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N.Borhani, T. and Wang, M. [orcid.org/0000-0001-9752-270X](https://orcid.org/0000-0001-9752-270X) (2019) Role of solvents in CO2 capture processes : the review of selection and design methods. *Renewable and Sustainable Energy Reviews*, 114. ISSN 1364-0321

<https://doi.org/10.1016/j.rser.2019.109299>

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# Role of solvents in CO<sub>2</sub> capture processes: the review of selection and design methods

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## Abstract

Solvent selection and design are imperative in the CO<sub>2</sub> capture process. The efficiency and the overall cost of the process are directly affected by the solvent as a consequence of the effect of solvent on factors such as CO<sub>2</sub> absorption capacity, size of equipment, and solvent regeneration energy. This review paper aims to review the most important solvents and mixtures of solvents, absorbing CO<sub>2</sub> via chemisorption, physisorption and chemi-physisorption. Characteristic and structure of different solvents are presented with the advantages and disadvantages of each being highlighted. Mixtures of solvents include chemical or physical solvents only, and combinations of physical and chemical solvents are categorised. In addition to common solvents, phase change solvents are also described. Once a comprehensive list of solvents is presented, different methods of solvent selection and design are illustrated, namely methods involving experiments, process and equilibrium models, predictive models, and computer-aided molecular design (CAMD). The importance of integrated solvent and process selection and design is also discussed. The most recent and selected progress studies in each section are reviewed in detail.

**Keywords:** CO<sub>2</sub> capture, physical solvents, chemical solvents, mixture solvents, solvent selection and design, integrated solvent and process design, CAMD.

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## 1 Introduction

CO<sub>2</sub> capture, utilization and storage have been attractive and practical methods to decrease the amount of CO<sub>2</sub> emitted into the atmosphere. All these three methods are important in the aspect of CO<sub>2</sub> emission control. CO<sub>2</sub> capture methods are utilized to remove the CO<sub>2</sub> from different gas streams [1-3]. In utilization processes, the researchers tried to convert CO<sub>2</sub> into more valuable components such as methane and in storage processes, the captured CO<sub>2</sub> is stored by different methods [4, 5]. Anthropogenic sources of CO<sub>2</sub> can be classified into different sectors with electricity and heat generation sector contributing most of it at 42% as shown in **Figure 1**. Anthropogenic CO<sub>2</sub> from electricity and heat sector emanate from fossil fuel (i.e. coal, oil, and natural gas) combustion during the energy generation process. To put this in perspective, coal combustion in a 500 MWe coal-fired power plant produces 8000-10000 tons of CO<sub>2</sub> per day while a similar capacity natural gas combined cycle power plant produces about 4000 tons of CO<sub>2</sub> per day. As these fuels are predicted to remain the main source of

electricity and heat in the foreseeable future (EIA, 2016), the sector will, therefore, remain a significant source of anthropogenic CO<sub>2</sub> emission.

**Figure 1:** Sources of CO<sub>2</sub> (IEA, 2016).

Technologies to capture CO<sub>2</sub> are categorised to three approaches in literature as Pre-Combustion, Oxy-Combustion, and Post-combustion [3, 6]. There are different separation methods that can be used in the above-mentioned approaches. Absorption, adsorption, membrane, chemical looping, hydrate based separation, and cryogenic [7-9]. The hybrid process attracts attention in recent years to overcome the disadvantages of the standalone method [10]. The choice of CO<sub>2</sub> capture method considerably related to the type of the plant which is producing CO<sub>2</sub> and the type of fuel utilized.

### **1.1 Motivation of the study**

Solvent-based absorption methods are the most well-known and applicable techniques between different methods of CO<sub>2</sub> capture [11, 12]. The available solvents that utilized for CO<sub>2</sub> capture processes possess a number of weaknesses such as solvent degradation, solvent loss, high corrosiveness, and high regeneration energy. Therefore, there are four activities to decrease the operating and capital cost of solvent-based CO<sub>2</sub> capture processes [13]:

- i. utilization of alternative solvents
- ii. utilization of alternative process configurations
- iii. optimization of process flowsheet
- iv. Integration of energy with other sections of the power plant

The first activity is the main subject of the current study. In order to make the CO<sub>2</sub> absorption process more effective and commercially viable, it is necessary to recognise and design more energy efficient and environmentally friendly solvents that are specialized for the solvent-based CO<sub>2</sub> capture processes. Continues literature reviews indicate the sparsity of academics literature related to the current subject of study. Mumford et al. [14] reviewed solvent based CO<sub>2</sub> capture technologies. They revised a number of common physical and chemical solvents and briefly had a discussion about mixed solvents and their applications. Budzianowski [15] discussed and reviewed the different type of available solvents and the criteria for their selection. The authors introduced eight important criteria for solvent selection and illustrated that the future studies in this area should be conducted to presenting novel single and blend solvents. PZ, ammonia and amino acids were recommended by the author as promising solvents. Papadopoulos et al. [16] discussed the design and identification of amine-based solvents of CO<sub>2</sub> capture using CAMD. The authors demonstrated the importance and effectiveness of CAMD method as a powerful tool for solvent screening and selection for CO<sub>2</sub> capture. Available studies are devoted to a few numbers of solvents and there is not an exhaustive study which covers all the solvents in a classified manner. In addition, in this review paper, the authors tried to cover methods of solvent selection and

design with proper organization. It will be a helpful document for all the researchers working in this area.

This review paper reviewed most of the available solvents and listed the advantages and disadvantages of each solvent. The characteristics of each solvent are also presented which provides a framework to compare the solvents for CO<sub>2</sub> absorption. The criteria to select the chemical and physical solvents are illustrated in a systematic manner. This classification will help the reader to recognise different type of selection methods and use them in future studies.

## **1.2 Objectives of the study**

The aims and objectives of the current review paper can be summarized as follow:

1. To review most of the available chemical, physical, chemical-physical, and mixture solvents.
2. To list the advantages and disadvantages of each solvent.
3. To present the characteristics of each solvent.
4. To illustrate the criteria to select the chemical and physical solvents.
5. To review the selection and design of solvents using experiments.
6. To review the selection and design of solvents using process and equilibrium models.
7. To review the selection and design of solvents using predictive models.
8. To review the selection and design of solvents using CAMD problems.

## **1.3 Outline of the paper**

After the current section, in Section 2 available solvents are reviewed. Details about solvents and their characteristics are provided. The solvents are classified into three class namely chemical, physical, and the mixture of solvents. The main criteria that must be considered to select the chemical and physical solvents are presented in Section 3. Section 4 is devoted to solvent selection or design using experiments. In Section 5, the solvent selection or design using process and equilibrium models are discussed. Section 6, is related to solvent selection or design using predictive models (such as quantum mechanical based models). In Section 7 the systematic method of solvent selection and design is described. In addition to single and mixture solvent design, the integrated solvent and process design also considered in this section. In Section 8, the prospects of the study is illustrated. In Section 9, the conclusions and summary of the study are emphasized.

## **2 Available solvents**

The most important part of the absorption process is solvent and its selection. In general, solvents can be classified based on properties [17] but in studies related to CO<sub>2</sub> absorption, solvents are usually classified based on their type of reactivity in solution [18, 19]. Different families of solvents are chemical, physical, and mixture solvents. ILs are another family of solvents which can be used as both physical and chemical solvents. In addition to usual solvents, phase change solvents (biphasic solvents) are also reviewed in related sub-sections.

## 2.1 Chemical solvents

Due to chemical reactions between solvents and carbon dioxide, these solvents are well-known as “chemical solvents”. Amines, salt solutions, ammonia are some examples of this type of solvents. There are two reasons that chemical reaction increases the CO<sub>2</sub> absorption rate [20]:

- i. The chemical reaction between CO<sub>2</sub> and solvent during the liquid phase reduces the equilibrium partial pressure and thereby increases the mass transfer driving force.
- ii. The chemical reaction causes the CO<sub>2</sub> to be consumed at the interface and hence increase the CO<sub>2</sub> concentration gradient at the interface.

The main advantages of chemical solvents are relative insensitivity to acid gases partial pressure, capture level of acid gases up to ppm, and high absorption and desorption mass transfer coefficients. The main disadvantages of these solvents are high energy requirement for solvent regeneration, poor selectivity between acid gases, the high price of materials, high heat of absorption, high corrosion, existence of side reactions, environmental damages, and occasionally due to using aqueous solution the treated gas will be saturated with water [21]. The energy requirement for solvent regeneration is a critical issue in using the absorption-desorption system which required around 20-30% of the power produced by a power plant [13]. The majority of energy consumption is related to the regeneration unit [22, 23]. Therefore, the design and operation of the regeneration unit have high importance in the chemical absorption process. Several researchers focused on reducing the energy consumption of the stripper using by doing new design [24], optimization [25, 26] and by considering different configurations for strippers [27, 28].

The most important chemical solvents are reviewed and discussed in the following sections. At the end of Section 2.1, the characteristics of the most important chemical solvents are summarized in **Table 1**. In **Table 2**, the advantages and disadvantages of different type of chemical solvents are summarized.

### 2.1.1 Amines

Alkanolamines are the most well-known solvents used for CO<sub>2</sub> absorption over the years [29]. There are numerous studies on different aspects of them from chemistry and kinetic reactions to thermodynamic analysis and process modelling in the different type of unit operations [8, 18, 30, 31]. Amines contain hydroxyl (-OH) and amino (-NH<sub>2</sub>, -NHR, and -NR<sub>2</sub>) functional groups on an alkane group.

#### 2.1.1.1 Primary and secondary amines

In this type of amines, one of the three hydrogen atoms in ammonia is substituted by an alkyl or aromatic. Secondary amines have two organic substituents (alkyl, aryl or both) bound to the nitrogen together with one hydrogen.

### **2.1.1.2 Tertiary amines**

In the structure of tertiary amines, nitrogen has three organic substituents [32]. The reaction mechanism for Tertiary amines is different from primary and secondary amines and no carbamate is formed when dealing with Tertiary amines. Tertiary amines are thought to catalyse the absorption of CO<sub>2</sub> by water through the production of hydroxyl radicals and hence does not have a direct reaction with CO<sub>2</sub> [33]. Therefore, water must be present for the reaction to proceed.

### **2.1.1.3 Hindered amines**

A sterically hindered amine is defined structurally as a primary amine in which the amino group is attached to a tertiary carbon atom or a secondary amine in which the amino group is attached to a secondary or a tertiary carbon atom [34].

### **2.1.1.4 Cyclic amines**

Piperazine (PZ) is a very well-known cyclic secondary amine [35, 36]. The 8 m solution of this amine showed volatility similar to MEA but the advantage of faster kinetics (more than twice) and higher capacity (double) than MEA [37]. It is also more resistant to oxidative and thermal degradation and can be used to high temperatures (up to 150 °C) [38]. This amine used as an additive to many other amines. Morpholine (MOR) is another famous cyclic amine that has been used as a solvent in commercial process well-known as Morphysorb<sup>®</sup>. This solvent can remove the acid gases from raw natural gas or syngas, selectively.

### **2.1.1.5 New amines**

New amines are primary, secondary, tertiary, and hindered ones and more and more of them introducing in recent years. The structural modification of a solvent has a great effect on the effectiveness of new amines in CO<sub>2</sub> capture processes. 2-((2-aminoethyl)amino)ethanol (AEEA), 1-diethylamino-2-propanol (1DEA2P), 2-(diethylamino)ethanol (DEEA), and 4-diethylamino-2-butanol (DEAB) are some examples of new amines [39]. Benzylamine (BZA) is a medium-strong base consisting of a primary amine functional group attached to a benzyl group [40]. More information about new amines and other types of amines can be found elsewhere [41, 42].

## **2.1.2 Ammonia**

The use of Ammonia as an absorber to capture CO<sub>2</sub> and H<sub>2</sub>S from gas streams is the subject of research for many years [43-45]. Depending on the temperature the CO<sub>2</sub> capture by using ammonia can be classified into two types.

### **2.1.2.1 Conventional ammonia system**

The first type is the absorption of CO<sub>2</sub> at ambient temperature (25–40 °C) and does not allow precipitation [46]. The kinetics of CO<sub>2</sub> absorption in unloaded aqueous ammonia solution with 0.9–5.4



M concentration and temperatures ranging 25–49 °C were measured using a string of discs contactor [47]. A rigorous rate-based model for CO<sub>2</sub> absorption using aqueous ammonia in a packed column has been developed and validated using pilot plant data [48]. Absorption and desorption of CO<sub>2</sub> in aqueous ammonia solution is simulated using a rate-based model in Aspen Plus and validated utilizing pilot plant data [49]. The VLE behaviour of absorption of CO<sub>2</sub> in aqueous ammonia solution is modelled using the species-group Pitzer activity coefficient model and compared with E-NRTL, extended UNIQUAC and original Pitzer model [50]. The equilibrium behaviour of CO<sub>2</sub> in aqueous ammonia at low temperatures was studied using experiments and modelling [51]. A novel process for ammonia based CO<sub>2</sub> capture was suggested to reduce the energy requirement. The authors integrated CO<sub>2</sub> absorption, CO<sub>2</sub> regeneration, product purification, SO<sub>2</sub> absorption, NH<sub>3</sub> abatement and recovery [52]. The effect of SO<sub>2</sub> loading (0.1–0.3 mol SO<sub>2</sub>/mol NH<sub>3</sub>) on VLE of CO<sub>2</sub> was measured in 2.5–7.5 wt.% aqueous ammonia at 20, 40, 60 °C using a Fourier transform infrared (FT-IR) gas analysis method with a pressure determination stirred tank apparatus [53]. The double film theory was utilized to investigate the mass transfer coefficient to evaluate the ammonia escape (which is a serious problem in this system) utilizing in CO<sub>2</sub> capture [54]. An organic solvent (acetone, dimethoxymethane, or acetaldehyde) added to a CO<sub>2</sub> rich, aqueous ammonia/CO<sub>2</sub> solution under room temperature and pressure conditions. The organic solvent and CO<sub>2</sub> absorbing solution are then regenerated using low-temperature heat [55]. A promising process modification of the ammonia (NH<sub>3</sub>) based CO<sub>2</sub> capture process is proposed that involves an advanced flash stripper with a cold rich split [56].

#### **2.1.2.2 Chilled (precipitating) ammonia system**

The second process is CO<sub>2</sub> absorption at low temperature (about 2–10 °C) and desorption of CO<sub>2</sub>-rich stream at a temperature range of 100–150 °C and pressures of 30–2000 psi. This process is called the chilled ammonia process and precipitation of some ammonium carbonate compounds is occurred in the absorber. Therefore, in this process phase change happen. The low-temperature process helps to reduce the ammonia slip in the absorber and the flue gas volume [46].

The chilled ammonia system also attracted a lot of attention in recent years. A selected number of recent progress in this process are reviewed. In order to evaluate the mass, energy, and entropy flows of the chilled ammonia process, an approximate model of the CO<sub>2</sub>-H<sub>2</sub>O-NH<sub>3</sub> system is coupled with a proposed process [57]. An aqueous ammonia process is modelled using a rate-based approach. The model is validated using experimental data and modified to a chilled ammonia process model. The model was then scaled up to process flue gas from a 580 MW supercritical coal-fired power plant [58]. A process for CO<sub>2</sub> capture from flue gas by using ammonia is developed. In order to increase the CO<sub>2</sub> concentration in the regeneration section of the process, solid ammonium bicarbonate is generated in the process. Precipitation, separation, and dissolution of the solid phase are considered in a separate section, hence the packed columns remain free of solids [59].

#### **2.1.3 Salt solutions**

Salt solutions are another family of chemical solvents which are salt in nature and can produce electrolyte solution when dissolving in water. The main feature of this family is the low price of them.

### **2.1.3.1 Carbonate/Bicarbonate**

Carbonate solutions (potassium and sodium) are chemical solvents and have considerable positive characterisations such as low cost, low toxicity, ease of regeneration, slow corrosiveness, low degradation, high stability, and CO<sub>2</sub> absorption capacity. The carbonate system has been applied in more than 700 plants worldwide for CO<sub>2</sub> and hydrogen sulphide removal from streams like ammonia synthesis gas, crude hydrogen, natural gas, and town gas [60]. Similar to CO<sub>2</sub> capture using ammonia the CO<sub>2</sub> capture by using carbonate solutions can be done in two main categories.

#### **2.1.3.1.1 Conventional carbonate/bicarbonate system**

The reaction of CO<sub>2</sub> with potassium carbonate solution is an exothermic reaction. The hot potassium carbonate process is useful for gas mixtures containing a high amount of CO<sub>2</sub>. The CO<sub>2</sub> absorption by using potassium carbonate solution is a slow rate reaction. Consequently, promoters (activators) have been used in different studies to improve process efficiency [34]. The promoters for potassium carbonate solution can be classified as organic and inorganic [60]. Characteristics and behaviour of sodium carbonate are very similar to potassium carbonate because both of them produce considerable carbonate in solution [61, 62].

#### **2.1.3.1.2 Precipitating carbonate solvent system**

The precipitating carbonate/bicarbonate system is proposed by Shell which this process utilizes K<sub>2</sub>CO<sub>3</sub> with a crystallization and concentration step and then CO<sub>2</sub> absorption step [63, 64]. The authors named the process as Shell carbonate slurry process and reported that a high amount of energy can be reduced in regeneration and the lower amount of nitrosamine emitted in compare with the amine process. Sodium carbonate/bicarbonate solution also used as precipitating solvent. In a study, the researchers allowed to form the solid bicarbonate is and hence forming slurry increased the capacity of the solvent [65]. The authors reported that the energy requirement for solvent regeneration that is used to capture CO<sub>2</sub> is about 3.22 MJ/kg of captured CO<sub>2</sub>.

### **2.1.3.2 Hydroxides**

Different types of hydroxides such as potassium, calcium, and sodium hydroxides are utilized to remove CO<sub>2</sub> from different gas streams [66-68]. As NaOH is a strong alkaline Na<sup>+</sup> and OH<sup>-</sup> are almost completely ionized in pure water. Then, the gaseous CO<sub>2</sub> is absorbed physically in the NaOH solution and change to aqueous CO<sub>2</sub>. After that, aqueous CO<sub>2</sub> reacts with OH<sup>-</sup> to generate HCO<sub>3</sub><sup>-</sup> and CO<sub>3</sub><sup>2-</sup>.

### **2.1.3.3 Amino acid salts solutions**

Amino acids are organic components, which include amine (-NH<sub>2</sub>) and carboxyl (-COOH) groups and an amino acid-specific side chain (R group). Amino acid salts (AAS) which are produced commonly by reacting amino acids with an inorganic base (e.g. KOH [69] and NH<sub>3</sub> [70]) utilized in a different study to perform the CO<sub>2</sub> capture [71]. They can be considered as a subset of amines. Potassium Salt of Taurine, Potassium Salt of Glycine, Potassium salt of Sarcosine are prominent examples of amino acid salts [72-75]. Amino acid salt solutions similar to the carbonate solution can be used in two different approaches. In addition to amino acid salts, if amino acids are neutralized using an organic base the product name is amine amino acid salt (AAAS). AAAS showed better behaviour in compare with AAS [76, 77].

#### **2.1.3.3.1 Conventional amino acid salt system**

Reaction kinetic between CO<sub>2</sub> and potassium salt of sarcosine solution and also the VLE for both unloaded and CO<sub>2</sub> loaded aqueous potassium salt of sarcosine at different temperatures are investigated in the literature [73, 78]. Kumar et al. [72] measured the reaction kinetic between CO<sub>2</sub> and aqueous potassium salts of taurine and glycine at 22 °C. They also experimentally examined the effect of temperature on reaction kinetics at the range of 12-32 °C. Aronu et al. [73] worked on reaction kinetic between CO<sub>2</sub> and potassium salt of sarcosine solution. Aronu et al. [78] measured the VLE for both unloaded (concentration 1-5 M and the total pressure of 4.08-97.8 kPa) and CO<sub>2</sub> loaded (concentration 3.5 M and the total pressure of 0.03-971 kPa) aqueous potassium salt of sarcosine at different temperatures. The authors also used the Extended UNIQUAC thermodynamic model to express the data. Aldenkamp et al. [75] measured the VLE of CO<sub>2</sub> in potassium salt of taurine and glycine at two concentrations namely 1 and 1.8 mol/kg and four different temperatures. These AAASs are utilized in a pilot plant rig and it was realized that it required around half of the stripping steam of the MEA system [79].

#### **2.1.3.3.2 Precipitating amino acid salts systems**

Amino acids could be presented in solutions in different forms. This happens because of the presence of both an amine group (cause protonation), and a carboxyl group (cause deprotonation) [80]. Kumar et al. [81] observed crystallization in the reaction between CO<sub>2</sub> and aqueous potassium taurate solutions at 25 °C. Majchrowicz et al. [82] investigated the tendency of alkaline (sodium, potassium, and lithium) salts of taurine, β-alanine, sarcosine and L-proline to form solid phase by changing the operating conditions of the CO<sub>2</sub> capture process. They reported that higher temperatures and lower CO<sub>2</sub> partial pressures lead to higher solubility limits and at higher amino acid salt concentration precipitation starts at lower CO<sub>2</sub> partial pressures. In addition, the effect of the counterion on the solubility limit appears to be: potassium > sodium > lithium. Finally, the precipitates formed can be the amino acid itself (as in the case of taurate), or more complex (CO<sub>2</sub>-containing) species (as for proline, sarcosine, and β-alanine).

The precipitation characteristics of fourteen aqueous amino acid salt systems are investigated experimentally [83]. The authors reported that at 40 °C, high concentrated amino acid salt systems precipitate in the presence of CO<sub>2</sub> and form two or three solid-liquid phases.

**Table 1:** Physical Characteristics, the molecular structure of selected chemical solvents.

**Table 2:** Advantage and disadvantage of selected chemical solvents.

## 2.2 Physical solvents

In physical absorption processes, Henry's law is applied and the gas absorption is achieved at high-pressure conditions. In this type of processes, the solvent regeneration may be done by reduction of pressure and in contrast to the chemical absorption addition of heat is not necessary [14]. In comparison with chemical absorption, physical solvents have greater absorption capacity and hence resulted in lower solvent recirculation rates. Another advantage of the physical solvent is their selectivity between acid gases. The disadvantages of physical solvents are their sensitivity to acid gas partial pressures (it must be high), necessity to have a low concentration of inert gases, and difficulty in meeting H<sub>2</sub>S specification [21]. The physical characteristics, molecular structure, and applications of well-known physical solvents are presented in **Table 3**. In **Table 4**, the advantages and disadvantages of a selected number of physical solvents are listed.

### 2.2.1 Dimethyl Ether of Polyethylene Glycols (DEPG or DMEPEG)

The Selexol<sup>®</sup> is the commercial process which uses DEPG. This solvent is a mixture of Dimethyl Ether of Polyethylene Glycols. The solvent can be utilized to absorb H<sub>2</sub>S and CO<sub>2</sub>, physically. Selexol has the low vapour pressure, high operating temperature, high CO<sub>2</sub> solubility, non-corrosiveness, relatively non-toxic, and well-characterized performance as compared with the other physical solvents [84]. The favorable operating temperature for the absorbers that use this solvent fall in the range of -20 to 40°C. The Selexol process is utilized in pre-combustion integrated gasification combined cycle (IGCC) systems to capture CO<sub>2</sub> [85]. Kapetaki et al. [86] simulated a common two-stage Selexol process to absorb the CO<sub>2</sub> and H<sub>2</sub>S from a synthesis gas system, simultaneously. They found that in order to capture 95% of CO<sub>2</sub> the required energy is 65% more than the energy necessary for 90% CO<sub>2</sub> capture. Gatti et al. [87] performed multi-objective optimization of a Selexol<sup>®</sup> process for the selective removal of CO<sub>2</sub> and H<sub>2</sub>S from coal gasification-derived syngas. Im et al. [88] added dimethyl carbonate (DMC), diethylcarbonate (DEC), and triacetin (TAT) to DEPG solution to improve the economics of the Selexol<sup>®</sup> process. The process used TAT additive is revealed to be competitive with the Selexol<sup>®</sup> process without additive in the aspect of both operating and equipment costs. In contrast, DMC and DEC exhibited a serious solvent loss. CO<sub>2</sub> absorption performance of DMEPEG solvent by considering a rate based mass transfer model is studied in ProTreat<sup>®</sup> simulator [89]. Dual-stage Selexol<sup>®</sup> process in the IGCC system for removing CO<sub>2</sub> as well as H<sub>2</sub>S from the syngas is simulated [90]. The authors

reported that by changing the operating conditions, 95% CO<sub>2</sub> capture can be obtained by the conventional, integrated dual-stage Selexol unit.

### **2.2.2 Methanol**

Methanol used as the physical solvent in two well-known processes: Rectisol<sup>®</sup> and Ifpexol<sup>®</sup>. Rectisol<sup>®</sup> process is the first process that used an organic component (Methanol) as the solvent. The abilities of the Rectisol process to separate impurities that are produced in the gasification of coal or heavy oil, including hydrogen cyanide, aromatics, organic sulfur compounds, and gum-forming hydrocarbons has been confirmed already. Dehydration and formation of ice and hydrate at the low temperatures of the process can be prevented by using Methanol. The operating temperature of Rectisol<sup>®</sup> process is low as -59.5 to -73.3 °C and the solvent's capture capacity for both CO<sub>2</sub> and H<sub>2</sub>S becomes very high (higher than that of other physical solvents). This characteristic cause to attain a very high amount of capture. The process is presented in a very different arrangement to meet specific requirements and feed conditions but there are two important configurations which are the nonselective standard process and the selective version [18].

Sun and Smith [91] simulated and analyzed a single-stage and a two-stage Rectisol<sup>®</sup> wash configurations in aspects of the acid gas removal ability, heat recovery, equipment requirement, power consumptions, and environmental emission and costs. They utilized revised PC-SAFT in the process simulation. Gatti et al. [92] reviewed Rectisol process configurations and applications. They also calibrated the PC-SAFT equation of state (EOS) for the Rectisol<sup>®</sup> process. The authors gave the details of process simulation and optimized heat integration, and utility design and optimized alternative Rectisol<sup>®</sup> configurations for CO<sub>2</sub> Capture. Gao et al. [93] predicted the thermodynamic behaviour of the Rectisol<sup>®</sup> process by using SAFT EOS. They used a method of equation oriented strategy. Sharma et al. [94] optimized the energy penalty and CO<sub>2</sub> capture rate simultaneously in standalone Rectisol<sup>®</sup> process to get the best-operating conditions for various CO<sub>2</sub> capture rates.

Ifpexol<sup>®</sup> process uses methanol as the agent for treating natural gas to perform dehydration, natural gas liquids recovery, and acid gas removal in one overall process. Selective removal of H<sub>2</sub>S or removal of essentially all the acid gas can be obtained by using this process [18].

### **2.2.3 Polyethylene glycol methyl isopropyl ethers (MPE)**

The commercial name of the process that used a mixture of polyethylene glycol dialkyl ethers (MPE) is Sepasolv-MPE<sup>®</sup> process. The process resembles the Selexol in the aspect of utilized solvent and the mode of operation. Initially, the process is designed for selective removal of H<sub>2</sub>S from natural gas and thereafter the same process was applied for CO<sub>2</sub> capture from synthesis gases [95]. Following the extensive literature review, our findings suggest that there are no studies on this process.

### **2.2.4 Propylene carbonate**

The commercial name of the process that used propylene carbonate (PC) is Fluor<sup>®</sup> process. Fluor<sup>®</sup> process is suitable for gas streams comprising of CO<sub>2</sub> partial pressures higher than 60 psig. The operating temperature for this solvent is between -17 °C to 65 °C. The process provides high solubility of CO<sub>2</sub> in the solvent. This process can be used to perform sweetening and dehydration simultaneously. In addition, it is useful to remove very low amounts of H<sub>2</sub>S (e.g. 20 ppmv) and also can operate at lower temperatures by good mass transfer without increasing its viscosity considerably [96].

### 2.2.5 N-Methyl 2Pyrrolidone (NMP)

The commercial name of the process that used NMP as the solvent is Purisol<sup>®</sup> process. The process can be operated at ambient and very low temperatures (about -15°C). The solvent has a higher vapour pressure in comparison to DEPG or propylene carbonate and hence it required to be washed by water. It must be mentioned that, due to the high selectivity for H<sub>2</sub>S, the process is mainly suitable to purify the high pressure, high CO<sub>2</sub> contains synthesis gas from gas turbine IGCC systems.

### 2.2.6 Glycerol

Glycerol which also well-known as glycerine or glycerin is a simple polyol compound. This component is a colorless, odorless, sweet-tasting, non-toxic and viscous liquid. Nunes et al. [97] only used glycerol solution and measured the CO<sub>2</sub> solubility in glycerol at three different temperatures i.e. 80, 120, and 150 °C and pressures up to 32 MPa. They reported that the CO<sub>2</sub> solubility increased by the pressure increase and by the temperature decrease. They also compared the performance of glycerol with some components having the same chain length. Medina-Gonzalez et al. [98] used in situ FT-IR methods to measure the CO<sub>2</sub> solubility in glycerol solution at a wide temperature range (40-200 °C) and pressures up to 35 MPa.

### 2.2.7 Sulfolane

Sulfolane (also well-known as tetramethylene sulfone (TMS) and 2,3,4,5-tetrahydrothiophene-1,1-dioxide) is an organosulfur colorless liquid with the chemical formula (CH<sub>2</sub>)<sub>4</sub>SO<sub>2</sub>. The solubility of gases including CO<sub>2</sub> is determined in sulfolane solution at temperatures in the range of 25-130 °C at pressures up to 7.6 MPa [99]. Solubilities and diffusivities of N<sub>2</sub>O and CO<sub>2</sub> in aqueous and pure sulfolane solution were measured and correlated for a range of temperature of 20-85 °C [100]. In order to find a microscopic picture of the utilization of sulfolane as the solvent for CO<sub>2</sub> and H<sub>2</sub> capture, the properties of this solvent as the physical solvent is studied using density functional theory (DFT) and molecular dynamics (MD) computational chemistry methods [101].

**Table 3:** Characteristics and molecular structure of selected physical solvents.

**Table 4:** Advantage and disadvantage of selected physical solvents.

## 2.3 Physical-Chemical solvents

ILs are solvents that showed both physical and chemical behaviour [102] and hence we considered them in a separate section in the title of physical-chemical solvents. These solvents are composed of cations and anions and have wide application in different areas due to their unique properties namely low vapour pressure, low melting point, modifiable solvation behaviour, staying liquid over a wide range of temperature, inflammability, and thermal stability [103, 104]. A lot of combination of anions and cations are possible, giving flexibility to the solvent design. Therefore, desired characteristics can be obtained by design of different ILs [105]. However, it must be mentioned that some of the ILs showed detrimental properties such as toxicity and corrosiveness [106]. Conversely, as the number of possible designed ILs is too high, it is challenging, time-consuming, and expensive to explore synthesis by a trial-and-error approach.

In physical absorption, the solubility of CO<sub>2</sub> in ILs is determined by free volume, IL size, cation and anion, while the structure of the amino function group attaching IL dominates the solubility of CO<sub>2</sub> in chemical absorption. This kind of IL is well-known as task-specific ionic liquid (TSIL) because IL is produced with the favorite properties [107]. Boot-Handford et al. [108] classified a different type of ILs and described the applicability of each group properly. According to literature, different classified type of ILs is Room Temperature ILs (RTILs); Task-Specific ILs (TSILs); Reversible ILs (RILs). These different type of ILs can be used with the support of membranes and this process name is supported ionic liquid membranes (SILMs) [109-111]. There is a considerable number of review papers on the utilization of ILs for CO<sub>2</sub> capture [112-118]. Lei et al. [116] described the applications of different thermodynamic models for ILs and also reviewed the solubility of CO<sub>2</sub> and some more gases in the ILs. Zeng et al. [118] reviewed all the important review papers related to ILs utilized for CO<sub>2</sub> capture. They recognized four main aspects that covered by review papers namely design of new ILs particularly task-specific ones, mixing of ILs with other components, determination of physicochemical properties, and determination of transport properties, kinetics and etc. They also covered structures effects, microscopic integration, transport behaviours, and scale up and process design for IL-based CO<sub>2</sub> separation from the viewpoint of industrialization.

It is noteworthy that ILs are utilized in non-aqueous (pure), aqueous (mixed with water), and mixed with amine for CO<sub>2</sub> capture. Recently a new idea is proposed to use a blend of ILs [119]. By this method, the undesired property can be overcome and a balanced and optimum characteristic in aspect of economic, environmental, and performance can be obtained. General advantage and disadvantage of ILs is listed in **Table 5**.

**Table 5:** Advantage and disadvantage of ILs.

### 2.3.1 Room Temperature ILs (RTILs)

RTILs are also well-known as conventional ILs in the literature. These ILs are very common which act as physical solvents in the absorption of CO<sub>2</sub> and most of them have imidazolium-based cations. The cations in these ILs are organic and anions can be organic or inorganic [120]. CO<sub>2</sub> is sufficiently soluble in RTILs. Prominent examples of RTILs that utilized in CO<sub>2</sub> capture are [bmim][PF<sub>6</sub>], [bmim][BF<sub>4</sub>], [bmim][Tf<sub>2</sub>N], [emim][Tf<sub>2</sub>N], [emim][MDEGSO<sub>4</sub>], [bmpy][Tf<sub>2</sub>N], and [hmim][BF<sub>4</sub>].

### **2.3.2 Task Specific ILs (TSILs)**

Functionalization of ILs by a proper component like amines can improve the ILs performance in CO<sub>2</sub> capture [121]. These type of ILs act as chemical solvents in absorption of CO<sub>2</sub>. Different examples of TSILs that utilized in CO<sub>2</sub> capture are [pabim][BF<sub>4</sub>], [Ambim][BF<sub>4</sub>], [Ambim][DCA], [3Amim][BF<sub>4</sub>], [bmim][acetate], [AHA][tbp], and [thtdp][2-CNpyr].

### **2.3.3 Reversible ILs (RILs)**

A new class of ILs, well-known as reversible ionic liquids (RILs) [122]. These ILs are obtained by reaction between CO<sub>2</sub> and a special type of amines or alcohols (such as silylamines). Then, the generated ILs could be used as a solvent for the physical absorption of CO<sub>2</sub>. Therefore, RILs enabling a dual CO<sub>2</sub> capture mechanism [123]. These solvents eliminate the energy penalty necessary in common amine solutions, increase the selectivity of CO<sub>2</sub> over N<sub>2</sub>, and increase the CO<sub>2</sub> loading.

### **2.3.4 Deep Eutectic Solvents (DESSs)**

This type of ILs is easy to prepare and no further purification steps are required which resulted in low cost, and hence this ILs is more economical than the other ILs [124]. Using DESSs as CO<sub>2</sub> absorbents were firstly reported by Li et al. [125]. Between the synthesized DESSs, choline chloride/urea (ChCl/Urea) is considered as one of the promising solvents to attain large-scale applications [124]. ChCl/Urea (1:2 on a molar basis) consists of natural compounds, i.e. choline chloride and urea, and hence it is easily biodegradable and with low toxicity. The viscosity of ChCl/Urea (1:2) is much higher than the conventional organic solvents. Therefore, the addition of water as a co-solvent can decline the viscosity significantly but still can maintain the high CO<sub>2</sub> capacity, making aqueous ChCl/Urea (1:2) a promising CO<sub>2</sub> absorption solvent [126].

## **2.4 Mixture of solvents**

Each solvent has some favorable characteristics, hence the researchers find out that by combining them they could use the positive features of each solvent. For example, by combining primary/secondary with tertiary/hindered amines the benefit of fast reaction kinetics with high absorption capacity and low energy requirement for regeneration will be achieved. The mixture of solvents can be classified as two main categories namely mixture of chemical solvents and mixture of physical and chemical solvents. In addition to the usual mixture of solvents, some solvent mixtures showed phase change behaviour.

### **2.4.1 Mixture of chemical solvents**



#### **2.4.1.1 Promoted carbonate**

As mentioned before, carbonate solutions have disadvantages of the slow rate of reaction with CO<sub>2</sub>. Addition of promoters to carbonate solutions can enhance the rate of reactions [127]. Different type of chemicals utilized as promoters of carbonate solution but the most important family of promoter components are amines [60]. Amine-promoted potassium carbonate solution has industrial applications and reported in several studies [128]. In addition to amines, amino acids also exploited as a promoter and added to carbonate solutions [129, 130].

The phase change behaviour also reported for promoted potassium carbonate solutions. Similar to the precipitating of the ammonia system, precipitating of promoted carbonate solution can improve the system in the aspect of energy utilization [129, 130]. There are a number of studies and research on promoted potassium carbonate system at the University of Melbourne. The researchers named the process as UNO MK3 which is commercialized by UNO Technology Pty Ltd [131]. In this precipitating system, the potassium bicarbonate precipitates from a promoted potassium carbonate solvent following CO<sub>2</sub> absorption and subsequent cooling. The precipitate is then separated from the liquid phase. It has been demonstrated that potassium glycine as a promoter can improve the CO<sub>2</sub> recovery rate of potassium carbonate solution by up to 6 times [103].

#### **2.4.1.2 Promoted Ammonia**

PZ due to its fast reaction rate is one of the best chemicals that can be used as an additive to ammonia solution. This component considerably improves the CO<sub>2</sub> absorption rate. Liu et al. [132] performed experiments on CO<sub>2</sub> absorption into a mixture of ammonia and PZ at 10–40 °C in a wetted wall column under the driving force of 8–25 kPa. Yu et al. [133] studied the CO<sub>2</sub> absorption process using NH<sub>3</sub>-PZ blended solutions in a packed column, and developed and validated a rate-based model for the NH<sub>3</sub>-PZ-CO<sub>2</sub>-H<sub>2</sub>O system. In addition to PZ, other components also utilized as a promoter for the ammonia solution [134].

#### **2.4.1.3 Mixture of amines**

Mixtures of amines show acceptable performance in plenty of studies and substantial number of various combinations of amines have been examined in recent years.

##### **2.4.1.3.1 Common mixtures of amines**

The tertiary amines which are proper for selective absorption of CO<sub>2</sub> in presence of H<sub>2</sub>S and has high absorption capacity and low cost of regeneration have the weakness of slow reaction rate with CO<sub>2</sub> due to lack of formation of Carbamate. Therefore, primary and secondary amines, that has fast kinetic, are added to them as additives in many studies. Chang and Shih utilized an aqueous mixture of DGA and MDEA to model the CO<sub>2</sub> absorption in an absorber-stripper system [135]. Rayer et al. [136] compared the experimental data from the literature to find the effect of different amines on MDEA as a ternary

amine at a constant temperature (40 °C). They reported that adding a hindered amine to MDEA could have the highest amount of CO<sub>2</sub> loading and increase the reaction rate with CO<sub>2</sub>.

PZ which is polyamine-based solvents has more than one active site to react with CO<sub>2</sub> and hence can potentially have a high absorption rate, high absorption capacity, and low volatility. Therefore, there are a number of studies on the application of PZ as an activator to ternary amines [137, 138] and also to hindered amines [139, 140] to perform CO<sub>2</sub> capture studies. Rayer et al. [136] compared the experimental data at a constant temperature (40 °C) from literature to illustrate the effect of adding PZ as a promoter to other amines. The authors reported that the mixture of PZ with hindered amines shows high absorption capacity and absorption rate for CO<sub>2</sub>.

In addition to PZ, the other polyamine which showed an effective application in combination with common amines (ternary and hindered) is N-(2-aminoethyl) ethanolamine (AEEA) [141, 142]. AEEA shows proper absorption rate among amines that are added as an activator to the tertiary amines. Further, as it is a Diamine compound, one mole of it is able to absorb 2 moles of CO<sub>2</sub>, thus has a high absorption capacity for CO<sub>2</sub> but it increases the regeneration cost [143]. Zoghi [144] considered five additives and reported that AEEA-MDEA aqueous solution has the highest absorption rate of CO<sub>2</sub>. In general, it can be said that considerable improvement can be obtained by using blends of amines in the aspect of reaction kinetics, solubility, mass transfer, and regeneration energy requirement [42].

#### **2.4.1.3.2 Phase change mixtures of amines**

In addition to mentioned amine mixtures, some amine mixtures act as phase change solvents. Arshad et al. [145, 146] measured heat of absorption of CO<sub>2</sub> and equilibrium total pressures in a mixture of 2-(diethylamino)-ethanol (DEEA) and 3-(methylamino) propylamine (MAPA) solution as a function of CO<sub>2</sub> loading at different temperatures. Pinto et al. [147] also worked on DEEA-MAPA solution. They found that MAPA is first loaded in the heavy phase with a subsequent reaction between DEEA and CO<sub>2</sub>. They also mentioned that the system has the potential for a significant reduction in the required heat for regeneration. Xu et al. [148] reported that 1,4-butanediamine (BDA) blended with DEEA resulted in phase change solvent. There is a non-aqueous amine solvent process which is well-known as Self-Concentrating Absorbent CO<sub>2</sub> Capture Process and presented by 3H Company [149]. Thermomorphic biphasic solvent (TBS) systems are another phase changing mixtures of amines which resulted by blending lipophilic amines to release CO<sub>2</sub> in the regeneration in lower temperatures (about 80 °C) in comparison with usual amines (about 120 °C) [150].

#### **2.4.1.4 Hydroxides-Carbonate**

A small fraction of research focused on a mixture of hydroxides and carbonates. Gondal et al. [151] studied the solubility of N<sub>2</sub>O in aqueous solutions of hydroxides (containing lithium, sodium and potassium ions) and the hydroxide blends with carbonates in temperatures (25–80 °C) and concentrations (0.08–3 M). Gondal et al. [152] measured the CO<sub>2</sub> absorption rate in the hydroxide-

carbonate mixture in the temperature range of 25-64 °C. They also presented a kinetic model for the system that can predict the kinetic by 12% AARD.

#### **2.4.1.5 Amino acids-Amine**

The mixture of amino acids and amines also attracted the researcher's attention. The speciation is determined for several amino acids including L-Proline (PRO), L-Alanine (ALA), L-Serine (SER), Taurine (TAU), Glycine (GLY) and Sarcosine (SAR), mixed with MEA and with different CO<sub>2</sub> contents [153]. The solubility of CO<sub>2</sub> in a blend of the aqueous solution of potassium proline (KPr) with PZ and AMP studied experimentally and theoretically [154].

#### **2.4.2 Mixture of physical and chemical solvents**

In this type of processes, the physical solvent captures the acid gas bulk and the chemical solvent purifies the gas stream to rigorous levels, simultaneously [18].

##### **2.4.2.1 Sulfolane-Amine**

Tetrahydrothiophene dioxide is an organic component well-known as Sulfolane. The commercial name of the process that used the mixture of amine and sulfolane as the solvent is Sulfinol process. One of the main benefits of sulfolane-amine solution to capture acid gases is the ability to simultaneously remove mercaptans and COS, which cannot be absorbed by using pure chemical solvents [155]. The Sulfinol process can strip CO<sub>2</sub> down to 50 ppm at LNG plants. The physical features of the aqueous solution of sulfolane-amine allow the relative quantities of water and sulfolane to vary and the energy of regeneration to be reduced [156].

##### **2.4.2.1.1 Common mixtures of Sulfolane-Amine**

In this type of solvents, there is not any solid precipitating. Zong and Chen [156] utilized ENRTL for the liquid phase and PC-SAFT for the gas phase to model CO<sub>2</sub> and H<sub>2</sub>S solubilities in sulfolane-DIPA and sulfolane-MDEA solution. Ghanbarabadi and Khoshandam [157] compared the applicability of sulfolane-MDEA-water, DGA, MDEA-AMP, and MDEA in the capture of CO<sub>2</sub>, H<sub>2</sub>S and more components in process simulation. Their results show that more than 30-40% of mercaptans along with sour gas is absorbed with a sulfolane-MDEA-water solution of lower flow rate, boasting 10-25% reduction in energy consumption associated with solvent regeneration. In addition, very little waste of solvent is observed in comparison with amine solvents (MDEA-AMP, DGA, and MDEA). Dash and Bandyopadhyay [158] worked on a mixture of MDEA-PZ-sulfolane and measured the VLE data and modelled them by using ENRTL thermodynamic model.

##### **2.4.2.1.2 Phase change mixtures of Sulfolane-Amine**

A mixture of DETA, sulfolane and water exhibited phase change behaviour at different temperatures and CO<sub>2</sub> partial pressures [159]. The results showed that DETA and CO<sub>2</sub> were placed mainly in the

upper stage and sulfolane mainly remained in the lower stage. During the reaction of DETA with CO<sub>2</sub> in sulfolane, the carbamate, dicarbamate, and tricarbamate will be produced that all of them have low solubility in the solution and hence cause biphasic separation.

#### **2.4.2.2 Amine-alcohol**

Primary amine-methanol. The commercial name of the process that used this mixture as the solvent is Amisol process. Yu et al. [160] proposed a non-aqueous mixture of PZ and diethylene glycol (DEG) in RPB. It was reported that the 40.8 wt% PZ could be dissolved in DEG at 20 °C without precipitation. The regeneration energy could be reduced because the heat capacity of DEG is lower than water. A study focused on the solubility of CO<sub>2</sub> in the mixture of MEA and glycerol [161]. The authors found that at lower pressures the solubility of CO<sub>2</sub> in glycerol solution is higher. In another study, the solubility of CO<sub>2</sub> was measured at atmospheric pressure and different temperatures in the mixture of MEA and Glycerol [162]. In order to decrease the vapour ization of methanol its mixture with MEA, TEA and Glycerol are investigated namely MEA-TEA-Methanol, MEA-Glycerol-Methanol. By increasing the concentration of TEA and decreasing the concentration of MEA, the absorption rate, CO<sub>2</sub> capture efficiency, and absorption capacity all decreased [163].

Some non-aqueous mixtures of amines and alcohols show phase change behaviour, e.g. a mixture of AMP and Ethylene Glycol (EG) [164]. The authors reported that in comparison with AMP-DEG or AMP-triethylene glycol (TEG) solutions, the loading of CO<sub>2</sub> in AMP-EG solution is higher especially at a lower partial pressure of CO<sub>2</sub>. In addition, the viscosity of the AMP-EG solution is also lower.

#### **2.4.2.3 Amines-ILs**

The main reason for blending amines with ILs is related to the reduction of high viscosity of ILs which cause problems for the CO<sub>2</sub> capture process, improvement of CO<sub>2</sub> capacity and selectivity [165].

##### **2.4.2.3.1 Common mixtures of amines-ILs**

In the case of mixing amines with ILs, it was reported that the increase of amine concentration leads to an increase in the solubility of CO<sub>2</sub> in the mixed solvent. The solubility of CO<sub>2</sub> in this mixture is more than standalone IL solutions [166]. However, it must be mentioned that this mixture has a high viscosity [167].

Zhao et al. [167] measured viscosities, CO<sub>2</sub> capture rate and the capacity of 16 various absorbents. They reported that one gram of MDEA-[MDEA][Cl]-H<sub>2</sub>O-PZ could capture 0.158 gram of CO<sub>2</sub>. Feng et al. [166] added different amounts of tetramethylammonium glycine ([N1111][Gly]) in MDEA aqueous solutions of higher concentration. An aqueous solution of 15 wt% [N1111][Gly] and 15 wt% MDEA has significant regeneration efficiency. Yang et al. [168] proposed 30 wt % MEA-40 wt % [bmim][BF<sub>4</sub>]-30 wt % H<sub>2</sub>O solution for CO<sub>2</sub> capture. They illustrated that the energy consumption of the proposed solution for regeneration and MEA loss per ton of captured CO<sub>2</sub> was lower than that of aqueous MEA solution. Bernard et al. [169] reported corrosion and CO<sub>2</sub> absorption behaviour of the

mixed IL–amine solutions. The authors performed the absorption tests at 45 °C and at a pressure of 0.1–2.7 MPa. The corrosion tests were carried out at 45 °C under 2.7 MPa. They found that addition of [bmim][BF<sub>4</sub>] in aqueous alkanolamine solutions reduces corrosion rate for MEA by up to 72%. Yang et al. [170] reported that addition of IL to MEA aqueous solution reduced the losses of MEA and water. In addition, the thermal energy at stripper of IL mixed absorbent is 33.8% lower than that of aqueous MEA solution.

#### **2.4.2.3.2 Phase change mixtures of amine-ILs**

In addition to the usual mixtures of amines and ILs, there are some mixtures that operate as phase change solvents. Hasib-ur-Rahman et al. [171] mixed DEA with ILs. The result was a proper solvent that can capture CO<sub>2</sub> by producing DEA-carbamate crystals without any equilibrium limitations. This enabled easy separation by having a reasonably smaller solid carbamate volume and promising cost-effective regeneration.

#### **2.4.3 Mixture of physical solvents**

Mixture of different alcohols as a solvent for carbon capture is reported in literature [172-174]. Carrera et al. [172] blended glycerol with three alcohol namely ethanol, propanol, and butanol in the temperature range of 40-60 °C and pressure up to 12 MPa. The authors used the PR equation of state to correlate the results of CO<sub>2</sub>-glycerol-ethanol and showed good agreement between predicted and experimental values. Pinto et al. [173] mixed glycerol with methanol in the temperature range of 30-70 °C and pressure up to 22 MPa. They presented phase equilibrium data for the system. They considered three different methanol to glycerol ratios. Araújo et al. [174] considered glycerol with ethanol in 30-70 °C and pressures up to 26 MPa. They worked by three different glycerol to ethanol molar ratios.

The mixture of Sulfolane and alcohols also attracted attention. Xu et al. [175] correlated density, viscosity and the dissociation constant and solubility of N<sub>2</sub>O in the mixture of Sulfolane, 2-piperidineethanol (2-PE), and water. The authors illustrated that in addition to the tertiary system their correlations are useful for binary solvents like 2-PE-Water and Sulfolane-Water systems. Li and Mather [176] correlated the solubility of CO<sub>2</sub> and H<sub>2</sub>S in a mixture of 2-PE, Sulfolane, and water by using Clegg-Pitzer equations at different temperatures. Li et al. [177] combined ionic liquid and polyethylene glycol (PEG) to absorb and desorb the CO<sub>2</sub>. The authors reported that both chemical and physical absorption exists in the system and IL enhances the kinetics of the absorption and desorption of CO<sub>2</sub> significantly. Recently, Aghaie et al. [178] evaluated the solubility of ILs at various operating conditions and the influence of impurities/additives such as water and toluene.

### **3 Criteria to select and design of solvents**

#### **3.1 Chemical solvents**

Tennyson and Schaaf [179] illustrated that the criteria to choose the best solvent for CO<sub>2</sub> capture depends on the composition, temperature, and pressure of the feed gas and the desired specification on the treated gas. They presented a logarithmic diagram and located partial pressure of CO<sub>2</sub> in the product in the horizontal axes and partial pressure of CO<sub>2</sub> in feed in the vertical axes. Veawab et al. [180] illustrated that the essential elements of solvent selection criterion are feed gas characteristics (composition, pressure, temperature, etc.) and the treated gas specifications (i.e. the process requirements). Hoff et al. [181] discussed fourteen different criteria that must be considered when selecting and screening solvents for CO<sub>2</sub> capture. The authors divided these criteria into two main families: criteria based on kinetics, thermodynamics, and mass transfer properties and criteria based on health and safety executive (HSE) and operability. Liang et al. [42] addressed by details three important aspects that must be considered during evaluating reactive solvents and selecting optimum operating conditions namely solubility, reactive kinetics and chemical species analysis for CO<sub>2</sub> capture. Liang et al. [182] reviewed ten of these criteria with considerable details. Mota-Martinez et al. [183] indicated the importance of accounting transport and kinetic properties of solvents that have a significant effect on the size of equipment and capital cost. They mentioned that within the research community, the focus was more on equilibrium properties that are related to operating cost of CCS units.

#### **3.2 Physical solvents**

Different parameters must be considered during physical solvent selection: capital cost, purity of treated gas, the concentration of CO<sub>2</sub>, and hydrocarbon loss. Experience and inventiveness of the designer in adjusting the process to the case at hand, and method of dealing with impurities that may be present (such as COS, NH<sub>3</sub>, aromatic hydrocarbons) also play important role in selecting physical solvents. Other different parameters such as corrosion, foaming, or other operating problems which cause to replace the initial solvent, vapour pressure of the solvent, solvent stability, energy loss, stripping gas necessities, and the cost of process royalty should be considered as well [18]. When the process is operating in high pressure the physical solvents are more suitable because they can be regenerated by reducing the pressure. The physical solvents are also more efficient for concentrated CO<sub>2</sub> streams.

### **4 Selection and design of solvents using experiments**

#### **4.1 Description of method**

The experimental VLE data has high importance on the selection of the best solvent for CO<sub>2</sub> capture process [136]. High-pressure conditions are suitable for the reaction between CO<sub>2</sub> and chemical solvents, hence the challenge is finding an effective solvent at low partial pressure conditions. They demonstrated that the best choice of solvent depends on the partial pressure of CO<sub>2</sub>. In the selection of

solvents using experiments, the authors compared the effectiveness of two or more solvents or their mixtures together, experimentally. Different type of apertures are utilized with the method such as wetted wall columns, pilot plant packed columns or any other type of unit operations to contact the phases. This method is used to compare and select chemical, physical, and ILs.

#### **4.2 Advantages and disadvantages of the method**

The advantages of the method are related to its ease of application. The main weakness of the method is that a few numbers of solvents are utilized in the study. Experiments are always time consuming and expensive. Therefore, it cannot be said that the selected solvent is the best option.

#### **4.3 Review of related studies**

Ma'mun et al. [184] compared seven amines experimentally. They also considered some mixtures as well. The authors reported that AEEA is a potentially good absorbent for capturing CO<sub>2</sub> from low-pressure gases. Singh et al. [185] compared different alkanolamines in the aspect of the effect of structure on and capacity for CO<sub>2</sub> absorption. They found that decrease of the rate of absorption and increase of capacity of absorption will be obtained by increasing the chain length between the amine and various functional groups. Aschenbrenner and Styring [186] conducted experiments that investigated several non-toxic and low-cost solvents for CO<sub>2</sub> capture. They compared the mentioned solvents in the aspect of thermal stability, CO<sub>2</sub> solubility, and selectivity over N<sub>2</sub>. They reported that poly (ethylene glycol) is the best solvent in comparison with the other ones due to high stability, low solvent loss and low stripping energy. Chowdhury et al. [187] selected AMP and MDEA as the base case for comparison and synthesized nine new amines. They reported three high-performance amines with the high rate of absorption and low heats of reactions in comparison to AMP and MDEA. Freeman and Rochelle [35] calculated Maximum Estimated Stripper Temperature (MEST) parameter based on experimental data from the literature for comparison of 46 pure amines and 11 mixtures of amines in the aspect of thermal stability. The authors reported morpholine, piperidine, and piperazine as the most thermally stable amines. On the other hand, alkyl chain or alkanolamines with changing combinations of methyl substitution, hydroxyl substitution, and amino functions were found as unstable amines. Chowdhury et al. [188] compared twenty-four different tertiary amines by considering MDEA as the base case in terms of absorption rate, the amount of CO<sub>2</sub> absorbed, cyclic CO<sub>2</sub> capacity and heat of reaction for each solvent. Three of these amines were synthesized by authors. Barzagli et al. [189] experimentally compared the usefulness of several solvent-free amines. The authors stated that is not necessary to use any organic or aqueous diluent for these types of amines as they are in the liquid state prior to the experiment and after the CO<sub>2</sub> uptake. Zhang et al. [190] collected seventy-six conventional ILs and screened them for energy consumption to identify potential ILs for CO<sub>2</sub> capture. They selected seven ILs and calculated the energy consumptions of them. The amount of required energy and characteristics of seven screened ILs were compared with those of 30 wt% MEA, MDEA and DEPG.

They reported that the energy consumption of all seven ILs is less than three mentioned solvents. Muchan et al. [191] tested and compared amines in the aspect of the rate of absorption and desorption, pKa, the partial pressure of CO<sub>2</sub>, the heat of regeneration, and heat of absorption. They reported that due to the negative electron withdrawing effect of the hydroxyl groups, amines with more hydroxyl groups showed lower performance in all the CO<sub>2</sub> capturing activities. They also selected amines with only one hydroxyl group and blended them as binary and ternary mixtures and illustrated better performance in the initial rate of desorption and energy efficiency compared to 5 M MEA solution.

## **5 Selection and design of solvents using process and equilibrium models**

### **5.1 Description of method**

In this type of studies, the authors developed a process model [192] and evaluated the effect of a few numbers of solvents on the carbon capture level of the system, heat of absorption, and CO<sub>2</sub> capture capacity. Therefore, this type of studies also could be considered comparison studies. Different types of assumptions can be considered in the modelling and the models are from simple to rigorous. According to our literature review, this method is used for both chemical and physical solvents.

### **5.2 Advantages and disadvantages of the method**

The advantages of the method are that it is economical and after developing model they can be used for different conditions and operations. However, it must be mentioned that the models must be validated using appropriate experimental data. Similar to selection and comparison of solvents using experiments a limited number of components can be used in these type of studies.

### **5.3 Review of related studies**

MEA solution (30 wt%) is compared with mixtures of MEA-PZ and MDEA-PZ by using the equilibrium-based model of stripper [13]. The authors also considered four types of configurations for the stripper in their study. They showed that matrix configuration and MDEA-PZ offers 22% energy saving compared to MEA solution. In an interesting study Burr et al. [193] the four physical solvents (DEPG, Methanol, NMP, and propylene carbonate) are compared with each other in terms of acid gas removal ability, equipment required and power requirements by using the process simulator ProMax. Kothandaraman et al. [194] compared MEA with potassium carbonate solution using simulation in ASPEN PLUS®. Urech [195] compared three CO<sub>2</sub> capture processes by using process simulation. They considered Selexol, UNO (participating potassium carbonate solution), and MEA (or MDEA). Borhani et al. [128] worked on the industrial absorption of CO<sub>2</sub> into DEA-potassium carbonate solution in a packed column in ASPEN PLUS®. They changed DEA with other amines and compared the effectiveness of them as a promoter on carbonate solution. The authors reported that MEA shows promising performance as a promoter for CO<sub>2</sub> removal. Sharifzadeh and Shah [196], compared amine-promoted buffer salt solution with MEA solution in a rate-based model in gSAFT toolboxes. In another



study [197], they compared a new developed solvent GCCmax with MEA and reported that GCCmax has features superior performances compared to MEA. In addition, the authors introduced a new methodology to assess the performance of CO<sub>2</sub> capture solvents [197]. They faced the problem as retrofitting an existing pulverized coal power plant with post-combustion carbon capture using two solvents namely CDRMax (an amine-promoted buffer salt (APBS)) and MEA. They reported that the CDRMax offers high CO<sub>2</sub> loading capacity and thus reduces the circulation rate significantly as compared to MEA.

Chen et al. [198] compared the performance of Selexol, Rectisol, and water by using a theoretical method. This method was established to evaluate the mass transfer of CO<sub>2</sub> in a stationary single droplet. Rectisol had the highest absorption rate and capacity to capture CO<sub>2</sub> among the three solvents. Koysoumpa et al. [199] compared Rectisol, Selexol, potassium carbonate and MDEA in the aspect of efficiency and feasibility. The study presents a comparison among the conceptual designs and mass and energy analyses of the four processes integrated with the coal-to-SNG system, based on ASPEN PLUS<sup>®</sup>. A comprehensive comparison between ammonia and amines as CO<sub>2</sub> absorption solvents performed [200]. The authors used information such as energy consumption in regeneration and CO<sub>2</sub> capture efficiency to compare solutions. The solubility of CO<sub>2</sub> and carbamate concentration in DEA, MDEA, and DEA-MDEA mixture is modelled using equilibrium models based on Deshmukh-Mather thermodynamic models by [201]. The performance of DEA, MDEA, and DEA-MDEA solutions in CO<sub>2</sub> absorption is evaluated and compared using the electrolyte-UNIQUAC thermodynamic model in a rigorous equilibrium model [202].

## **6 Selection and design of solvents using predictive models**

### **6.1 Description of method**

In this approach, the predictive models act as screening tools. There is a different type of predictive models that can be used to perform screening and selection of solvents. Group contribution models (SAFT, UNIFAC,...), Quantitative Structure-Property Relationship (QSPR) models, computational chemistry methods (quantum mechanical based models and molecular dynamic) are some examples of predictive models that used to predict different properties for different components and purposes. These methods are used to select the ILs in the majority of studies.

### **6.2 Advantages and disadvantages of the method**

The advantages of using predictive models as a screening tool are their ease of application for a large number of components. In general, it can be said that these models are "forward problems" namely a desired property for a list of components can be calculated using a different type of properties related to chemical structure and other properties of components. Therefore, they must be applied for all the generated or collected components as solvents which cause sometimes extensive calculations.

## **6.3 Review of related studies**

### **6.3.1 Group contribution models applications**

The Statistical Associating Fluid Theory for potentials of variable range (SAFT-VR) is utilized as an EOS to model and evaluate the behaviour of alkanolamines, water, and CO<sub>2</sub> system [203]. A more predictive approach is the development of group parameters for these mixtures to use with the group contribution (GC) SAFT- $\gamma$  SW (square well) approach [204]. UNIFAC model is utilized for the first time by Lei et al. [205] to predict the CO<sub>2</sub> solubility in 22 pure ILs and in the binary mixture of ILs at high and low temperatures. Therefore, their study showed that UNIFAC can be used as a proper predictive model for screening the ILs.

### **6.3.2 Computational chemistry models applications**

Between quantum mechanical based models CSOMO-based models utilized widely in thermodynamic studies especially in CO<sub>2</sub> capture studies [206, 207]. These predictive thermodynamic models are utilized to predict some key properties that can help to select the best candidates between solvents. COSMO-based methods do not have adjustable parameters and therefore, experimental data are not required for them. They are particularly appropriate for the screening of potential ILs for CO<sub>2</sub> capture [103].

Zhang et al. [208] used the COSMO-RS model to predict Henry's constant of ILs. They had a pool of 24 cations and 17 anions and hence 408 ILs. As higher Henry's constant means the lower solubility, the authors used Henry's constant as a criterion for ILs selection. Finally, they selected three ILs which are not solid at room temperature and obtained them from Merck KGaA. They measured the solubility of CO<sub>2</sub> in [hmim][FEP], [bmpyrr][FEP], and [ETT][FEP] at three temperatures namely 283.5 K, 298.6 K, and 323.3 K and different pressures up to 1.8 MPa. Palomar et al. [206] illustrated that the van der Waals forces accompanying with the solute in the liquid phase control the CO<sub>2</sub> absorption capacity in ILs, which is measured in terms of Henry's Law constants. They screened over 170 ILs with COSMO-RS to design new ILs that increase physical absorption of CO<sub>2</sub>. Liu et al. [209] proposed a screening method to select the best ILs between 90 classes of ILs, based on COSMO-RS model, an absorption mechanism, and experimental data. The author considered CO<sub>2</sub> solubility, CO<sub>2</sub>-CH<sub>4</sub> selectivity and toxicity and viscosity of ILs as selection criteria. Retief [210] utilized the Hansen solubility parameters (HSPs) as the only parameter to screen a large number of amines and ILs solutions.

### **6.3.3 Chemometric model applications**

The chemometric methods are based on molecular structure and use chemical structure-based parameters to predict any type of properties [211, 212]. The QSAR/QSPR method has been used in several solvent designs and selection studies, the majority of which are related to ILs design [213-215]. The first attempt in this area was the work of Matsuda et al. [213]. They used QSPR methods coupled with descriptors of group contribution to design new ILs for applications other than CO<sub>2</sub> capture.

Furthermore, to predict the property of viscosity and ionic conductivity of ILs, some models are developed. In order to predict the pseudo acidity constant and the absorption isotherms for amines, a statistical neural network model is presented by Porcheron et al. [216]. Venkatraman et al. [214] used evolutionary de novo design to obtain imidazole-based solvents for CO<sub>2</sub> capture. The authors used QSPR methods to compute the density, viscosity, biodegradability, and acid dissociation constant (pKa) which is a proper criterion for solvent reactivity.

## **7 Selection and design of solvents using CAMD problem**

### **7.1 Description of method**

Due to the existence of non-ideal interactions between solvents, CO<sub>2</sub>, and water, the selection of the best solvent for such a system is very challenging. In order to select the most proper solvent, several properties such as thermodynamic, kinetic, and sustainability must be considered as criteria simultaneously [181, 217] but the mentioned methods in sections 3-5 only consider a few number or in some cases only one criterion to select the solvents. On the other hand, the three described methods in sections 3-5 expect some predictive models are screening methods, not design methods.

Therefore, a systematic method is proposed and developed in recent years to select or design of the best single and mixture solvents for CO<sub>2</sub> capture and also for selection and design of solvent integrated with the process. In a systematic selection of solvents, there is a large pool of candidates and a predictive model that is described in Section 5 must be used to identify useful solvent candidates. This approach is well-known as computer-aided molecular design (CAMD) and tries to select the best and optimum components for a special purpose from a pool of molecules and structures. The CAMD problem is known as “Reverse Problem” in which the component structure is design by giving the desired properties. There are three main approaches to dealing with CAMD problems [218, 219].

#### **7.1.1 Generate and search (test) approach**

In this approach, the molecular groups and target properties are identified first. After that, a feasible set of compound structures are generated. Then the properties of generated structures are predicted. The desired solvents can be selected from the identified components with predicted target properties [220]. This method can often result in finding optimum solvents or products over a pool of molecules without solving a potentially complex optimization problem [221].

#### **7.1.2 Algebraic modelling approach**

In this approach, a set of algebraic equations representing the property and structural constraints are solvent at the same time to generate the target molecules [222].

#### **7.1.3 Mathematical optimization approach**

In addition to two mentioned approaches, the CAMD problems can be expressed as optimization problems. The solvent selection and design optimization problem is a mixed integer nonlinear problem

(MINLP) in most of the cases [218]. Most of the studies on CO<sub>2</sub> capture are performed by using this method and it is described by the detail in Section 6.3.

## 7.2 Advantages and disadvantages of the method

The numerous number of molecules and components can be evaluated systematically using this method. The challenges of CAMD method are related to the availability of predictive models for all properties, numerical issues related to generated components, the high degree of nonlinearity of the problem, and generation of a large number of components [223].

## 7.3 Review of related studies

### 7.3.1 Single and mixture solvent selection and design

In this problem, the structure of the solvent is the only design objective. The schematic diagram of single and mixture solvent and selection design is shown in **Figure 2**.

**Figure 2:** Single and mixture solvents selection and design problem framework.

The single solvent selection and design can be formulated as follow:

$$\begin{aligned}
 & \min C(n, p) \\
 & n \\
 & p = f(n) \quad \text{Solvent predictive model} \\
 & h_1(p, n) \leq 0 \\
 & h_2(p, n) = 0 \\
 & s_1(n) \leq 0 \\
 & s_2(n) = 0 \\
 & p_{min} \leq p \leq p_{max} \\
 & n_{min} \leq n \leq n_{max}
 \end{aligned} \tag{1}$$

where  $C$  is objective or cost function which depends on two set of variables namely vector  $n$  and vector  $p$ . Vector  $n$  demonstrates relevant structural information of the designed molecules and vector  $p$  is the vector of properties. The constraints  $h_1$  and  $h_2$  are related to property values and desired structural features.  $s_1$  and  $s_2$  ensure structural feasibility. The similar formulation can be considered for mixture selection and design:

$$\begin{aligned}
 & \min C(n, p, q) \\
 & n, x \\
 & q = f(x, n, p) \quad \text{Solvent, property, and mole fraction relation model} \\
 & \sum_i x_i = 1 \\
 & h_1(p, q, n) \leq 0 \\
 & h_2(p, q, n) = 0 \\
 & s_1(n) \leq 0 \\
 & s_2(n) = 0 \\
 & p_{min} \leq p \leq p_{max} \\
 & n_{min} \leq n \leq n_{max} \\
 & q_{min} \leq q \leq q_{max}
 \end{aligned} \tag{2}$$

where here  $C$  is a function of  $n$ ,  $p$ , and  $q$  which  $q$  is the mixture property variables. The main elements of the single and mixture solvents selection/design optimization problem are:

- (i) **Design space:** This space contains different molecules and mixtures and a wide range of operations.
- (ii) **The solution of the problem:** Different type of algorithms can be utilized to solve CAMD problems such as deterministic algorithms and stochastic (heuristics) ones. In addition, large optimization problems can be solved as a series of optimization sub-problems by using decomposition methods.
- (iii) **Predictive property models:** These models relate molecular structure to physical properties and estimate property. In general, the predictive models must predict phase equilibria, caloric values, transport properties, kinetic properties, and the impact on product morphology or toxicity.

Papadopoulos et al. [217] considered several criteria and developed a systematic screening method. They selected the best solvent candidates based on the criteria from 126 commercially available amine-based solvents which had enough data required for GC or other methods to calculate properties. The authors used the SAFT-VR and SAFT- $\gamma$  equation of states to predict the vapour -liquid equilibrium behaviour of solvent-CO<sub>2</sub>-H<sub>2</sub>O for the selected solvents. Chong et al. [106] developed a systematic approach to design an optimal IL to capture CO<sub>2</sub>. The significant contribution of the presented approach in their work is the introduction of disjunctive programming to identify optimal operating conditions of the process involved while solving the IL synthesis problem. Chong et al. [224] presented a simple yet systematic visual approach to design IL solvents for carbon capture. A systematic two-stage approach has been proposed to discover the proper CO<sub>2</sub> capture solvents [225]. This approach initiates with a fast screening stage in which the solvent structures are evaluated based on the simultaneous consideration of important pure component properties reflecting thermodynamics, kinetics, and sustainability. In the second step of the approach, the solvents are further selected and evaluated using SAFT- $\gamma$  SW to predict the non-ideal chemical and phase equilibrium of the solvent-water-carbon dioxide mixtures. Zarogiannis et al. [226] repeated their methodology [217] with a few changes to select the binary mixture of amines and reported that a mixture of DEAB and 2A1H was promising among the other options.

### 7.3.2 Integrated solvent and process selection and design

Design and selection of a representative set of solvents without attention to the CO<sub>2</sub> capture processes is not a proper strategy due to the strong interaction between solvent properties and the process [227, 228]. Therefore, the best goal can be an integration of solvent and process design. Establishment of a direct connection between solvents and process is challenging. The method is based on combining CAMD with process synthesis methods in the form of an optimization framework which is MINLP

[223] and is well-known as computer-aided molecular and process design (CAMPD) [229]. Such a framework has been shown in **Figure 3**.

**Figure 3:** Integrated solvent and process selection/design problem framework.

It can be seen that the framework presented in **Figure 3** is more complex than the framework of **Figure 2**. Integrated solvent and process selection/design (for single solvent) can be formulated as follow [221]:

$$\begin{aligned}
 & \min C(n, p, \mu) \\
 & n, \mu \\
 & p = f(n) \quad \text{Solvent predictive model} \\
 & h_1(p, \mu, n) \leq 0 \\
 & h_2(p, \mu, n) = 0 \\
 & s_1(n) \leq 0 \\
 & s_2(n) = 0 \\
 & p_{min} \leq p \leq p_{max} \\
 & n_{min} \leq n \leq n_{max} \\
 & \mu_{min} \leq \mu \leq \mu_{max}
 \end{aligned} \tag{3}$$

where here  $C$  is a function of  $n$ ,  $p$ , and  $\mu$  which  $\mu$  is the process variables.  $h_1$  and  $h_2$  here representing process model. The main elements of the integrated solvent and process selection/design optimization problem are:

- (iv) **Design space:** Same as Section 7.3.1.
- (v) **The solution to the problem:** Same as Section 7.3.1.
- (vi) **Predictive property models:** Same as Section 7.3.1.
- (vii) **Predictive process models:** These models are used to relate physical properties to process performance. This model can be equilibrium-based or rate-based models with different type of assumptions and complexity [60].

Eden et al. [230] presented a systematic framework for the simultaneous solution of process/product design problems related to separation. By using this method, the properties of the desired product that offer optimum process performance are identified. Lots of studies on the integrated design of solvent and process were performed using SAFT family EOS as a predictive model. Mac Dowell et al. [231] find out the optimal composition for the mixture of AMP and Ammonia integrated with optimal operating conditions for the CO<sub>2</sub> absorption process. They calculated VLE using SAFT-VR and also utilized a rate-based model as the process predictive model. Pereira et al. [232] applied SAFT-VR to separate CO<sub>2</sub> from the methane-utilizing physical solvent. They considered n-alkane blends as a proper solvent for CO<sub>2</sub> capture and used a simple flowsheet to maximize the purity and net present value. They reported the best sizes of equipment, operating conditions, and the average chain length of the solvent (n-alkane). The results suggest that n-alkane solvents are promising alternatives. Bardow et al. [233] utilized PCP-SAFT and proposed a two-step procedure for the integration of solvent and process design. In the first step, they considered a hypothetical target molecule and reported that this continues-molecular-targeting (CoMT) approach attains the direct coupling between solvent and process

properties. In the second step, they mapped the hypothetical target molecule to the real solvent molecules. This method is applied by the same research group for CO<sub>2</sub> capture processes by [234] and [218] which in both studies the selection of physical solvents are integrated with the process.

Salazar et al. [235] proposed a method to select the novel solvents between 50 primary amines and solvent stripping for CO<sub>2</sub> capture from flue gas of fossil-fired power plants. The method is based on CAMD for solvent selection and integrating with solvent stripping process design to achieve better CO<sub>2</sub> capture and reduce energy consumption. Qadir et al. [236] presented an optimization method that simultaneously targets an optimal solvent and optimal process conditions for pre-combustion carbon capture processes (by physical solvents). The authors' utilized PPC-SAFT equation of state is used to determine solvent properties and made a connection between MATLAB (for MINLP problem) and ASPEN PLUS® (for process model).

Burger et al. [229] proposed a novel two-step method to solve CAMPD problems that are used for physical CO<sub>2</sub> capture. In the first step, is to have a set of initial guesses for the MINLP problem, they derived reduced models for the unit operations of the process. In the case that is not possible to calculate the original objective function from the reduced model, some surrogate objectives are defined which represent different contributions to the original objective. The Pareto-optimal set of best compromises between these objectives is determined using multi-objective optimization step (MOO). In the second step, the original MINLP problem is solved. The Pareto-optimal solutions are then used as initial guesses for the solution of the full MINLP. In order to predict the required physical properties, they used SAFT- $\gamma$  Mie. Papadokostantakis et al. [237] combined CAMD, GC method, superstructure based process synthesis, and multicriteria sustainability assessment to screen a big number of chemical solvents and process configurations for post-combustion CO<sub>2</sub> capture. Zhou et al. [238] demonstrated that the majority of the earlier studies utilized decomposition solution strategies to solve the CAMD problems. They proposed a hybrid stochastic-deterministic algorithm to solve the integrated design problem of absorption/desorption. They also used their method to show its effectiveness and strength on a gas absorption process. In the absorption process solvent, molecular structures and process operating conditions are optimized simultaneously to maximize the overall economic performance of the process. The authors utilized high-level GC predictive models to predict the required properties. Recently, Papadopoulos et al. [239] added an assessment of controllability to the integrated solvent and process design. Therefore, their proposed framework contains three main stages: solvent-process screening stage (contains CAMD and analysis of obtained solvent set), solvent-process design (contains rigorous models and operating targets), and solvent-process control (integrates the controllability and economic performance).

## **8 Prospective**

In this review paper, we illustrated the importance and role of different solvents in capturing CO<sub>2</sub>. There are many attempts to find methods to screen and select the best solvents. By all the available studies still, there are some demands that must be addressed in future studies.

### **8.1 Evaluation of technical and economic performance of solvents**

So far, no detailed and systematic and comparison studies were presented on the technical and economic performance of different solvents and the studies are devoted to one solvent [240]. In addition, the economic criteria should be considered more in studies to reduce the capital and operation cost of carbon capture processes for all type of solvents.

### **8.2 Life cycle assessment of different solvents**

There are eleven studies focused on LCA of CCS [241]. Most of these studies are focused on the method of separation and compared these methods using LCA. A few LCA studies have been done to compare the solvents [242, 243]. Thereby there is a gap in the literature that requires further research to be conducted in comparing solvents using LCA.

### **8.3 Solvent selection using experiments**

Future efforts should be directed towards performing more experimental comparison between solvents especially using the newly designed solvents. By this method, the newly designed solvents can be validated in the aspect of energy consumption, degradation and corrosion problems. In addition, in order to predict the physical property of new solvents, more experimental data are required.

### **8.4 Solvent selection using process and thermodynamic models**

Majority of process and thermodynamic modelling and simulation studies are performed using well-known solvents in literature. More studies are required by using more diverse solvents such as new amines, new ILs, and comparison of physical and chemical solvents. This will help to find out the applicability and effectiveness of new solvents.

### **8.5 Solvent selection using predictive models**

Development of more applicable, accurate, and effective predictive models which are integrated with the CAMD and CAMPD problems can be helpful in the initial screening of the solvents. In addition, the predictive and molecular-based methods such as quantum chemistry, molecular dynamic, Monte Carlo, SAFT, and UNIFAC showed high potential to perform microscopic characterization of CO<sub>2</sub> capture using solvents [101, 244].

### **8.6 Solvent selection and design using CAMD**

More studies on integrated solvent and process design are required as these activities are still in the infant stage. As ILs attracted a lot of attention in recent years and showed desirable characteristics they



should be used in CAMPD problems by considering the different type of unit operations such as packed columns, rotating packet bed columns, wetted wall columns and etc. After screening and design of proper ILs candidates, they should be the synthesis in laboratory scales and test in the mentioned above unit operations. In addition, the mixed solvents could be considered a serious alternative for single solvent systems and more studies are necessary for them, especially in the aspect of CAMD problems.

## 9 Conclusions

Available solvents for CO<sub>2</sub> absorption are reviewed and classified. The paper classified available solvents as chemical, physical, and chemical-physical solvents. The mixture of solvents also reviewed in this paper based on three groups which are a mixture of chemical solvents, a mixture of physical solvents, and a mixture of chemical and physical solvents. The recent progress and researches in each group are reviewed and mentioned in the study. In addition to the review of available solvents, different methods for solvent selection and design are reviewed. Four groups of methods are categorized in this study which is solvent selection and design using experiments, using process and equilibrium models, using prediction models, and using optimization problems. For each method, a number of selected studies and recent progress are reviewed.

## Acknowledgment

The authors acknowledge financial support from UK Engineering and Physical Sciences Research Council (EPSRC) (Ref: EP/M001458/2).

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