Literature Review of Tracer Partition Coefficients

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Milestone 2 - "Literature review and presentation of tracers with partition coefficients with error bars currently reported in literature" to the Australian National Low Emissions Coal Research and Development (ANLEC R&D)

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1   Chemical Tracers in CCS Projects

1.1   Introduction

As the first deliverable of Project 3-1110-0125 Fundamentals of tracer applications for CO_2 Storage, the following report titled "Literature Review and Presentation of Tracers with Partition Coefficients with Error Bars Currently Reported in Literature" (Milestone 2) has been prepared. At the onset of this project it is important to review the current literature to obtain any relevant information that may have been published on tracer compound partition coefficients between supercritical (and other forms of) CO_2 and water (with or without added minerals). It has been noted by various researchers examining the potential use of tracer compounds in carbon storage projects that quantified partition coefficients are greatly lacking in the literature (Myers et al., 2012a). As such, the Commonwealth Scientific Industrial Research Organisation (CSIRO) has invested in new equipment designed to make these measurements for various tracer applications. This project aims to measure partition coefficients for tracers that have already been deployed at various carbon storage sites. For example, the CO2CRC granted the project access to use the tracer data set generated at the CO2CRC Otway Stage 1 and Stage 2B projects in Victoria. With quantified partition coefficients, it will be possible to provide better constrained interpretations of observed tracer data and contribute towards reducing uncertainty in model forecasting. The following is a short summary of particular chemical tracers applied to various recent CCS projects globally with the goal of identifying a set of tracers that will be characterised as a part of this study. This will serve to validate the usefulness of the results that will be generated by the laboratory experiments that comprise the main research component of this project. Furthermore, this study will focus exclusively on chemical tracers that are added to the formation during injection and will not examine naturally occurring tracers (i.e. chemical species already previously present in the formation mobilized as a result of CO_2 injection).

Predicting and understanding the behaviour of CO_2 is challenging due to its complex phase behaviour (i.e. CO_2 can exist in the subsurface as a liquid, gas, supercritical fluid or a solute in water depending on the physical/chemical conditions) and the wide range of possible trapping mechanisms (i.e. residual, solubility, structural and mineral). Commonly proposed storage scenarios involve pumping CO_2 into reservoir rock formations at depths greater than 800 metres, where the pressure/temperature typically exceeds the critical point of carbon dioxide (7.38 MPa, 31.1°C).   Chemical tracers represent a complimentary reservoir characterisation and monitoring tool to alternative approaches such as geophysical measurements (e.g. time lapse seismic) and have been used extensively worldwide at carbon capture and storage (CCS) sites. The majority of tracer applications within CCS are related to either understanding the subsurface movement of carbon dioxide (Boreham et al., 2011; Freifeld et al., 2005; Underschultz et al., 2011; Vandeweijer et al., 2011), quantifying the trapping capacity (Zhang et al., 2011) or determining containment and leakage rates for monitoring and verification programs (Strazisar et al., 2009; Wells et al., 2010; Wells et al., 2007).   Chemical stability, cost effectiveness, ease of detection, toxicity, injection/sampling protocols and subsurface behaviour, together dictate the choice of tracer for a particular application or scenario.

1.2   Tracers Relevant to the CO2CRC Otway Project and Frio Brine Projects

Perdeuterated methane (CD_4), krypton (Kr) and sulphur hexafluoride (SF_6) were used as tracer gases for the CO2CRC Otway Stage 1 Project (Boreham et al., 2011). The breakthrough of the injected CO_2 plume was identified by the presence of the tracer compounds, an increase in CO_2 concentration over background

levels and a change in the $\delta^{13}C$ of the measured CO_2. From the available publications on this project, reservoir simulation of tracer behaviour within the relevant geological formations is currently lacking (Boreham et al., 2011; Jenkins et al., 2012; Underschultz et al., 2011). Although, some activity has been directed at reservoir simulation of the results, a full synthesis has not yet been published. This can be partially attributed to a distinct lack of fundamental information on tracer behaviour (derived from laboratory based experiments) with which to develop accurate models. Also in this case, the effect of methane (both within the storage reservoir and as component of the injected gas which contains approximately 20% methane) on tracer behaviour adds additional complexity to the system and its effect is largely unknown. In this case, these uncertainties in the physical properties of the tracer compounds translate into uncertainty in the interpretation of the final observations.

For the Frio Brine Projects in Texas, various perfluorocarbons, SF_6, Kr and CD_4 were injected as tracers to detect CO_2 breakthrough in an interwell (injector/producer) configuration (Hovorka et al., 2006). For similar reasons as with the CO2CRC Otway Project, a detailed reservoir simulation of tracer behaviour has not been published. Although tracer injections were useful in the case of both the Otway and Frio Brine projects for limited/qualitative interpretations (i.e. determining breakthrough of injected CO_2), for other purposes such as monitoring for leaks into the atmosphere, knowledge of the partitioning behaviour between water and CO_2 under a variety of geological conditions is instrumental. As such an understanding of tracer behaviour in CO_2/CH_4 and water would not only be very helpful for modelling tracer behaviour for the Otway and Frio Brine field trials, it would also provide critical information for interpreting tracer behaviour in future projects. Furthermore, tracer partition coefficient often determines the suitability of a tracer for a particular application (e.g. for estimating sweep volumes, non-partitioning tracers are appropriate whereas partitioning/reactive tracers are not).

Table 1 summarises the application of particular chemical tracers at various CCS sites around the world including at the Otway and Frio Brine sites. Not surprisingly, inert tracers which include perfluorocarbons (e.g. perfluorocyclohexane, perfluoromethylcyclopentane), krypton, xenon, sulphur hexafluoride, R134a and deuterated methane are the dominant choices due to their limited interaction with the reservoir rocks and formation water. Tracers with reactive functional groups are much less common.

Table 1 - Tracers Implemented at CCS Projects

Tracers (*tracers chosen for characterisation as part of this ANLEC project)	CCS site / Application
Sulphur hexafluoride*, perdeuterated methane* and krypton*	Otway Stage 1 / understanding the migration of a CO_2/CH_4 mixture between a producer 300 metres up-dip from an injector and the influence of a natural gas-water contact on mixing (Boreham et al., 2011; Underschultz et al., 2011)
Sulphur hexafluoride *, krypton*, perfluorocarbons (perfluoromethylcyclohexane, perfluorotrimethylcyclohexane, perfluoromethylcyclopentane, perfluorodimethylcyclohexane) perdeuterated methane*	Frio Brine I / understanding the migration of carbon dioxide between a producer 30 metres up-dip from an injector (Freifeld et al., 2005) Frio Brine II / CD_4 and other tracers were tested to understand evolution of a CO2 plume in an interwell configuration.
Perfluorocarbons (perfluorodicyclohexane, perfluorotricyclohexane and	West Pearl Queen / surface gas samples are taken to assess formation-to-surface CO_2 leakage

perflurodimethylcyclobutane)	rates (Wells et al., 2007)
Krypton* and xenon*	Otway Stage 2B / in a single-well "push-pull" test to determine residual CO_2 saturation (Zhang et al., 2011)
Perfluoromethylcyclopentane and perfluorodimethylcyclohexane	K12B/to understand the migration of CO_2 between wells in a compartmentalized field
Reactive esters (propylene glycol diacetate, triacetin and tripropionin) and their hydrolysis products*	Otway Stage 2B / in a single-well "push-pull" test to determine residual CO_2 saturation

2   Part II Tracer Partition Coefficients

Partition coefficients describe the equilibrium behaviour of a given chemical species between two immiscible phases (e.g. oil/water and air/water). For sufficiently dilute solution conditions (i.e. the concentration of the chemical species in each phase is much lower than the solubility limit), it is defined as the ratio of the chemical concentrations in each of the two phases (Srebrenik and Cohen, 1976). As tracers are typically utilized at low concentrations (i.e. ppm or lower concentration), partition coefficients are essential for accurately characterizing their behaviour in multi-phase systems. Both theory and practice have demonstrated that partition coefficients often exhibit Arrhenius type temperature dependence (i.e. log K vs. 1/T where T is the thermodynamic temperature and K is the partition coefficient) (Bahadur et al., 1997; Moreira et al., 1993).

Octanol-water partition coefficients have been used extensively in understanding and predicting the bioaccumulation and environmental fate of organic species (Cronin et al., 2003). Henry's Law coefficients (otherwise known as air/water partition coefficients) have been used to understand the interaction of atmospheric chemicals with bodies of water (Rathbun, 2000).

For CCS projects, the two most dominant phases within the formation are typically supercritical CO_2 and water. However, there is currently limited fundamental information on the supercritical CO_2/water partitioning behaviour for organic compounds (see Table 2 for a list of reported values) (Timko et al., 2004). Notably, there is no existing supercritical CO_2/water partition coefficient data for any inert gases used inthe referenced CCS tracer test applications. Furthermore, there are currently no reports of any of the compounds in Table 2 (where the partition coefficients have been measured for supercritical CO_2/water partitioning) being used as tracers for either CCS or oil and gas projects. Rather, other partition coefficients (namely air/water [Henry's] and octanol/water) are often used as parameters in modelling tracer behaviour. In particular, the EOS7C module in the TOUGH2 dynamic reservoir simulation software has a parameter for the inverse Henry's coefficients which is used to describe tracer partitioning behaviour between CO_2 and water (Oldenburg et al., 2004). Octanol and air have very different chemical properties than supercritical carbon dioxide and as such these alternative parameters may not be representative or indicative of actual subsurface behaviour (Zhang et al., 2011).

The overall aim of this project is to address this knowledge gap through a variety of laboratory based experiments with the goal of determining the partitioning behaviour for a variety of chemical tracers under a range of physical conditions. This will result in more accurate modelling and interpretation of tracer data leading to reduced risk and uncertainty for site characterisation, insurance/permitting, well drilling/operation and monitoring/verification assessments. Generally this lack of fundamental information on tracer behaviour has resulted on a reliance on other types of partition coefficient (as described above) potentially resulting in inaccuracies or flaws in the interpretation of chemical tracer data.

Clearly there is a need to determine the partition coefficients of tracers in regards to their partitioning behaviour between supercritical CO_2 and H_2O or formation fluids for CCS projects. An estimation technique has been achieved (Fredenslund et al., 1975; Magnussen et al., 1981) for determining octanol/water partition coefficients uses structure activity relationships (SARs), which involves assigning a "contribution value" to chemical bonds and functional groups present in a molecule and summing these to obtain a partition. Although SARS has been used extensively, there is uncertainty in whether these estimates are sufficiently accurate for certain applications (Renner, 2002). Timko et al. (2004) measured the supercritical CO_2/water partition coefficients for a variety of organic compounds (e.g. aldehydes, ketones, esters, halides, phenols, alkanes and aromatic hydrocarbons) and showed that there is no adequate correlation with octanol/water partition coefficients, where the values are known for a much larger number of compounds (Haynes, 2011; Timko et al., 2004). They also looked at correlations with solubility parameters

(e.g. Hansen solubility indices) and other solvent/water partition coefficients (e.g. carbon disulfide/water) and found that none of these methods were sufficient for prediction. Currently, the limited data of partition coefficients precludes the development of even a rudimentary SARs type method for predicting supercritical CO_2/water partition coefficients. Consequently, in order to accurately model subsurface partitioning behaviour, an appropriate experimental protocol must be designed and conducted to actually determine the supercritical CO_2/water partition coefficients for relevant tracers.

Table 2 List of Known Supercritical CO_2/Water Mole-Fraction Based Partition Coefficients in the Literature (from Timko et al. 2004 and references therein)*

Compound	Partition Coefficient	Compound	Partition Coefficient
Acetophenone	48.5 ± 4.6	Propiophenone	121 ± 13
Benzaldehyde	39.1 ± 3.7	Propylbenzoate	1050 ± 220
Bromobenzene	1090 ± 100	Tetrahydrofuran	8.5 ± 1.0
3-buten-2-one	7.8 ± 1	Toluene*	1200 ± 250.5
Chlorobenzene	1140 ± 110	Acetylacetone	3
Cyclohexane	4900 ± 600	Aniline	2.1
Cyclohexene	1900 ± 300	Benzene	2756
Cyclopentene	1400 ± 180	Benzoic acid	1.3
Ethylbenzoate	550 ± 100	Benzyl alcohol	1.9
Fluorobenzene	770 ± 150	Caffeine	0.15
Hexane	9000 ± 3000	2-chlorophenol	14
2-methoxyacetophenone	47.3 ± 4	4-chlorophenol	3
3-methoxyacetophenone	84.0 ± 7	Cyclohexanone	41
Methylbenzoate	205 ± 21	1,2–dichloromethane	154
Naphthalene	347	2,4–dichlorophenol	70
2-nitrophenol	80	2,4–dichlorophenoxacetic acid	0.1
4-nitrophenol	0.2	2,4–dimethylphenol	10.7
Parathion	18.3	Hexafluoroacetylacetone	0.7
Pentachlorophenol	80	2–hexanone	118
Phenol	1	3–methyl–4–chlorophenol	6
Salicylic acid	0.3	2-methyl-4,6-dinitrophenol	55
1,1,2,2-tetrachloroethane	84	2-methyl-5-hexyloxymethyl-8-	500
2,3,4,5-tetrachlorophenol	15	3-methylphenol	4
1,1,2-trichloroethane	28	Vanillin	1.5
2,4,6-trichlorophenol	150		

* Errors associated with partition coefficients have been added to the table where available. Partition coefficients were determined at 300 K at a variety of densities (or pressures). Mole-based partition coefficients are used as they are invariant with respect to density.

2.1 Currently Known Information on the Partitioning Behaviour of Inert Gas Tracers

Unfortunately, as mentioned earlier, there is a complete lack of data available for the supercritical CO_2/water partition coefficients for inert gas tracers. Consequently Henry's Law coefficients have been used instead of supercritical CO_2/water partition coefficients as input parameters in reservoir simulations to characterise the subsurface partitioning behaviour of krypton and xenon (Zhang et al., 2011). Henry's

Law coefficients have been determined for sulphur hexafluoride from 25 °C to 230 °C (Mroczek, 1997), krypton from 0 °C to 75 °C (Wilhelm et al., 1977), xenon from 0 °C to 75 °C (Wilhelm et al., 1977), R134a from 0 °C to 60 °C (Zheng et al., 1997) and perdeuterated methane from 12 °C to 42 °C (Gomes and Grolier, 2001) (see Table 3). These studies show that for these compounds, as expected, there is generally Arrhenius type temperature dependence. Furthermore, octanol-water partition coefficients have been determined for a very large number of non-gaseous chemical compounds (Haynes, 2011). A search of the literature has revealed that information on the octanol/water partitioning behaviour of many relevant fluorinated organic compounds (e.g. R134a and most perfluorocarbons) is also not currently available presumably due to their low solubility. It seems then that there is a distinct lack of data regarding the octanol/water partitioning behaviour of inert tracers as well. Given that the behaviour of tracer compounds from both of these classes will need to be interpreted for a number of geosequestration projects and are an important indicator of the effectiveness of a site for CO_2 storage, it is critical that the behaviour of these tracers in the conditions present in typical underground storage reservoirs is understood. Obtaining the partitioning behaviour over relevant geological pressures and temperature regimes for supercritical CO_2/water interfaces is therefore an important step in developing this understanding.

Table 3. Temperature Dependence of Henry's Coefficients for Inert Gas Tracers. Data amalgamated from (Mroczek, 1997, Wilhelm et al., 1977 and Gomes and Grolier, 2001.

Compound	Temperature (°C)	Henry's coefficient (MPa)
Krypton	0	663
	20	1150
	40	1850
	60	2830
	75	3760
Xenon	0	1250
	20	2010
	40	3040
	60	4380
	75	5600
R134a	5	155
	35	454
	65	823
CD_4	11.7	0.0640
	25	0.0424
	35	0.0733
	44.5	0.0528
	51.2	0.0874
SF_6	25	22900
	50	34900
	75	42200
	100	43500
	125	40100
	150	33900

175	27200
200	20700
225	15500
230	14600

2.2 Currently Known Information on the Partitioning Behaviour of Reactive Ester Tracers

For several years, we have been developing a class of reactive ester tracers capable of quantifying the residual carbon dioxide saturation in a formation and have determined the supercritical CO_2/water partitions coefficients for propylene glycol diacetate, triacetin, tripropionin and their hydrolysis products (Myers et al., 2012b). The partition coefficients were determined at the reservoir temperature and pressure intended for the CO2CRC Otway Stage 2B "Residual Saturation and Dissolution Test" (Table 4), where they have been recently utilised in the field as part of a larger test sequence (Paterson et al., 2010; Zhang et al., 2011). However, to extend the utility of these tracers to other field trails, further tests need to be performed over a larger range of geologically appropriate pressures and temperatures.

Table 4. Supercritical CO_2/water Partition Coefficients for Reactive Ester Tracers at 62 °C

Compound	Partition coefficient based on mole fraction of solute in solvent, k_i^x	Partition coefficient based on concentration at 15 MPa, k_i
Propylene glycol diacetate	54.5 ± 5.3	8.77 ± 0.86
Propylene glycol monoacetate 1	1.04 ± 0.12	0.167 ± 0.019
Propylene glycol monoacetate 2	9.79 ± 2.22	1.57 ± 0.36
Triacetin	27.7 ± 5.6	4.46 ± 0.90
Diacetin 1	0.837 ± 0.214	0.135 ± 0.034
Diacetin 2	0.769 ± 0.107	0.124 ± 0.017
Monoacetin 1	0.876 ± 0.272	0.141 ± .044
Monoacetin 2	0.163 ± 0.057	0.0263 ± 0.0093
Tripropionin	313 ± 58	50.3 ± 9.3
Dipropionin 1	5.09 ± 0.85	0.820 ± 0.137
Dipropionin 2	4.83 ± 1.06	0.778 ± 0.170
Monopropionin 1	8.72 ± 1.64	1.40 ± 0.26
Monoproprionin 2	0.349 ± 0.089	0.0562 ± 0.0143
Acetic acid	0.914 ± 0.256	0.147 ± 0.041
Propionic acid	1.50 ± 0.60	0.241 ± 0.097
Glycerol	[a]	[a]
Propylene glycol	[a]	[a]

[a] Glycerol and propylene glycol were not detected in the supercritical carbon dioxide phase. This is presumably due to their low solubility in supercritical carbon dioxide

Conclusions

In order to successfully determine the partitioning behaviour of chemical species in the subsurface environment, the methodology used for determining partition coefficients for tracers must be accurate and robust (Renner, 2002). As a result, we are currently testing and optimizing several new methodologies for determining the supercritical CO_2/water partition coefficients (Ramachandran et al., 1996; Robbins et al., 1993). In the next milestone report, we will report on this work and provide a preliminary analysis of the

supercritical CO_2/water partitioning behaviour for krypton, xenon, sulphur hexafluoride, R134a, perdeuterated methane and reactive ester tracers over a range of temperatures and pressures.

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