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# Solubility of sulfur compounds in commercial physical solvents and an ionic liquid from Monte Carlo simulations

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## Abstract

Natural gas, synthesis gas, and flue gas typically contain a large number of impurities (e.g., acidic gases), which should be removed to avoid environmental and technological problems, and to meet customer specifications. One approach is to use physical solvents to remove the acidic gases. If no experimental data are available, the solubility data required for designing the sweetening process can be obtained from molecular simulations. Here, Monte Carlo (MC) simulations are used to compute the solubility of the gas molecules, i.e., carbonyl sulfide, carbon disulfide, sulfur dioxide, hydrogen sulfide, methyl mercaptan, carbon dioxide, and methane in the commercial solvents tetraethylene-glycol-dimethyl-ether (Selexol), n-methyl-2-pyrrolidone, propylene carbonate, methanol (Rectisol), and the ionic liquid 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([bmim][$Tf_2N$]). Henry coefficients of the gases in the investigated solvents are obtained from the computed solubilities. The ratio of Henry coefficients is used to compute ideal selectivities of the solvents. The solubilites and selectivities computed from MC simulations are compared with available experimental data. Some guidelines are provided to remove acidic gases using the investigated solvents. Rectisol is the best solvent for acid gas removal, but it should be used at low

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temperatures. Selexol and the ionic liquid have similar selectivity of sulfur compounds with respect to methane and may be used at elevated pressures and temperatures since both have low vapor pressures. The solubility of carbon disulfide, sulfur dioxide, and methyl mercaptan in these solvents is the highest. Hence, these components can be removed easily prior to hydrogen sulfide, carbonyl sulfide, and carbon dioxide in a pre-absorber.

*Keywords:* Molecular Simulation, Natural Gas, Carbon Capture, Acidic Gases, Sulfur Compounds, Osmotic Ensemble

## 1. Introduction

Natural gas typically contains a wide range of light hydrocarbons, sulfur and nitrogen compounds, and other inorganic molecules [1]. The presence of acidic gases in natural gas, in particular sulfur compounds, is a major concern because of their corrosivity, toxicity, and ability to deactivate catalysts [2, 3]. Therefore, it is essential to remove these components before the natural gas is further processed. Typical sulfur compounds in natural gas are hydrogen sulfide ($H_2S$), sulfur dioxide ($SO_2$), carbonyl sulfide (COS), carbon disulfide ($CS_2$), and organic sulfur compounds such as mercaptans (RSH) [1]. These components can be inherently present in natural gas or can be produced during the processing of the gas or after burning sulfur-containing fuels. The aim of natural gas separation is to obtain pure light hydrocarbons [3]. This means that the acidic gases, i.e., $CO_2$ and sulfur compounds, have to be reduced substantially without removing valuable products such as methane.

Typically, these acidic components are removed using physical, chemical, or hybrid solvents [4] as well as other methods like membrane separation and cryogenic fractionation [5]. Chemical solvents react with solutes ($CO_2$, $H_2S$, etc.) and the solute-rich solvent is regenerated by applying heat. In contrast, physical solvents do not react, but physically absorb acidic gases. At high pressures, the acidic gases dissolve in the solvent, which is regenerated by reducing the pressure (flashing) or applying heat. Compression of the feed gas for acid gas removal is not economic unless the acidic gases have high partial pressures [4]. Therefore, physical solvents are attractive when acidic gases constitute a large fraction of the feed gas with high partial pressures (50-100 psi) whereas chemical solvents are appropriate for removing acidic gases with low partial pressures (10-15 psi) [4].

The main industrial chemical solvents for removing acidic gases cover a wide range of fluids such as amines (e.g., monoethanolamine (MEA), dimethylethanolamine (DMEA), and diisopropylamine (DIPA)), activated hot potassium carbonate [4]. The main industrial physical solvents considered for acid gas removal are propylene carbonate (PC, Fluor solvent process), N-methyl-2-pyrrolidone (NMP, Purisol process), methanol (Rectisol process), and polyethylene-glycol-dimethyl-ether (Selexol process) [1]. Hybrid processes utilize physical and chemical solvents to combine the advantages of both types. For instance, in the Sulfinol process, sulfolane is used as a physical solvent to remove the bulk of the acidic gases while DIPA chemically absorbs the remaining impurities.

A comprehensive discussion about commercial solvents, their processes along with their advantages and disadvantages is available in the book by Kohl and Nielsen [1]. Polyethylene-glycol-dimethyl-ether (DEPG) with the structural formula $CH_3O(C_2H_4O)_nCH_3$ (n between 3 and 9) is a solvent used in various commercial processes such as Selexol and Coastal AGR. Here, whenever the term Selexol is used, it refers to DEPG. Selexol has not only a high affinity for $H_2S$, but also absorbs $CO_2$, mercaptans, COS, and other sulfur compounds [1, 5]. Selexol has a high viscosity, so it is preferably used at high temperatures. The operating temperature of the process ranges from 0 °C up to 175 °C. In the Purisol process, NMP is used as a physical solvent to remove acidic gases. NMP has the highest $H_2S/CO_2$ selectivity among the commercial physical solvents [5]. Unfortunately, NMP has the highest vapor pressure at its working temperature compared to the other physical solvents, which is a major drawback. Therefore, NMP recovery may be necessary to prevent solvent losses through the process [5]. The working temperature of NMP ranges from -15 °C up to ambient temperatures. The processes known as “Rectisol”, “Ifpexol”, etc. use methanol as the physical solvent [1]. Hereafter, whenever the term Rectisol is used, it refers to methanol. Rectisol is mainly used for synthesis gas purification, and it can separate $H_2S$ from $CO_2$ [1]. The vapor pressure of methanol at room temperature is high. Therefore, Rectisol is often applied at relatively low temperatures between -70 °C and 0 °C [5]. This requires a huge refrigeration load, which makes the process expensive. Unless a high $H_2S$ selectivity is required, this process is not economically appealing because of its high capital and operational costs [5]. PC is the physical solvent of the Fluor solvent$^{SM}$ process [1]. PC is an appropriate solvent if $CO_2$ is the main component to be removed and if little $H_2S$ is present in the raw gas. PC has a higher vapor pressure than Selexol, but it is not necessary to utilize solvent recovery. Typical operating temperatures of this process are between -18 °C and 65 °C.

In recent years, ionic liquids (ILs) have been extensively investigated for natural gas or syngas sweetening purposes [6, 7] as well as for carbon capture [6, 8–13]. Most of the ILs have a very low vapor pressure, high chemical and thermal stability, low flammability, and relatively high acid gas capacities [6]. One of the prominent properties of ILs is their tunability that allows the design of application-specific ILs by changing the nature of the cations and anions. Here, we selected [bmim][$Tf_2N$] as a reference IL and a comparison of its performance for acid gas removal with respect to the commercial solvents is provided.

The design of an acid gas removal process requires solubility data of all the components present in the natural gas or syngas for a wide range of temperatures and pressures. As stated in the book by Kohl and Nielsen [1]: "The key requirement is adequate liquid/vapor equilibrium data covering all components and conditions encountered in the process." However, for some of the components such as mercaptans, there is little or no experimental vapor-liquid equilibrium (VLE) data available. In general, it is difficult to experimentally measure the VLE of toxic and corrosive compounds (i.e., sulfur compounds) [6]. In these cases, computational methods, e.g., Monte Carlo simulations, play an important role in providing the required VLE data. This study is a supplement to our previous experimental and simulation work, focused mainly on $CO_2$/$CH_4$ solubilities and selectivities [6, 8–13]. Here, we focus on the solubility and the selectivity of sulfur compounds. As it will be shown later, there is almost no experimental data for some of the sulfur compounds in conventional physical solvents. Obtaining solubility data for these compounds can be helpful for designing more accurate processes.

In this work, we investigate the solubility of sulfur compounds ($H_2S$, $CS_2$, COS, $SO_2$, and methyl mercaptan ($CH_3SH$)) as well as their ideal selectivities with respect to methane and $CO_2$ in physical solvents by Monte Carlo (MC) simulations using RASPA, a molecular simulation software package [14, 15]. The commercial physical solvents considered in this study are PC, NMP, Selexol, and methanol. Since the main component of Selexol is tetraethylene-glycol-dimethyl-ether (TTEGDME, n=4), simulations are carried out exclusively for this component. The results of MC simulations are compared with available experimental data and predictions from the Peng-Robinson equation of state (PR EoS).

This paper is organized as follows. In Section 2, we describe the details of the conducted MC simulations. In Section 3, the simulation results are presented and compared with available experimental data. The solubility data are used to compute the Henry coefficient of the gases in the solvents. Subsequently, the Henry coefficients are used to calculate ideal selectivities, which are required to assess the performance of a solvent. Based on the computed data, we provide some guidelines to remove acidic gases from natural gas or flue gas.

## 2. Simulation Details

Monte Carlo simulations are performed in the osmotic ensemble where the number of solvent molecules, temperature, and pressure of the simulation box are kept constant [7, 12, 13, 16–23]. The vapor pressure of the investigated solvents at their operating temperature is negligible which makes it possible to consider them as non-volatile liquids in simulations. The solute molecules can be exchanged with an open reservoir having the same pressure, temperature, and fugacity of the solute in the simulation box [16]. Three types of trial moves are considered for the solvent: translation, rotation, and partial reinsertion (to take into account the internal degrees of freedom of flexible molecules). There are three types of trial moves for the solute: translation, rotation, and exchange with the open reservoir. The exchange trial move is performed by the Continuous Fractional Component MC (CFCMC) method since the high density of the mixture makes it difficult for efficient insertion of new solute molecules [17–20, 24]. When computing the loading, the fractional molecule is disregarded [25]. A volume change trial move is used to regulate the pressure of the system. For more details on the Monte Carlo simulation methodology, the reader is referred to the book by Frenkel and Smit [26].

The simulation temperature is fixed at 60 °C, except for Rectisol which is -25 °C due to its high vapor pressure at the ambient temperature. All simulations are started with an equilibration run to ensure that the number of solutes, the energy level, and other properties of the system fluctuate around their average values. After reaching equilibrium, the Wang-Landau scheme [27, 28] is applied to obtain the biasing factors for the CFCMC method [17]. Once the biasing factors are fixed, production simulations with at least half a million MC cycles are carried out to obtain the statistical averages such as the average number of the solute molecules dissolved in the solvent. The number of MC moves in each MC cycle is equal to the total number of molecules in the simulation box. The size of the box is more than twice the cutoff radius, which is on average 26 Å. The number of solvent molecules in the simulation box is computed from the box size and experimental densities of the solvents.

Various force fields have been used for the solutes ($CH_3SH$ [29], $CO_2$ [30], COS [31], $CS_2$ [32], $H_2S$ [33], $SO_2$ [34], and $CH_4$ [35]) and the solvents (Rectisol [36], Selexol [37], PC [38], NMP [39], and [bmim][$Tf_2N$] [40]). Intramolecular interactions for all gas molecules are omitted (the solutes are considered rigid with fixed bonds and bond angles). The solvents NMP and PC are considered rigid while Selexol, Rectisol, and the ionic liquid are flexible in this study. Nonbonded interactions are described by electrostatic and Lennard-Jones (LJ) potentials. The Ewald summation method is used with a relative precision of $10^{-5}$ for long-range electrostatic interactions [26]. All LJ potentials are truncated at a cutoff radius of 12 Å including analytical tail corrections. The Lorentz-Berthelot mixing rules are applied for the interaction between dissimilar atoms. We note that, for instance, the TraPPE force field uses a cutoff radius of 14 Å and analytical tail corrections [41]. However, we use a cutoff radius of 12 Å for nonbonded interactions in this work. The advantage of using a cutoff radius of 12 Å over 14 Å is the substantial decrease in computational time. We show in Section S3 of the Supplementary Content that MC simulations using a cutoff radius of 12 Å including analytical tail corrections can correctly reproduce experimental vapor-liquid equilibrium (VLE) diagrams of the pure components. For COS and PC, some missing force field parameters (i.e., partial atomic charges and positions) have been obtained from standard DFT (quantum mechanics) calculations as discussed in Section S3 of the Supplementary Content. The force field functional forms are shown in Section S2 of the Supplementary Content and all force field parameters for bonded and nonbonded interactions are listed in Tables S1 to S12.

## 3. Results and Discussion

We computed the solubility of $H_2S$, COS, $CS_2$, $CH_3SH$, $SO_2$, $CO_2$, and $CH_4$ in the 4 conventional physical solvents and the ionic liquid using Monte Carlo simulations. As mentioned in Section 2, the VLE diagrams and densities of pure components are calculated to validate the employed force field using MC simulations in the Gibbs and NPT ensembles, respectively [42–44]. The results of these simulations are illustrated in Figures S4 to S16 of the Supplementary Content. In general, the VLE diagrams of the pure components are in good agreement with experimental data. The same force field parameters have been used for the simulation of the binary mixtures in the osmotic ensemble.

Only a selected number of systems will be presented in the main text, but all solubility results can be found in Tables S16 to S20 of the Supplementary Content. Simulations performed with or without analytical tail corrections, see Figures S4 to S16 of the Supplementary Content, yield a significant difference in the solubility results. Therefore, we use analytical tail corrections in all simulations as prescribed in the original force fields. In Figure 1, the solubility of the sulfur compounds in the ionic liquid is shown as an example. It is clearly visible that the solubility of $H_2S$ and COS is lower than the solubility of $SO_2$, $CH_3SH$, and $CS_2$ in the ionic liquid. This difference in solubility provides the required selectivity to efficiently separate $H_2S$ and COS from the rest of the sulfur compounds.

The solubilities of $H_2S$ and $SO_2$ in all solvents are shown in Figures 2 and 3, respectively. It is clear that all solvents are more selective towards $SO_2$ than $H_2S$. Likewise, all solvents are more selective towards $CS_2$ and $CH_3SH$ than COS. Therefore, COS and $H_2S$ have the lowest solubility in all solvents. $CS_2$ is the highest soluble compound, followed by $CH_3SH$, and $SO_2$ in NMP, PC, Rectisol, and [bmim][$Tf_2N$]. This trend is reverse for Selexol ($CS_2 < CH_3SH < SO_2$). Little experimental data are available for these highly soluble compounds; thus, it is difficult to assess this trend quantitatively.

Typically the solubility of a gas in a solvent is evaluated in terms of Henry coefficients, specifically when the gas partial pressure is low:

$$H_{g,i} = \lim_{x_i \to 0} \frac{f_i}{x_i} \tag{1}$$

where $f$ is the fugacity of the gas phase at a specific temperature, which is calculated from the PR EoS. We computed the Henry coefficients of all gases from the solubility data. In Table 1, the Henry coefficients of the solutes in the investigated solvents are presented. It is difficult to verify the calculated Henry coefficients of the highly soluble gases (e.g., $CS_2$ and $CH_3SH$) since no experimental data are available for these systems. From Table 1, it can be seen that there is a good agreement between most of the experimental data and the simulation results. Note that in our previous work, $H_2S$ solubilities in [bmim][$Tf_2N$] were computed with a different force field. The new set of force field parameters and settings for $H_2S$, $CO_2$, and $CH_4$ provide more accurate results. For consistency reasons, we have repeated the solubility simulations of these solutes in [bmim][$Tf_2N$] including analytical tail corrections, which were excluded in our previous work [7]. For example, the experimental Henry coefficient of $H_2S$ in the ionic liquid is 22.8 bar. The simulated Henry coefficients of $H_2S$ in the previous work and the current study are 11.7 and 23.9, respectively [7]. This shows the superiority of the current force field of $H_2S$ over the previous one. Nevertheless, the MC simulation data for $SO_2$ in NMP and PC show considerable deviation from the experimental data. A possible reason for this discrepancy is the assumption of rigid molecules for PC and NMP in the simulations. Only NMP and PC show large deviations between the simulated and experimental Henry coefficients (more than 500% and 100%, respectively) while this is not the case for the other solvent molecules. $SO_2$ has the largest van der Waals volume among the solutes followed by $CS_2$ and $CH_3SH$ [45]. It seems that the solubility of these large solutes in the rigid solvents is underpredicted since the internal degrees of freedom of the solvents, i.e., NMP and PC, are not taken into account. This is due to the ring in their structures which cannot be considered flexible in RASPA. Therefore, the solvent molecule cannot deform to provide further space for absorption of the large solutes. The other reason for this large discrepancy may be due to the used Lorentz-Berthelot mixing rules. The properties of pure components (the VLE of $SO_2$ and the densities of NMP and PC) are reproduced accurately with this set of force field parameters, as shown in Figures S12, S13, S21, and S22 of the Supplementary Content, but these mixing rules may not correctly predict the cross-interactions between $SO_2$ and the solvent molecules. Due to the lack of experimental data, it is not possible to validate this hypothesis for the other highly soluble gases (i.e., $CS_2$ and $CH_3SH$).

The Henry coefficient can be used to define the ideal selectivity:

$$S_{1,2}^{\text{ideal}} = \frac{H_{g,1}}{H_{g,2}} \tag{2}$$

The selectivity describes the performance of a solvent to separate two fluids. In Table 2, the ideal selectivity of the sulfur compounds with respect to $CO_2$ as well as $CO_2/CH_4$ selectivities are provided. The partial pressures of the sulfur compounds, except $H_2S$, in natural gas or flue gas are relatively low. Therefore, ideal selectivities calculated from the ratio of Henry coefficients (Equation (2)) are expected to be close to the real selectivities. As mentioned in the introduction, NMP has the highest $CO_2/H_2S$ selectivity, which is also predicted by the MC simulations. Rectisol is preferred when a high $CO_2/H_2S$ selectivity is required. The high $CH_4/CO_2$ and $CH_4/H_2S$ selectivities in Rectisol reduce the loss of valuable products. However, the disadvantage of this process is the low operating temperature and the required refrigeration. According to the MC simulations, Selexol and the ionic liquid [bmim][$Tf_2N$] have similar but lower selectivities for removing acidic gases. It should be pointed out that both solvents have a very low vapor pressure for a wide range of temperatures. Hence, the related processes do not need any solvent recovery. In addition, they can be used at high temperatures without significant degradation or solvent losses.

According to Tables 1 and 2, $CO_2$ has the lowest solubility (the largest Henry coefficient) among the acidic gases. The sulfur compounds can be categorized into two groups: "medium" and "highly" soluble gases. $H_2S$ and COS belong to the former while $SO_2$, $CS_2$, and $CH_3SH$ belong to the latter. This difference can be observed for $H_2S$ and $SO_2$ in Figures 2 and 3. Based on this classification, it is possible to propose guidelines for separating a hypothetical mixture containing all these sulfur compounds. Due to the high solubility of the second group, they can be separated in an initial stage of an acid gas removal process, which can be carried out at relatively high temperatures or low pressures. Either Selexol or the ionic liquid may be used if the operating temperature is high for their low vapor pressures. However, if the temperature is low, Rectisol provides the highest selectivity followed by NMP. The solubility of the other sulfur compounds and the valuable gases is very low for these operating conditions. If further removal is required, it can be achieved by using molecular sieves [46]. In the next stage, $H_2S$ and COS can be removed. In contrast to the previous stage, high pressures and low temperatures are required. Depending on the application, both $CO_2$ and $H_2S$ can be separated at the same time, so PC can be chosen in this case. Nonetheless, if two separate streams of $H_2S$ and $CO_2$ are required, $CO_2$ should be removed from the gas in a third stage by using a highly selective solvent such as Rectisol or NMP. If deep $CO_2$ removal is required, a chemical solvent should be used to decrease the $CO_2$ concentration to ppm levels. Note that in the presence of COS and $CS_2$, it is better not to use MEA which irreversibly reacts with those solutes [1]. All acidic gases are removed by this stage and the remaining gas would mainly consist of valuable products like methane.

## 4. Conclusions

The acidic gases present in natural gas or post-combustion products can be detrimental to industrial apparatus and the environment. In the absence of experimental data, Monte Carlo simulations can be used to compute the solubility of corrosive and toxic compounds, which are difficult to measure experimentally. The solubilities of the acidic gases ($H_2S$, COS, $CS_2$, $CH_3SH$, $SO_2$, and $CO_2$) as well as $CH_4$ in four commercial solvents (PC, NMP, Selexol, and Rectisol) and an ionic liquid ([bmim][$Tf_2N$]) were calculated from MC simulations in the osmotic ensemble. The force field parameters of PC and COS were adjusted to reproduce the experimental density and VLE of the pure components, respectively. Good agreement between the available experimental data and the computed solubilities was observed. For all solvents, the solubility of the sulfur compounds is much higher than for the other compounds, i.e., methane and $CO_2$. In few cases, the MC simulations underpredict the solubility of highly soluble compounds, e.g., $SO_2$, which may be related to the use of rigid molecules for NMP and PC in the simulations or the inadequacy of the Lorentz-Berthelot mixing rules. A 2-stage (or 3-stage) process for removing the acidic gases is proposed based on the solubility of the solutes. $SO_2$, $CS_2$, or $CH_3SH$ can be removed in the initial stage of the process due to the very high solubilities of these compounds in all solvents. This is followed by $H_2S$, COS, or $CO_2$ removal, which requires a higher pressure than the previous stage. If a separate stream of $CO_2$ is required, a third stage using NMP or Rectisol as physical solvents can be added. Overall, the results show that in the absence of experimental data Monte Carlo simulations can be used to predict the solubility of toxic or corrosive compounds, which are relevant for the industry but difficult to measure experimentally.

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## Supplementary Content

Tables and figures containing force field parameters, partial charges from standard DFT calculations, validation of the force field by comparing the pure compounds VLE diagrams and densities, the fitted PR EoS parameters, and $p - x$ data the investigated systems.

Table 1: Henry coefficients ($H_g$/bar, Equation (1)) of the investigated solutes in PC, NMP, selexol, and the ionic liquid [bmim][$Tf_2N$] at 333.15 K and Rectisol at 248 K. The available experimental Henry coefficients are provided for comparison.

| | | PC | NMP | Selexol | Rectisol | [bmim][$Tf_2N$] |
|---|---|---|---|---|---|---|
| $CS_2$ | Sim. | 2.3 | 1.6 | 3.2 | 0.42 | 1.2 |
| | Exp. | - | - | - | - | - |
| $CH_3SH$ | Sim. | 3.5 | 1.9 | 2.4 | 0.51 | 2.4 |
| | Exp. | - | - | - | - | - |
| $SO_2$ | Sim. | 9.8 | 6.1 | 1.2 | 1.01 | 3.3 |
| | Exp. | 4.69 [47], 4.89 [48] | 0.94 [48] | 0.84 [49] | 0.72 [50] | - |
| COS | Sim. | 36.8 | 33.7 | 27.0 | 9.1 | 18.0 |
| | Exp. | - | - | - | 10.97 [5] | - |
| $H_2S$ | Sim. | 43.2 | 33.8 | 19.7 | 11.1 | 23.9 |
| | Exp. | 44.2 [47], 42.2 [51] | 16.5 [52] | - | 6.09 [5] | 22.8 [53] |
| $CO_2$ | Sim. | 156 | 135 | 68.6 | 42.9 | 62 |
| | Exp. | 154 [47], 142.6 [52] | 115 [52] | 65 [54] | 43.0 [55], 40.8 [56] | 64.2 [57], 56.0 [58] |
| $CH_4$ | Sim. | 1500 | 1320 | 765 | 950 | 470 |
| | Exp. | 1340 [59], 1390 [60] | 1100 [61] | 394 [61] | 840 [5], 990 [62] | 522 [63] |

Table 2: The ideal selectivity (Equation (2)) of the acidic gases in the investigated solvents computed from MC simulations at a temperature of 333.15 K, except for Rectisol at 248.15 K.

| Selectivity | PC | NMP | Selexol | Rectisol | IL [bmim][Tf$_2$N] |
|---|---|---|---|---|---|
| $CH_4$ / $CO_2$ | 9.6 | 9.8 | 11 | 22 | 7.6 |
| $CO_2$ / $H_2S$ | 3.6 | 4.0 | 3.5 | 3.9 | 2.6 |
| $CO_2$ / COS | 4.2 | 4.0 | 2.5 | 4.5 | 3.4 |
| $CO_2$ / $SO_2$ | 16 | 22 | 59 | 42 | 18 |
| $CO_2$ / $CH_3SH$ | 44 | 70 | 28 | 84 | 25 |
| $CO_2$ / $CS_2$ | 71 | 85 | 21 | 103 | 52 |

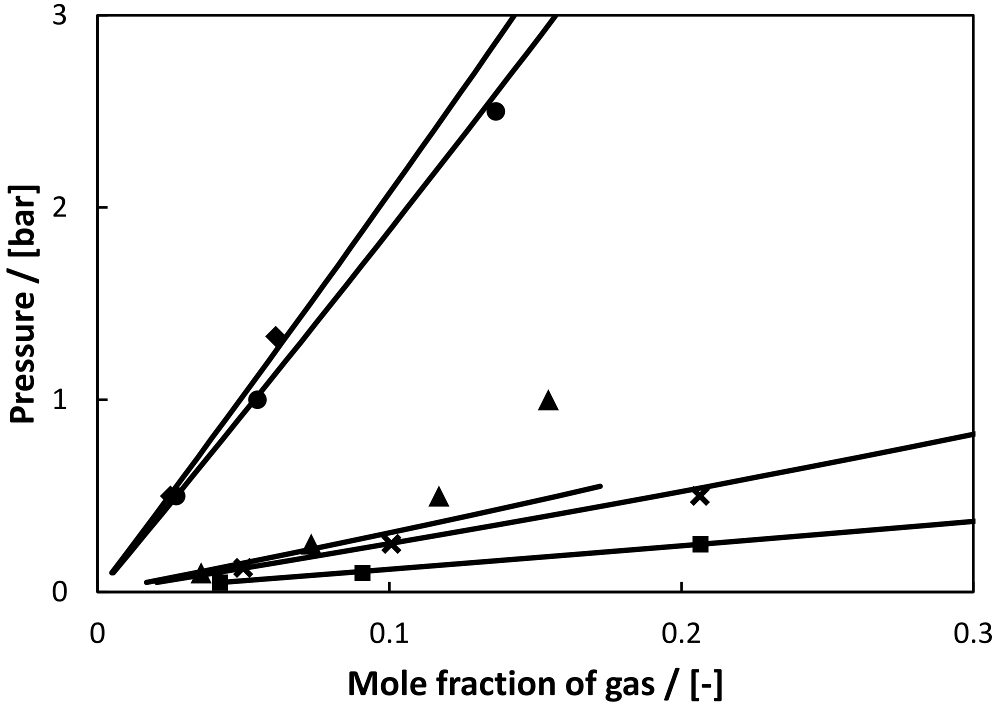

Figure 1: Solubility of acidic gases, COS (closed circles), $SO_2$ (closed triangles), $CS_2$ (closed squares), $CH_3SH$ (crosses), and $H_2S$ (closed diamonds) molecules, in the ionic liquid [bmim][$Tf_2N$] at 333.15 K. The lines are fitted to the PR EOS. The fitted parameters are available in Table S15 of the Supplementary Content. The PR EOS with the van der Waals mixing rule is not able to accurately model the $SO_2$ solubility in the ionic liquid and Selexol [49].

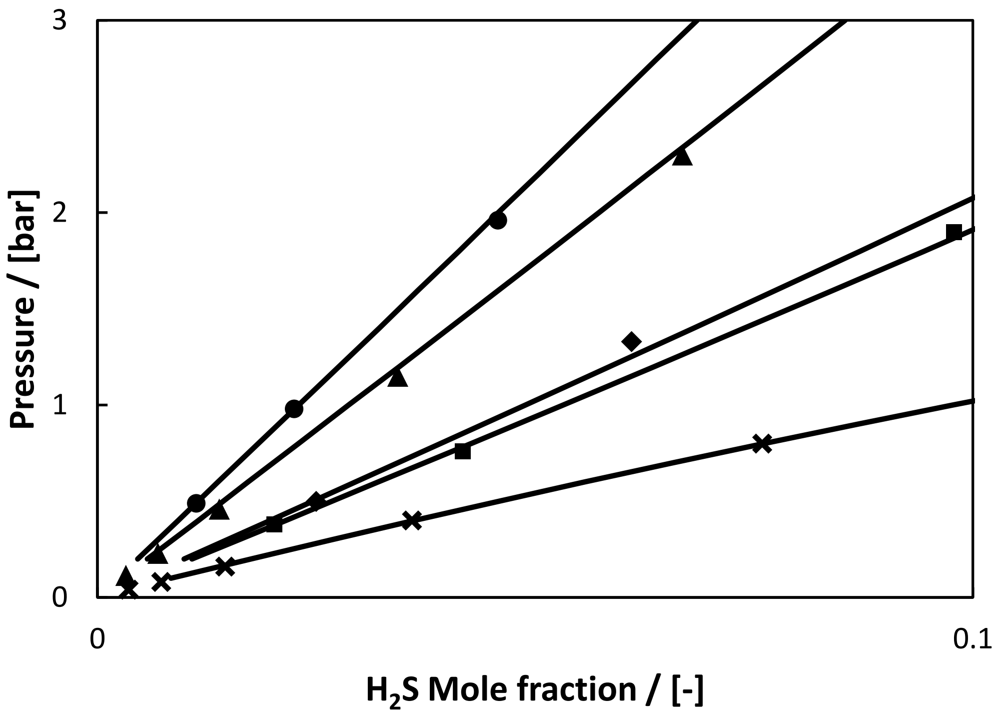

Figure 2: Solubility of $H_2S$ in PC (closed circles), NMP (closed triangles), Selexol (closed squares), Rectisol (crosses), and [bmim][$Tf_2N$] (closed diamonds) molecules at 333.15 K (except Rectisol at 248.15K). The lines are fitted to the PR EOS. The fitted parameters are available in Table S15 of the Supplementary Content.

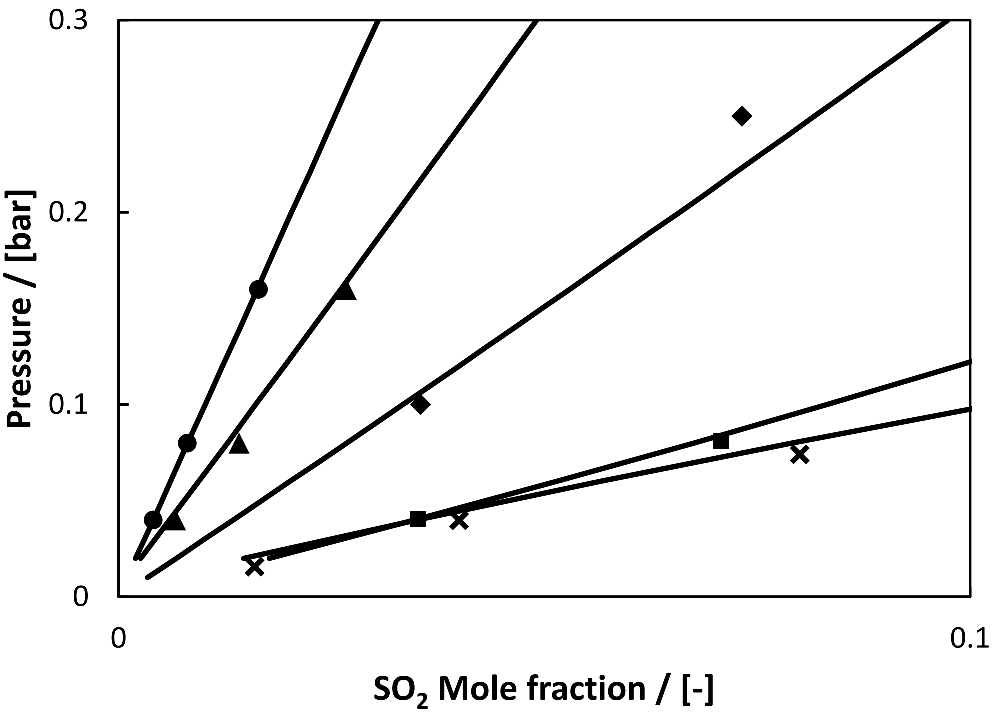

Figure 3: Solubility of $SO_2$ in PC (closed circles), NMP (closed triangles), Selexol (closed squares), Rectisol (crosses), and [bmim][$Tf_2N$] (closed diamonds) molecules at 333.15 K (except Rectisol at 248.15K). The lines are fitted to the PR EOS.The fitted parameters are available in Table S15 of the Supplementary Content.

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