Influence of ionic liquid on polar organic compounds solubility in dense CO_2 phase

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HIGHLIGHTS

- solubility of 1,2-butanediol and butylene carbonate in dense CO_2.
- phase behaviour of ternary and quaternary CO_2-IL biphasic mixtures.
- 1-hexyl-3-methylimidazolium tris(pentafluoroalkyl)trifluorophosphate ionic liquid as solubility modifier.

GRAPHICAL ABSTRACT
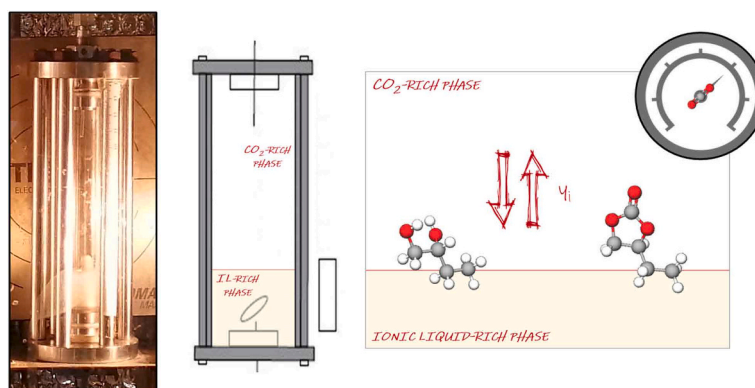
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ABSTRACT

Accurate measurement and prediction of the phase behaviour of mixtures involved in a chemical process are crucial for its optimisation. Given the importance of CO_2 conversion technologies and considering possible benefits of CO_2-ionic liquid biphasic systems, i.e., facilitating a product separation, we investigated the high-pressure behaviour of components of interest in a recently developed process of cyclic carbonate synthesis directly from CO_2 and potentially bio-based alcohols. The solubility of 1,2-butanediol and 1,2-butylene carbonate in a dense carbon dioxide phase was determined experimentally at the temperature of 313.2 K and pressures between 6 and 18 MPa. The influence of 1-hexyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate ionic liquid, [hmim][FAP], as a solvent, on the solubility of these compounds in CO_2-rich phase, in ternary (CO_2 + 1,2-butanediol + [hmim][FAP]), CO_2 + butylene carbonate + [hmim][FAP]) and quaternary (CO_2 + 1,2-butanediol + butylene carbonate + [hmim][FAP]) mixtures was investigated. The experimental results of the two binary systems were correlated using the density-based Chrastil equation. The knowledge of phase equilibria

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behaviours reported in this work will be useful for designing chemical conversions of carbon dioxide using [hmim][FAP] ionic liquid as reaction solvents.

1. Introduction

Increasing demand for biodegradable plastic materials revived the interest in aliphatic polycarbonates due to their biocompatibility and low toxicity [1,2]. Virtually ignored in the role of thermoplastics due to their poor thermal stability and high susceptibility to hydrolysis, aliphatic polycarbonates attracted increasing attention in biomedical fields. They can be degraded in vivo by surface erosion into neutral diols and carbon dioxide, in contrast to aliphatic polyesters, i.e., poly(lactic acid) – PLA, poly(lactic-co-glycolic acid) – PLGA, or poly(ε-caprolactone) – PCL, which upon decomposition give rise to diols and carboxylic acids leading to increased acidity of the surrounding tissue and inflammatory response, or affecting the loaded drug [3].

Aliphatic polycarbonates can be synthesised either by condensation polymerisation of dialkyl or diphenyl carbonate and aliphatic diols, copolymerisation of carbon dioxide with epoxides or by ring-opening polymerisation (ROP) of cyclic carbonates [4,5]. Cyclic carbonates themselves can be produced through a coupling reaction of carbon dioxide and cyclic ethers such as oxiranes or oxetanes, with alternative pathways including, i.e., carboxylation of olefins with carbon dioxide or

transformation of diols: transesterification with dialkyl carbonate/urea, oxidative carbonylation with carbon monoxide, or diols dehydrative condensation with carbon dioxide [6–8]. The last method is particularly relevant as it satisfies the requirements of green chemistry, such as lower production costs (single-step reaction) and eco-friendly properties (hazardless reagents and water as the sole by-product). Moreover, it involves carbon dioxide conversion, which gains further advantages in light of global concerns over greenhouse gas pollution and means to alleviate the shortage in conventional petroleum fuel supplies [9,10].

High-pressure CO_2 combined with an ionic liquid in a biphasic system has been proposed as an efficient and greener medium for many chemical processes [11–13], owing to the peculiar phase behaviour of ($scCO_2$+IL) mixtures first described by Brennecke and co-workers [14]. While the solubility of carbon dioxide in the ionic liquid-rich phase is significant, the molten salt does not dissolve in the pure carbon dioxide phase, even at high pressures. The discovery of this phenomenon led to a new method to separate ionic liquid from organic solvent [15–17], using CO_2 as a separation switch. As a further advance, high-pressure CO_2 allowed for an attractive integration of chemical reaction and separation unit operations by extracting the desired product from the ionic liquid
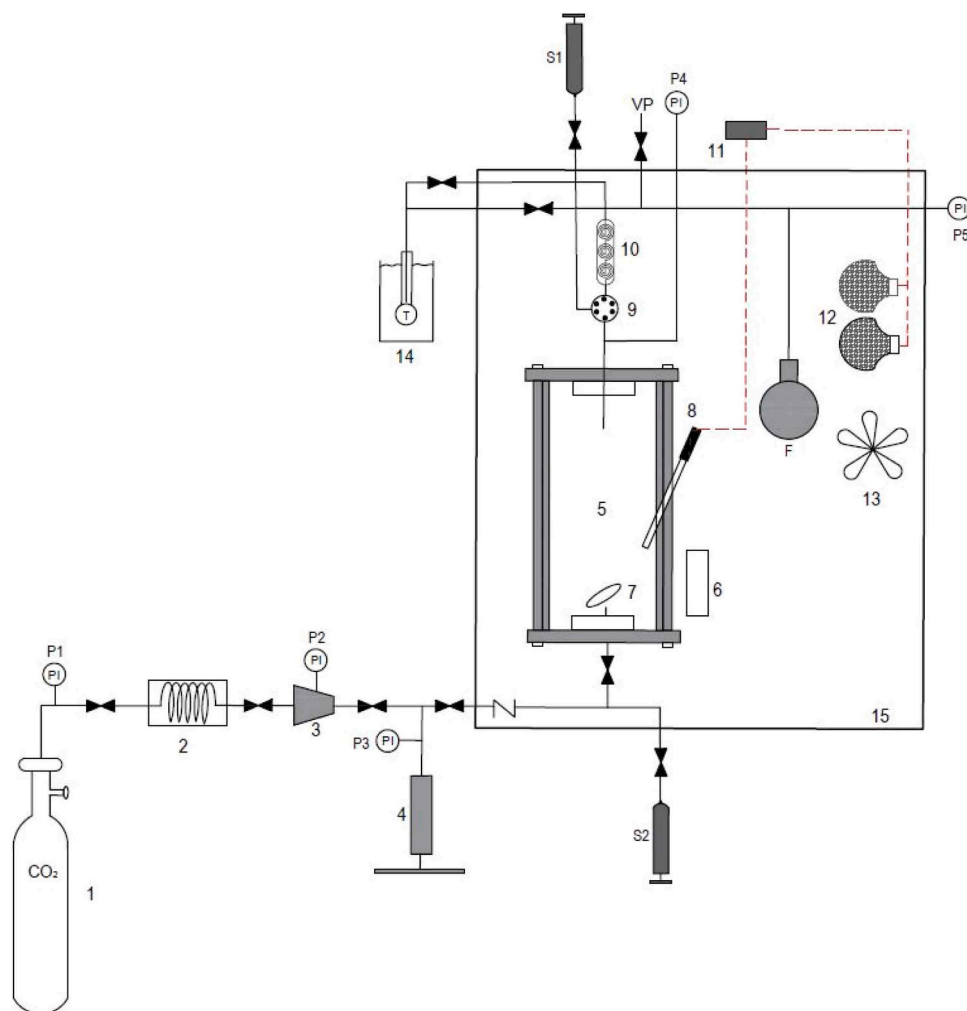
Fig. 1. Scheme of the experimental apparatus: 1 – CO_2 tank; 2 - ice bath; 3 – compressor; 4 – manual compressor; 5 – high-pressure cell; 6 – magnetic stirrer; 7 – magnetic stirring bar; 8 – temperature probe; 9 – HPLC valve; 10 – sampling loop; 11 – temperature controller; 12 – heating lamps; 13 – ventilator; 14 – ice bath; 15 – air bath; T – glass trap; F – calibrated expansion volume flask; VP – vacuum pump; P1 – P5 – pressure indicator; S1 and S2 – washing syringes.

phase, leaving behind not only ionic liquid but also the catalyst to reuse, permitting thus a continuous mode of operation.

In this context, in our ongoing project, we explore the possibility of synthesis of cyclic carbonates through a direct coupling of CO_2 and potentially biomass-derived alcohols in a biphasic system comprising one of the most CO_2-philic ionic liquid with physical absorption mechanism – 1-hexyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate, [hmim][FAP] [18,19]. This work discusses the influence of the ionic liquid on the solubility of cyclic carbonate and diol in the CO_2-dense phase. Here, the phase behaviours of binary, ternary, and quaternary mixtures containing dense carbon dioxide, [hmim][FAP], 1,2-butanediol (1,2-BDO) and/or corresponding butylene carbonate (BC) are reported at 313.2 K and pressures between 6 and 18 MPa. High-pressure fluid-phase equilibrium studies of (scCO$_2$ +IL) systems continue to play a secondary role in the undergoing research on carbon dioxide - ionic liquids interactions, and the data is limited, particularly for multicomponent mixtures [20,21]. To the best of our knowledge, the high-pressure solubility data of these organic compounds in (CO_2 +IL) multicomponent systems has not been reported in the literature.

2. Materials and methods

2.1. Materials

1,2-butanediol and butylene carbonate (4-ethyl-1,3-dioxolan-2-one) ($\geq$ 98.0 % purity) were purchased from Fluka Analytical and Fluorochem, respectively, and dried over molecular sieves (Fluka Analytical, 0.3 nm pore diameter) for at least 24 h prior to their use. The ionic liquid, 1-hexyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate, [hmim][FAP], was purchased from Merck KgaA, Germany, ($\geq$ 99.0 % purity) and used without further purification (water content < 300 ppm as confirmed with Karl Fischer titration method). Carbon dioxide (99,998 % purity) was supplied by Air Liquid and also used as received. Absolute anhydrous ethanol of 99.9 % purity (Carlo Erba, Barcelona, Spain) was used as a solvent to collect the vapour samples and for gas chromatography analysis. The following chemicals: hexadecane (Sigma-Aldrich, $\geq$ 99.0 % purity), n-nonane (Sigma-Aldrich, $\geq$ 99.0 % purity) and 1-octanol (Alfa Aesar, $\geq$ 99.0 % purity) were used as internal standards, depending on the systems analysed.

2.2. Apparatus and experimental procedure for phase behaviour studies

The phase behaviour investigation was carried out in a high-pressure apparatus described for the first time in 1993 [22], with the most current version including all the posterior modifications reported, in detail, in the work of Rebocho et al. [23]. Briefly, the experimental system is built around a 30 cm^3 high-pressure cylinder-shaped sapphire cell placed inside a thermostatic air bath with a high-power ventilator for uniform heat distribution (Fig. 1). A transparent window allows for real-time visual surveillance of phase behaviour, i.e., for an inspection of the number of coexisting phases. The temperature is regulated by the Hart Scientific temperature controller (model 2100) coupled with an RTD probe (model 2622) from the same supplier (uncertainty of 0.1 K), and the pressure is measured by the Setra pressure transducer (model 204/C204), with an accuracy of $\pm$ 0.007 MPa.

The experiment begins with removing of all gases from the apparatus using a vacuum pump (Edwards, model RV3). Then, a certain amount of liquid sample (approximately 4 cm^3 for each system) of known composition (weight was determined using KERN ABT 220–5DNM balance (uncertainty of 0.01 mg) and reported in Table S2 of the Supplementary Material) is loaded into the cell and heated up to the experimental temperature. Overall mole ratios of components investigated were kept constant and equalled to 0.3 for [hmim][FAP]:1,2-butanediol or [hmim][FAP]:butylene carbonate, and 1 for 1,2-

butanodiol:butylene carbonate. These ratios were selected to mimic a reaction mixture with a 50 % conversion of diol to carbonate. When the temperature of 313.2 K is reached, the required CO_2 pressure is slowly introduced into the reactor using a CO_2 compressor. To accelerate the equilibration of liquid and vapour phases, the entire content of the cell is mixed with a magnetic stirrer for 1.5 h and then left to settle for 30 min. The sample from the gas phase is taken into the previously evacuated sampling loop (0.1 cm^3) and then expanded to a low-pressure calibrated volume (276.5 cm^3) using an HPLC valve. The loop is linked to an expansion zone through a glass trap immersed in an ice bath, ensuring precipitation of all components except CO_2. Next, a solvent (ethanol) is pumped through the tubing leading from the HPLC valve to the glass trap in order to collect any solute that might have precipitated along the way to the trap. Due to the limitations of the apparatus regarding highly viscous mixtures (very small inner diameter of tubing), it was impossible to take representative samples from the liquid phase. Each data point reported is the average of three replicate sampling measurements. In order to avoid the disturbance of the equilibrium upon sampling, only a small amount of sample was collected as verified by the pressure drop in the cell always smaller than 0.4 MPa. The validity of the experimental method for the phase behaviour determination was confirmed by carrying out replicas of the assays at random conditions of composition and pressure. The average standard deviation of mole fractions of alcohol and cyclic carbonate in the CO_2-rich phase is $\pm$ 0.0002.

The amount of CO_2 in each sample is calculated by examining the pressure change in the calibrated sampling volume. The average standard deviation of the mole fraction of carbon dioxide is $\pm$ 0.0002. The concentration of organic compounds, 1,2-BDO and BC, was analysed by a gas chromatographer coupled with a flame ionisation detector (GC-FID), using ZB-1HT Inferno capillary column (15 m, 0.25 ID, 0.1 film). Helium served as the carrier gas and 1-octanol (for samples with 1,2-BDO), n-nonane (for samples with BC) and hexadecane (for samples with 1,2-BDO and BC) were used as internal standards.

2.3. Correlation of solubility of polar compounds in dense CO_2

The density-based model proposed by Chrastil [24] was used to correlate experimental equilibrium data of the binary (CO_2 + 1,2-butanediol and CO_2 + butylene carbonate) systems:

$$S = \rho^k \exp\left(\frac{a}{T} + b\right) \quad (1)$$

where S is the solubility of a solute in CO_2 (g L^{-1}), ρ is the density of CO_2 (g L^{-1}) and T is the temperature (K), while k, a and b are constants. For a constant temperature, Eq. (1) can be written as:

$$\ln(S) = k\ln(\rho) + c \quad (2)$$

where c is a constant. The density of carbon dioxide was taken from the literature [25]. Parameters k and c were obtained by linear regression.

Root mean square deviation (*RMSD*) was used to compare the experimental data and data predicted by the Chrastil equation, according to:

$$RMSD = \sqrt{\frac{\sum_i \left(S_i^{calc} - S_i^{exp}\right)^2}{N}} \quad (3)$$

where S_i^{exp} and S_i^{calc} are the experimental and calculated values of the solubility of either 1,2-butanediol or butylene carbonate in the vapour phase, respectively, while N is the number of data points.

3. Results and discussion

Table S1 (Supplementary Material) shows the experimental phase equilibrium data for the vapour phase of binary (CO_2 + 1,2-butanediol) and CO_2 + (butylene carbonate), ternary (CO_2 + 1,2-butanediol +
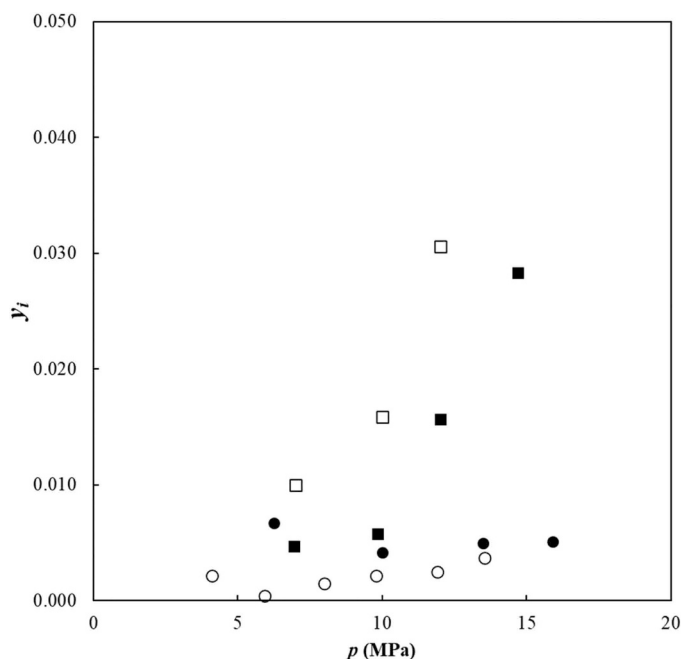
Fig. 2. Solubility data in dense CO_2 for 1,2-butanediol (filled circles – this work, empty circles – data from the literature [26]), butylene carbonate (filled squares-this work) and propylene carbonate (empty squares- data from literature [27]) at 313.2 K, expressed in mole fraction of solute in the gas phase.

[hmim][FAP]) and (CO_2 + butylene carbonate + [hmim][FAP]) and quaternary (CO_2 + 1,2-butanediol + butylene carbonate + [hmim][FAP]) at 313.2 K. These data were used to construct Figs. 2 and 3. Fig. 2 presents a vapour-liquid equilibrium diagram for the two binary systems and their comparison with the previously reported equilibrium data for the (CO_2 + 1,2-butanediol) [26] and (CO_2 + propylene carbonate) [27] systems, showing a relatively good agreement. The observed discrepancies in solubility values could be due to the difference in the methods

used – here, the static sampling method was used, while Inomata et al. [26] employed a flow flow-type apparatus. The authors have noted that their results are characterised by small discrepancies compared to a static method, particularly at lower pressures.

The solubilities of 1,2-butanediol and butylene carbonate in the vapour phase are similar at lower pressures. At elevated pressures, the solubility of butylene carbonate in the CO_2 phase is enhanced, probably due to the π-π interactions present in the carbonyl group, which forms a more stable complex [28]. Additionally, the affinity between CO_2 and carbonate is reflected in a high solubility of CO_2 in the butylene carbonate, leading to a significant expansion of the liquid phase up to the point of creating one phase at pressures exceeding 15 MPa. The strong hydrogen bonds between the hydroxyl groups of diol in the liquid phase as well as weaker CO_2-diol interactions might be responsible for the lower solubility of the alcohol in the CO_2 phase.

The Chrastil equation (Eq. (2)) was used to correlate the experimental solubility data of the two binary systems. Table 1 presents obtained constants (k and c) and root mean square deviation ($RMSD$), obtained from Eqs. (2) and (3). Figs. S1 (a) and S1 (b) presented in Supplementary Material show the fitting results.

Fig. 3(a) shows the solubility of 1,2-butanediol and butylene carbonate in the vapour phase of their ternary mixtures with CO_2 and [hmim][FAP] as a function of pressure at 313.2 K. We did not detect the presence of [hmim][FAP] in the vapour phase in all experiments. Very similar solubilities for the two ternary systems were observed in the whole pressure range. For comparison, Fig. 3(a) also contains data

Table 1
Summary of the parameters of Chrastil Eq. (1) fitted to the experimental solubility data for binary (CO_2 + 1,2-butanediol) and (CO_2 + butylene carbonate) system. The data are provided in Table S1 (Supplementary Material). *RMSD* stands for the root mean square deviation.

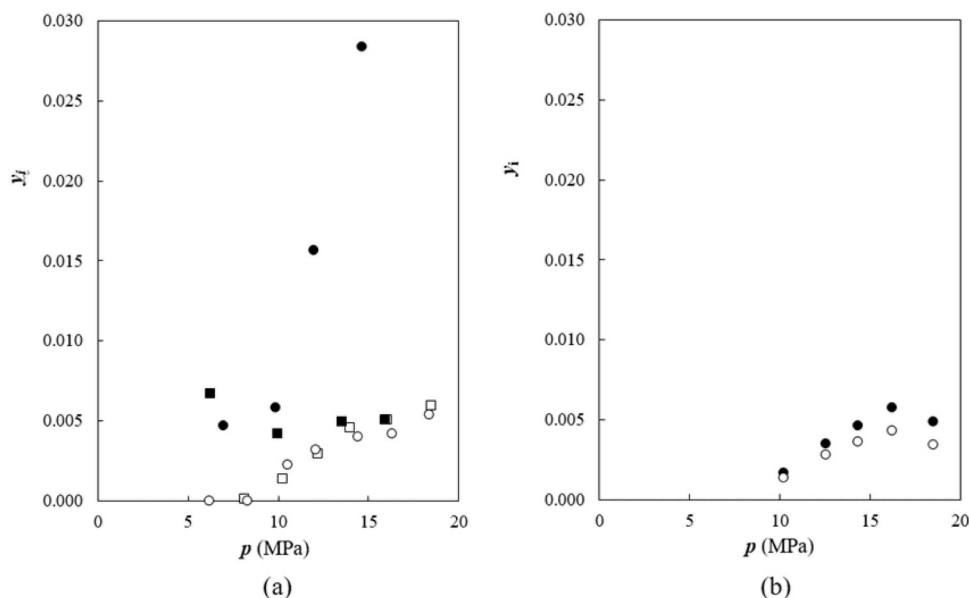|	CO_2 + 1,2-butanediol	CO_2 + butylene carbonate
k	0.560	4.412
c	−8.77	−32.62
$RMSD$ (g L^{-1})	0.0004	0.0075

Fig. 3. (a) Solubility of solutes (1,2-butanediol or butylene carbonate) as a function of pressure at 313.2 K in the vapour phase of the following systems: CO_2 + 1,2-butanediol (filled squares), CO_2 + 1,2-butanediol + [hmim][FAP] (empty squares), CO_2 + butylene carbonate (filled circles) and CO_2 + butylene carbonate + [hmim][FAP] (empty circles), in mole fraction (y_i). Overall mole ratios [hmim][FAP]:1,2-butanediol and [hmim][FAP]:butylene carbonate were kept at 0.3. **(b)** Solubility of 1,2-butanediol (full circles) and butylene carbonate (empty circles) as a function of pressure at 313.2 K in the vapour phase of the quaternary system composed of CO_2 + 1,2-butanediol + butylene carbonate + [hmim][FAP], in mole fraction (y_i). Overall mole ratios were: [hmim][FAP]:1,2-butanediol = 0.3, [hmim][FAP]:butylene carbonate = 0.3, and 1,2-butanediol:butylene carbonate = 1.

points for the solubilities in the corresponding binary systems. It can be observed that the solubility of 1,2-butanediol in the binary system is higher than in the corresponding ternary system at lower pressures but becomes very similar at higher pressures. A similar trend is observed when comparing the solubilities of butylene carbonate at low pressure. However, at higher pressures, the solubility of butylene carbonate is much lower in its ternary mixture than in binary, demonstrating the effect of the ionic liquid present in the liquid phase.

Finally, we studied the solubilities in the quaternary system composed of carbon dioxide, 1,2-butanediol, butylene carbonate and [hmim][FAP] and these results are presented in Fig. 3(b). In this system, the overall mole ratios [hmim][FAP]:1,2-butanediol and [hmim][FAP]: butylene carbonate were kept at 0.3, the same as in their corresponding ternary systems (Fig. 3(a) in order to allow comparisons. The solubility of both solutes in the vapour phase was enhanced by increasing the pressure until reaching the maximum at 16 MPa, while a further increase in pressure resulted in lower solubility. The maximum solubility was 0.0043 and 0.0057 for butylene carbonate and 1,2-butanediol, respectively. These values are similar to their maximum solubilities observed in ternary systems (0.0054 and 0.0060). These results highlight the significant effect that the presence of an ionic liquid exerts on solute solubilities in dense CO_2, which, in this case, hinders the utilisation of CO_2 for an effective separation between the diol and the carbonate at the studied conditions.

4. Conclusions

The results show that the solubility of both organic compounds, 1,2-butanediol and butylene carbonate, in dense CO_2, in binary systems, increases with the increasing pressure in the entire measured range, with the effect being more pronounced in the case of cyclic molecule with carbonyl moiety. The strong affinity between CO_2 and butylene carbonate is reflected in a high solubility of CO_2 in the butylene carbonate, leading to a significant expansion of the liquid phase up to the point of creating one phase at pressures exceeding 15 MPa. For both organic compounds, the presence of fluorinated ionic liquid in the ternary systems leads to a decrease of the solubility values to almost to the same level within the whole pressure range studied. When present in the quaternary (CO_2 + 1,2-butanediol + butylene carbonate + [hmim] [FAP]) mixture, at conditions of the example given, both organic molecules show increased solubility in the condensed phase, but only to approximately 16 MPa of pressure, after which their solubility starts to synchronically decrease.

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.

Data availability

Data will be made available on request.

Acknowledgements

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.supflu.2023.106089.

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