Review

Viscosities, thermal conductivities and diffusion coefficients of CO_2 mixtures: Review of experimental data and theoretical models

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ABSTRACT

Accurate experimental data on the thermo-physical properties of CO_2-mixtures are pre-requisites for development of more accurate models and hence, more precise design of CO_2 capture and storage (CCS) processes. A literature survey was conducted on both the available experimental data and the theoretical models associated with the transport properties of CO_2-mixtures within the operation windows of CCS. Gaps were identified between the available knowledge and requirements of the system design and operation. For the experimental gas-phase measurements, there are no available data about any transport properties of CO_2/H_2S, CO_2/COS and CO_2/NH_3; and except for $CO_2/H_2O(/NaCl)$ and $CO_2/amine/H_2O$ mixtures, there are no available measurements regarding the transport properties of any liquid-phase mixtures. In the prediction of gas-phase viscosities using Chapman–Enskog theory, deviations are typically <2% at atmospheric pressure and moderate temperatures. The deviations increase with increasing temperatures and pressures. Using both the Rigorous Kinetic Theory (RKT) and empirical models in the prediction of gas-phase thermal conductivities, typical deviations are 2.2–9%. Comparison of popular empirical models for estimation of gas-phase diffusion coefficients with newer experimental data for CO_2/H_2O shows deviations of up to 20%. For many mixtures relevant for CCS, the diffusion coefficient models based on the RKT show predictions within the experimental uncertainty. Typical reported deviations of the CO_2/H_2O system using empirical models are below 3% for the viscosity and the thermal conductivity and between 5 and 20% for the diffusion coefficients. The research community knows little about the effect of other impurities in liquid CO_2 than water, and this is an important area to focus in future work.

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1. Introduction

Currently operating commercial projects about CO_2 capture and storage (CCS) have raised many research & development requests to improve the health, safety and environmental issues and reduce the costs in existing and future CCS chains. Accurate knowledge about thermo-physical properties of fluids plays an important role in cost-effective design and operation of chemical and biochemical plants. Broadly speaking, the thermodynamic properties determine the feasibility of a given process, while the transport properties have a major impact on sizing of the equipment (Hendriks et al., 2010). As discussed in (Li et al., 2011; Jiang, 2011), the knowledge about thermo-physical properties is essential to the design and operation of CO_2 conditioning and transport. The knowledge about the behavior of the mixture under the conditions of a particular process will allow:

- Identification of possibly encountered problems.
- Specification of safe concentration limits for involved impurities.
- Defining the requirements for purification if necessary.
- Designing efficient and safe processes.

The thermo-physical properties include thermodynamic properties such as vapor liquid equilibrium behaviors and densities; and transport properties such as viscosities, thermal conductivities and diffusion coefficients. Our previous work (Li et al., 2011) contains a review of the experiments and theoretical models available in the literature concerning important thermodynamic properties. In this work, the focus will be on the transport properties of fluids in the CCS-chain.

The transport properties of CO_2 rich mixtures are important properties closely connected to heat, momentum and mass transfer in CCS. This fact may be illustrated by considering the straight-forward example of CO_2 transport in pipelines. The pressure drop is directly related to the power consumption and dimensioning of pumps/compressors to maintain flow through the pipelines. The pressure drop in laminar and transitional flow has been observed to be approximately inversely proportional to the Reynolds number of the flow. The Reynolds number is again inversely proportional to the viscosity of the particular mixture. In practice, this means that a viscosity model which predicts a 30% too low viscosity, will lead to a 30% underestimation of the pump/compressor power consumption. In addition, the Reynolds number is also proportional to velocity, which is further related to mass flow rate and density. In order to predict mass flow and density precisely, heat and mass balance equations must be solved, which may include additional transport properties such as the thermal conductivity and the diffusion coefficients. Another example of the importance of transport properties is in the development, design and simulation of amine-based chemical absorption columns where it is essential to provide accurate predictions of viscosities, thermal conductivities and diffusion coefficients (Hoff et al., 2004).

The CO_2 captured from an energy-conversion process always contains impurities and the existences of impurities will clearly change the properties compared to pure CO_2. Therefore, the thermo-physical properties of CO_2-mixtures attract more and more attention in both the industry and the academia (Hendriks et al., 2010). The properties of CO_2-rich mixtures have been partly reviewed previously with the purpose of understanding supercritical fluid processes and technology (Ely et al., 1987; Magee, 1991). This work contains a more comprehensive literature review concerning both the experimental data and the mathematic models about the transport properties of CO_2-mixtures relevant for CCS. The purpose of the work is to summarize and evaluate the available experimental data, identify knowledge gaps and investigate the available models that have been proposed and tested in the literature. The work will also provide suggestions for future research on the transport properties of CO_2 rich mixtures.

2. Operating windows and possible impurities in CCS processes

The operating windows of CCS processes determine the relevant ranges of temperature, pressure and composition, in which experimental data are required and property models should preferably be validated to minimize the uncertainties in the design criteria of the different steps of the CCS chain. A typical CCS chain normally consists of four main steps: CO_2 capture, CO_2 conditioning (dehydration, non-condensable gas separation and/or liquefaction, and compression/pumping), CO_2 transport and CO_2 storage. The operating conditions of the CCS processes have been estimated in previous work (IPCC, 2005; Li, 2008; Li et al., 2009) and show that to cover the whole CCS-chain, available experimental data and models should ideally cover a temperature range of 218.15–1620 K and a pressure range of ∼0–50 MPa. This range will herby be referred to as the temperature and pressure (T&P) window of CCS. The type and amount of impurities in the CO_2 depend on the fuels used and the choice of capture technology. The CO_2 streams captured from post-combustion with an amine solution are relatively clean, with H_2O as the main impurity. Relatively high levels of impurities are, however, expected in the CO_2 streams captured from oxy-fuel combustion, and a more complicated composition of the CO_2 streams is expected in the integrated gasification combined cycles. Based on the different oil industry and fuel conversion processes, the possible impurities and ranges for these are summarized in Table 1.

There are no strong technical barriers to provide high purity CO_2 from the flue gas of fossil fuel fired power plants. However, high purity requirements are likely to induce additional costs and energy requirements resulting in a high loss of power plant efficiency. It is thus important to find an optimal balance between the requirements with respects to safety, legal and environmental aspects of transport and storage and the costs concerning CO_2 sequestration. Knowledge about the behavior of CO_2 with impurities is vital to achieve this.

Nomenclature

A_{ij}	adjustable parameter in Wassiljewa's model
c	total mole number
D	diffusion coefficient
f_D	correction term
K	thermal conductivity
k	Boltzmann's constant
J	mole flux
M	molar mass
M_{AB}	function of the molar weights of component A and B
n	number density of molecules in the mixtures
P, p	pressure
R	gas constant
r	radius of the solute
T	temperature
v	special diffusion parameters
X	transport property of pure CO_2
x	mole fraction
z	spatial length
η	viscosity
ρ	density
σ	collision diameter
σ_{AB}	Lennard-Jones characteristic length
ε_{AB}	Lennard-Jones characteristic energy
Ω_D	collision integral for diffusion

Abbreviations

AAD	average absolute deviation
CCS	CO_2 capture and storage
CE	Chapman–Enskog
CS	corresponding state
DEA	diethanolamine
Dev	deviation
Emp	empirical
FSG	Fuller-Schettler-Giddings
L-J	Lennard-Jones
MDEA	methyldiethanolamine
MEA	monoethanolamine
RKT	rigorous kinetic theory

Subscripts

1, 2, A, B, i, j	component labels
c	critical
int	internal contribution
sat	saturated

Superscripts

0	property at zero density

Table 1

Ranges in concentration for the relevant impurities (IPCC, 2005; Li, 2008; Li et al., 2009).

Component	Min mol%	Max mol%
CO_2	75	99
N_2	0.02	10
O_2	0.04	5
Ar	0.005	3.5
SO_2	<0.001	1.5
$H_2S + COS$	0.01	1.5
NO_x	<0.002	0.3
CO	<0.001	0.2
H_2	0.06	4
CH_4	0.7	4
H_2O	0.005	6.5
Amines (MEA, DEA, MDEA)	<0.001	0.01
NH_3	<0.001	3

chain, there are large gaps between available experimental data and requirements. Except for the mixtures CO_2/H_2O, CO_2/H_2O/amines and $CO_2/NaCl/H_2O$, there are no available measurements for any of the transport properties of liquid mixtures. Liquid mixtures are, however, important in many parts of the CCS-chain, for instance when CO_2 is transported in pipelines. For the gas-phase, there are no available measurements for the mixtures CO_2/H_2S, CO_2/NH_3 and CO_2/COS. Table 2 reveals the knowledge gaps for the transport properties of CO_2 rich mixtures. In general, most of the transport property data are available only at atmospheric pressure. The pressure dependency of transport properties such as the viscosity is, however, large in particular in vicinity of the critical point. The lack of data for the most important binary mixtures of CO_2 is presented below:

- CO_2/O_2

There are some experimental data about viscosity and diffusion coefficients of CO_2/O_2 and the temperature could cover most of the temperature window of CCS. However, data at higher pressures than one bar should be provided. Compared to the viscosity and the diffusivity, much less data are available for the thermal conductivity. 4 points have been measured at 369 and 370 K, without a specified pressure.

- CO_2/N_2

The transport properties of the gas mixture, CO_2/N_2, have been well studied. The available data can satisfy the requirements of CCS, except for diffusion coefficients at pressures larger than one bar.

- CO_2/SO_2

More measurements about the viscosity at high temperatures and pressures should be provided. Few experimental points are available for the thermal conductivities (9 points) and the diffusion coefficients (5 points).

- CO_2/Ar

All of the data about the transport properties of CO_2/Ar are measured at temperatures below 673 K. Therefore, experimental data for the properties at high temperatures should be provided.

- CO_2/CH_4

The experimental data about the viscosity and thermal conductivity of CO_2/CH_4 are available at both low and high pressures. However, more data in a larger temperature range are desirable. In

3. Experimental data

3.1. Knowledge gaps

Accurate experimental data are not only important to assess whether already established models are reliable for applications in CCS, but also essential in the development of better theoretical models. Details such as temperature, pressure range and uncertainty for all available data on the transport properties of mixtures relevant for CCS may be found in 3 tables in Appendix A (Tables A1–A3). Table 2 is a summary of the available experimental data and shows the TPX ranges. Compared to the possible ranges in pressure, temperature and composition encountered in the CCS

Table 2
Summary of the PTx ranges of the available experimental data about the transport properties of CO_2-mixtures.

Mixtures	Phase	Viscosity				Thermal conductivity				Diffusion Coefficient		
		T (K)	P (MPa)	x_{CO_2}	Exp. Points	T (K)	P (MPa)	x_{CO_2}	Exp. Points	T (K)	P (MPa)	Exp. Points
CO_2	G	220–1500	0.1–350	1	300	186–1450	0.1–200	1	300	194.8–1680	0.1	21
	L	219–303	0.6–453	1	300	NA				NA		
Binary mixtures												
CO_2/O_2	G	297–673	0.1	0–1	24	369 & 370		0.2224–0.7301	4	297–1680	0.1	39
CO_2/N_2	G	289–873	0.1–120	0–1	150	273–1033	0.1–300	0–1	257	290–1100	0.1	19
CO_2/SO_2	G	238–353	0.1	0–1	69	323 & 373		0.1–0.9015	9	263–473	0.1–2	5
CO_2/H_2S	G/L	NA				NA				NA		
CO_2/Ar	G	293–673	0.1–2.5	0–0.92	135	273–473	0.1–11.3	0–1	170	273–473	0.1	11
CO_2/CH_4	G	293–673	0.1–68	0–1	230	228.13–433	0.1–17.68	0.075–0.878	210	NA		
CO_2/H_2O	G	303	0.1	0.962–0.985	8	298–603	0.1	0–1	41	307–352	0.1	5
	L	273–313	0.1–30	0–0.0295	71	NA				279–348	0.1–0.4	40
CO_2/CO	G	298–473	0.1	0.3141 & 0.7654	10	NA				296–473	0.1	9
CO_2/HCl	G	291	0.1	0–1	8	NA				NA		
CO_2/N_2O	G	298–550	0.1	0–1	34	300.65–723	0.1–4.25	0–1	90	194.8–362.6	0.1	6
CO_2/H_2	G	291–1100	0.1–0.3	0–1	65	258–893	0.1–7.5	0–1	120	291–1100	0.1	25
Multi-component mixtures												
$CO_2/N_2/O_2$	G	291–1100	–	0.062–0.507	34	370	–	0.304	1	NA		
$CO_2/H_2/O2$	G	296–299	–	0.092–0.78	12	NA				NA		
$CO_2/N_2/Ar$	G	298–873	0.1	0.2551–0.5289	20	NA				NA		
$CO_2/N_2/CH_4$	G	298–473	0.1	0.1953–0.5588	12	NA				NA		
$CO_2/H_2O/NaCl$	L	273–278	0.1–30	0–0.913[a]	90	NA				NA		
$CO_2/N_2/O_2/N_2O$	G	313–413	–	0.1–0.25	12	NA				NA		
$CO_2/O_2/N_2/H_2$	G	300.5–1279	–	0.108	4	NA				NA		
$CO_2/O_2/N_2/CO/H_2$	G	307.5–1287	–	0.06–0.067	12	NA				NA		
$CO_2/CH_4/N_2/CO/H_2$	G	293	–	0.087–0.106	3	NA				NA		
$CO_2/O_2/CH_4/CO/N_2/H_2$	G	293–1282	–	0.017–0.048	14	NA				NA		
CO_2/Air	G	NA				NA				273–317.2	–	3
$CO_2/MEA/H_2O$	L	295	–	0–0.5[b]	44	NA				NA		
$CO_2/DEA/H_2O$	L	295	–	0–0.5[b]	44	NA				NA		
$CO_2/MDEA/H_2O$	L	295	–	0–0.64[b]	44	NA				NA		
$CO_2/MEA/H_2O$	L	295	–	0–0.5[b]	44	NA				NA		
$CO_2/DEA/MDEA/H_2O$	L	295	–	0–0.5[b]	33	NA				NA		

[a] mol/kg H_2O.

[b] CO_2 loading (mol/mol).

addition, no measurements were published concerning the binary diffusion coefficient.

- CO_2/H_2

The transport properties of the gas mixture, CO_2/H_2, have been well investigated. In order to cover the whole T&P window of the CCS chain, some data about the viscosity and the thermal conductivity at high pressures are still required.

- CO_2/NO_x

There are some data available for the transport properties of CO_2/N_2O at temperatures below 500 °C and moderate pressures, but measurements at high temperatures and high pressures are required for all transport properties, and all the components (NO, NO_2 and N_2O).

- $CO_2/H_2O(/NaCl)$

The experimental data about the properties of both liquid and gas mixtures with CO_2/H_2O are only available at low temperatures (<80 °C) and atmospheric pressure, except the data for the thermal conductivity of gaseous mixtures. Considering the T&P window of CCS, the transport properties of gas mixtures are needed also at high temperatures and high pressures.

- CO_2/HCl

Experimental data are only available regarding the viscosity of CO_2/HCl at one temperature (291 K).

- CO_2/CO

There are no available data about the thermal conductivity of CO_2/CO. Meanwhile, all of the data about the viscosity and diffusivity of CO_2/CO are measured at temperatures below 473 K at atmospheric pressure.

- $CO_2/amines$

The measured viscosities of $CO_2/monoethanolamine$ (MEA), $CO_2/diethanolamine$ (DEA) and $CO_2/N-methyldiethanolamine$ (MDEA) are only available at 298 K. No experimental data have been published about the thermal conductivity and diffusion coefficients of $CO_2/amine$ mixtures.

- Multi-component CO_2-mixtures.

Most of the experimental data for the multi-component mixtures are about the viscosity. Since the data about multi-component CO_2-mixtures are important to verify the property calculations, more data in large temperature and pressure ranges are desired.

3.2. The precision, consistency and reliability of the experimental data

As experimental measurements are used for model calibration and parameter fitting, it is of great importance to have reliable measurements in order to develop high accuracy models (Reid et al., 1987; Hendriks et al., 2010). 'Despite the fact that measurements have been conducted over a period of at least 150 years, it was not until around 1970 that techniques of an acceptable accuracy were developed for the measurement of any of the transport properties' (Wakeham, 1996). Tables A1–A3 in Appendix A show that many of the measurements are published before 1960, for instance more than 60% of the gas-phase viscosity measurements.

There is ample evidence in the literature of very large discrepancies among measurements made prior to that date (Wakeham, 1996). In order to check the precision, consistency and reliability of the published literature, experimental data available in the same ranges of composition, pressure and temperature were compared. Figs. 1–3 show comparisons of the experimental data which are in the same range in temperature, pressure and composition.

Fig. 1 presents a comparison of the viscosity data. According to the details of the experiments shown in Table A1, the reported experimental uncertainty is below 3% for all the published data. Fig. 1 shows that the experiments published for CO_2/N_2 (Fig. 1a) and CO_2/H_2 (Fig. 1d) are consistent within the experimental uncertainty. The viscosity measurements for CO_2/CH_4 show minor inconsistencies (1.4%). However, deviations up to 5% were found in the data for CO_2/O_2 (Fig. 1b). More accurate measuring techniques were used and a lower experimental uncertainty reported by Kestin et al. (1977). The data by Gururaja et al. (1967) should therefore be used with care, and uncertainties up to 5% expected. The data for CO_2/SO_2 also show inconsistencies up to 5%. Here, both publications report uncertainties below 1%, which is much smaller than the deviations shown in Fig. 1(e). The data by Bhattacharyya and Ghosh (1970) should be preferred, because of the more up to date measuring techniques.

Fig. 2 presents the comparison of the thermal conductivity data. The experimental data from different sources are consistent for CO_2/H_2 and CO_2/H_2O at high CO_2 concentrations as shown in Fig. 2a and b. Some minor discrepancies were identified in the experimental data of CO_2/Ar as shown in Fig. 2c. Compared to Yorizane's data (Yorizane et al., 1983), the values measured by Kestin et al. (1982) are about 5% higher at pressures lower than 3 MPa and at pressures higher than 7 MPa. Considering the slight difference in CO_2 concentration, the deviations may be acceptable. Larger inconsistencies are observed in the experimental data of CO_2/H_2O mixtures at low CO_2 concentrations. For CO_2/H_2O, the deviation is up to 4% based on Kulakov's data (Kulakov, 1955). More experiments are necessary to verify the accuracy of these data.

Fig. 3 presents a comparison of the diffusion coefficient data. Few of the sources for the diffusion coefficient data have presented the experimental inaccuracy in their results (Table A3). According to the comparison of the experimental data for CO_2/CO_2 (Fig. 3c), CO_2/Ar (Fig. 3d), CO_2/SO_2 (Fig. 3e), and CO_2/N_2O (Fig. 3f) the experimental data for these mixtures are observed to be consistent. For the mixture CO_2/H_2, the published data from Gavril et al. (2004) and Ivakin and Suetin (1964a, 1964b) are consistent, while the data by Boyd et al. (1951), on the other hand, display deviations over 20% (Fig. 3a), which shows that this source should be avoided. For CO_2/N_2 at temperatures close to 300 K, the diffusion coefficients measured by Boyd et al. (1951) agree with the measurement by Walker and Westenberg (1958a). However, compared to the measurements by Giddings and Seager (1962), discrepancies of 15–20% are observed. In addition, the diffusion coefficients of CO_2/H_2O have been studied by many researchers. In general, the measured values are consistent, except for that of Nijsing et al. (1959). As shown in Fig. 3g, the difference between the data by Unver and Himmelblau (1964) and the data by Nijsing et al. (1959) may be up to 85%.

4. Available transport property models

In this section, a review of the existing transport property models which have been proposed, tested and evaluated for CO_2 and CO_2-mixtures in the literature will be presented. An overview of the investigated models is shown in Appendix B (Table B1).
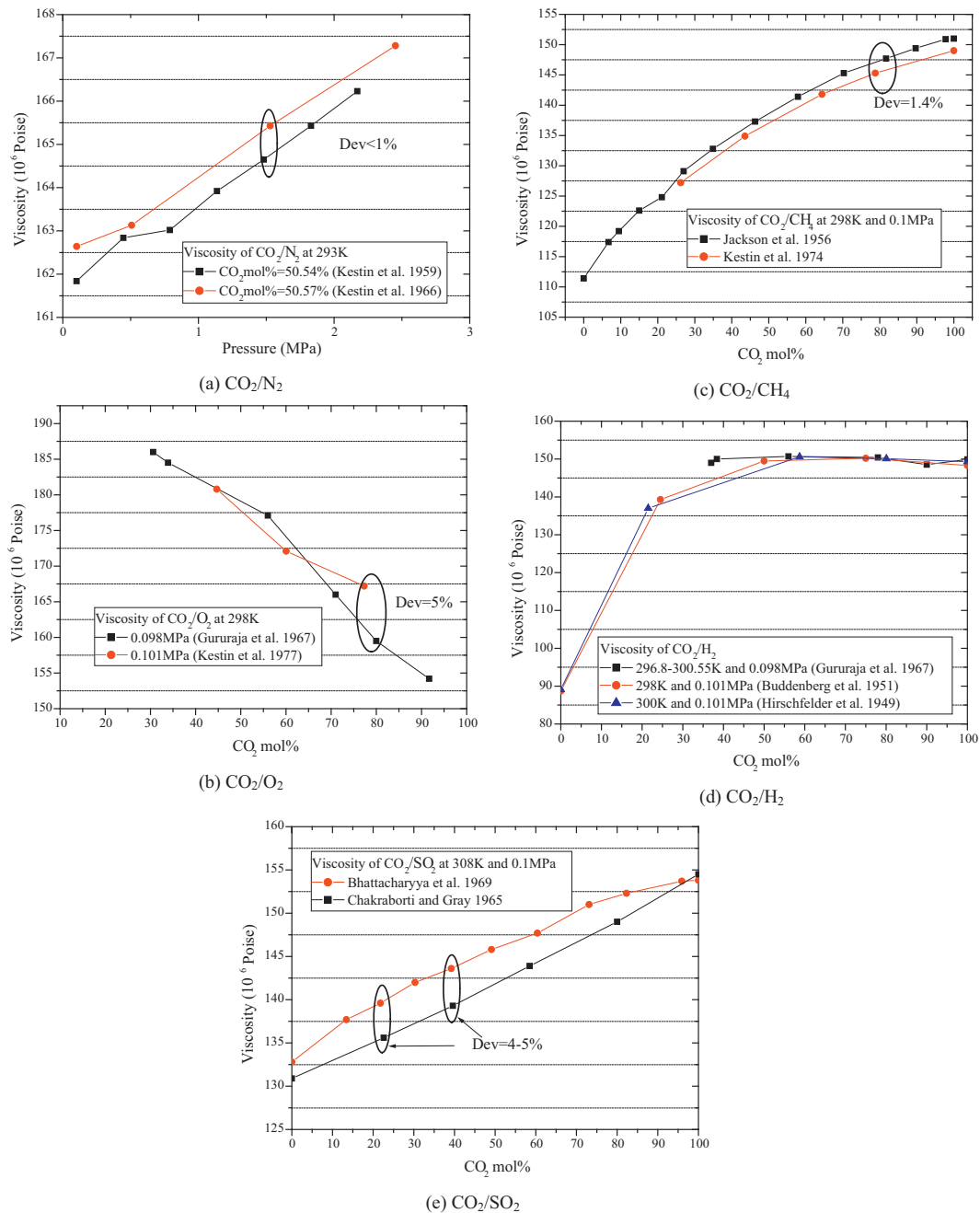
Fig. 1. Comparison of experiments about the viscosities of CO_2-mixtures.

4.1. Transport property models for pure CO_2

Models for the viscosity and thermal conductivity of pure CO_2 were developed by Vesovic et al. (1990). The model equations have the following functional form:

$$X(\rho, T) = X^0(T) + \Delta X(\rho, T) + \Delta_C X(\rho, T) \qquad (1)$$

Here, the first term, $X^0(T)$, is the contribution to the transport property in the limit of zero-density, where only two-body molecular interactions occur. The final term, $\Delta_C X(\rho,T)$, is the critical enhancement that arises from the long-range fluctuations which occur in a fluid near its critical point and contribute to divergences of both the viscosity and thermal conductivity at that singular point. Finally the term $\Delta X(\rho,T)$, the excess property, represents the contribution of all other effects to the transport property of the fluid

at elevated densities including many-body collisions, molecular-velocity correlations, and collisional transfer. The correlation by Vesovic et al. (1990) covers a temperature range of 200 K–1500 K and a pressure range of 0.1–100 MPa. In general, the estimated deviation for the viscosity of pure CO_2 is less than 5% for gas and supercritical phases. Owing to the inconsistencies between the available experimental liquid viscosity data, the uncertainty for the liquid-phase was originally around 7%. In 1998, Fenghour and Wakeham (1998) revised the published equations by including new reliable measurements and omitting inconsistent sources for the liquid CO_2 viscosity. The resulting overall viscosity representation for pure CO_2 covers the temperature range of 200–1500 K and pressures up to 300 MPa. The uncertainties associated with the proposed representation vary from ±0.3% for dilute gas near room temperature to ±5.0% at the highest pressures. Figs. 1–3 show that

(a) CO_2/H_2

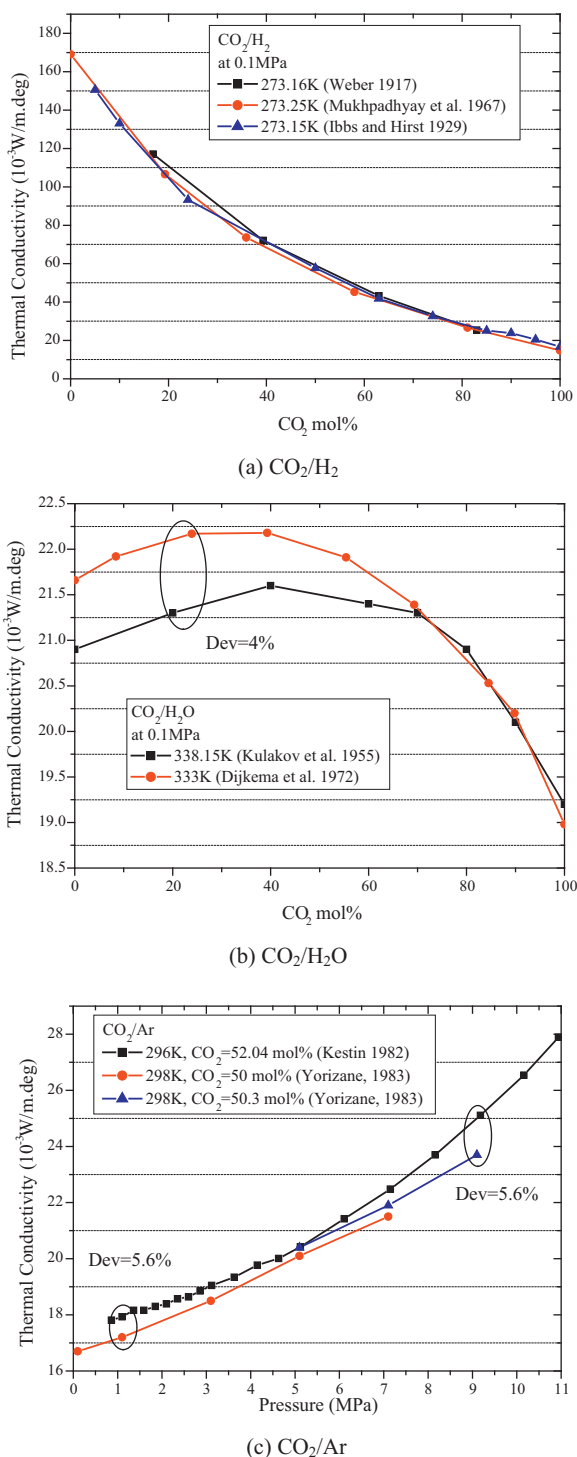(b) CO_2/H_2O

(c) CO_2/Ar

Fig. 2. Comparison of experiments about the thermal conductivities of CO_2-mixtures.

the transport properties of mixtures may be considerably different from those of pure CO_2, and for high accuracy, mixture models should be preferred.

4.2. Viscosity models for mixtures

4.2.1. Gas mixtures

The viscosities of gases are strong functions of pressure near the critical point and at reduced temperatures of about 1–2. For diluted gases, the viscosity will increase with temperature. At high reduced

pressures however, there is a wide range of temperatures where the viscosity decreases with temperature. In this region the behavior of the viscosity more closely resembles the liquid state. At very high reduced temperatures, there is again a condition in which pressure has little effect and viscosities increase with temperature. Acceptable models for gas-phase viscosities should be able to handle all these features. The theoretical models are mainly divided in two categories. One approach is based on the principle of corresponding states, in which the reduced viscosity is linked to a reduced pressure and temperature. The other approach has its foundation in kinetic gas theory and is known as Chapman–Enskog theory.

Once the viscosities of the pure components are available, several techniques have been developed to estimate the viscosity of mixtures. Examples are the method by Reichenberg (1974, 1975, 1977) and the method by Wilke (1950) which neglects second order effects. In corresponding state-methods for mixtures, it is common to estimate mixture properties from the pure properties, the composition and various mixing rules. Examples are the procedure by Lucas (1980), Lucas et al. (1984), and the procedure by Chung et al. (1984, 1988).

4.2.1.1. Chapman–Enskog theory for the gas-phase viscosity of CO_2-mixtures. The Chapman–Enskog (CE) theory requires an estimate of the collision diameters and the collision integrals to evaluate the viscosity of gases. The first applications of the CE-theory evaluated the collision integrals with simplified functions of temperature. Chapman and Cowlings expression for the viscosity (Chapman and Cowling, 1939) was for instance used by Heath (1948) to calculate the viscosity of binary mixtures, including H_2/Ar, He/N_2, He/CO_2, H_2/Ar, H_2/N_2 and CO_2/H_2. The calculations based on CE-theory were in good agreement with experiments conducted at 291 K and 0.1 MPa.

Since the simplified collision integrals used in the first applications of the CE-theory were considered artificial and unrealistic, Hirschfelder developed a new method using the more realistic 6-12 Lennard-Jones energy potential (Hirschfelder et al., 1948, 1954) to estimate the collision integrals. The new method is based on the solution of the Boltzmann equation for the molecular distribution, as carried out by Chapman and Enskog. The results obtained by this method are applicable at low pressure and apply strictly only to monatomic gases. Buddenberg and Wilke (1951) used Hirschfelder's equation to calculate the viscosity of CO_2/H_2 mixtures at 298 K and 0.1 MPa. The calculated results from both equations agreed very well with the experimental data, with an AAD of <1%. Hirschfelder's equation was also used to calculate the viscosities of CO_2/H_2 by Keyes and Mass (1951). In all cases, the agreement was satisfactory. For example, almost perfect accordance was obtained at 299 K, while at 550 K the viscosity in a mixture with 19.93% H_2 was 2.7% larger than the calculated. The mixture with 41.29% H_2 was 2.5% larger, and the mixture with 78.5% H_2 was 2.1% larger than the calculations.

The viscosities of CO_2/Ar and CO_2/N_2 at 293 and 303 K were studied by Kestin et al. (1966) using Hirschfelder's approach. The analysis of the experimental data showed that for CO_2/N_2, it is possible to obtain a single set of optimum values of the mixture parameters which correlate the variation of viscosity with composition, when the viscosities of the pure components are known. For CO_2/Ar, a separate set must be used for each temperature. Moreover, it was also concluded that Hirschfelder's approach provides an excellent approximation to the viscosity of the binary mixtures CO_2/Ar and CO_2/N_2. If the viscosity of a binary mixture was computed with known values for the viscosities of the pure substances and an interaction term, the calculations revealed deviations in the order of 0.1% and reproduced the measured data with an uncertainty which is comparable to that of the measurements. In 1968, Kestin and Yata did a similar work regarding the CO_2/CH_4 mixture.
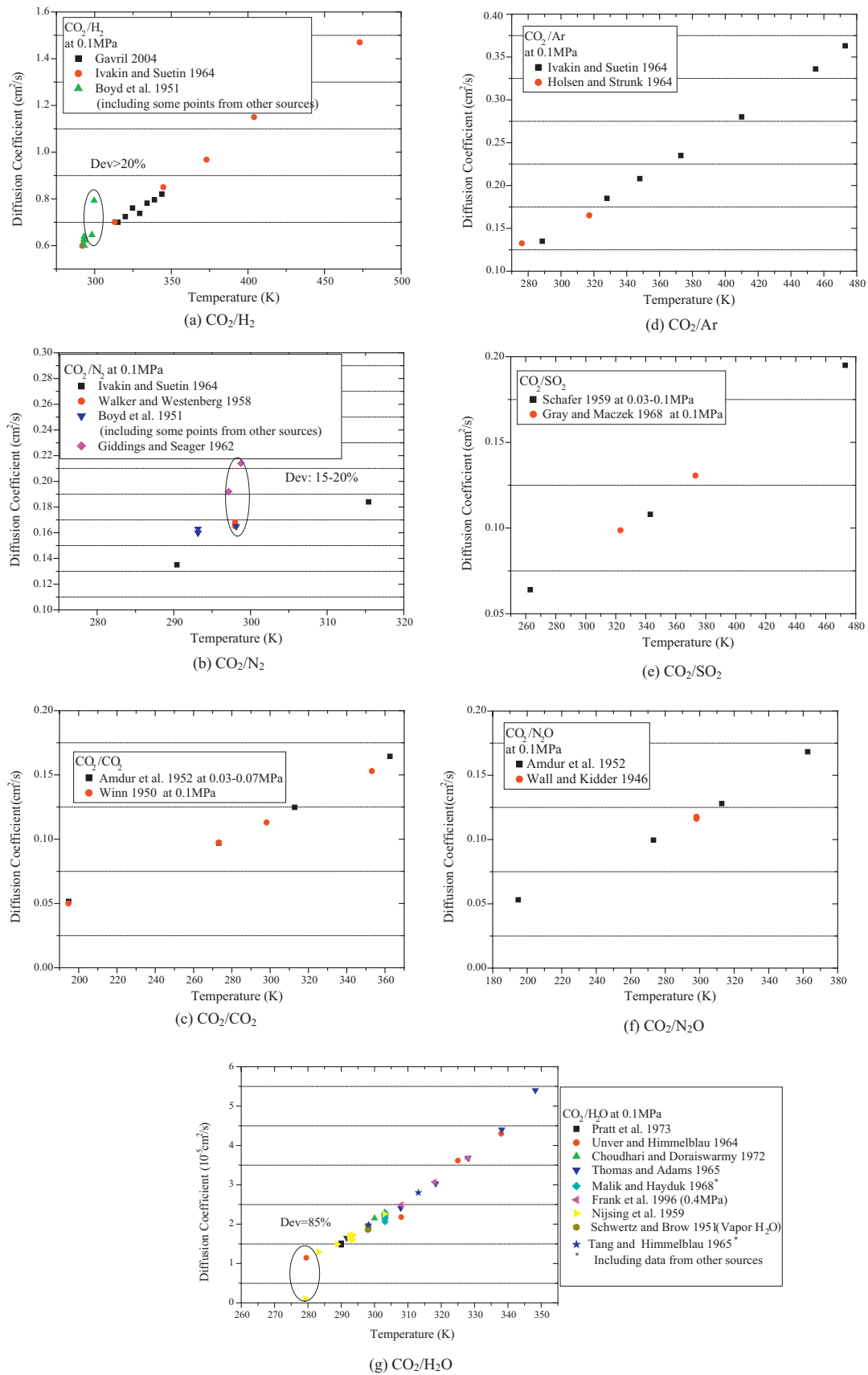
Fig. 3. Comparison of experiments about the diffusion coefficients of CO_2-mixtures.

Their results also showed good agreement between experimental data and predicted values.

Bhattacharyya and Ghosh (1970) studied the viscosities of polar–quadrupolar gas mixtures. Their results show that the viscosity of binary polar–quadrupolar gas mixtures can be represented satisfactorily by Hirschfelder's approach without taking into consideration the inelastic collisions. The average absolute deviation (AAD) of the viscosities of the CO_2/SO_2 mixture in the temperature range 238–308 K was <1%. In addition, the agreement between the experimental and the calculated values was more or less the same for the Lennard-Jones (6-12) and the 12-6-4 representations of the unlike interactions.

The changes in the viscosity of CO_2 resulting from the addition of a defined fraction of water vapor have been investigated at 303 K and at atmospheric pressure, by Munczak and Sedlacek (1970). Here, Hirschfelder's approach did not successfully predict the viscosity of water vapor and CO_2, since the theoretical curves did not follow the relatively large changes in the viscosities occurring with a small variation of the water vapor concentration.

Boushehrl and Najafi (1979) studied the viscosity of the four component mixture $N_2/CO_2/O_2/N_2O$ in the temperature range 313–413K. Compared to the measurements, the deviations of the values predicted by the CE-theory and its extension to multicomponent mixtures are within ±2%. By comparing the method with the experimental data of some multi-component mixtures involving CO_2, the agreement in more than half of the examples is excellent. However, in some of the other mixtures there is a considerable discrepancy which might be explained on the basis of errors in the experimental gas analysis. For ternary mixtures containing CO_2, O_2 and N_2, Kenney et al. (1956) found that the same model gave values which agreed with experimental data with an accuracy of about 1% in the temperature range 317–1161 K. Here it was concluded that the Hirschfelder method may be used to calculate accurately the viscosity of gas mixtures within and also outside this interval, since the model was accurate over a wide range of temperatures.

For polar gas-mixtures, the properties of the mixtures may be more difficult to predict, mainly because the interactions between polar molecules are so complex that a suitable potential function is difficult to obtain. Furthermore, collision integrals containing orientation dependence are difficult to compute. Alternatives to the Lennard-Jones energy potential have, thus, been used in the Hirchfelder approach. The most extensively used potential for polar molecules has been the Stockmayer potential in which the angle-dependent dipole-dipole interaction is added to the Lennard-Jones (6-12) potential. The canonically angle-averaged pair potential energy with temperature dependent parameters can also be used to calculate the viscosity and diffusion coefficients of polar–polar and polar–nonpolar gas mixtures, for example CO_2/SO_2. The canonically angle-averaged pair potential proved to be as successful as the Stockmayer potential in correlating the transport properties of polar gases (Bae and Reed, 1971). For CO_2/SO_2 mixtures, the absolute deviations were 1.8% and 3.0% compared to the experimental data from Jung and Schmick (1930) and Schafer (1959) respectively.

In a further simplification of the kinetic theory approach, Wilke neglected second order effects and proposed a general equation for the viscosity as a function of molecular weights and the viscosities of the pure components of the mixture (Wilke, 1950). Wilke's equation was also used by Jackson to calculate the viscosity of CO_2/CH_4 (Jackson, 1956). At 298 K, the AAD was <1%. Kestin and Leidenfrost (1959) tested Wilke's equation regarding the viscosity calculations of the CO_2/N_2 mixture at 293 K in 1959. The average deviation was about 1.7%. However, Gururaja et al. (1967) also evaluated Wilke's equation based on the experimental data of CO_2/N_2. Their results showed that the AAD in the temperature range 296–303 K was only 0.57%. A comparison of the experimental data from both references shows some discrepancies as shown in Fig. 1b. In addition,

Gururaja et al. (1967) studied the viscosities of CO_2/O_2, CO_2/H_2, $CO_2/O_2/N_2$ and $CO_2/O_2/H_2$. The results show that the AAD of Wilke's equation in the temperature range 296–303 K is 1.91% for CO_2/O_2, 0.57% for CO_2/N_2, 0.62% for CO_2/H_2, 1.77% for $CO_2/O_2/H_2$, and 0.79% for $CO_2/O_2/N_2$. Mal'tsev et al. studied the viscosity of CO_2/H_2 at high temperatures (500, 800 and 1100 K) (Mal'tsev et al., 2004). At a pressure of 0.3 MPa, the results calculated by Wilke's equation are higher than the measurements and the maximum deviation is almost 8%.

4.2.1.2. Corresponding state theory for the gas-phase of CO_2-mixtures. The Kestin-Ro-Wakeham (KRW) law of corresponding states was developed by Kestin et al. (1972a,b) based on the working hypothesis that the inter-molecular force potentials of all monatomic gases and of their binary mixtures differ so little that they can be shrunk to a single diagram with the aid of a linear scaling factor and an energy scaling factor. It follows that all equilibrium and transport properties of monatomic gases and of their mixtures can be calculated on the basis of the Chapman–Enskog solution of Boltzmann's equation with the aid of universal, empirically determined collision integrals. The KRW scheme was used to calculate the viscosity of the mixtures CO_2/N_2, CO_2/Ar, CO_2/CH_4, CO_2/N_2O, $CO_2/N_2/Ar$, and $CO_2/N_2/CH_4$ (Kestin and Ro, 1976, 1982). The agreement between the KRW law and the experiments was within a maximum error of 1% in the temperature range 298–873 K.

Another corresponding states procedure used to predict the viscosity of CO_2/N_2 was proposed by Hanley in 1976. The work showed that the transport properties can be calculated to within the experimental error given only corresponding values for a reference fluid and equation of state data. With methane as the reference fluid, the viscosity of CO_2/N_2 was calculated at 289 K and in the pressure range 2–12 MPa. The deviations rose with pressure, from 0% at 2 MPa to 7.8% at 12 MPa.

The viscosities of eighteen binary gaseous systems, including CO_2/O_2, were described with the aid of the CE-solution of the Boltzmann equation, supplemented by an extended law of corresponding states, and three pairs of scaling parameters by Kestin et al. in 1977. They claimed that the standard deviation between the experimental data and the calculated values was about ±0.3% in the temperature range 298–674 K, which is comparable to the experimental uncertainty.

4.2.1.3. Empirical models and other models for the gas-phase of CO_2-mixtures. In addition to the semi-empirical methods above, some empirical correlations have been developed. A special correlation was proposed by DeWitt and Thodos (1966) for the CO_2/CH_4 mixture with $\rho_R < 1.5$. 128 experimental viscosities for methane, carbon dioxide and three compositions in the temperature range of 323–473 K produced an average deviation of 1.83%, with a maximum deviation of 3.82%.

Dean and Stiel (1965) developed a model for the calculation of the viscosity of nonpolar gas mixtures at moderate and elevated pressures from the molecular weights and critical constants of the components. Using available experimental data and appropriate pseudocritical constant rules, results obtained previously for the viscosity of pure gases have been extended to mixtures. The average deviations of CO_2/N_2 and CO_2/CH_4 are in the ranges 1.32–3.28% and 3.23–3.68% depending on the different methods used to calculate the pseudocritical critical constants and viscosity parameters.

4.2.1.4. Comparison of methods from different categories. Chakraborti and Gray (1965) investigated the viscosity of CO_2/SO_2 at temperatures between 25 and 80 °C. Four methods, including Hirschfelder's approach, Brokaw's equation (Brokaw, 1965), the empirical Herning and Zipperer's equation (Herning and Zipperer, 1936) and Wilke's equation (Wilke, 1950), were evaluated. The

results show that Hirschfelder's approach underestimated the experimental values by about 2%. Brokaw's equation gave the best accuracy, with an AAD of less than 2%. The AAD of Herning and Zipperer's equation and Wilke's equation were about 3.5%.

4.2.2. Liquid mixtures

For a temperature range from the freezing point to somewhere around the normal boiling temperature, it is often a good approximation to assume that the logarithm of the viscosity of liquids is linear in the reciprocal absolute temperature (Reid et al., 1987).

In general, pure liquid viscosities at high reduced temperatures are usually correlated with some variation of the law of corresponding states, such as the model by Sastri and Rao (1992). At low temperatures, most methods are empirical and involve a group contribution approach. Current liquid mixture correlations are essentially mixing rules relating pure component viscosities to composition. Little theory has been shown to be applicable to estimating liquid viscosities within a reasonable accuracy (Reid et al., 1987). Generally, almost all methods to estimate or correlate liquid mixture viscosities assume that values of the pure component viscosities are available. Thus the methods are, in reality, interpolative. Nevertheless, there is no agreement on the best way to carry out the interpolation. Irving (1977) surveyed more than 50 equations for binary liquid viscosities and classified them by type. He pointed out that only very few do not have some adjustable constant that must be determined by experimental data and the few that do not require such a parameter are applicable only to systems of similar components with comparable viscosities. He recommended the one-constant Grunberg–Nissan equation as being widely applicable with reasonable accuracy except for aqueous solutions (Grunberg and Nissan, 1949).

To evaluate quantitatively the results of gas–liquid absorption experiments, accurate liquid-phase viscosities are vital. For this purpose, Frank et al. (1996) measured the viscosities of CO_2/H_2O mixtures, from 293 to 333 K. The measured viscosity of CO_2/H_2O was correlated to Arrhenius type functions, with an AAD <1%. Kumagai and Yokoyama (1998) studied the viscosity of aqueous solutions of CO_2 along three isotherms at 273, 276 and 278 K for pressures up to 30 MPa. The experimental values were compared with the correlation proposed by Kanti et al. (1991) derived from the Bloomfield–Dewan equation (Bloomfield and Dewan, 1971) and the theory by Flory et al. (1964), Flory (1965). The results show that the equation is in poor agreement with the experimental data, but the equations of Kanti et al. (1991) and of Grunberg and Nissan (1949) with one adjustable parameter give good agreement. The AAD was for many cases <1%, with a maximum deviation of −2.2%. Kumagai and Yokoyama (1999) measured the viscosity of aqueous NaCl solutions containing CO_2 along three isotherms at 273, 276 and 278 K at pressures up to 30 MPa. The experimental values were correlated in terms of pressure, temperature and concentrations of NaCl and CO_2. The correlation reproduced the experimental values within ±1.3%. The viscosity of aqueous NaCl solutions with dissolved CO_2 was measure at conditions representing an underground aquifer at a depth of 1000–2000 m for the geological storage of CO_2 (i.e., 30–60 °C and 10–20 MPa) at a mass fraction of NaCl between 0 and 0.03 by Bando et al. (2004). On the basis of the experimental data, an empirical equation for predicting the viscosity of $CO_2/H_2O/NaCl$ was correlated as a function of the temperature and mole fraction of CO_2. The correlation has deviations of ±5%.

4.3. Thermal conductivity models

The first approximation to the rigorous kinetic theory of gases accounts successfully for the thermal conductivity of mixtures containing monatomic gases (Hirschfelder et al., 1954). For binary mixtures of polyatomic gases Hirschfelder (1957) suggested that the total thermal conductivity of each constituent can be written as a sum of a translational contribution and an internal (rotational and vibrational) contribution. The translational contribution to the thermal conductivity of a mixture is calculated as if the individual gases were all monatomic. The internal contribution to the thermal conductivity of the mixture is then calculated from the equation:

$$K_{\text{int}} = \frac{K_{1,\text{int}}}{1 + (D_{11}x_2/D_{12}x_1)} + \frac{K_{2,\text{int}}}{1 + (D_{22}x_1/D_{12}x_2)} \tag{2}$$

Here, x_i is the mole fraction of component i and D is the diffusion coefficient. In addition to several attempts to extend the approximations to a rigorous theory, several formulas have been suggested. One of the most successful expressions with a theoretical foundation which accounts for the thermal conductivity of mixtures was purposed by Wassiljewa (1904):

$$K_{mix} = \sum_i \frac{K_i}{1 + \sum_j A_{ij}(x_j/x_i)} \tag{3}$$

Here K_{mix} and K_i are the thermal conductivities of the mixture and pure component i respectively and A_{ij} is one of a set of adjustable parameters. The simple physical interpretation of A_{ij} is that it is a measure of the ratio of the efficiencies with which molecules j and i impede the transport of heat by molecule i. It has also been shown that the first approximation to a rigorous theory reduces to the Wassiljewa form (Eq. (3)) (Wassiljewa, 1904) with A_{ij} depending only slightly on composition. In practice, A_{ij} can be treated as if independent of composition and could be calculated from the approximation of Lindsay and Bromley equation (Lindsay and Bromley, 1950), or it could be estimated from experiments.

4.3.1. Semi-empirical models

4.3.1.1. Hirschfelder's equation.
Based on Hirschfelder's equation (Eq. (2)), Brokaw (1959) calculated the thermal conductivity of CO_2/N_2 in the temperature range 273–1033 K. The force constants characterizing the CO_2/N_2 interaction were computed in two ways: (i) using the standard combining rules and (ii) using Walker and Westenberg's methods (1958). Compared with experimental data, method (i) gave good agreement at low temperatures and method (ii) gave good agreement at high temperatures.

Westenberg and Dehaas (1962) evaluated two methods regarding the calculations of the thermal conductivity of the CO_2/N_2 mixture. Both methods were based on Hirschfelder's equation. For the first method (i) all the parameters involved in Hirschfelder's equation were from experiments, either directly or indirectly through experiments combined with established relations form kinetic theory. Unfortunately, the experimental values were typically not available. For the second method (ii), they used viscosity force constants to compute the necessary quantities as outlined, together with the theoretical Eucken correction. For CO_2/N_2 in the temperature range of 294–1000 K, method (i) gave much better results than method (ii), especially at high temperatures. Method (i) did however always overestimate the thermal conductivity, and its average deviation exceeded slightly 10%.

Mathur and Saxena (1966) studied the thermal conductivities of 59 mixtures of 13 different gas pairs, including CO_2/N_2 and CO_2/H_2, based on Hirschfelder's theory. The results showed good overall agreement. However, compared to the experimental data, the deviations of the CO_2/N_2 mixture were between 6.4 and 7.8% at the temperature 323.16 K and the deviations of CO_2/H_2 were between 2.2 and 3.5% at the temperature 273.16 K.

Mukhopadhyay et al. (1967) used Hirschfelder's equation to calculate the thermal conductivity of CO_2/H_2. The experimental values in the temperature range 258–473 K were 5–8% lower than the calculated results, assuming local chemical equilibrium. The situation

could be improved when the experimental values for the thermal conductivities of the pure components were used and in this case the mean deviation increased only from 1% to 5% as the temperature increased from −15 to 200 °C.

Barua et al. (1968) used Hirschfelder's equation to calculate the thermal conductivities of CO_2/Ar and CO_2/N_2. In the temperature range 273–473 K, the deviations were, on average, about 3% for the CO_2/Ar system and about 4% for the CO_2/N_2 systems. A modified Hirschfelder's equation, which includes the experimental values for the thermal conductivities of the pure components instead of calculated values, was also evaluated. It gave slightly better results than the original Hirschfelder's equation. The improvement of the AAD was about 0.3%. Later, Saxena and Gupta (1970) conducted experiments to measure the thermal conductivities of CO_2/N_2O. A comparison of Hirschfelder's equation with Lennard-Jones potentials showed that the deviations were −2.0–9% in the temperature range 300–750 K.

The thermal conductivity of 126 different binary mixtures, including CO_2/SO_2, was investigated by Maczek and Gray (1970) with Hirschfelder's equation. The deviation was, on average, −3.45% for all the mixtures. For CO_2/SO_2, the deviations were in the range 0–3%. The modified Hirschfelder–Eucken equation with realistic estimates of the inelastic collisions provided even better predictions (<2%). The Saksena formulation (Maczek and Gray, 1969) gave the best results for CO_2/SO_2, with average deviations <1%.

The equation developed by Mason, Monchick and Pereira (Monchick et al., 1965) based on kinetic-theory was used by Kestin et al. (1983) to calculate the thermal conductivity of CO_2/H_2 at 297 K. The results showed that this equation represented the experimental thermal conductivity data with an absolute deviation up to 4%. This is much higher than the uncertainty (±0.4%) of the empirical equation which correlates the density to calculate the thermal conductivity. In addition, Monchick et al. (1965) extended the treatment of Mason and Monchick's method (1962) to the case of polyatomic gas mixtures incorporating both relaxation and cross-relaxation into the general frame work of the theory. This new method gave the same accuracy as the modified Hirschfelder's equation for both CO_2/Ar and CO_2/N_2. The same method was used by Johns et al. (1988) to calculate the thermal conductivity of CO_2/N_2 with some modifications regarding the combination rule for the pseudoradial distribution function, second virial coefficients and the ratios of collision integrals. Deviations larger than 5% were identified in a temperature range of 302–470 K and a pressure range of 0.9–30.8 MPa.

4.3.1.2. Wassiljewa's equation. An alternative to Hirschfelder's equation is to use the Wassiljewa equation (Eq. (3)). Here, Lindsay and Bromley (1950) developed a correlation for the A_{ij}-factors. The Lindsay–Bromley correlation was first used to calculate the thermal conductivity of CO_2/H_2. At 273 and 296 K, the deviations were between −0.2 and 8.4%. In 1951, Bromley and Wilke used the correlation to calculate the thermal conductivity of CO_2/N_2. Compared to the experimental thermal conductivity of CO_2/N_2 measured by Rothman and Bromley (1955) in the temperature range 369–688 °C, the maximum deviations for the Lindsay–Bromley equation values were −1% at 642 K, −1.1% at 645 K, −1.9% at 648 K, −1.5% at 745 K and about −3% at higher temperatures. Keyes and Mass (1952) studied the thermal conductivity of the CO_2/N_2 mixture between 323 and 623 K. They found that the semi-empirical formula of Lindsay and Bromley (1950) (AAD = 1.36%) had a better accuracy than the Enskog theory (Keyes and Mass, 1952) (AAD = 3.43%). Gilmore and Comings (1966) arrived at the same conclusion at high pressures. At a pressure of 17.6 MPa, even though the maximum deviation of the Lindsay–Bromley correlation can be up to 30%, the results are 'significantly better than those calculated by Enskog equation'.

Gray and Maczek (1968) calculated the thermal conductivity of CO_2/SO_2. The method of Wassiljewa with experimental A_{ij} gave the best accuracy, and the average discrepancy was <0.5% at 50 and 100 °C. It was better than Hirschfelder approximation and the combination of Wassiljewa method and A_{ij} calculated from the Lindsay–Bromley formula, which had average discrepancies between −1.16 to −1.56% and 2.17 to 2.53% at 323 and 373 K respectively.

4.3.1.3. Other methods. An approximate formula for the thermal conductivity of multicomponent gas mixtures was derived from the rigorous kinetic theory by well defined approximations by Mason and Saxena (1958). Numerical calculations with the formula are relatively simple, and the only data needed are the molecular weights, thermal conductivities, and either viscosities or heat capacities of the pure components at the same temperature as the mixture. The form of the formula is quite similar to the previously described semi-empirical Lindsay–Bromley correlation. The formula was tested by comparing it to experimental results for multiple binary and ternary mixtures involving both monatomic and polyatomic nonpolar gases. For CO_2/N_2 systems, the viscosities needed in the calculations were obtained from Keyes's empirical equations (Keyes, 1951). The AAD was 4.6% in the temperature range 323–961 K, which is similar to the behavior of the Lindsay–Bromley formula (1950).

Based on the formal kinetic theory developed by Monchick et al. (1963), Monchick et al. (1965) calculated the thermal conductivity of polyatomic and polar gas mixtures, including CO_2/N_2. Two assumptions were necessary to obtain usable mixture-models. They neglected complex collisions and assumed no correlation between the internal energy states and the relative velocities. With these assumptions plus suitable definitions of the internal diffusion coefficients and relaxation times, the model was obtained. For the CO_2/N_2 systems, the experimental data agreed well with the calculations at 300 K and 500 K, and was within the experimental uncertainty (2%). At high temperatures like 1000 K however, the deviations became larger.

Johns et al. evaluated the corresponding-states method by Ely and Hanley (1983) called the TRAPP methodology, which is analogous to the extended corresponding states viscosity model (Ely and Hanley, 1981) for the thermal conductivity of CO_2/CH_4. In a temperature range of 302–470 K and a pressure range of 0.9–30.8 MPa, the comparison showed that all the predictions by the TRAPP methodology were within ±3% of the experimental points.

4.3.2. Empirical models

An approximate method, an empirical one, a semi-theoretical one, and the procedure by Lindsay and Bromley were examined for the prediction of the thermal conductivity of polar/non-polar gas mixtures by Tondon and Saxena (1968). With a modification of the approximate method, the deviations could be reduced to 2%. The study was about 12 different systems, including the gaseous mixture CO_2/H_2O.

The experimental data for the thermal conductivity of six binary gaseous mixtures containing water as a component, including CO_2/H_2O, were compared to a Wassiljewa-type formula (Dijkema et al., 1972). No agreement was, however, obtained with values calculated from four different theories based on this formula, Gruss and Schmick (1928), Lindsay and Bromley (1950), Mason and Saxena (1959) and Brokaw (1961), at temperatures between 298 and 333 K.

Experimental results for the thermal conductivities of CO_2/Ar and CO_2/CH_4 were compared by Yorizane et al. (1983) with the values calculated by the Wassiljewa equation, in which the Mason-Saxena equation (1958.) was used as a combination factor with values predicted by the Stiel and Thodos (1964) equation extended

to binary gas mixtures. Both methods were found to represent the measurements within a maximum deviation of 5% at temperatures 25 and 35 °C and pressures up to 9 MPa.

Correlations based on equations derived from kinetic theory have been developed by Cheung et al. (1962) for the thermal conductivity of gas mixtures. For mixtures of polyatomic molecules, the energy transport is divided in two parts, where one comes from collisions and the other from diffusion. When compared with the experimental data for 226 binary mixtures, including CO_2/O_2 and $CO_2/N_2/O_2$, for temperatures between 273.15 and 1047 K, the obtained average deviation was 2.1%.

The resulting thermal conductivities for the dense gaseous state and the corresponding thermal conductivities of the dilute gas at atmospheric pressure for the binary system CO_2/CH_4 were correlated to a unique formula for this system by Rosenbaum and Thodos (1969). This formula was applied for the calculation of thermal conductivities which, when compared with corresponding experimental values, produced an average deviation of 2.24% in the temperature range 333–433 K and in the pressure range 3.28–6.89 MPa.

Andreev and Mal'ter (1975) correlated an empirical equation for the calculation of the thermal conductivities of gas mixtures. It was tested for 47 mixtures, including CO_2/H_2. The mean-square deviation for these data was 4.3% (maximum deviation was 13.7%). The absolute deviations for CO_2/H_2 (50/50 mol%) were slightly above 1% at 273 and 893 K.

Kestin et al. proposed an empirical correlation for the calculations of thermal conductivities of CO_2/Ar (1982), CO_2/H_2 (1983) and CO_2/N_2O (1984). Their conductivity data have been used in a statistical analysis (de Groot et al., 1978) to extract optimum values for the coefficients in a virial expression for the density. Compared to the experimental data, the deviations are within ±0.5% for CO_2/Ar in the density range 10–250 kg/m³, ±0.4% for CO_2/H_2 in the density range 8–75 kg/m³ and ±0.7% for CO_2/N_2O in the density range 10–100 kg/m³ at 296 K.

Johns et al. (1988) also fitted the thermal conductivity data of CO_2/N_2 to polynomials of different degrees using increasing number of points by a procedure described by Kestin et al. (1971) to obtain coefficients for the density expansion of the thermal conductivity in a temperature range of 302–470 K and a pressure range of 0.9–30.8 MPa. The scatter of the experimental points around the density expansion was seen to be <0.2%.

4.4. Diffusion coefficient models

The diffusion coefficient of a binary mixture has been defined as:

$$D_{AB} = -\left(c \frac{dx_A}{dz} \right)^{-1} J_A \tag{4}$$

Here, J_A is the mole flux of component A in the mixture, c is the total concentration, x is the mole fraction and z is a spatial length. From a theoretical perspective, the driving force of diffusion is the chemical potential. Diffusion coefficient models for mixtures which deviate considerably from ideality, such as liquids, polar or high density gas mixtures should thus be corrected with a term containing the derivative of the activity coefficient. The theory describing diffusion in binary gas mixtures at low to moderate pressures has been well developed. The theory results from the solution of the Boltzmann equation and the results are usually credited to both Chapman and Enskog, who independently derived the following equation:

$$D_{AB} = \frac{3}{16} \frac{(4\pi kT/M_{AB})^{1/2}}{n\pi\sigma_{AB}^2 \Omega_D} f_D \tag{5}$$

Here, n is the number density of molecules in the mixtures, k is Boltzmann's constant and M_{AB} is a function of the molar weights of components A and B. Ω_D is the collision integral for diffusion, which is a function of the temperature. This quantity depends on the choice of the intermolecular force law between the colliding molecules. The 6–12 Lennard-Jones potential is a popular choice of force law in the literature. σ_{AB} is a characteristic length which also depends on the intermolecular force law selected. f_D is a correction term which is of the order of unity (Marrero and Mason, 1972). To use Eq. (5), some rules must be chosen to obtain the interaction values σ_{AB} from σ_A and σ_B. For liquids, the Stokes–Einstein equation which has been developed on the basis of hydrodynamic theory for large spherical molecules diffusing in a dilute solution has been the starting point of several correlations:

$$D_{AB} = \frac{RT}{6\pi\eta_B r_A} \tag{6}$$

Here, R is the universal gas constant; r_A is the radius of the solute and η_B is the viscosity of the solvent. Correlations for diffusion coefficients in non-dilute liquids, often uses the dilute diffusion coefficients correlated with the derivative of the activity coefficient discussed previously. Reid et al. (1987) however, claim that no single correlation is always satisfactory in the estimation of the concentration effect on the diffusion coefficients of non-dilute liquid mixtures.

4.4.1. Semi-empirical models

The methods by Wilke and Chang (1955) and by Othmer and Thakar (1953) were used to calculate the diffusion coefficient of CO_2 in liquid water by Unver and Himmelblau (1964). The method by Wilke and Chang uses Eq. (6) as the foundation, whereas the method by Othmer and Thakar is derived by linking the temperature dependency of the viscosity and the diffusion coefficient. 'Both methods represented the overall experimental results well'. In addition, a convenient way to calculate the diffusion coefficient was provided. The measurements were used to correlate a quadratic equation, using the lease square method. The liquid diffusion coefficients computed in this way were within ±11% of the experimentally measured values. The methods by Wilke and Chang (1955) were also used by Thomas and Adams (1965) to calculate the diffusion coefficients of CO_2 in water. In the temperature range 291.6–348.2 K, the values by Wilkes method were approximately 20% lower than the experimental data at each temperature.

The measured data for the diffusion coefficient of CO_2/O_2 have been analyzed in terms of the intermolecular potential energies and the rigorous kinetic theory. Four methods were used to approximate the actual potential energy needed in Eq. (5), including the Lennard-Jones potential (12-6), the potential modified by Buckingham, the point center of repulsion (inverse power), and the exponential repulsion potential energy functions (Walker and Westenberg, 1960). Their results showed that all four of the energy functions are capable of fitting the diffusion data with about the same precision. No significant concentration effects are, however, expected for CO_2/O_2 since the molecular weights are not widely different.

The importance of using the right energy potential in the estimation of collision integrals has been recognized by several authors. Holsen and Strunk (1964) studied the diffusion coefficients of CO_2/Ar and CO_2/Air in the temperature range 276–317 K. Within this range, the temperature dependency of the coefficients was found to be inconsistent with the theoretical values predicted with Chapman–Enskog's expression for the first approximation, in which the Lennard-Jones potential parameters are derived from viscosity data. Hirschfelder has shown that at a given temperature, the collisions most effective in promoting diffusion occur at closer distances than those most effective in the transfer of momen-

tum and energy (viscosity and thermal conductivity). Holsen and Strunk, thus, found it necessary to correlate a correction factor for the Lennard-Jones potential to make the model represent the experimental data.

Instead of using a correction factor for the Lennard-Jones potential, other energy potentials have been tested. The experimental diffusion coefficients of 22 pairs of gas mixtures, including CO_2/CO, were compared with theoretical values from a potential of Lennard-Jones and from the modified potential of Buckingham by Ivakin and Suetin (1964a). The theoretical values calculated by the Lennard-Jones potential deviate from the experimental values by no more than 6% at 296 K. The empirical coefficient proposed by Wilke and Lee (1955) permitted improvement in the accuracy to 5.5%. Buckingham's potential gave an even better description than the Lennard-Jones potential. On the average, the theoretical values obtained with Buckingham's potential deviate from the experimental data by 3%. Ivakin and Suetin (1964b) also used the obtained experimental data to calculate the potential parameters of the intermolecular interaction for the Lennard-Jones (6-12) potential, the modified Buckingham potential and the point center of repulsion. Here, the first approximation of the strict kinetic gas theory was used to calculate the diffusion coefficient of gas mixtures, including CO_2/N_2 and CO_2/H_2. In the temperature range 573–1100 K, the calculations using the point center of repulsion potential showed the best accuracy for both CO_2/N_2 and CO_2/H_2 (AAD = 3% for CO_2/N_2 and AAD < 10% for CO_2/H_2), while the Lennard-Jones (6-12) potential with parameters fitted from viscosity data showed the worst accuracy (AAD = 10% for CO_2/N_2 and AAD = 13% for CO_2/H_2).

4.4.2. Empirical models

The most widely used empirical equation for the prediction of binary diffusion coefficients in gaseous mixtures at low concentrations is that of Fuller–Schettler–Giddings (FSG). This equation is the result of the correlation of more than 340 experimental diffusion coefficients for 153 different binary mixtures (Fuller et al., 1966):

$$D_{AB}^{FGS} = \frac{10^{-3} T^{1.75} \sqrt{1/M_A + 1/M_B}}{p \left[\left(\sum v \right)_A^{1/3} + \left(\sum v \right)_B^{1/3} \right]^2} \tag{7}$$

Here, T is the absolute temperature, p is the pressure (atm) and Σv are special diffusion parameters to be summed over atoms, groups and structural features of the diffusion species, called diffusion volumes and having dimensions of atomic volumes. This method has the advantage of being able to overcome the general lack of accuracy associated with other category methods. It has been used to calculate the diffusion coefficients of several mixtures, including CO_2/H_2, CO_2/Ar, CO_2/N_2, CO_2/N_2O and CO_2/H_2O (gas). The average deviations were between −3.4 and 14.3% (Fuller et al., 1966).

The FSG method was used to estimate the diffusion coefficients of binary CO_2-mixtures including the impurities N_2, O_2, H_2, H_2O and CO (Todd and Young, 2002). By comparing the results with experimental data, the obtained mean deviations were between −2.44 and −4.71% except for CO_2/H_2O. This method displayed poor accuracy for the CO_2/H_2O system, with a mean deviation of 20.91% and a maximum deviation of 34.1%. Gavril et al. (2004) used the FSG equation to calculate the diffusion coefficients of CO_2/H_2. In the temperature range 315.2–343.9 K, the absolute deviations were <0.5%.

An Arrhenius-type equation by Versteeg (1986) and Frank et al. (1996) was used to represent the diffusion coefficient of liquid CO_2/H_2O mixtures. Compared to the measurements by Frank et al. (1996) in the temperature range 298–328 K, Frank's correlation has an AAD of <1%, while Versteeg's correlation has an AAD of 1.67%. Frank et al. (1996) also evaluated the modified Stokes–Einstein

equation and the Wilke–Chang equation. Both of them showed typical errors larger than 5%.

4.5. Models for multi-component properties

Some models are able to handle several transport properties. Bzowski et al. (1990) for instance, used results from statistical-mechanical theory applied through a combination of an extended principle of corresponding states with some knowledge about intermolecular potentials, to calculate the transport and equilibrium properties of gas mixtures at low densities, including the second virial coefficients, viscosities, diffusion coefficients and thermal diffusion coefficients. For the diffusion coefficients, the deviations are within ±1% for CO_2/N_2O, within ±5% for CO_2/CH_4 and CO_2/CO, within ±7% for CO_2/O_2, within ±18% for CO_2/N_2 and within ±22% for CO_2/Ar. For viscosity: the deviations are within ±2% for CO_2/N_2, CO_2/CO and CO_2/N_2O, within ±2% for CO_2/CH_4 and within ±4% for CO_2/O_2 and CO_2/Ar.

Second virial coefficients, viscosities, thermal conductivities and diffusion coefficients of binary gas mixtures have been computed for the Morse potential in conjunction with a set of combination rules for the unlike interactions (Bahethi et al., 1964). For the viscosity of CO_2/H_2, Bahethi calculated values which differ 2.3% on average from the experimental values. The comparison of experimental diffusion coefficients with the theory leads to very notable discrepancies for CO_2/N_2, which is up to 20% at temperatures over 900 K. Moreover, the viscosities, diffusion coefficients, thermal conductivities and diffusion coefficients of natural gas components were determined based on the principle of corresponding states for the viscosity together with an inversion technique (Moghadasi et al., 2007). The method developed by Schreiber et al. (1997) and the Chapman–Enskog approach have also been used to calculate the viscosity, the thermal conductivities and the diffusion coefficients with average accuracies within ±3%, ±5% and ±14% respectively.

4.6. Discussion of the transport property models

Several models and governing theories have provided the engineers with a large variety of expressions, and many comparisons with experimental data have been presented in the literature as displayed in Table B1. A major issue is that only few of the comparisons have been published after 1970. As discussed in Section 3.1 and displayed in the Figs. 1–3, poor accuracy is expected for many of the experiments conducted before 1970. A wrong impression of the accuracy may be the result of comparing models to inaccurate experimental data. Another issue is that few comparisons have investigated the pressure dependency of the transport properties. Operation conditions at high pressures, however, are expected in several parts of the CCS-chain.

For the prediction of gas-phase viscosities, the two competing methodologies have been the one based on Chapman–Enskog theory, and the theory based on the principle of corresponding states. Few comparisons in the literature have evaluated corresponding state methods for calculation of the viscosity of CO_2 rich mixtures (Kestin and Ro, 1976, 1982; Hanley, 1976; Mal'tsev et al., 2004) and the comparisons do not lead to any conclusions with respect to which theory that is most suitable for viscosity predictions in CCS. More model evaluation is necessary at larger temperatures and pressures and the performance of corresponding state methods should be more carefully evaluated.

Two different approaches are common in the estimation of both gas-phase thermal conductivities and diffusion coefficients, namely the methodology based on the Rigorous Kinetic Theory (RKT) and empirical models. The best results with empirical models are obtained when the A_{ij} factor is adapted to experiments. The predictive abilities of these models outside the range of the

experiments are questionable. The better extrapolative properties of models based on the RKT is a clear advantage for CCS applications which involve a large range in temperature and pressure. Few sources have evaluated the accuracy of thermal conductivity models at high pressures.

One of the most popular models often recommended for use in prediction of gas-phase diffusion coefficients is the empirical model by Fuller et al. (1966). Comparison with newer data for the CO_2/H_2O mixture has, however, shown that up to 21% inaccuracy should be expected. A serious concern with the very popular equation by Fuller et al., is that the data forming the basis of the model-regression were obtained before 1950. Data of this age are expected to contain inaccuracies due to obsolete measuring techniques as discussed by (Wakeham, 1996). A new regression of the functional form presented by Fuller et al. for mixtures relevant for CCS may be an attractive possibility. When the RKT is used to predict the diffusion coefficients, several intermolecular force-laws have been tested in the estimation of the collision integral. The variation in results by choosing different energy potentials in estimation of the diffusion coefficients was displayed by Ivakin and Suetin (1964b). More energy potentials should be tested to obtain even better accuracy for CO_2 rich mixtures. For many mixtures, the diffusion coefficient models based on the RKT show predictions within the experimental uncertainty according to Table B1.

For the prediction of liquid-phase transport properties of CO_2-mixtures, only $CO_2/H_2O(/NaCl)$ mixtures were investigated and only empirical models have been tested. The research community knows little about the effect of other impurities in liquid CO_2 than water. However, liquid properties are of importance in the processes of amine-based chemical absorption, CO_2 pipeline transport and sub-sea CO_2 storage. The existence of accurate data and models for the calculation of liquid-phase transport properties of pure CO_2 (see Section 4.1), points in the direction of corresponding state approaches as an alternative for future modelling of liquid CO_2-mixtures with high accuracy. In addition, some general liquid property models are available (Reid et al., 1987) under different temperature and pressure conditions. Due to the shortage of experimental data, it is currently not possible to evaluate their performance for liquid CO_2-mixtures. Therefore, more experiments are needed to asses which models that are most suitable for the prediction of liquid-phase transport properties.

5. Conclusion and suggestions for future work

The literature containing both experimental data and theoretical models about the transport properties of CO_2-mixtures has been reviewed. Based on the pre-defined operating windows of CCS, gaps in the knowledge about the transport properties of CO_2-mixtures have been identified.

In general, except for the $CO_2/H_2O(/NaCl)$ and $CO_2/amine/H_2O$ mixtures, there are no available measurements regarding the transport properties of liquid-phase mixtures. For gas mixtures, there are no available experimental data about any transport properties of CO_2/H_2S, CO_2/COS and CO_2/NH_3. Few data are available for the transport properties at high temperatures and pressures over 1 bar, and the situation is particularly scarce for the mixtures CO_2/O_2,

CO_2/SO_2 and CO_2/CO. Another major concern is that there are no available data for the diffusion coefficients of the CO_2/CH_4 mixture.

Several models and governing theories have been compared to experimental data and presented in the literature. A major issue is that most of the comparisons have been published before 1970 and poor accuracy is expected for the experimental data. A comparison with more reliable data and also an investigation of models at higher pressures should be conducted in the future. For the prediction of gas-phase viscosities using Chapman–Enskog theory, deviations are typically <2% at atmospheric pressure and moderate temperatures, except for the CO_2/H_2O mixture. The deviations increase with increasing temperatures and pressures. Few sources in the literature have evaluated corresponding state methods for calculation of the viscosity of CO_2 rich mixtures.

Using both the rigorous kinetic theory and empirical models in the prediction of gas-phase thermal conductivities will result in deviations with experimental data of 2.2–9% with atmospheric pressure and modest temperatures. The predictive abilities of empirical models outside the range of the experiments are questionable, and the better extrapolative properties of model based on RKT is a clear advantage for use in CCS.

Comparison of the popular empirical model by Fuller et al. (1966) for estimation of gas-phase diffusion coefficients with newer experimental data for CO_2/H_2O shows that deviations over 20% should be expected. A serious concern with Fuller's equation is that the data which is the basis for the model are from before 1950. A new regression of Fuller's equation for mixtures relevant for CCS may be an attractive possibility. For many mixtures, the diffusion coefficient models based on the RKT show predictions within the experimental uncertainty.

For the prediction of liquid-phase transport properties, empirical models have only been tested for $CO_2/H_2O(/NaCl)$. Typical reported deviations for the viscosity and the thermal conductivity of the $CO_2/H_2O(/NaCl)$ system using empirical models are below 3%. Models for prediction of liquid-phase diffusion coefficients have typical reported deviations between 5 and 20%. Here, the research community knows little about the effect of other impurities in liquid CO_2 than water. The existence of accurate data and models for the calculation of liquid-phase transport properties of pure CO_2, points in the direction of corresponding state approaches as an alternative for future modelling of liquid CO_2-mixtures with high accuracy.

Appendix A.

Details about all available experiments for the viscosity, the thermal conductivity and the diffusion coefficients are given in Tables A1–A3 respectively.

Table A1
Available experimental data on the viscosities.

Source	Year	Phase	Substance	T (K)	P (MPa)	No. of data	Uncertainty
White and Twining	1913	L	CO_2/H_2O	293			
Jung and Schmick	1930	G	CO_2/HCl, CO_2/SO_2	289 and 291		16	
Trautz and Kurz	1931	G	CO_2/H_2	300 and 551		16	
Trautz and Sorg	1931	G	CO_2/N_2O	300–550		24	
Herning and Zipperer	1936	G	$CO_2/O_2/CO/H_2/CH_4/N_2$	293–1287		17	

Table A1 (*Continued*)

Source	Year	Phase	Substance	T (K)	P (MPa)	No. of data	Uncertainty
Schmid	1942	G	$CO_2/O_2/CO/H_2/CH_4/N_2$	300–1279		19	
Heath	1948	G	CO_2/H_2	291	0.1	11	
Buddenberg and Wilke	1951	G	CO_2/H_2	298	0.1	5	
Swindells et al.	1952	L	CO_2/H_2O	293–313			
Weber	1955, 1963	L	CO_2/H_2O	303–313			
Kenney et al.	1956	G	$O_2/N_2/CO_2$	317–1161		20	2%
Jackson	1956	G	CO_2/CH_4	298		14	
Kestin and Leidenfrost	1959	G	CO_2/N_2	293	0.1–2.14	45	±0.05%
Chakraborti and Gray	1965	G	CO_2/SO_2	298–353		37	1%
DeWitt K.J., Thodos	1966	G	CO_2/CH_4	323–473	3.4–68	>100	
Kestin et al.	1966	G	$CO_2/N_2, CO_2/Ar$	293 and 303	0.1–2.6	12	±0.1%
Gururaja et al.	1967	G	$CO_2/O_2, CO_2/N_2, CO_2/H_2, CO_2/O_2/N_2, CO_2/O_2/H_2$	295–303	0.098	41	
Kestin and Yata	1968	G	CO_2/CH_4	293 and 303	0.1–2.6	48	±0.05%
Bhattacharyya and Ghosh	1970	G	CO_2/SO_2	238–308		24	±0.6%
Golubev	1970	G	CO_2/N_2	289	2–12	4	
Munczak and Sedkacek	1970	G	CO_2/H_2O	303		8	±0.15%
Kestin and Ro	1974	G	$CO_2/N_2, CO_2/Ar, CO_2/CH_4, Ar/ CO_2/N_2, CH_4/CO_2/N_2$	298–873		117	
Kestin and Ro	1976	G	$Ar/N_2/CO_2, CH_4/N_2/CO_2$	298–873		40	
Kestin et al.	1977	G	CO_2/O_2	298–674	0.1	15	±0.3%
Boushehrl and Najafi	1979	G	$N_2/O_2/CO_2/N_2O$	313–413		12	
Kestin and Ro	1982	G	CO_2/N_2O	298–473		10	±0.3%
Kestin et al.	1983	G	CO_2/H_2	295–303	0.1	6	±0.1%
Kestin and Ro	1983	G	CO_2/CO	298–473	0.1	10	±0.1–0.2%
Hobley et al.	1989	G	CO_2/Ar	310–521	0.1	19	<0.7%
Frank et al.	1996	L_{sat}	CO_2/H_2O	293–313	0.4	6	±2%
Kumagai and Yokoyama	1998	L	CO_2/H_2O	273–278	0.1–30	41	±1.5%
Weiland et al.	1998	L	$CO_2/Amines$	298		165	±0.2%
Kumagai and Yokoyama	1999	L	$CO_2/H_2O/NaCl$	273–278	0.1–30	90	±0.8%
Uchida et al.	2003	L	CO_2/H_2O	273–282	0.7–5	30	±2.3%
Bando et al.	2004	L	$CO_2/H_2O/NaCl$	303–333	0.1–20	53	±2%
Mal'tsev et al.	2004	G	CO_2/H_2	500, 800, 1100	0.3	21	±3%

Table A2
Available experimental data on the thermal conductivities.

Source	Year	Phase	Substance	T (K)	P (MPa)	No. of data	Uncertainty
Weber	1917	G	CO_2/H_2	273.16	0.1	4	
Ibbs and Hirst	1929	G	CO_2/H_2	273	0.1		
Kornfeld and Hilferding	1931	G	CO_2/H_2	298		5	
Keyes and Mass	1952	G	CO_2/N_2	273–623	0.1	22	
Vargaftik and Timroth	1952	G	CO_2/H_2O	338		5	
Rothman and Bromley	1955	G	CO_2/N_2	642–961	0.1	19	
Kulakov	1955	G/L	$CO_2/H_2O, CO_2/N_2$	338–1047	0.1	39	
Von Lehmann	1957	G	$CO_2/H_2, CO_2/N_2, CO_2/H_2O$	273–623		6	
Vines	1960	G	CO_2/N_2	1033		5	
Cheung et al.	1962	G	$CO_2/N_2, CO_2/O_2$	369–370		5	
Westenberg and Dehaas	1962	G	CO_2/N_2	300–2000		25	
Gilmore and Comings	1966	G	CO_2/N_2	348	0.1–300	24	
Mukhpadhyay et al.	1967	G	CO_2/H_2	258–573	0.1	42	±1%
Barua et al.	1968	G	$CO_2/Ar, CO_2/N_2$	273–473		87	
Rosenbraum and Thodos	1969	G	CO_2/CH_4	333–433	3.28–6.89	130	
Maczek and Gray	1970	G	CO_2/SO_2	323–373		18	±0.4%
Saxena and Gupta	1970	G	CO_2/N_2O	323–723		27	
Dijkema et al.	1972	G	CO_2/H_2O	298, 333	0.1	18	
Vargaftik	1972	G	CO_2/H_2	273, 893		2	
Christensen and Fredenslund	1979	G	CO_2/CH_4	228.13–272.07	0.26–1.76	14	
Kestin et al.	1982	G	CO_2/Ar	300.5	0.85–11.29	48	±0.3%
Kestin et al.	1983	G	CO_2/H_2	300.65	0.85–7.47	44	±0.3%
Yorizane et al.	1983	G	$CO_2/CH_4, CO_2/Ar$	298 and 308	0.1–9	130	±3%
Imaishi et al.	1984	G	CO_2/N_2O	300.65	0.62–4.25	63	
Johns et al.	1988	G	CO_2/N_2	320–470	0.9–30.8	93	<0.2%

Appendix B.

This Appendix contains a summary of the models which have been tested for the transport properties in the literature in Table B1.

Table A3
Available experimental data on the diffusion coefficients.

Source	Year	Phase	Substance	T (K)	P (MPa)	No. of data	Uncertainty
Boardman and Wild	1937	G	CO_2/O_2, CO_2/N_2, CO_2/H_2	293	0.1	3	
Chapman and Cowling	1939	G	CO_2/O_2	273	0.1	1	
Waldman	1944	G	CO_2/N_2, CO_2/H_2	293	0.1	2	
Wall and Kidder	1946	G	CO_2/N_2O	298	0.1	1	
Winn	1950	G	CO_2	197–350	0.1	4	
Boyd et al.	1951	G	CO_2/H_2, CO_2/N_2	293–298	0.1	4	
Schwertz and Brow	1951	G	CO_2/H_2O	307–353	0.1	5	
Amdur et al.	1952	G	CO_2/N_2O, CO_2	194.8–362.6	0.03–0.07	5	
Walker and Westenberg	1958b	G	CO_2/N_2	298	0.1	4	
Nijsing et al.	1959	L	CO_2/H_2O	279–303	0.1		
Schafer	1959	G	CO_2/SO_2	263–273	0.1		
Walker and Westenberg	1960	G	CO_2/O_2	300–3000	0.1	7	
Walker et al.	1961	G	CO_2/N_2	573–1100		7	
Ember et al.	1962	G	CO_2/CO_2	1180–1680		12	
Giddings and Seager	1962	G	CO_2/N_2, CO_2/H_2	297–299	0.085	3	
Clarke	1964	L	CO_2/H_2O	298	0.1	1	
Holsen and Strunk	1964	G	CO_2/Ar, CO_2/Air	273–317	0.1	6	
Ivakin and Suetin	1964b	G	CO_2/H_2, CO_2/N_2, CO_2/CO, CO_2/Ar	291.9–473	0.1	28	1.5–2.5%
Ivakin and Suetin	1964a	G	CO_2/CO	296	0.1	2	
Unver and Himmelblau	1964	L	CO_2/H_2O	280–338	0.1	5	
Tang and Himmelblau	1965	L	CO_2/H_2O	298	0.1	1	
Thomas and Adams	1965	L	CO_2/H_2O	292–378	0.1	7	1%
Duda and Vrentas.	1968	L	CO_2/H_2O	298, 313	0.1	2	
Gray and Maczek	1968	G	CO_2/SO_2	323–373	0.1	2	
Malik and Hayduk	1968	L	CO_2/H_2O	303	0.1	1	
Choudhari and Doraiswarmy	1972	L	CO_2/H_2O	298–303	0.1	3	
Marrero and Mason	1972	G	CO_2/Ar, CO_2/O_2, CO_2/N_2			3	
Pratt et al.	1973	L	CO_2/H_2O	290	0.1	3	±8%
Robjohns and Dunlop	1984	G	CO_2/Ar, CO_2/O_2, CO_2/N_2	300		3	0.2–0.3%
Versteeg	1986	L	CO_2/H_2O		0.1		
Frank et al.	1996	L_{sat}	CO_2/H_2O	293–313	0.4	4	
Gavril et al.	2004	G	CO_2/H_2	315.2–343.9	0.1	7	

Table B1
Summary of mathematic models of transport properties.

Model	Year	Phase	Type	T (K)	P (MPa)	Mixture	Dev (%)	Ref.
Viscosity								
Herning–Zipperer	1936	G	Empirical (Emp)	298–353		CO_2/SO_2	3.5	Chakraborti and Gray (1965)
				291	0.1	CO_2/H_2	Good agreement	Heath (1948)
Chapman–Enskog	1939	G	Chapman–Enskog (CE)	298–353		CO_2/SO_2	2	Chakraborti and Gray (1965)
				313–413		$CO_2/O_2/N_2O/N_2$	2	Boushehrl and Najafi (1979)
				299–550		CO_2/H_2	2–3	Keyes and Mass (1951)
				288	0.1	CO_2/H_2	<1	Buddenberg and Wilke (1951)
				317–1161		$CO_2/O_2/N_2$	1	Kenney et al. (1956)
Hirschfelder	1948	G	CE	293–303		CO_2/N_2, CO_2/Ar	0.1	Kestin et al. (1966)
				293–303		CO_2/CH_4	Good agreement	Kestin and Yata (1968)
				238–308		CO_2/SO_2	<1	Bhattacharyya and Ghosh (1970)
				303	0.1	CO_2/H_2O	Poor agreement	Munczak and Sedlacek (1970)
Runberg and Nissan	1949	L	Emp	273–278	0–30	CO_2/H_2O	<1	Kumagai and Yokoyama (1998)
				298		CO_2/CH_4	<1	Jackson (1956)
				293		CO_2/N_2	1.7	Kestin and Leidenfrost (1959)
				298–353		CO_2/SO_2	3.5	Chakraborti and Gray (1965)
Wilkes equation	1950	G	CE			CO_2/N_2	0.57	
						CO_2/O_2	1.91	
				296–303		CO_2/H_2	0.62	Gururaja et al. (1967)
						$CO_2/O_2/H_2$	1.77	
						$CO_2/O_2/N_2$	0.79	
				500–1100	0.3	CO_2/H_2	Max 8	Mal'tsev et al. (2004)
Brokaw	1965	G	CE	298–353		CO_2/SO_2	<2	Chakraborti and Gray (1965)
Dean and Stiel	1965	G				CO_2/N_2, CO_2/CH_4	1.32–3.65	Dean and Stiel (1965)
DeWitt and Thodos	1966	G	Emp	323–473	$\rho_R < 1.5$	CO_2/CH_4	1.83	DeWitt and Thodos (1966)
Canonically angle–average pair potential energy function	1971	G	CE	289	0.1	CO_2/SO_2	1.8–3.0	Bae and Reed (1971)
Bloomfield–Dewan equation and Flory theory	1971	L	Flory	273–278	0–30	CO_2/H_2O	Poor agreement	Kumagai and Yokoyama (1998)
KRW law	1972	G	Corresponding State (CS)	298–873		CO_2/N_2, CO_2/Ar, CO_2/CH_4, CO_2/N_2O, $CO_2/N_2/Ar$, $CO_2/N_2/CH_4$	1	Kestin and Ro (1976, 1982)
Hanley	1976	G	CS	289	2–12	CO_2/N_2	0–7.8	Hanley (1976)
Kumagai and Yokoyama	1999	L	Emp	273–278	0.1–30	$CO_2/H_2O/NaCl$	1.3	Kumagai and Yokoyama (1999)
Bando	2004	L	Emp	303–333	10–20	$CO_2/H_2O/NaCl$	5	Bando et al. (2004)
Boltzmann		G	CE + CS	298–674		CO_2/O_2	0.3	Kestin et al. (1977)
Arrhenius type function		L	Emp	293–333		CO_2/H_2O	1	Frank et al. (1996)
Thermal conductivity								
Wassiljewa	1904	G	Semi–Emp	323–373		CO_2/SO_2	0.5	Gray and Maczek (1968)
				273–298		CO_2/H_2	−0.2–8.4	Lindsay and Bromley (1950)
				642–961		CO_2/N_2	−3∼-1	Rothman and Bromley (1955)
Wassiljewa + Lindsay–Bromley A_{ij}	1950	G	Semi–Emp	348	0.1–300	CO_2/N_2	Max = 30%	Gilmore and Comings (1966)
				323–373		CO_2/SO_2	−1.16–2.53	Gray and Maczek (1968)
				338		CO_2/H_2O	1.4	Tondon and Saxena (1968)
				298–333		CO_2/H_2O	No agreement	Dijkema et al. (1972)
Enskog	1951	G	Rigorous kinetic theory (RKT)	323–623	0.1	CO_2/N_2	3.43	Keyes and Mass (1952)

Table B1 (*Continued*)

Model	Year	Phase	Type	T (K)	P (MPa)	Mixture	Dev (%)	Ref.
				273–1033		CO_2/N_2	Good agreement	Brokaw (1959)
				294–1000		CO_2/N_2	10	Westenberg and Dehaas (1962)
				323.16		CO_2/N_2	6.4–7.8	Mathur and Saxena (1966)
				273.16		CO_2/H_2	2.2–3.5	
Hirschfelder	1957	G	RKT	258–473		CO_2/H_2	5–8	Mukhopadhyay et al. (1967)
				273–473		CO_2/Ar	3	Barua et al. (1968)
						CO_2/N_2	4	
				300–750		CO_2/N_2O	−2–9	Saxena and Gupta (1970)
				323 & 373		CO_2/SO_2	0–3	Maczek and Gray (1970)
				300	0.85–7.5	CO_2/H_2	>0.3	Kestin et al. (1983)
Mason and Saxena	1958	G	RKT	323–961		CO_2/N_2	4.6	Mason and Saxena (1958)
				298–333		CO_2/H_2O	No agreement	Dijkema et al. (1972)
Wassiljewa + Mason–Saxena	1958	G	Semi-Emp	298–308	0–9	CO_2/CH_4, CO_2/Ar	<5	Yorizane et al. (1983)
Cheung	1962	G	Emp	273–1047		CO_2/O_2, CO_2/O_2N_2	2.1	Cheung et al. (1962)
Monchick	1964	G	RKT	300–1000		CO_2/N_2	2 (≤500 K)	Monchick et al. (1965)
Tondon and Saxena	1968	L	Emp	338		CO_2/H_2O	2.2	Tondon and Saxena (1968)
Rosenbaum and Thodos	1969	G	Emp	333–433	3.3–6.9	CO_2/CH_4	2.24	Rosenbaum and Thodos (1969)
Andreev and Mal'ter	1975	G	Emp	273 & 893		CO_2/H_2	1	Andreev and Mal'ter (1975)
Mason	1978	G	RKT		0–75 kg/m³	CO_2/H_2	≈5	Kestin et al. (1983)
					10–250 kg/m³	CO_2/Ar	0.5	Kestin et al. (1982)
Kestin		G	Emp	300	8–75 kg/m³	CO_2/H_2	0.4	Kestin et al. (1983)
					10–100 kg/m³	CO_2/N_2O	0.7	Kestin et al. (1984)
Ely and Hanley	1983	G	CS	302–470	0.9–30.8	CO_2/N_2	6	Johns et al. (1988)
Johns	1988	G	Emp	302–470	0.9–30.8	CO_2/N_2	5	Johns et al. (1988)
Diffusion coefficient								
				273–293	0.1	CO_2/O_2	Within the experimental error	Walker and Westenberg (1960)
			Lennard–Jones potential	296.1		CO_2/CO	1.3	Ivakin and Suetin (1964a)
				Up to 1000		CO_2/N_2, CO_2/H_2, CO_2/Ar, CO_2/CO	Good agreements	Ivakin and Suetin (1964b)
RKT		G		276–317		CO_2/Air, CO_2/Ar	Inconsistent	Holsen and Strunk (1964)
			Modified–Buckingham potential (Hirschfelder et al. 1954)	273–293	0.1	CO_2/O_2	Within the experimental error	Walker and Westenberg (1960)
				276–317		CO_2/Air, CO_2/Ar	Inconsistent	Holsen and Strunk (1964)
				296.1		CO_2/CO	0	Ivakin and Suetin (1964b)
			Wilke–Lee (1955)	296.1		CO_2/CO	7.3	Ivakin and Suetin (1964b)
			Point center of repulsion	273–293	0.1	CO_2/O_2	Within the experimental error	Walker and Westenberg (1960)
			Exponential repulsion	273–293	0.1	CO_2/O_2	Within the experimental error	Walker and Westenberg (1960)
			Canonically angle–average pair potential energy function	263–473	0.1	CO_2/SO_2	3	Bae and Reed (1971)
				279–338		CO_2/H_2O	<11	Unver and Himmelblau (1964)
Wilke–Chang	1955	L	Semi-Emp	291–348		CO_2/H_2O	−20	Thomas and Adams (1964)
				298–328	0.4	CO_2/H_2O	5	Frank et al. (1996)
Othmer–Thakar	1960	L	Semi-Emp	279–338		CO_2/H_2O	<11	Unver and Himmelblau (1964)
Stokes–Einstein	1960	L	Hydrodynamic theory	298–328	0.4	CO_2/H_2O	5	Frank et al. (1996)
				194.8–1200	0.1	CO_2/H_2, CO_2/N_2 CO_2/Ar, CO_2/H_2O	−3.3–14.4	Fuller et al. (1966)
Fuller–Schettler–Giddings	1966	G	Emp	300–1500	0.1	CO_2/N_2, CO_2/O_2, CO_2/H_2, CO_2/H_2O, CO_2/CO	−2.44–4.71 (20.91 for CO_2/H_2O)	Todd and Young (2002)
				315.2–343.9		CO_2/H_2	<0.5	Gavril et al. (2004)
Arrhenius–type (Versteeg)	1986	G	Emp	298–328	0.4	CO_2/H_2O	1.67	Frank et al. (1996)
Arrhenius–type (Frank)	1996	G	Emp	298–328	0.4	CO_2/H_2O	1	Frank et al. (1996)

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