

# Calculating thermophysical fluid properties during geothermal energy production with NESS and Reaktoro



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## ABSTRACT

We investigate how subsurface fluids of different compositions affect the electricity generation of geothermal power plants. First, we outline a numerical model capable of accounting for the thermophysical properties of geothermal fluids of arbitrary composition within simulations of geothermal power production. The behavior of brines with varying compositions from geothermal sites around the globe are then examined using the model. The effect of each brine on an idealized binary geothermal power plant is simulated, and their performances compared by calculating the amount of heat exchanged from the fluid to the plant's secondary cycle.

Our simulations combine (1) a newly developed Non-linear Equation System Solver (NESS), for simulating individual geothermal power plant components, (2) the advanced geochemical speciation solver, Reaktoro, used for calculation of thermodynamic fluid properties, and (3) compositional models for the calculation of fluid-dynamical properties (e.g., viscosity as a function of temperature and brine composition). The accuracy of the model is verified by comparing its predictions with experimental data from single-salt, binary-salt, and multiple-salt solutions.

The geothermal power plant simulations show that the brines considered in this study can be divided into three main categories: (1) those of largely meteoric origin with low salinity for which the effect of salt concentration is negligible; (2) moderate-depth brines with high concentrations of Na<sup>+</sup> and K<sup>+</sup> ions, whose performance is well approximated by pure NaCl solutions of equivalent salinity; and (3) deeper, high-salinity brines that require a more detailed consideration of their composition for accurate simulation of plant operations.

## 1. Introduction

Optimal geothermal energy extraction requires an understanding of both the thermodynamic (e.g., heat capacity, thermal conductivity) and fluid dynamical (e.g., dynamic viscosity) properties of the geothermal reservoir fluid, hereafter collectively referred to as thermophysical properties. These thermophysical properties depend not only on temperature, but also on fluid composition, which typically varies from site to site, and may also change over time as a result of, for example, the introduction of fluids into the geothermal reservoir, geochemical reactions between fluid species and rock minerals, and temperature variation as the fluid flows through the reservoir (Richards et al., 1992). It is, therefore, important to understand the extent and manner in which fluid composition affects the efficiency of geothermal energy production and associated power (i.e. electricity) generation of geothermal power plants.

Several models exist for calculating the thermophysical properties of fluids of predefined composition (e.g. Laliberté, 2007; Laliberté, 2009; Sharqawy et al., 2010a; Wang and Anderko, 2012; Sharqawy, 2013; Bell et al., 2014; Lei et al., 2016). However, in general, these properties are expressed as a function of solute mass fraction for pre-designated solute mixtures, usually single-salt solutions. To properly analyze how fluid composition can impact energy production from the subsurface and eventually electricity generation, descriptive models are needed that are capable of determining the thermophysical properties of fluids of arbitrary chemical composition.

We present such a simulation framework that can be extended to geothermal fluids with a wide range of compositions. This could eventually be extended to include fluids other than water, such as carbon dioxide and nitrogen, which have enjoyed increasing popularity, at least theoretically, both in Hot-Dry Rock or Enhanced Geothermal Systems (Brown, 2000; Luo et al., 2014; Pruess, 2006,

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2008; Ram Mohan et al., 2013) and in sedimentary-basin geothermal systems (Randolph and Saar, 2011; Adams et al., 2015; Garapati et al., 2015; Buscheck et al., 2016). For this initial contribution, we focus on determining the thermophysical properties of geothermal brines.

Our numerical framework enables the determination of accurate fluid (e.g. brine) properties directly from the aqueous species in the fluid. These properties can be incorporated into simulations of subsurface fluid flow and heat transfer, and also (particularly pertinent for this paper) into calculations (and optimization) of the thermodynamic cycle of electricity generation in geothermal power plants. The power plant simulations are performed with our Non-linear Equation System Solver (NESS), first introduced here, which provides a common framework for coupling the power plant components with functions describing their thermophysical and thermodynamic properties. We employ our geochemical solver, Reaktoro (Leal et al., 2015, 2016) to determine how the thermodynamic quantities (density, enthalpy, heat capacity, etc.) depend on the concentrations of the aqueous species within the brine. Additional thermophysical models are introduced to calculate brine viscosity and thermal conductivity as a function of the aqueous species concentrations.

Assessing the impact of brine composition in the production of electricity requires accurate fluid property calculations. Thus, after outlining the different model components of the simulation framework, we show that our calculated thermodynamic and thermophysical brine properties, composed of different salts with different concentrations, agree well with experimental observations (with less than 3% deviation for multiple-salt solutions) and to predictions from mass-fraction-based calibrations of single-fluid models. Good agreement is obtained not only for single-salt solutions, but also for multiple-salt solutions for all thermophysical and thermodynamic properties considered.

Finally, we show how our method can be applied to realistic, real-world scenarios. This is done by examining the effects of brine composition on power production for systems from different geothermal sites employing brine as the subsurface heat extraction fluid. Here, we consider the fluid composition effect on the well-bore flow and on the power plant only, and ignore such effects during geofluid flow through the geothermal reservoir. This latter assumption is adopted to focus on the effects the brine composition has on the power plant, including its wells, in isolation. The results we obtain, even with such simplifications, already show that brine composition can have a major effect on electricity generation. This provides a motivation to conduct more detailed fluid flow simulations that account for the effects of brine composition during geofluid flow in the geothermal reservoir, which will be addressed in the future.

The results of the present study reveal that the investigated geothermal fluids may be divided into three main categories with regard to their thermophysical properties: (i) low salinity geothermal fluids of largely meteoric origin; (ii) moderate- to high-salinity NaCl-dominated geothermal fluids; and (iii) deeper geothermal brines with more varied chemical makeup. The first two groups of fluids are shown to be well represented by approximating the brine as a pure NaCl solution. At low concentrations, the effects of the salt on the thermophysical properties of the fluid are minor. At moderate concentrations and when sodium dominates, this is also frequently accompanied by significant concentrations of other dissolved salts (KCl in particular) with similar thermophysical characteristics to NaCl. However, at large depths, the possibility exists that other ions are present due to the influence of diagenetic and formation waters, which can significantly affect brine properties.

## 2. Numerical model description

The simulations described in this paper involve three coupled numerical models: (i) a component model capturing the different stages of the power plant cycle; (ii) a geochemical model to determine the speciation of the geothermal brine; and (iii) thermophysical models for

calculating the material properties of the brines. These three models are briefly outlined next.

Coupling between the components of the power plant cycle and the other simulators is conducted using our Non-linear Equation System Solver (NESS), a software platform for the solution of nonlinear equation systems. NESS is introduced here for the first time. It provides a simple programming interface to simultaneously or sequentially solve systems of equations. It also includes the ability to integrate results from external simulators.

Our calculation of brine speciation is accomplished by coupling NESS to Reaktoro (Leal et al., 2014, 2015, 2016). Based on a Gibbs energy minimization (GEM) formulation, Reaktoro is a C++ library that provides efficient methods for simulating chemical systems. Reaktoro includes methods for obtaining thermodynamic quantities (e.g. enthalpy, heat capacity, and density) for both pure and multi-component fluids based on the fluids' chemical compositions.

Additional thermophysical properties, namely brine viscosity and thermal conductivity, are also required as part of the power plant simulation. Thus, we supplement our thermodynamic quantity calculations in Reaktoro with composition-based viscosity and thermal conductivity calculations. This, in combination with similar formulations in Reaktoro for the other thermophysical properties, enables the response of the system as a whole to be related directly to the chemistry of individual brines. The details of these calculations are further outlined in the sections below.

In addition to the composition-based thermophysical properties available in Reaktoro, NESS also includes methods that allow coupling to the CoolProp thermophysical library (Bell et al., 2014). Unlike the Reaktoro formulation, the thermophysical properties in CoolProp are specific to particular fluids, or predefined mass-fraction based solutions. While they are less versatile than the fluid property models provided in Reaktoro, they nevertheless provide a baseline against which to compare the Reaktoro results for specific fluid examples.

### 2.1. Plant model

The geothermal power plant considered in this paper is a simple binary system, where the heat from the geothermal fluid (e.g. a brine) is transferred to a secondary working fluid (e.g. CO<sub>2</sub>, R245fa) through a counter-flow heat exchanger that drives the secondary Rankine cycle. A schematic cartoon, illustrating the model of the geothermal power plant, is given in Fig. 1. The reservoir pressure and temperature at the base of the production well (State 1) are determined by assuming a constant hydrostatic pressure gradient,  $\nabla P$ , and a constant geothermal temperature gradient,  $\nabla T$ , in the subsurface, i.e.

*State 1:*

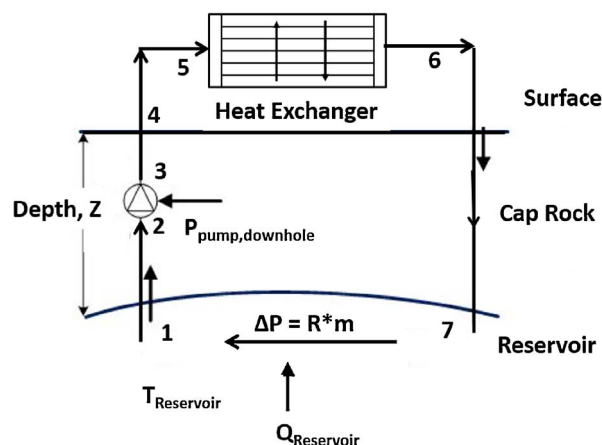


Fig. 1. Components of the geothermal power plant model. Numbers denote thermodynamic state points, discussed in the main text.

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