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Abstract

For injection and storage of CO_2, knowledge on thermodynamic properties of all components and the mixture of them is important to ensure stable storage conditions. Therefore, a predictive property model for brines in contact with CCS fluids is presented. This model combines a brine model in terms of the Gibbs energy, namely the seawater standard approved by the International Association for the Properties of Water and Steam (IAPWS), and a Helmholtz mixture model for mixtures common for CCS applications for consistent thermodynamic calculations. Consistent calculations for transport and storage of CO_2-rich mixtures are necessary to avoid errors in mass and energy balances as different types of equations will, e.g., lead to different densities with temperature and pressure as input.

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1   INTRODUCTION

Over the last few years, mathematical models for the CCS-chain got more and more detailed. In the past, the CCS-fluids were regarded as pure carbon dioxide. Later on, natural gas models were used to calculate thermodynamic properties of the relevant CO_2-rich mixtures. With the EOS-CG 2016 model [1] the basis for an accurate and more detailed calculation of the main CCS-components in contact with pure water was created. New extensions to more components, which represent the impurities of CCS-fluids, were developed within the EOS-CG 2019 model [2–4]. As the impurities coming from the combustion part of the CCS-chain are considered quite well in the mentioned models, the storage part is still restricted to water when it comes to the interaction of CCS-gases with the liquid phase in saline aquifers.

Enabling calculations of the most accurate equations of state explicit in Helmholtz energy in combination with models for the representation of brines is one part of work package 2 in ELEGANCY. This combination of the models will lead to a consistent description of the CCS-chain as transport, injection and storage can be described with the most accurate set of equations available for the components. Furthermore, this combination simplifies consistent calculations regarding mass and energy balances within the transport, injection and storage part of the CCS-chain.

2   EQUATIONS OF STATE FOR DIFFERENT COMPONENTS

For modeling brines with a seawater-like composition the equation of state (EOS) for seawater by Feistel [5] is used to model brines with a seawater-like composition. This EOS is documented as IAPWS standard [6]. Formulated in the specific Gibbs energy, the EOS adds a saline contribution to the pure water EOS by Wagner and Pruß (IAPWS-95) [7]. For the description of the gaseous components related to CCS-mixtures like carbon dioxide (CO_2) and nitrogen (N_2), the EOS-CG Helmholtz mixture model by Gernert and Span [1] is used because it is the most accurate model in the literature for the representation of CO_2-rich mixtures containing water.

2.1   Brine model

The seawater EOS of Feistel [5,6] is formulated in terms of the specific Gibbs energy with the natural variables temperature T, pressure p, and absolute salinity S_A. The absolute salinity describes the mass fraction of salt in seawater, see Equation (1). The Gibbs energy of pure water is calculated from the pure water EOS (IAPWS-95) by Wagner and Pruß [7].

$$S_A = \frac{m_S}{m_S + m_W} \tag{1}$$

Based on the Gibbs energy of water $g^W(T,p)$ derived from the Helmholtz equation for pure water [7], the seawater equation [5,6] adds a saline contribution $g^S(S,T,p)$ to the water part, see Equation (2). As described by Feistel [5], the Gibbs energy obtained by the saline contribution and the Gibbs energy of the seawater is a specific property referring to one kilogram of the mixture.

$$g(S,T,p) = g^W(T,p) + g^S(S,T,p) \tag{2}$$

The saline contribution of the Gibbs energy is calculated with a polynomic expression as function of temperature and pressure, and further depends on the amount of salt dissolved in water:

$$g^S(S,T,p) = g^* \sum_{k=0}^{5} \sum_{j=0}^{6} \left(g_{1jk}\, \xi^2 \ln \xi + \sum_{i=2}^{7} g_{ijk}\, \xi^2 \right) \tau_s^j\, \pi^k . \tag{3}$$

The coefficients g_{ijk} are given in the publications describing the seawater EOS [5,6], g^* equals 1 J/kg, ξ is the reduced absolute salinity, τ_s is the reduced temperature, and π is the reduced pressure:

$$\xi = \sqrt{\frac{S}{S^*}} \qquad \text{with} \qquad S^* = 0.03516504 \text{ kg} \cdot \text{kg}^{-1} \frac{40}{35} \tag{4}$$

$$\tau_S = \frac{T - T_0}{T^*} \qquad \text{with} \qquad T_0 = 273.15 \text{ K}, \quad T^* = 40 \text{ K} \tag{5}$$

and

$$\pi = \frac{p - p_0}{p^*} \qquad \text{with} \qquad p_0 = 101325 \text{ Pa}, \quad p^* = 10^8 \text{ Pa}. \qquad (6)$$

The thermodynamic properties of seawater can be obtained by combining derivatives of Equation (2) according to Table 1, which was taken from [6]. The index p stands for the Gibbs energy derived with respect to pressure at constant temperature, the index T for the derivative with respect to temperature at constant pressure. Properties of the pure water part based on the Helmholtz EOS [7] are given in Table 2. Properties different from the independent variables are calculated by a combination of derivatives according to the independent variables of the type of equation. Density and speed of sound are calculated by a nonlinear combination of derivatives. The density is the inverse specific volume and for the speed of sound the ratio of derivatives below the radical needs to be calculated correctly. Thus, for a combination of two different types of equations the mixture property has to be calculated with the derivatives of the combined mixture description and must not be calculated by a combination of the property itself.

Since the basic mathematical concept of the seawater EOS [5,6] is a summation of two parts, this approach is also valid for each derivative of these two parts. Therefore, the equivalent for the Gibbs energy derivative needs to be calculated with the corresponding combinations of derivatives of the Helmholtz energy as described by Feistel and the IAWPS Advisory [5,6]. The derivatives according to the publications of the seawater model [5,6] equivalently show this in form of the Helmholtz energy. Consequently, for the implementation in reduced Helmholtz energy mixture models, adaptions of these derivatives are necessary in order to transform derivatives with respect to T and ρ into derivatives with respect to $\tau = T_r(\bar{x})/T$ and $\delta = \rho/\rho_r(\bar{x})$, see Table 2.

Table 1: Calculation of thermodynamic properties from the Gibbs energy. For Index description see text.

Property	derivatives
$\rho(T,p)$	$g_p^{-1}(T,p)$
$g(T,p)$	$g(T,p)$
$a(T,\rho)$	$g - pg_p$
$u(T,\rho)$	$g - Tg_T - pg_p$
$s(T,\rho)$	$-g_T$
$h(T,p)$	$g - Tg_T$
$w(T,p)$	$g_p\sqrt{\dfrac{g_{TT}}{g_{Tp}^2 - g_{TT}g_{pp}}}$
$c_v(T,\rho)$	$\dfrac{T(g_{Tp}^2 - g_{TT} - g_{pp})}{g_{pp}}$

The calculation of seawater in equilibrium with water ice Ih and water vapor is given in the publications describing the equation for seawater [5,6]. In case of thermodynamic equilibrium, the

chemical potential of water in seawater is equal to the Gibbs energy of water in ice or pure water vapor.

2.2   Helmholtz equations of state

For several fluids and mixtures, accurate fundamental equations of state in terms of the Helmholtz energy are available. The Helmholtz energy is split into two parts. The first part a^o represents the behavior of the hypothetical ideal gas, whereas the second part a^r takes the residual behavior of the fluid deviating from the ideal gas into account. The independent variables of these equations are temperature T and density ρ. For a fluid mixture with the composition $\overline{x}$, the Helmholtz energy is calculated according to [1,8]:

$$a(T,\rho,\overline{x}) = a^o(T,\rho,\overline{x}) + a^r(T,\rho,\overline{x}). \tag{7}$$

δ represents the reduced density and τ the inverse reduced temperature. The reducing parameters depend on the composition when properties of a mixture are calculated:

$$\tau = \frac{T_r(\overline{x})}{T} \text{ and } \delta = \frac{\rho}{\rho_r(\overline{x})}. \tag{8}$$

For mixtures, composition dependent reducing functions as proposed in the GERG-2004 [8] are applied. In most cases, the reduced Helmholtz energy $\alpha = a/RT$ is obtained by dividing the Helmholtz energy by the gas constant and the temperature:

$$\alpha(T,\rho,\overline{x}) = a^o(T,\rho,\overline{x}) + a^r(\tau,\delta,\overline{x}). \tag{9}$$

In mixtures the ideal part represents the ideal mixture of the ideal gas:

$$\alpha^o(T,\rho,\overline{x}) = \sum_{i=1}^{N} x_i \left[\alpha_{oi}^o(T,\rho) + \ln x_i \right]. \tag{10}$$

The residual part shown in Equation (11) can consist out of two parts, where the second one is optional. The first part is the sum over the residual Helmholtz energy of the N components, which represents the residual behavior of the single components in the mixture, whereby the substance specific formulations are evaluated using common reduced temperatures and densities of the mixture. The second part is the departure function $\Delta\alpha^r$. For comprehensively investigated mixtures, this optional and additional departure function can be applied. The departure function considers binary mixing effects of each pair of components in a multi-fluid mixture and belongs to real part of the Helmholtz energy.

$$\alpha^r(\tau,\delta,\overline{x}) = \sum_{i=1}^{N} x_i\, \alpha_{oi}^r(\tau_{o,i}, \delta_{o.i}) + \Delta\alpha^r(\tau,\delta,\overline{x}) \tag{11}$$

For more detailed information regarding the different possibilities of reducing functions and more capabilities of the departure function, see [1,8].

In a homogenous phase all thermodynamic properties can be calculated from derivatives of the fundamental equation of state with respect to its independent variables. An overview how thermodynamic properties can be derived from Helmholtz and Gibbs equations is given in Table 3.

Table 2: Equivalents of Helmholtz derivative in Gibbs derivatives. A subscript δ denotes a derivative with respect to δ, a subscript τ a derivative with respect to τ.

Property	Helmholtz
$p(T,\rho)$	$\rho RT(1 + \delta\alpha_\delta^r)$
$g(T,p)$	$RT(1 + a^o + a^r + \delta\alpha_\delta^r)$
$u(T,\rho)$	$RT\tau(\alpha_\tau^o + \alpha_\tau^r)$
$s(T,\rho)$	$RT[\tau(\alpha_\tau^o + \alpha_\tau^r) - a^o - a^r]$
$h(T,p)$	$RT[1 + \tau(\alpha_\tau^o + \alpha_\tau^r) + \delta\alpha_\delta^r]$
$w(T,p)$	$\sqrt{\left[1 + 2\delta\alpha_\delta^r + \delta^2\alpha_{\delta\delta}^r - \frac{\left(1 + \delta\alpha_\delta^r - \delta\tau\alpha_{\delta\tau}^r\right)^2}{\tau^2(\alpha_{\tau\tau}^o + a_{\tau\tau}^r)}\right]\frac{RT}{M}}$
$c_v(T,\rho)$	$RT[-\tau^2(\alpha_{\tau\tau}^o + \alpha_{\tau\tau}^r)]$

2.3 Combination of Gibbs and Helmholtz equations

While the independent variables of Gibbs equations of state are temperature and pressure, the independent variables of Helmholtz equations of state are temperature and density. Since both equations are fundamental equation of state, properties are calculated by a combination of derivatives as described in the previous sections, cf. Table 1 and Table 2.

For mixture calculations including brines, these models need to be linked to each other as brine models are explicit in Gibbs energy while the most accurate EOS for CCS fluids are formulated in Helmholtz energy. This combination is necessary for a consistent thermodynamic mixture model. A simple addition of the seawater or brine property to the gaseous components dissolved in the liquid phase would neglect the interaction between the gaseous components and water. Furthermore, the reducing function would not be used, which would disregard the reducing function for the mixture.

Since the Helmholtz energy of seawater can be calculated from the Gibbs equation, see Table 1, the first step of this combination is straightforward, if only the Helmholtz energy is needed. The remaining properties are calculated by derivatives of the Helmholtz energy; thus a correct differentiation of the Helmholtz energy has to be ensured. However, the Helmholtz energy is derived with respect to τ and δ, whereas the independent variables of the seawater or the brine model are

T and p. This means that a link between pressure and density is necessary for the correct derivatives in order to calculate thermodynamic properties. Numerical differentiation of this combined model is difficult because all three natural variables must be variated correctly and different boundary conditions for the derivatives have to be fulfilled. Furthermore, the concept of reduced density and temperature has to be respected. As no reducing functions depending on salinity are known, numerical differentiation is quite challenging for such a combination of different types of equations.

To overcome this problem, an analytical approach can be used to transfer a combination of Gibbs energy and its derivatives to the required Helmholtz expression. Since both EOS are fundament EOS, there is an equal combination of Helmholtz derivatives for every derivative of a Gibbs function and vice versa. This procedure is inspired by the calculation of the seawater EOS combining the derivatives in the other direction and in non-reduced Helmholtz energy, which leads to a different combination of derivatives.

The new analytical approach can be used to calculate the corresponding combination of derivatives for a fundamental equation in Gibbs energy, as needed to express a derivative of the reduced Helmholtz energy. The required correlations are given in Table 3. This consistent combination of both types of fundamental equation is an important step for the combination of different thermodynamic models, especially for property models formulated in the Gibbs excess energy, or for mixture components for which only EOS in terms of the Gibbs energy exists.

Table 3: Equivalent Gibbs-energy combinations for Helmholtz-energy derivatives.

Helmholtz derivative	Equivalent Gibbs combination
$a(T,\rho)$	$g - pg_p$
$\tau(\alpha_\tau^o + \alpha_\tau^r)$	$\dfrac{g - Tg_T - pg_p}{RT}$
$\delta\alpha_\delta^r$	$\dfrac{pg_p}{RT} - 1$
$\tau^2(\alpha_{\tau\tau}^o + \alpha_{\tau\tau}^r)$	$\dfrac{T(g_{Tp}^2 - g_{TT} - g_{pp})}{g_{pp}}(RT)^{-1}$
$\delta^2\alpha_{\delta\delta}^r$	$\dfrac{g_p^2}{-g_{pp}RT} - \dfrac{2pg_p}{RT} + 1$
$\delta\tau\,\alpha_{\delta\tau}^r$	$\sqrt{\left(-\dfrac{Tg_{TT}}{R} + \tau^2(\alpha_{\tau\tau}^o + \alpha_{\tau\tau}^r)\right)\left(1 + 2\,\delta\alpha_\delta^r + \delta^2\alpha_{\delta\delta}^r\right) + 1 + \delta\alpha_\delta^r}$

To ensure a proper mixture modeling in the Helmholtz framework, the fundamental equation in terms of the Gibbs energy should be related to a pure substance. Otherwise this could lead to a loss of thermodynamic information and problems with the proper integration in the Helmholtz framework can occur. If the Gibbs energy represents a mixture model itself, the combination of both models is much more challenging because mixing effects between all components in the mixture must be considered. Therefore, knowledge on the pure-fluid behavior is necessary for all

components in at least one of the two models. For the correct calculation, a comprehensive thermodynamic understanding of mixture models is indispensable.

2.4   Combination of the seawater EOS and CO_2-rich mixtures

For the combination of the brine with the CO_2-rich mixture, the brine contribution is added to the Helmholtz energy calculated from the EOS-CG model [1–4]. Therefore, the Gibbs energy obtained from the seawater EOS [5,6] is transferred to Helmholtz energy. The same procedure is used for the properties derived from the reduced Helmholtz energy.

The saline part of the seawater represents not only the salt part, but also contains every change in property related to the salt added to the water. Furthermore, the specific related addition of the different contributions makes it difficult to transfer the single contributions to a molar basis. To overcome this difference in the two models, the complete contribution of the brine is calculated and added to the CCS-mixture, while the contribution of the pure water part contained in the brine model was subtracted from the CCS-mixture simultaneously, see Equation (12). Thereby the index mix stands for the mixture of brines with CCS-fluids, the subscript Helm stands for the contribution coming for the Helmholtz model for the pure water-CCS-fluid mixture, seaw stands for the Helmholtz energy coming from the seawater EOS [5,6] and ow stands for only water:

$$\alpha_{\text{mix}}(\tau, \delta, \overline{x}, S) = a_{\text{Helm}}(\tau, \delta, \overline{x}, S) + \alpha_{\text{seaw}}(\tau_{\text{ow}}, \delta_{\text{ow}}, S) - \alpha_{\text{w}}(\tau_{\text{ow}}, \delta_{\text{ow}}). \tag{12}$$

This procedure allows for adding the brine properties to the model while respecting mixture effects of the Helmholtz multi-fluid approach for water and other CCS components. Since no properties for the pure salt can be obtained from the seawater EOS, it is not possible to take mixing effects between pure salt and CCS gases into account.

When considering a brine instead of water, the most significant effect is the change of the chemical potential caused by dissolved salts in the liquid phase. This has two different effects. On one hand, there is a shift of the freezing, melting, and bubble lines. On the other hand, there is a change of the gas solubility in the liquid phase. This change is caused by the shifted chemical potential in the liquid phase. According to the phase-equilibrium conditions, the chemical potential of each component in the vapor phase needs to be the same as in the liquid phase. Therefore, the composition of the vapor phase needs to be changed, as the chemical potential is related to the composition of the phase. This change of composition in the vapor phase finally leads to the change of composition in the liquid phase as the overall mass balance needs to be fulfilled in flash calculations. For flash calculations the concept of partial molar properties is applied.

The approach presented in the previous subsections is implemented in TREND 4.0 [9]. For further information about TREND and the software delivered with this report, please contact TREND@thermo.rub.de.

3   RESULTS

The implementation of the seawater EOS [5,6] was tested against the given check values [5,6] and further given values for freezing and boiling temperature in a separate IAWPS brine advisory [10]. Furthermore, triple points for different salinities from the brine advisory were used for testing the correct implementation.

The implementation of the new routines for the test of the Helmholtz Gibbs transformation were carried out by using the seawater routines with zero salinity. Results were compared to the results for pure water with CO_2, N_2, and O_2 calculations.

3.1   Seawater - carbon dioxide

With the new model the change of solubility in the system seawater-carbon dioxide can be described well within the range of validity of the equation for seawater. Reduced concentrations of carbon dioxide in comparison to the system water-carbon dioxide can be described as a function of absolute salinity as shown in Figure 1 for ambient pressure. The two shown isotherms illustrate the reduction of the concentration of solved CO_2 as a function of the salinity of seawater. Although the solubility of CO_2 is overestimated for the plotted isotherms, the reduction of the solubility of CO_2 is modeled quite accurately.
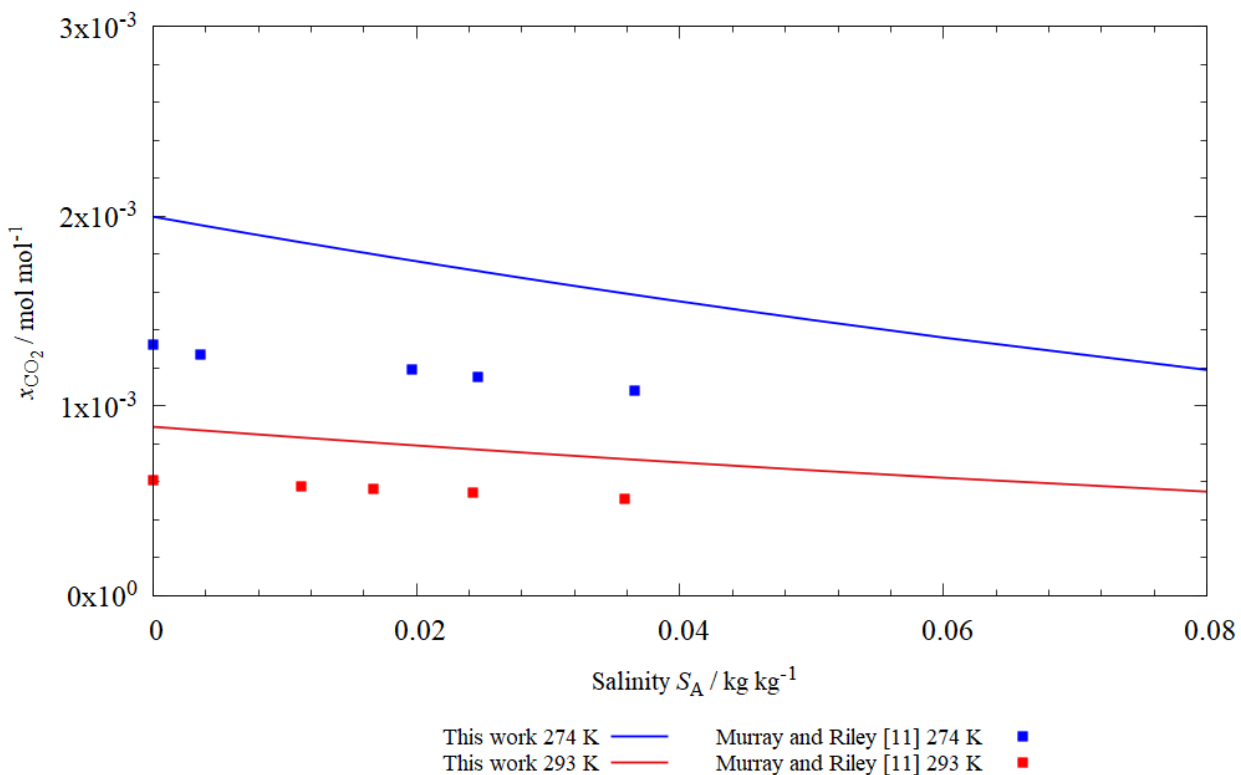

Figure 1: carbon dioxide solubility in seawater over absolute salinity. The effect of salinity can be described well, although shortcomings for the solubility of carbon dioxide in water become obvious.

The offset for the two isotherms to the experimental data by Murray and Riley [11] results from deficits of the description of the system water-carbon dioxide. Especially at lower temperature and

pressure the EOS-CG 2016 model [1] has some disadvantages in the exact determination of solubilities, although it is the most accurate model available for this mixture in general.

3.2   Seawater - nitrogen

The solubility of nitrogen in seawater is described like the system seawater - CO_2. As EOS-CG 2016 [1] seems to have less shortcomings for the solubility of nitrogen, the calculated solubilities better match the experimental values. In contrast to the system seawater - CO_2, the drop of gas solubility in the liquid phase is predicted to be a little bit higher than shown by the experimental data by Douglas [12] and Murray and Riley [13] for the lower isotherms (273 and 303 K) at ambient pressure. However, in general the influence of salinity on gas solubility is described well.
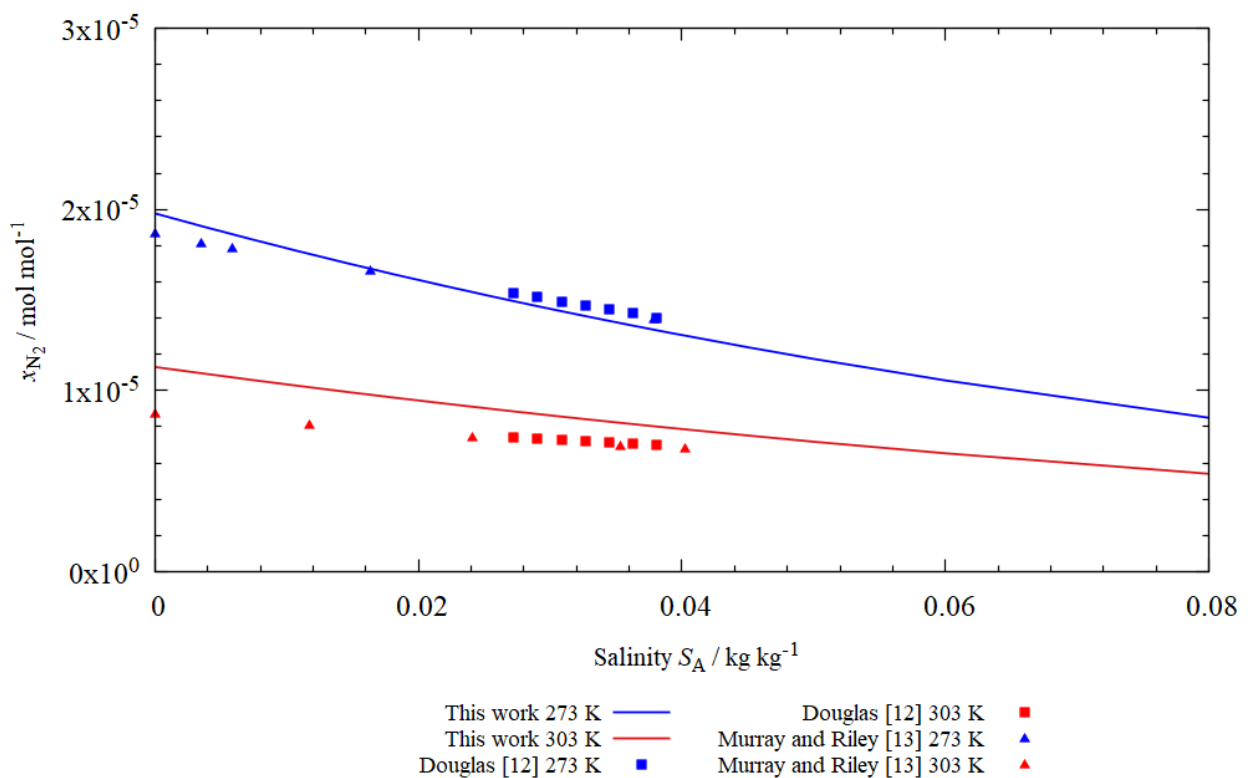

Figure 2: solubility of nitrogen in seawater. The effect of salinity is adequately described. Shortcomings of the Helmholtz model are not as significant as for carbon dioxide-water.

When the slope of the different isotherms is analyzed it gets obvious, that the effect of degassing is slightly overestimated at a temperature of 273 K. This overestimation becomes less pronounced for higher temperatures as can be seen at the 303 K isotherm.

3.3   Seawater - oxygen

Solubilities of oxygen in seawater are predicted like solubilities of the other two presented gases. The shortcomings of the Helmholtz model in the prediction of low solubilities becomes obvious again. The solubility of oxygen in water is over- or underestimated, depending on the isotherm. The change of solubility as function of salinity matches the experimental data by Green [14]; the

predicted change in solubility slightly exceeds the reduction of solubility indicated by the experimental data.
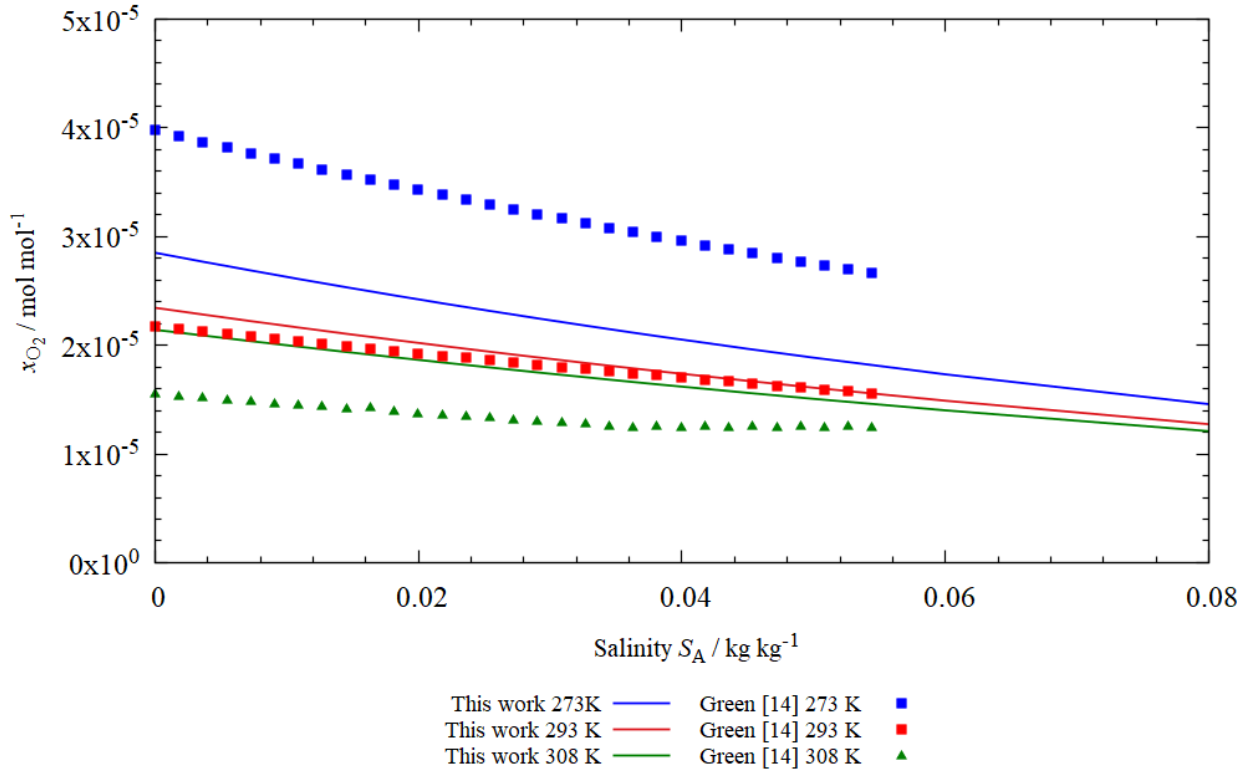

Figure 3: solubility of oxygen in seawater. The effect of salts on the solubility can be described well. Shortcomings of the Helmholtz mixture model for gas solubilities in the system oxygen-water become obvious.

3.4 High pressure and high salinity data

As the range of validity of the seawater EOS is limited to ambient pressure for salinities higher than standard salinity (~0.042 kg kg^{-1}), the solubility of gases cannot be calculated reliable for high salinities at elevated pressures [6]. In this case the reduction of solubility is overestimated as shown in Figure 4. The red graph shows the calculated solubility of CO_2 in pure water at a temperature of $T = 273$ K. For comparison the experimental values determined by Stewart and Munjal [15] are shown as red squares. An overestimation of the solubility by EOS-CG 2016 [1] is obvious. In blue, data for CO_2 in seawater with an absolute salinity of $S_A = 0.0344$ kg kg^{-1} are given. The comparison shows similar offsets for a mixture of pure water and CO_2 and for seawater-CO_2, which indicates that the salinity model can also predict data for higher pressures for salinities up to standard salinity.

The combination for seawater with high salinity ($S_A = 0.0966$ kg kg^{-1}) at pressures above ambient pressure is shown in green. A significant underestimation of the solubilities is obvious for all pressures higher than 1 MPa. This result was to be expected, as the seawater model exceeds its range of validity for salinity at these pressures.
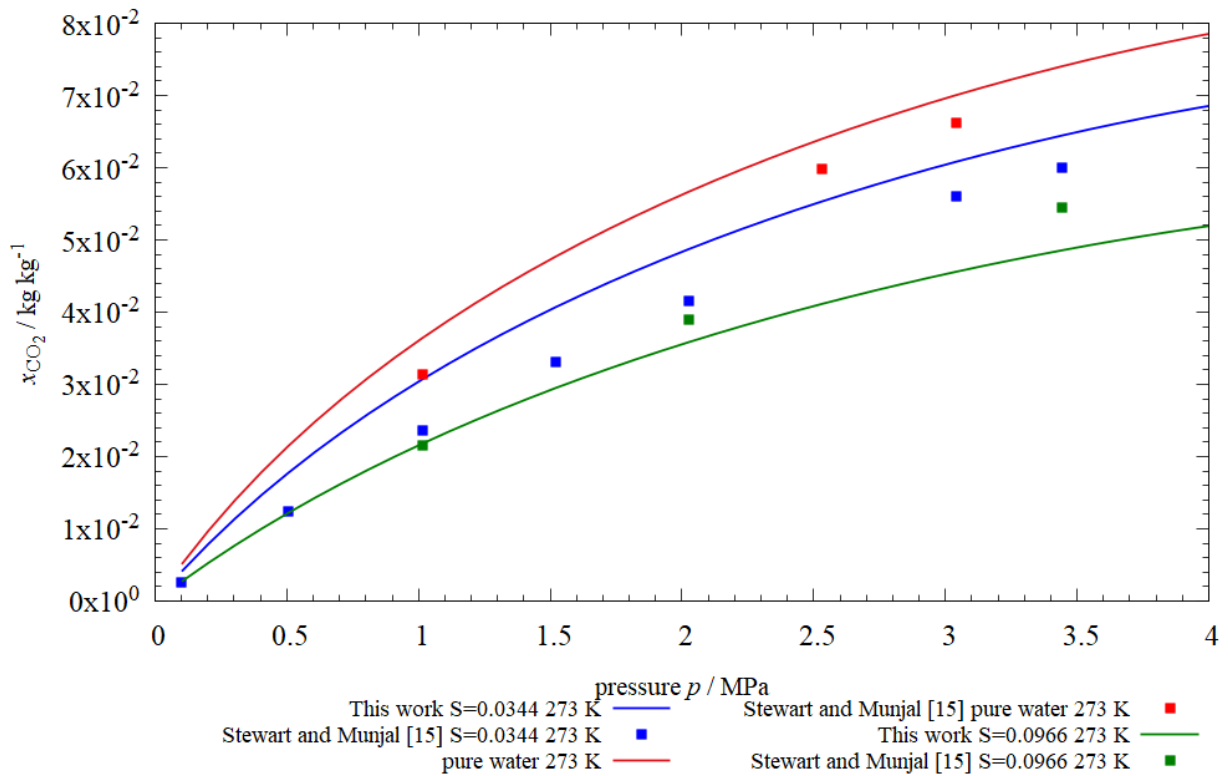
Figure 4: high pressure and high salinity data for the system seawater-carbon dioxide. High pressure data can be predicted well for standard salinities but data for higher salinities cannot be predicted well. The offset for pure water and for S = 0.0344 is mainly caused by shortcomings of the EOS-CG model, but the limits of the new model become visible for high salinities (S = 0.0966).

4   CONCLUSION AND OUTLOOK

In the first phase of our work in WP2 of ELEGANCY a property model for CO_2-rich mixtures in contact with brines with a seawater like composition was developed. The predictive property model (no parameters were adjusted to data for mixtures with brines) describes the change of solubility as a function of salinity. The influence of salinity can be described well with the model. Within the range of validity of the seawater EOS the degassing of the liquid phase can be described reasonably good for a predictive model. Nevertheless, the restriction of the seawater EOS with regard to high salinities at high pressures show, that a model for a broader range of salinities and different salt compositions needs to be coupled with the Helmholtz multi-fluid approach to describe all states relevant for CCS applications, and in particularly systems involving CO_2-rich mixtures and brines under typical storage conditions.

Known shortcomings of Helmholtz mixture models become obvious again. Systems with a solved gas at low pressure are typically characterized by very low concentrations of the gaseous component or mixture in a liquid phase. While phase equilibria at higher pressure can be described well by Helmholtz mixture models, cases with very low concentration of the gas are very often described unsatisfactory. Henry coefficients are not yet considered in fitting these models, but obviously the assumption that the limiting behavior is automatically predicted correctly from fitting phase equilibria at higher pressures is wrong. This point needs to be addressed in the development of Helmholtz-energy based mixture models.

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