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## Investigating the design of ORC heat introduction for single- and two-phase geofluid brines with and without non-condensable gases

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**Keywords:** geothermal, organic Rankine cycle, brine modelling, optimisation.

### ABSTRACT

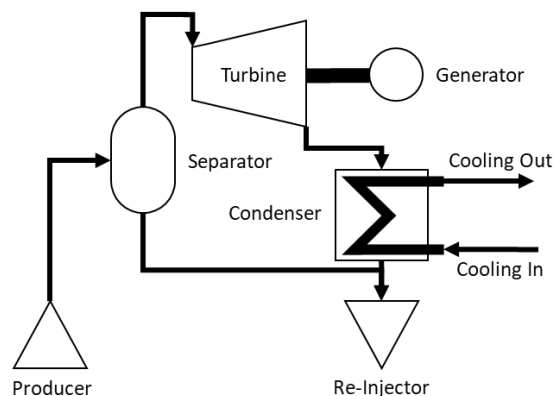
A modularised thermophysical property model for capturing single- and two-phase geothermal fluids of arbitrary composition (dissolved minerals and gases) has been developed, using amongst others Reaktoro, CoolProp and ThermoFun as the underlying partitioning and property estimation engines. The resultant model has been validated against some of the incompressible binary fluids implemented within CoolProp as well as field experimental data. Case studies are presented highlighting the importance of accurate thermophysical properties for the design of geothermal ORC power plants.

### 1 INTRODUCTION

Over the coming decades the global energy industry will be subject to significant external pressures. On the one hand energy demand is rising due to population growth and the continuing improvements in the global standard of living and quality of life. Simultaneously, supply is transitioning away from fossil fuels, due to concerns over global climate change. In light of this, technologies tapping into Earth's natural, vast and renewable energy reserves, such as wind, solar and geothermal energy have emerged as cost effective and clean alternatives for all final energy uses (IEA, 2021).

Humans have already harnessed geothermal energy for thousands of years, but it is only now proving an attractive option for grid-scale renewable baseload and dispatch-capable electricity and heat generation. So far geothermal energy utilisation has mostly been limited to geothermal "hot spots" typically located at tectonic boundaries. However, the adoption of ORC (Organic Rankine Cycle) and EGS (Enhanced Geothermal System) technologies is ever widening the applicability range (DiPippo, 2016).

Traditional Dry-Steam or Flash geothermal power plants (Figure 1) require significant volumes of steam, whereas ORC geothermal power plants (Figure 2) can generate power from much lower enthalpy resources. This is achieved by transferring the thermal energy to a low-boiling-point secondary fluid, which evaporates and then drives a turbine.

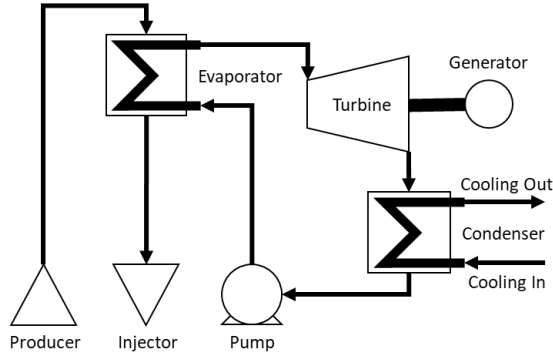


**Figure 1 Flash Plant. Hot geofluid is separated into liquid vapour streams; the latter driving the turbine to generate electricity.**

Besides opening-up otherwise uneconomical low-enthalpy sites for development, the decoupling of the geofluid from the power generation process also has several operational advantages.

ORC turbines can be smaller and therefore cheaper, as the changes in specific enthalpy across the turbine are generally smaller for organic fluids compared to steam. Moreover, the efficiency and lifetime of turbines used in ORCs also tend to be higher than for steam turbines. This can be attributed to the turbine being specially designed for a given pure working fluid and application, and organic working fluids have more favourable vapour domes, limiting liquid drop-out during the expansion and therefore damage to the turbine (DiPippo, 2016).

However, as for all low-temperature heat engines, the conversion efficiency of geothermal ORC plants is expectedly low.



**Figure 2 ORC Plant. Hot geofluid is cooled down to evaporate the secondary working fluid, which in turn drives the turbine**

Another important factor to consider is that indirect heat utilisation induces additional second law (from the Second Law of Thermodynamics) or exergetic losses. For ORCs the majority of exergetic losses occur in the primary heat exchanger and an effective design of this component results in the greatest gains in plant efficiency.

Fortunately, from the historical use of ORCs in applications like heat recovery, waste-to-energy and biomass, algorithms and expertise to aid the selection of working fluids, plant configurations and operating conditions have already been developed. However, reliable and robust models for the thermophysical properties of geofluids, which are a key input to these algorithms, remain limited (Macchi & Astolfi, 2016).

The thermophysical properties of pure water and some specific brines have been studied extensively and tabulated (Wagner & Pruß, 2002) (Sharqawy et al., 2010), however, the composition of brines is extremely site specific. Geofluids can range from low to extremely high amounts of dissolved minerals and non-condensable gases, and their composition may even change over a site's lifetime (DiPippo, 2016). Moreover, capturing the dissolution of minerals and gases is important from an operation perspective for scale prevention and NCG handling at the surface.

### 1.1 Objectives

The primary aim of this study is the development and validation of a thermophysical property model for brines of arbitrary composition, covering a wide range of specific enthalpies and pressures as well as allowing for the co-existence of aqueous, gaseous, liquid and mineral phases.

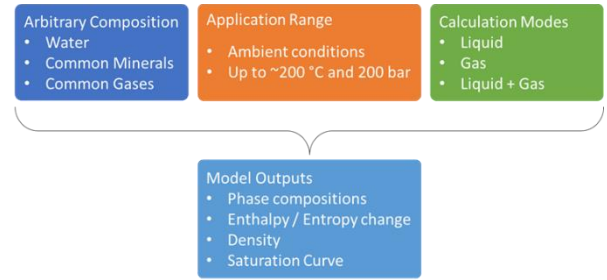
The secondary aim is to demonstrate the application of this new thermophysical property model for generating temperature heat content curves (T-Q curves) for some single and two-phase geofluids so that these T-Q curves

may be used in the design and optimisation of a geothermal binary cycle power plant.

## 2 METHODOLOGY

### 2.1 Thermophysical Property Model Scope

The thermophysical property model should be capable of capturing brines of any arbitrary composition and reliably predict the density, enthalpy, and entropy of the various phases over a wide range of temperature and pressure. Additionally, information on the phase transitions from liquid to vapour dominated and the associated latent heat are desired. Future studies may extend this to transport properties such as viscosity, thermal conductivity and interfacial tension. The requirements of such a thermophysical property model are summarised below in Figure 5.



**Figure 3 The requirements of a thermophysical property model of brines and NCG**

### 2.2 Theoretical Basis

Determining a fluid's thermophysical properties is a two-step process. First, the fluid is "partitioned" into its stable equilibrium phases, thereby determining the composition of each species in each phase; second, the thermophysical properties of each phase are evaluated.

Stable equilibrium is achieved when the Gibbs Free Energy associated with a given state is at a minimum, as this corresponds to a state of maximum entropy. The Gibbs Free Energy of a given state can be calculated from the species' amounts and chemical potential [1].  $G$  is the Gibbs Free Energy,  $P$  is the pressure,  $T$  is the temperature,  $\mathbf{n}$  is the vector of species amounts,  $n_i$  is the amount of species "i",  $\mu_i$  is the chemical potential of species "i" and  $\mathbf{y}$  is the vector of species mole fractions.

$$G(P, T, \mathbf{n}) = \sum_i^N n_i \mu_i(P, T, \mathbf{y}) \quad [1]$$

Besides its pure component chemical potential, in a mixture, a species' chemical potential is also dependent on its interactions with the other species, which can be captured via its activity, see [2]. Where  $R$  is the universal gas constant,  $a_i$  is the activity of species "i" and,  $P^\circ$  and  $\mathbf{y}^\circ$  refer to the reference pressure and composition.

$$\mu_i(P, T, \mathbf{y}) = \mu_i^\circ(T, P^\circ, \mathbf{y}^\circ) + RT \ln a_i(T, P, \mathbf{y}) \quad [2]$$

Conveniently, the partial molar properties of interest, enthalpy, entropy and volume (or density) can be calculated from the chemical potential using Maxwell's relations, see [3] to [5]. (Gyftopoulos & Beretta, 2005)

$$h_i(T, P, \mathbf{y}) = \frac{d(\mu_i(T, P, \mathbf{y})/T)}{d(1/T)}_{P, \mathbf{y}} \quad [3]$$

$$s_i(T, P, \mathbf{y}) = -\frac{d(\mu_i(T, P, \mathbf{y}))}{d(T)}_{P, \mathbf{y}} \quad [4]$$

$$v_i(T, P, \mathbf{y}) = \frac{d(\mu_i(T, P, \mathbf{y}))}{d(P)}_{T, \mathbf{y}} \quad [5]$$

### 2.3 Existing Tools

There are number of academic models and open-source computing frameworks for orchestrating partitioning and property estimation calculations.

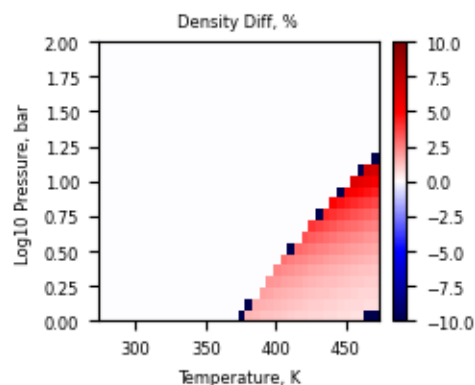
Spycher & Pruess or Duan & Sun provide models for predicting the partitioning of brine and CO<sub>2</sub> mixtures for a range of conditions. However, given that these models were developed in the context of carbon capture and storage, thermophysical properties are not included.

The open-source library CoolProp (Bell et al., 2014), provides implementations of equations of state (EOS) for a number of pure components (e.g. water, carbon dioxide, nitrogen, hydrogen sulphide and many more) or incompressible fluids (e.g. seawater, lithium bromide solution or calcium chloride). While mixtures of pure components (e.g. carbon dioxide and nitrogen) can be captured by means of binary interaction coefficients, mixtures of pure components and incompressible fluids (e.g. seawater and carbon dioxide) or a number of incompressible fluids (e.g. seawater and lithium bromide solution) are not implemented in the tool.

Similarly, ThermoFun (Miron et al., 2021) implements methods for evaluating the thermodynamic properties of a large number of chemical species from open-source databases such as SUPCRT92 (Johnson et al., 1992) or SUPCRTBL (Zimmer et al., 2016).

Reaktoro, a framework for geochemical computations, (Leal, 2015) implements standard thermodynamic and activity models for a large number of species from open-source databases (e.g. SUPCRTBL mentioned above or in fact ThermoFun) and provides the necessary numerical methods for equilibrating the fluid. Although Reaktoro's thermophysical property predictions are generally accurate for aqueous systems, they lack accuracy for vapour-liquid systems. This can

be attributed to the standard thermodynamic properties of important gaseous species like steam or carbon dioxide being calculated using non-industry standard EOS. In turn, the density and specific enthalpy are inconsistent with those reported by NIST. For steam (H<sub>2</sub>O(g) in Reaktoro) for example, density differences as high as 7.5% were observed in a direct comparison of Reaktoro and CoolProp, see Figure 4.

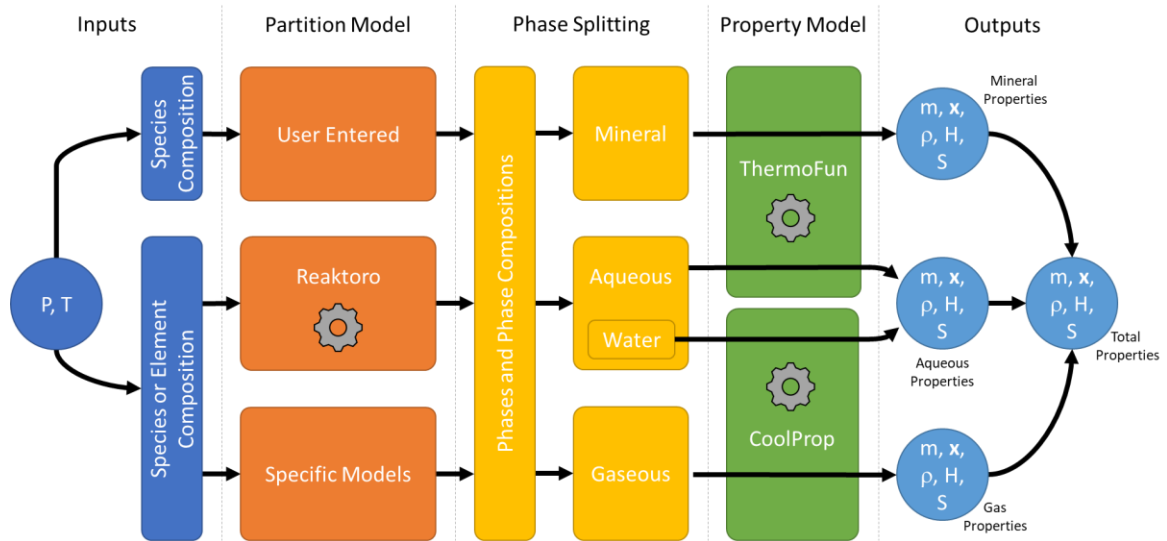


**Figure 4 Comparing the steam density reported by CoolProp and Reaktoro for various pressures and temperatures**

### 2.4 Selected Approach

A modularised approach was chosen to leverage the strengths of each of the aforementioned tools. As such, partition models are used to equilibrate the fluid and determine the composition of each phase (aqueous, gaseous and mineral) and then the property models are used to compute the phase properties, with the most appropriate model being used for each phase.

The architecture of this coupled thermophysical property model is shown in Figure 5. The user initially defines the main components of the fluid, this can be done by elemental composition or specific species. The partitioning model, by default Reaktoro, then determines the equilibrium phases and their composition at a specified temperature and pressure. The phase properties are then evaluated using the equilibrium composition and CoolProp or ThermoFun. CoolProp is used for the gaseous phase, while ThermoFun is used for the mineral phase, and both CoolProp and ThermoFun are used for the aqueous phase. The individual phase properties are then aggregated to the total fluid properties using a simple mass-based mixing rule.



**Figure 5** The architecture of the thermophysical property model for brines and NCG

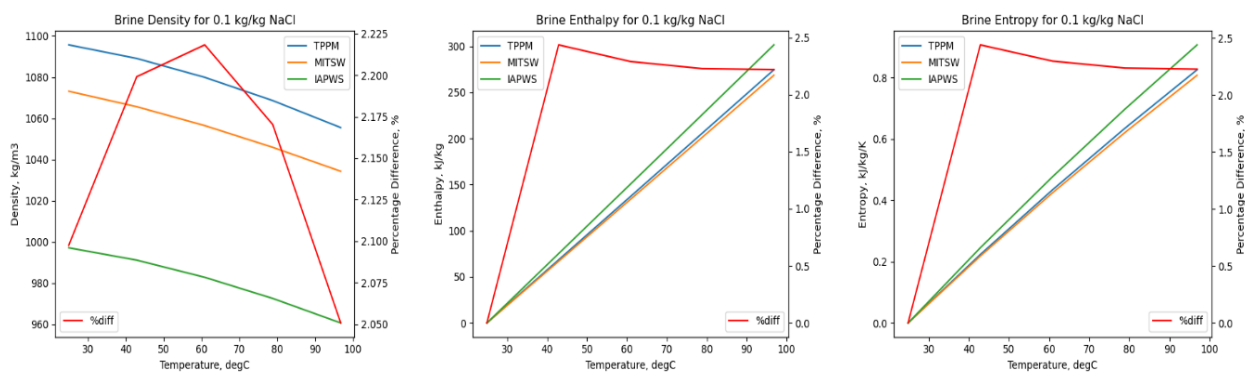
### 3 VALIDATION

Datasets on the thermophysical properties of geothermal brines are generally scarce (Walsh et al., 2017) and typically limited to either the equilibrium composition of a partitioned fluid (e.g. brine and carbon dioxide mixture) or the thermodynamic properties of specific brines.

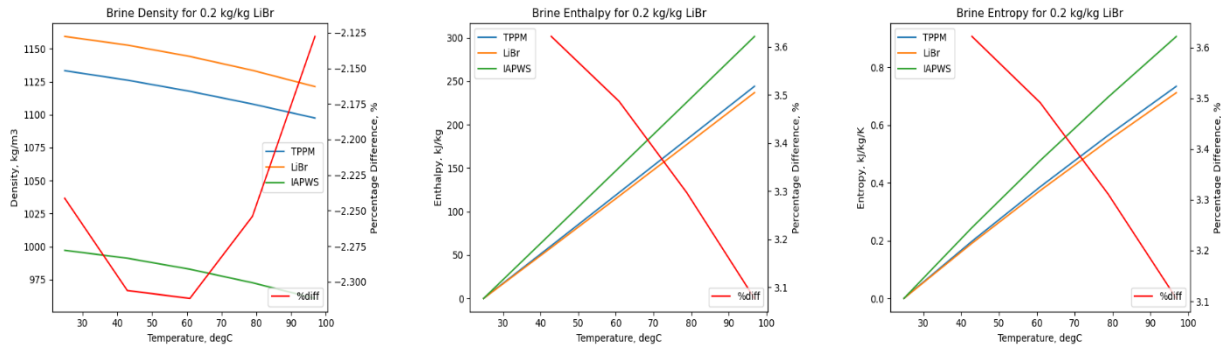
Some of the incompressible fluid models implemented in CoolProp, such as the MIT Seawater model (Sharqawy et al., 2010) or the Lithium Bromide model (Pátek & Klomfar, 2006), can serve as initial benchmarks for validating this new coupled thermophysical property model up to moderate temperatures and mineral content. Comparison of this thermophysical property model against the MIT Seawater model showed that differences remained below 3% at a salinity of 0.1 kgNaCl / kgH<sub>2</sub>O, see

Figure 6. This is close to the maximum salinity the MIT Seawater model considers. From a similar comparison against the aforementioned Lithium Bromide model, the deviations were observed to be less than 4% for salinities as high as 0.2 kgLiBr / kgH<sub>2</sub>O, see Figure 7.

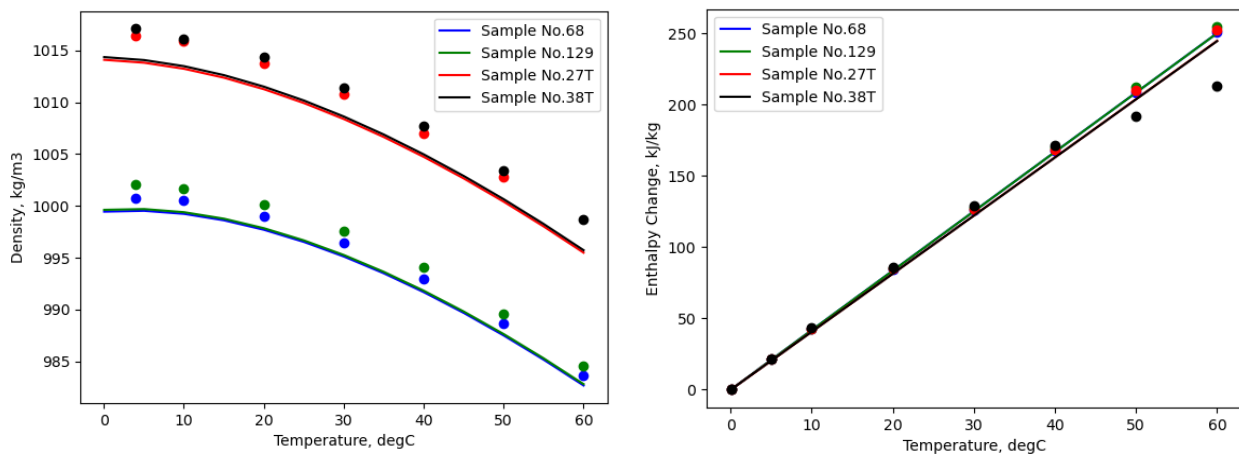
Further comparison against published data for fluids taken from four wells from a geothermal field near Makhachkala, the regional capital of Dagestan, Russia, (Abdulagatov et al., 2016) was performed. This dataset presents a rare example where thermophysical properties beyond the density and composition are reported. The enthalpy and entropy are not measured directly but are instead inferred from density and speed of sound measurements. The thermophysical property model presented in this work was found to reproduce the density within 2% and the enthalpy change within 0.5%, see Figure 8.



**Figure 6** Plots of the brine density as well as enthalpy and entropy change for a salinity of 0.1 kgNaCl / kgH<sub>2</sub>O, comparing the Thermophysical Property Model (blue) against the MIT Seawater model (orange) as well as the percentage difference (red). The enthalpy and entropy change of pure water is calculated using the industry standard IAPWS model (green). The reference conditions are 101325 Pa and 25°C.



**Figure 7** Plots of the brine density as well as enthalpy and entropy change for a salinity of 0.2 kg<sub>LiBr</sub> / kg<sub>H<sub>2</sub>O</sub>, comparing the Thermophysical Property Model (blue) against the Lithium Bromide model (orange) as well as the percentage difference (red). The enthalpy and entropy change of pure water is calculated using the industry standard IAPWS model (green). The reference conditions are 101325 Pa and 25°C.



**Figure 8** The density and enthalpy change for different temperatures at ambient pressure for four different fluid samples as determined in the lab (points) or calculated using this thermophysical property model (lines)

#### 4 CASE STUDIES

Using this thermophysical property model the temperature heat content relationship (T-Q curve) for a number of geofluids was investigated.

##### 4.1 Single-Phase Brine

The T-h and T-s curves for a single-phase geofluid consisting of water and NaCl (at 0.1 kgNaCl/kgH<sub>2</sub>O) as well as pure water were calculated, see Figure 9. Assuming a production and rejection temperature of 160 °C and 100 °C respectively for both fluids, and a constant pressure of 10 bar, the specific heat and exergy transferred were determined using [6] and [7]. T<sub>0</sub>, the temperature of the reference environment was assumed to be 25 °C.

$$Q = (h_{in} - h_{out}) \quad [6]$$

$$E = (h_{in} - h_{out}) - T_0(s_{in} - s_{out}) \quad [7]$$

The results showed that both the heat and exergy content of the brine were about 10% lower than pure

water, see Table 1. This highlights the importance of accurate models for capturing the thermophysical properties of geofluids, not only for correctly assessing the plant potential and productivity, but also sizing of plant components, in particular the primary heat introduction.

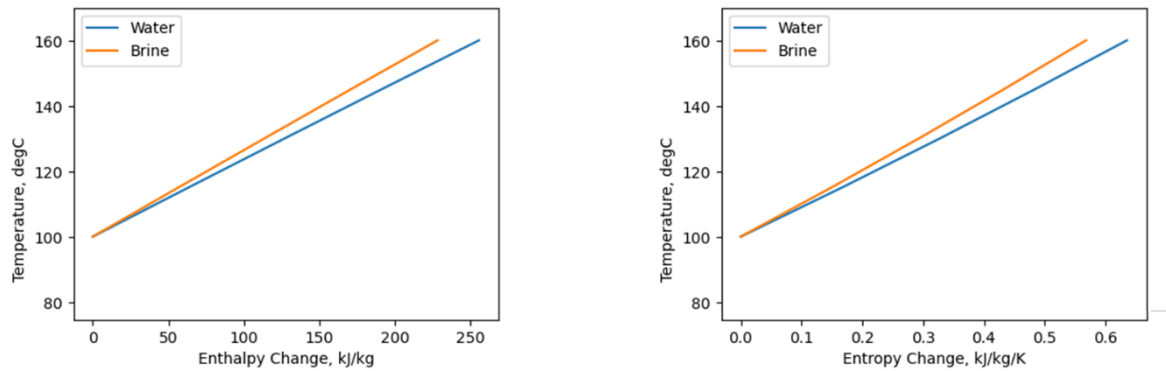
**Table 1** Comparison of the Heat and Exergy content of brine vs. pure water

	Brine	Water	Diff, %
Heat Content, kJ / kg	228.5	255.9	-10.7
Exergy Conent, kJ / kg	59.22	66.47	-10.9

##### 4.2 Two-Phase Brine

While the shape of the T-Q and T-s curves is relatively straightforward for single-phase sources, for two-phase sources, the presence of NCG introduces a temperature glide in the condensation. Capturing the shape of the T-Q curve is particularly important for optimising the primary heat introduction, which is achieved by aligning the geofluid and working fluid T-Q profiles and thus minimising the average temperature difference of heat introduction.

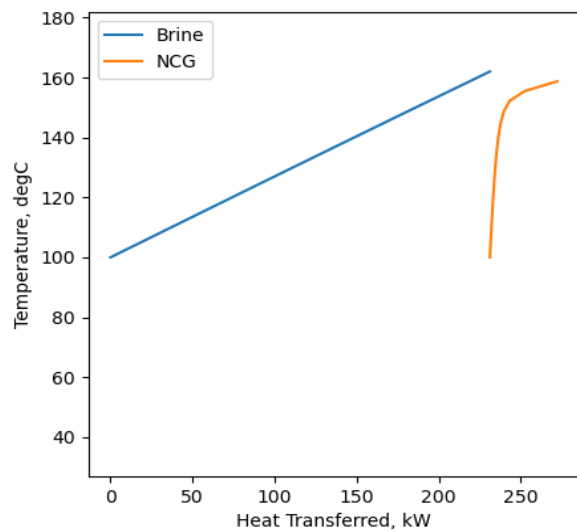




**Figure 9** The enthalpy and entropy content of water and brine (water + NaCl) geofluids

A geofluid comprised of water, NaCl (at 0.1 kgNaCl/kgH<sub>2</sub>O) and CO<sub>2</sub> (at 0.1 kgCO<sub>2</sub>/kgH<sub>2</sub>O) was considered. Assuming an arrival temperature and pressure of 162 °C and 10 bar respectively, the thermophysical property model was used to partition the fluid into its constituent liquid and vapour phase – the vapour quality was found to be around 2%. Assuming a reinjection temperature of 100 °C, the T-Q curve, see Figure 10, and in turn the heat and exergy content of the geofluid were calculated.

The heat and exergy content of this two-phase geofluid were found to be around 270 kJ/kg and 72.4 kJ/kg respectively.



**Figure 10** The T-Q diagram of a two-phase geofluid, assuming a mass rate of 1 kg/s.

## 5 CONCLUSIONS

The functionality of existing partitioning and property estimation tools has been extended by using a coupled modelling approach to leverage the strengths of the respective models. In its default configuration, this coupled model uses Reaktoro for the partitioning and ThermoFun and CoolProp to calculate the phase properties. That being said, this model’s modularised

architecture means that it is fully extendable with other partition or property models.

The calculated thermophysical properties are consistent with the investigated datasets. Moreover, the case studies shown above highlight the importance of using appropriate thermophysical property models, as compared to pure water the thermophysical properties of geothermal brines can be significantly different.

## 6 ACKNOWLEDGEMENTS

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## 7 NOMENCLATURE

### 7.1 Symbols

	Units	Description
$E$	kJ/kg	Exergy Content
$G$	kJ	Gibbs Free Energy
$P$	Pa	Pressure
$Q$	kJ/kg	Heat Content
$R$	kJ/kmol/K	Ideal Gas Constant
$T$	K	Temperature
$a$		Activity
$h$	kJ/kmol	Specific enthalpy
$n$	kmol	Moles
$s$	kJ/kmol/K	Specific entropy
$v$	m <sup>3</sup> /kmol	Specific volume
$y$		Mole fraction
$\mu$	kJ/kmol	Chemical Potential

### 7.2 Sub- and Superscripts

	Description
$i$	Species “i”
$^{\circ}$	Standard State

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