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A report that identifies knowledge gaps for thermodynamic properties of CO_2 mixtures with impurities

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History table

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Key word list

CO$_2$ mixtures, impurities, phase equilibria, derivative properties, transport properties, experimental data, knowledge gaps

Definitions and acronyms

Acronyms	Definitions
EoS	Equation of State
PC-SAFT	Perturbed Chain – Statistical Associating Fluid Theory
VLE	Vapor – Liquid Equilibria

Acknowledgements

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Disclaimer

1. Executive summary

CO2QUEST is a project funded by the EC FP7 Energy Programme, which addresses the fundamentally important issues regarding the impact of the typical impurities in the gas or dense phase CO_2 stream captured from fossil fuel power plants on its safe and economic transportation and storage.

This report forms Deliverable 1.7 of Work Package 1 and presents the results of an extensive literature review on available experimental data for systems that contain CO_2 and are of interest to CO2QUEST. Along with the collection of the data, an estimation of the knowledge gaps is given, as well as some first suggestions for experimental measurements to be obtained via this project.

2. Introduction

The Deliverable 1.7, titled “A report that identifies knowledge gaps for thermodynamic properties of CO_2 mixtures with impurities”, is an attempt to gather the available data in the literature that regard thermodynamic properties of CO_2 mixtures with other gases. This database will serve as the basis for validation of the thermodynamic models that are currently being developed in CO2QUEST. Moreover, the mapping of the available data will indicate the knowledge gaps and give general directions on what experimental data is needed to be measured.

2.1 General context

Properties such as phase equilibria, derivative properties, and transport properties are necessary for the design of pipelines that will be used for CO_2 transport. These properties are affected by the existence of impurities in the stream of CO_2, in a way that should be accurately predicted by any thermodynamic property model that is going to be used for the design. Offline basic experimental work that is available in the literature can give data for a number of properties of several CO_2-containing systems, but as the complexity of the models increases, more data is needed.

2.2 Deliverable objectives

The objectives of the Deliverable 1.7 are stated below:

- Form a collection of the available and relevant experimental data, for a number of systems and properties that are of interest to CO2QUEST.
- Identify the knowledge gaps, meaning the properties or systems that no data are reported in the literature, yet they are necessary for thermodynamic model development and validation.
- Give some sample suggestions for experiments to be performed.

3. Methodological approach

This deliverable was approached at four levels, closely linked to the objectives. For each level, a specific methodology was followed, which will be described in this part.

3.1 Literature Review

Extensive literature review was carried out, using widely acceptable search engines for scientific papers, including Scopus, ScienceDirect, Google Scholar, ACS Publications. The search was based on keywords that include the definition of the fluid systems that were under investigation, and the properties, or the family of properties of interest. Keywords such as “phase equilibria CO_2 mixture”, “speed of sound CO_2 mixture”, etc. were used as starting points to get access to the desired data. Databases that are closed to the public, proprietary, or not accessible within the premises of NCSR were not taken into account.

3.2 Database of experimental data

The research papers that included data for thermophysical properties of CO_2 mixtures with other gases, were processed further, in order to extract these data in tabulated format. In some cases, the data were only presented in figures, so they were extracted to tables with the use of specialized software. The already tabulated values were just copied to a Microsoft Excel file, which is actively indexed by the means of a customized macro. In other words, the database is easily expandable and user friendly.

3.3 Identification of knowledge gaps

Upon the completion of the data collection, the conditions and components range was compared to the desired respective ranges that are ultimately of interest to CO2QUEST. This gave rise to the missing data, in terms of conditions, properties, and impurities.

3.4 Suggestions for experimental measurements

Having identified the knowledge gaps, thermodynamic models that are currently developed in CO2QUEST, were used to produce predictions of unknown data, so as to potentially form the basis of experimental design.

4. Summary of activities and research findings

4.1 Literature Review

The literature review for thermodynamic properties data of CO2-containing mixtures of interest to CO2QUEST resulted in a large number of data, especially for binary mixtures (CO_2 with any given impurity from the list of Ar, CH_4, H_2S, N_2, SO_2, H_2O).
Figure 1 shows the conditions range of the binary mixtures VLE data. As a general comment, can be noted that there are enough data for VLE binary mixtures covering all the range where VLE exists. These data are necessary for the optimization of binary interaction parameters. Work on this topic has been published by Diamantonis et al. [1] reporting optimum binary interaction parameters for all these binary systems, and for a number of EoS.

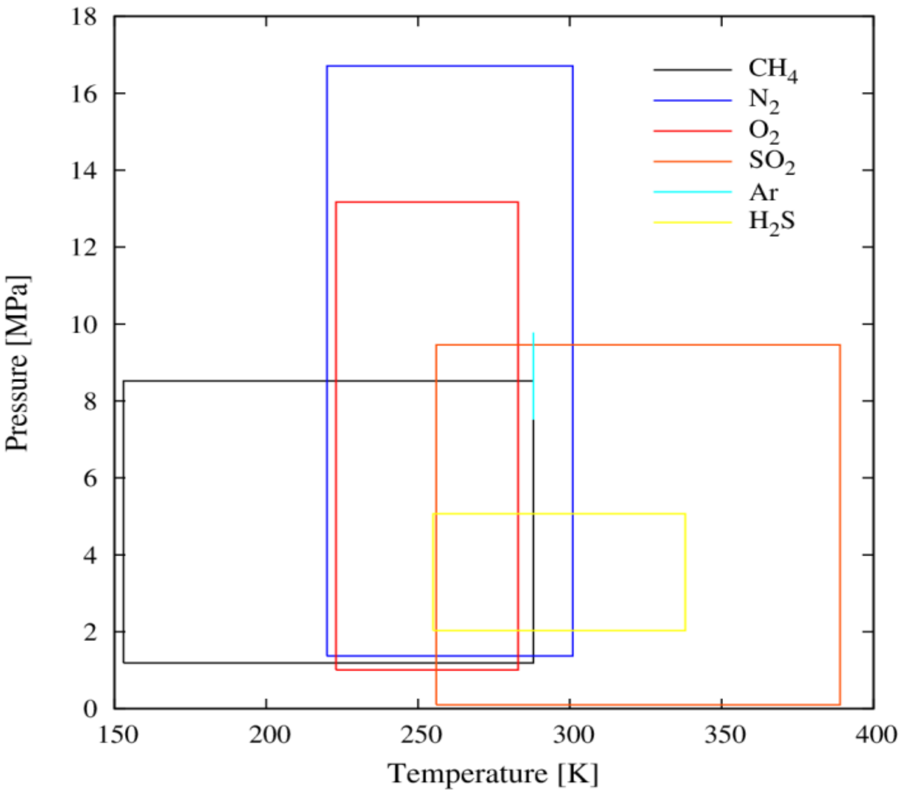

Figure 1. Range of conditions where binary VLE data exist in the literature.

For the sake of completeness, Table 1 summarizes the references of the available data for binary systems VLE.

Especially the system CO$_2$-H2O has been studied separately, because of its scientific and technological importance, and experimental data for its VLE is given from Valtz et al. [2], Wiebe and Gaddy [3], Nakayama et al. [4], King et al. [5]. The temperature range is 298K-533K, while the pressure reaches as high as 20MPa, with the addition of a single point at 50MPa.

Table 1. References for VLE data of binary mixtures containing CO_2 and 1 impurity. [1]

System	Temperature (K)	Pressure (MPa)	Reference
CO_2-CH_4	311 - 511	1.4 - 6.9	Reamer et al. [6]
CO_2-CH_4	167 - 301	2.0 - 7.4	Donnelly and Katz [7]
CO_2-CH_4	230 - 250	0.9 - 8.5	Davalos et al. [8]
CO_2-CH_4	89 - 208	0.5 - 6.3	Mraw et al. [9]
CO_2-CH_4	205 - 320	0.2 - 48.0	Esper et al. [10]
CO_2-CH_4	253 - 288	6.2 - 8.5	Arai and Saito [11]
CO_2-N_2	223 - 273	0.7 - 16.9	Dorau et al. [12]
CO_2-N_2	209 - 320	0.1 - 48.0	Esper et al. [10]
CO_2-N_2	253 - 288	3.5 - 14.1	Arai and Saito [11]
CO_2-N_2	220 - 270	1.8 - 14.0	Brown et al. [13]
CO_2-N_2	230 - 250	6.2 - 10.3	Al-Sahhaf [14]
CO_2-N_2	220 - 240	0.6 - 16.7	Al-Sahhaf et al. [15]
CO_2-N_2	273 - 293	4.5 - 12.0	Yorizane et al. [16]
CO_2-N_2	288 - 301	5.1 - 10.3	Krichevskii et al. [17]
CO_2-O_2	223 - 283	1.0 - 13.2	Frendeslund and Sather [18]
CO_2-SO_2	291 - 416	2.7 - 10.5	Caubet [19]
CO_2-SO_2	256 - 308	0.1 - 3.1	Blumcke [20]
CO_2-SO_2	263 - 233	0.1 - 9.0	Lachet et al. [21]
CO_2-Ar	288.15	5.7 - 9.8	Sarashina et al. [22]
CO_2-H_2S	273 - 370	1.0 - 8.0	Bierlein and Kay [23]
O_2-N_2	77 - 125	0.1 - 3.0	Dodge and Dunbar [24]

More complex mixtures measured for their VLE and reported in the literature are shown below:

Table 2. References for VLE data of ternary and quaternary mixtures containing CO_2.

System	Temperature (K)	Pressure (MPa)	Reference
CO_2-N_2-O_2	273	5.2 - 10.6	Muirbrook and Prausnitz [25]
CO_2-N_2-O_2-Ar	250 - 290	7 - 9	Chapoy et al. [26]

Table 3. References of data on thermodynamics derivative properties of CO_2 mixtures with impurities.

System	Temperature (K)	Pressure (MPa)	Reference
		Speed of sound	
CO_2-CH_4	268 K,301 K	8.8 - 38.1	Alsiyabi et al. [27]
CO_2-N_2	268 K, 301	9.5 - 38.2	Alsiyabi et al. [27]
CO_2-O_2	268 K,301K	10.4 - 40.9	Alsiyabi et al. [27]
CO_2-Ar-CO	268 K301K	13.1 - 41.1	Alsiyabi et al. [27]
		Joule-Thomson Inversion Curve	
CO_2-CH_4	275-950 K	23.1 - 70.1	Vrabec et al. [28]
CO_2-CH_4-N_2	200-875 K	15.0 - 59.4	Vrabec et al. [28]
		Isothermal Compressibility	
CO_2-Ar	268 , 301	9 - 37	Alsiyabi et al. [27]
CO_2-CH_4	268 , 301	9 - 37	Alsiyabi et al. [27]
CO_2-Ar-CO	268 , 278 , 301	7.5 - 39	Alsiyabi et al. [27]
CO_2-CH_4-N_2-H_2	268 , 301	7.5 - 35	Alsiyabi et al. [27]

Table 4. References of data on transport properties of CO_2 mixtures with impurities.

System	Temperature (K)	Pressure (MPa)	Reference
		Viscosity	
CO_2-CH_4	293 - 303	0.1 - 2.6	Kestin and Yata [29]
CO_2-N_2	293	0.1 - 2.3	Kestin and Leidenfrost [30]
CO_2-O_2	298 - 674	0.1	Kestin et al. [31]
CO_2-N_2-O_2	300	0.1	Gururaja et al. [32]
CO_2-Ar-N_2	298 - 873	low pressure gas	Kestin and Ro [33]
CO_2-CH_4-N_2	298 , 373 , 473	low pressure gas	Kestin and Ro [33]
CO_2-N_2-O_2-Ar	243 - 423	0 - 150	Chapoy et al. [26]
		Thermal conductivity	
CO_2-CH_4	335 - 435	3.4 – 68.9	Rosenbaum and Thodos [34]
CO_2-CH_4	298 , 308	0.1 - 9	Yorizane et al. [35]
CO_2-CH_4	212 - 267	0.2 – 1.8	Christensen and Fredenslund [36]
CO_2-N_2	320 - 470	1 - 31	Johns et al. [37]
CO_2-N_2	348	0.1 – 300	Gilmore and Comings [38]
CO_2-N_2	300 - 2000	low pressure gas	Westenberg and DeHaas [39]
CO_2-N_2	642 - 961	0.1	Rothman and Bromley [40]
CO_2-SO_2	323 - 373	gas state	Maczek and Gray [41]
CO_2-O_2	370	gas state	Cheung et al. [42]
CO_2-Ar	298 - 308	0.1 - 9.0	Barua et al. [43]
CO_2-Ar	298 , 308	0.1 – 9.1	Yorizane et al. [35]
CO_2-N_2-O_2	370	gas state	Cheung et al. [42]

4.2 Database of experimental data

The database that was initiated with the collection of the previously mentioned data, is based on Microsoft Excel and a macro that indexes the workbook, so as to easily find the needed data. A screenshot of the index is given in Figure 2 for illustration purposes.

25	CO2-N2 Visco Kestin
26	CO2-CH4 Visco Kestin
27	CO2-N2-O2 Visco Gururaja
28	CO2-N2-CH4 Visco Kestin
29	CO2-imp compositions Alsiyabi
30	Pure CO2 sound Alsiyabi
31	CO2-imp sound -5C Alsiyabi
32	CO2-imp sound 28C Alsiyabi
33	Pure CO2 isoT compr Alsiyabi
34	CO2-imp isoT compr Alsiyabi
35	CO2-imp isoT compr -5C Alsiyabi
36	CO2-imp isoT compr 28C Alsiyabi
37	Thermal Conductivity References
38	CO2-O2-N2-CH4 Th Cond Cheung
39	CO2-SO2 Th Cond Maczek
40	CO2-N2 Th Cond Rosenbaum
41	CO2-N2 Th Cond Johns
42	CO2-N2 Th Cond Gilmore
43	CO2-N2 Th Cond Westenberg

Figure 2. Part of the index of the Microsoft Excel based experimental data collection.

The data is contained in separate worksheets, tabulated in a way that depends on the kind of data that it contains. The reference of the paper from which the data are extracted is given explicitly, as well as the units and some notes regarding the experimental procedure that was followed.

Most of these data has already been taken into account when validating models for VLE, density, and viscosity, for the corresponding conditions ranges.

Also, during the modelling procedure, some inconsistent data were left out, so as to avoid discrepancies and convergence errors when performing thermodynamic modelling.

4.3 Identification of knowledge gaps

- Phase equilibria (VLE) and density
    - More ternary and quaternary systems, possibly containing SO_2 and H_2S
    - Multicomponent systems that approach real pipeline CO_2 mixtures
- Derivative properties of multicomponent mixtures
    - Speed of sound
    - Heat capacities (isochoric and isobaric)
    - Joule-Thomson Inversion Curves
- Transport properties
    - Viscosity and Thermal conductivity
        - Higher pressures, close to pipeline operation conditions
        - Multicomponent systems

4.4 Suggestions for experimental measurements

4.4.1 Phase equilibria of multicomponent systems

Previous studies of the NCSR "D" group [1, 44] provide a comprehensive analysis of phase equilibria of binary mixtures of CO_2 and a number of components, for a range of impurities that can occur in the CCS process. The data that were used for the validation of the thermodynamic models were obtained from reliable literature sources, thus, in most of the cases pressure – composition plots are constructed for some given values of temperature.

As complexity increases in terms of number of components in the mixture, less experimental data are available in the literature. Presently, apart from binary systems, only the system CO_2-O_2-N_2 was studied by NCSR "D" as there were some experimental data available. Needless to say, that quaternary, and even richer mixtures, were not found in the literature.

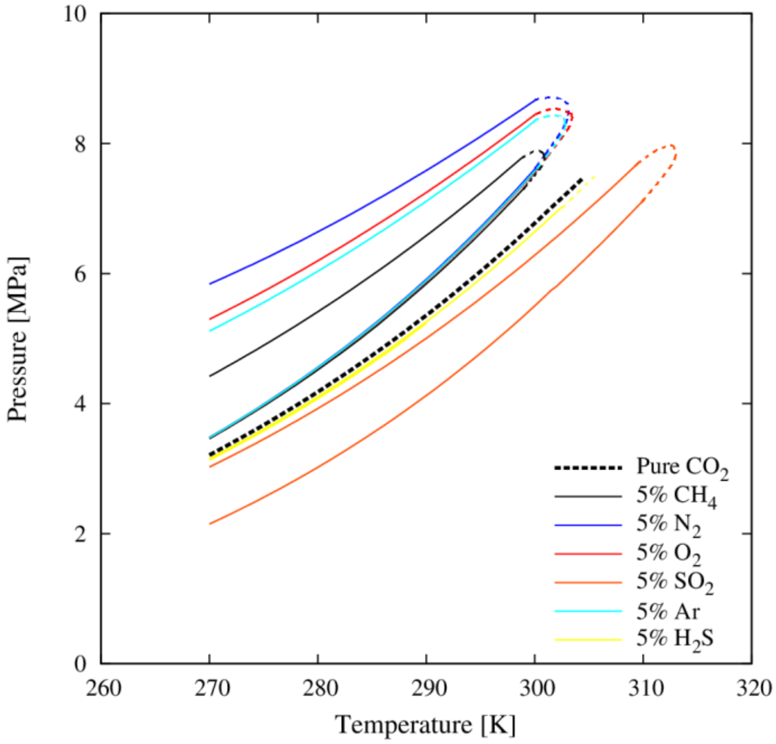

Figure 3. Predictions of phase envelopes for binary mixtures of CO_2 with 5 % (mole) of impurities, with PC-SAFT.

According to some reports [45, 46] that serve as international guidelines, the CO_2 content after the capture part should not be lower than 95% (mole fraction). It is suggested that the low limit, for the purpose of this document, of CO_2 is set to 90%, so as the effect of impurities has a significant contribution in the thermodynamic model calculations, in order to avoid numerical errors due to very low values of composition. Another constraint is that the content of N_2 should not exceed 4%. These constraints are taken into account in the design of the mixtures to be measured.

For this reason, the suggested experiments contain ternary and quaternary systems at a given feed composition that adheres to the aforementioned guidelines, so that the bubble (P^{bubble}) and dew pressures (P^{dew}) by varying temperature (T) shall be measured. This will give as result the phase envelopes of the mixtures (P-T plots), which are very important for process design, as well as for model validation and optimization.

From a previous study [47], the phase envelopes of CO_2 binary mixtures with impurities (Fig. 3), as calculated by PC-SAFT equation of state (EoS), show that the only impurity that moves the envelope to lower pressures is SO_2, while H_2S produces a very narrow phase envelope almost overlapping with the pure CO_2 VLE curve.

Ternary systems

Suggestions for ternary systems to be measured in terms of their phase envelope contain CO_2-CH_4-Ar, CO_2-CH_4-N_2. PC-SAFT calculations were performed for the prediction of those phase envelopes and are presented in Fig. 4.

Since all other impurities shift the envelope to higher pressures, it would be interesting to investigate the combined effect of two impurities with opposite effects, such as SO_2 and N_2. Therefore, the ternary system CO_2-SO_2-N_2 is one of the suggestions for measuring its phase envelope. Predictions from PC-SAFT EoS are shown in Fig. 4

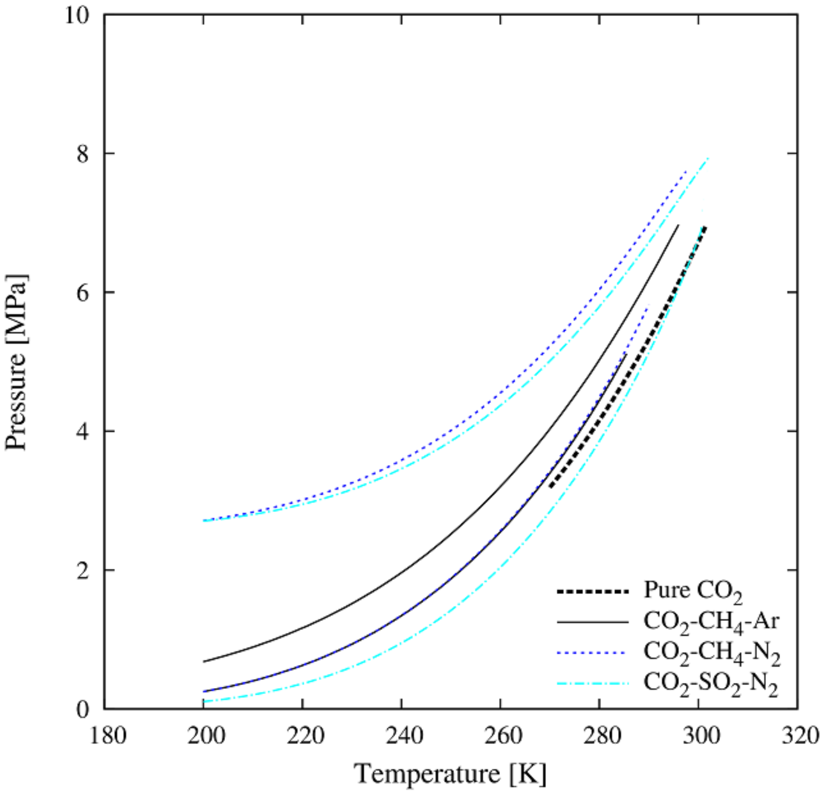

Figure 4. PC-SAFT EoS predictions of phase envelopes of ternary mixtures. Compositions reported in Table 5.

It can be drawn as a conclusion from Fig. 4 that the substitution of CH_4 with SO_2 in the ternary mixture that contains CO_2, N_2, and one of the CH_4 and SO_2, indeed has the desirable effect of shifting the phase envelope to lower pressures. It remains to be validated by experiment.

Quaternary systems

To the authors' knowledge, the mixture with the highest number of components that has been reported in the literature is that of CO_2-N_2-CH_4-H_2 [27]. Several properties were reported in that paper, except for the phase envelope. The isothermal compressibility of the mixture was modeled by NCSR "D" with the use of PR and PC-SAFT EoS, and good agreement between experimental data and model predictions was found (Fig. 5).

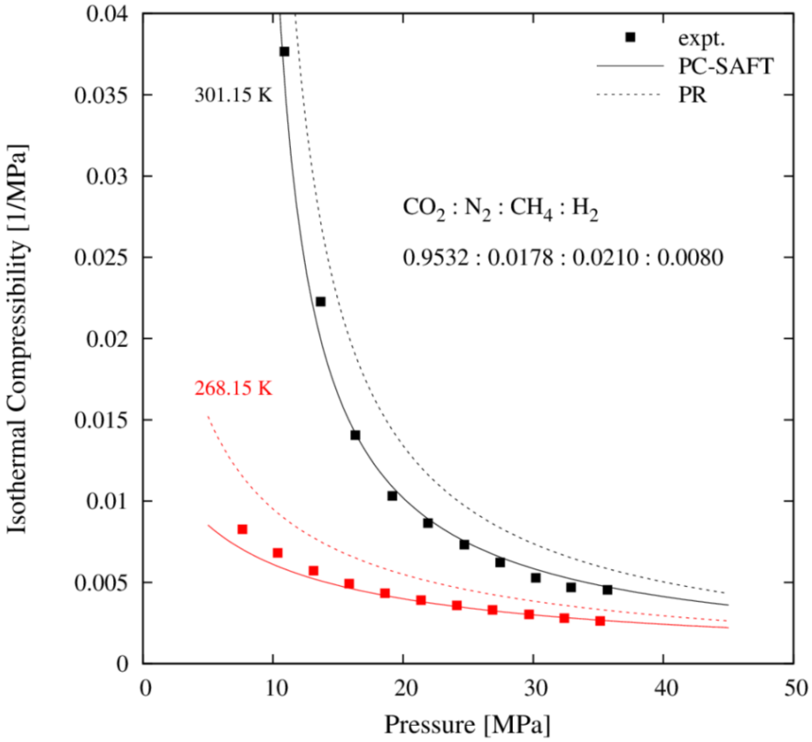

Figure 5. Isothermal compressibility of the quaternary system CO_2-N_2-CH_4-H_2. Experimental data [27] (points) and EoS predictions (lines).

With the experimental measurement of the phase envelope of this system, the thermodynamic models developed in the framework of CO2QUEST will be more thoroughly validated, as well as a very strong and useful literature publication with experimental data and modeling can be produced.

Another quaternary system that can be very useful for thermodynamic model validation is the CO_2-O_2-N_2-Ar. The composition of the system was calculated by assuming a 93% (mole) of CO_2 and the remaining 7% was distributed among O_2, N_2, and Ar, following the composition of atmospheric air (approximately 21%, 78%, and 1% respectively. Thus, the feed composition of CO_2-O_2-N_2-Ar is 0.9300:0.0546:0.0147:0.0007. The predicted phase envelopes of both quaternary systems discussed here are shown in Fig. 6.

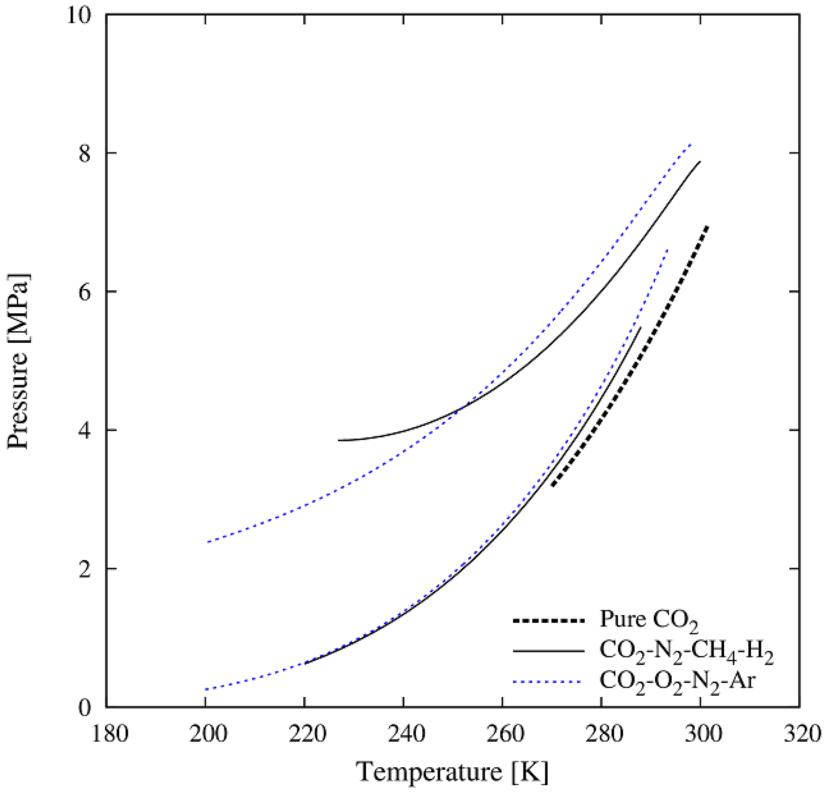

Figure 6. PC-SAFT EoS predictions of phase envelopes of quaternary mixtures. Compositions reported in Table 5.

Summary

A summary of the mixtures, compositions and conditions, is reported in Table 5. Of course, this is an open topic for discussion, according to the features of the available equipment.

Table 5. Compositions and conditions ranges for phase equilibria experiments on suggested CO_2 mixtures.

Mixture	Composition of liquid phase (mol %)	Temperature range (K)	Temperature step (K)	Pressure range (expected) (MPa)
CO_2-CH_4-Ar	95.0 : 4.9 : 0.1	200 – 300	20	0.5 – 8.0
CO_2-CH_4-N_2	95.0 : 1.5 : 3.5	200 – 300	20	0.5 – 8.0
CO_2-SO_2-N_2	95.0 : 1.5 : 3.5	200 – 300	20	0.5 – 8.0
CO_2-N_2-CH_4-H_2	95.32 : 1.78 : 2.10 : 0.80	220 – 300	20	0.5 – 8.0
CO_2-O_2-N_2-Ar	93.00 : 5.46 : 1.47 : 0.07	200 – 300	20	0.5 – 8.0

4.4.2 Derivative thermodynamic properties and transport properties

Especially for the pipeline transport part of CCS and the hazard assessment studies that accompany the process design, derivative thermodynamic properties and transport properties are necessary for different types of calculations.

Speed of sound and Joule-Thomson coefficient (or inversion curve), are two of the most widespread derivative thermodynamic properties. On the transport properties part, viscosity and thermal conductivity are also very important for studies that contain a fluid dynamics part.

Thus, it would be useful and quite innovative in terms of literature reported data, to have measurements of these properties for the mixtures that were mentioned in the previous section. As far as conditions are concerned, a collection of literature reported operating temperatures and pressures of CO$_2$ pipelines resulted in Fig. 7, and it is suggested that the measurements of derivative thermodynamic and transport properties, as a first step, should be inside the operating window.

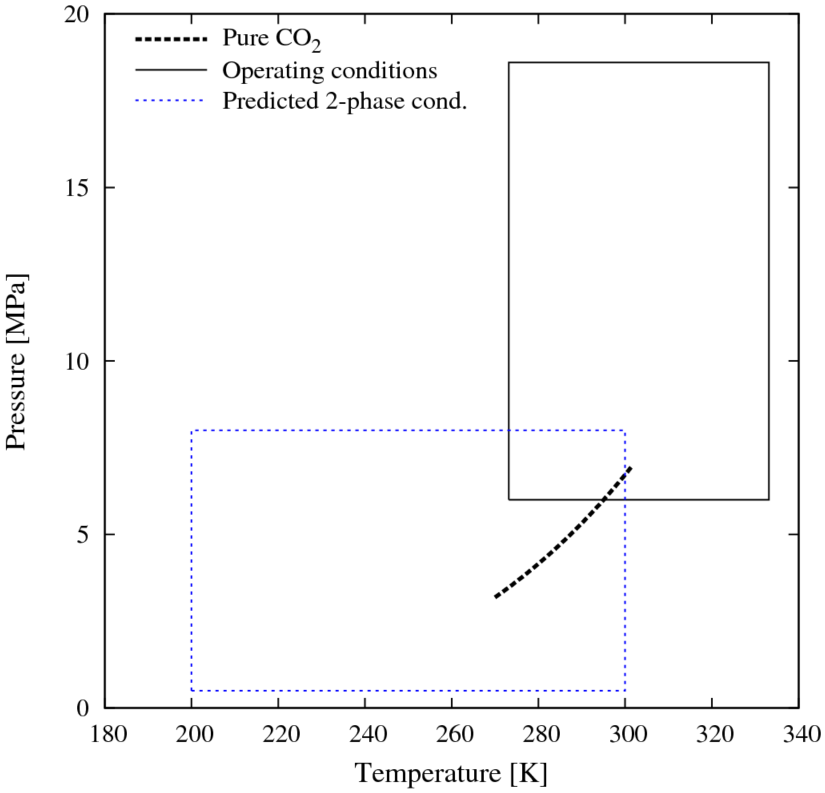

Figure 7. Predicted 2-phase conditions extreme values (approximate) as calculated by PC-SAFT EoS in this report. Operating conditions extreme values as reported in [48-50].

5. Conclusions and future steps

The work that has been carried out toward the achievement of Deliverable 1.7 and is documented in this report, has led to an extensive collection of thermophysical properties data from the literature, mainly regarding mixtures of CO$_2$ with other gases as they are of particular interest to CO2QUEST. A large part of these data has already been used for validating thermodynamic models and it will be continuously used for this purpose. Furthermore, the data collection can be used by other Work Packages that are in need for thermophysical properties data.

The mapping of the available data also assisted in identifying the need for experimental measurements for systems and conditions that either there are no data at all, or the existing data are not conclusive.

Based on the latter, as well as on some predictions from PC-SAFT EoS, a few suggestions for experimental measurements were made, with the outlook that they can serve as a basis for further discussions with the experimental groups involved in CO2QUEST. The convergence of the experimental capabilities and the model validation needs will definitely be of great benefit to the results of CO2QUEST.

6. Publications from the work described

None. This is a literature survey report.

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