2315	1.2338	0.18	284.35	0.97	227.99	2.21	1.043E-09	0.18
x_2 = 0.69872									
278.15	1.2572	1.2584	0.09	253.92	0.45	199.65	1.60	7.228E-10	0.09
283.15	1.2561	1.2572	0.09	255.27	0.44	200.90	1.58	7.458E-10	0.09
288.15	1.2548	1.2559	0.09	256.63	0.45	202.19	1.58	7.698E-10	0.09
293.15	1.2533	1.2545	0.10	258.00	0.47	203.51	1.61	7.947E-10	0.10
298.15	1.2517	1.2530	0.11	259.39	0.52	204.87	1.66	8.205E-10	0.11
303.15	1.2500	1.2513	0.11	260.80	0.54	206.27	1.67	8.474E-10	0.11
308.15	1.2480	1.2495	0.12	262.22	0.61	207.70	1.75	8.752E-10	0.12
313.15	1.2460	1.2477	0.14	263.66	0.68	209.17	1.83	9.042E-10	0.14
318.15	1.2438	1.2457	0.15	265.10	0.76	210.66	1.91	9.342E-10	0.15
323.15	1.2416	1.2436	0.17	266.57	0.85	212.19	2.01	9.654E-10	0.17
328.15	1.2393	1.2415	0.18	268.04	0.92	213.73	2.09	9.977E-10	0.18
x_2 = 0.79749									
278.15	1.2664	1.2672	0.06	238.81	0.28	186.83	1.20	6.895E-10	0.06
283.15	1.2653	1.2661	0.07	240.08	0.31	187.99	1.23	7.112E-10	0.07
288.15	1.2641	1.2649	0.06	241.37	0.29	189.19	1.21	7.337E-10	0.06
293.15	1.2627	1.2636	0.07	242.67	0.32	190.42	1.23	7.571E-10	0.07
298.15	1.2612	1.2621	0.07	243.99	0.32	191.68	1.23	7.814E-10	0.07
303.15	1.2596	1.2605	0.07	245.32	0.35	192.99	1.26	8.066E-10	0.07
308.15	1.2577	1.2588	0.09	246.66	0.41	194.32	1.33	8.328E-10	0.09
313.15	1.2558	1.2569	0.09	248.03	0.46	195.68	1.38	8.600E-10	0.09
318.15	1.2536	1.2550	0.11	249.39	0.53	197.07	1.46	8.882E-10	0.11
323.15	1.2515	1.2530	0.12	250.78	0.59	198.50	1.52	9.174E-10	0.12
328.15	1.2493	1.2509	0.13	252.17	0.65	199.94	1.60	9.477E-10	0.13
x_2 = 0.9021									
278.15	1.2802	1.2794	0.06	224.06	0.29	174.25	0.16	6.510E-10	0.06
283.15	1.2789	1.2782	0.06	225.06	0.26	175.20	0.18	6.710E-10	0.06
288.15	1.2773	1.2768	0.04	226.08	0.17	176.18	0.29	6.918E-10	0.04
293.15	1.2755	1.2753	0.02	227.11	0.08	177.20	0.40	7.134E-10	0.02
298.15	1.2736	1.2736	0.00	228.15	0.01	178.24	0.50	7.357E-10	0.00
303.15	1.2716	1.2719	0.02	229.20	0.08	179.32	0.59	7.590E-10	0.02
308.15	1.2694	1.2700	0.04	230.25	0.21	180.42	0.74	7.830E-10	0.04
313.15	1.2671	1.2680	0.07	231.33	0.33	181.55	0.88	8.080E-10	0.07
318.15	1.2647	1.2659	0.10	232.40	0.46	182.70	1.04	8.338E-10	0.10
323.15	1.2622	1.2637	0.12	233.49	0.58	183.88	1.18	8.606E-10	0.12
328.15	1.2595	1.2614	0.15	234.58	0.73	185.07	1.36	8.882E-10	0.15
x_2 = 0.94974									
278.15	1.2863	1.2852	0.09	217.05	0.41	168.42	0.22	6.319E-10	0.09
283.15	1.2849	1.2840	0.08	217.99	0.34	169.31	0.14	6.512E-10	0.08
288.15	1.2833	1.2826	0.05	218.95	0.25	170.23	0.02	6.712E-10	0.05
293.15	1.2816	1.2811	0.04	219.91	0.17	171.19	0.07	6.919E-10	0.04
298.15	1.2796	1.2794	0.02	220.89	0.07	172.17	0.19	7.134E-10	0.02
303.15	1.2776	1.2777	0.00	221.87	0.01	173.18	0.29	7.357E-10	0.00
308.15	1.2754	1.2758	0.03	222.87	0.12	174.21	0.42	7.587E-10	0.03
313.15	1.2731	1.2738	0.05	223.87	0.24	175.27	0.56	7.827E-10	0.05
318.15	1.2707	1.2717	0.08	224.88	0.37	176.36	0.71	8.074E-10	0.08

(*continued on next page*)

Table 3 (*continued*)

T/K	γ^{exp}	γ^{est}	%error	C_p^{est}	%error	C_V^{est}	%error	$\kappa_\tau{}^{est}$	%error
323.15	1.2681	1.2695	0.10	225.90	0.49	177.47	0.87	8.331E-10	0.10
328.15	1.2656	1.2672	0.13	226.92	0.61	178.59	1.00	8.595E-10	0.13
x_2 = 1.00000									
278.15	1.2928	1.2915	0.10	209.57	0.45	162.27	0.55	6.110E-10	0.10
283.15	1.2913	1.2903	0.08	210.40	0.36	163.07	0.44	6.294E-10	0.08
288.15	1.2895	1.2888	0.05	211.24	0.24	163.90	0.30	6.485E-10	0.05
293.15	1.2875	1.2872	0.02	212.09	0.09	164.76	0.11	6.683E-10	0.02
298.15	1.2855	1.2855	0.00	212.94	0.00	165.64	0.00	6.888E-10	0.00
303.15	1.2833	1.2837	0.03	213.80	0.12	166.55	0.15	7.100E-10	0.03
308.15	1.2810	1.2817	0.05	214.67	0.25	167.49	0.30	7.320E-10	0.05
313.15	1.2786	1.2796	0.08	215.55	0.38	168.45	0.47	7.547E-10	0.08
318.15	1.2760	1.2775	0.11	216.43	0.52	169.42	0.63	7.783E-10	0.11
323.15	1.2734	1.2752	0.14	217.33	0.65	170.43	0.79	8.026E-10	0.14
328.15	1.2706	1.2729	0.17	218.22	0.81	171.44	0.98	8.277E-10	0.17

*The measurement used in this work were determined under pressure of 0.1 MPa. The standard uncertainties u are u(p) = 0.04 MPa for pressure, u(T) = 4.07 K for temperature, u(x) = 0.5946 for molar fraction (0.68 level of confidence).

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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