An isenthalpic formulation for simulating geothermal systems with phase changes

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Introduction

Geothermal energy extraction requires detailed characterization of geological, physical, and geochemical properties of the reservoir and fluid properties of the geothermal fluids. For a proper understanding of the involved reservoir processes, robust and efficient numerical thermal simulation tools are essential (Zhu and Okuno, 2014, 2016; Connolly et al., 2021). Simulations of mass and heat transfer in porous media traditionally include temperature as an independent variable and the set of natural variables. This, however, requires variable substitution procedures to handle phase transitions, which add complexity to the implementation (Voskov and Tchelepi, 2012). In contrast, the overall composition formulation, has the advantage of well-defined equations and variables at each cell, so it does not require variable substitution procedures, (Voskov and Tchelepi, 2012). In this formulation, the coupled mass and heat transfer problem is solved at each time step by using pressure, enthalpy, and composition, requiring an isobaric and isenthalpic formulation to solve the local phase equilibrium problem. This study approaches the isenthalpic phase equilibrium problem from a unified perspective and ties it to equations of energy and mass conservation.

An isenthalpic formulation

The constitutive model is based on a cubic equation of state (EoS) and a unified formulation for computing isenthalpic phase behavior. As in the work of Gupta et al. (1990) and (Zhu and Okuno, 2016), the adopted approach is essentially meant to solve the stability and the isenthalpic flash. Our solution approach is based on recasting the equations as a minimization problem with complementary conditions or unilateral conditions (Lauser et al., 2011; Gharbia et al., 2021). The compositional multiphase equilibrium problem can be presented in an abstract form:

$$\begin{aligned} \Lambda(\mathbf{Y}) &= 0 \quad \in \mathbb{R}^{l-m}, \\ \min\left(G(\mathbf{Y}), H(\mathbf{Y})\right) &= 0 \quad \in \mathbb{R}^{m}, \end{aligned} \tag{1}$$

where $\mathbf{Y} \in \mathbb{R}^{l}$ is the unknown, the set of $l-m$ functions $\Lambda(\mathbf{Y})$ are algebraic equations representing the equilibrium of the compositional multiphase mixture (material balance and isofugacity constrains) and the last m functions $G(\mathbf{Y})$ and $H(\mathbf{Y})$ are complementary conditions representing the stability analysis in a similar way to the work by Gupta et al. (1990) and Zhu and Okuno (2016). Our research is an extension of the isobaric-isothermal analysis performed by Gharbia et al. (2021) to an isobaric-isenthalpic equilibrium problem. Such extension is performed by appending to $\Lambda(\mathbf{Y})$ an additional constraint, such that the equilibrium problem is composed of material balance, isofugacity, and enthalpy constraints. As an example of the unified formulation, we present the set of equations for the isenthalpic equilibrium problem for a two-phase (Gas, Liquid) two-component (H2O, Co2) mixture. Components are identified with roman numbers, *I* for water, and *II* for CO2.

$$\Lambda(\mathbf{Y}) = \begin{bmatrix} V\xi_G^I + (1-V)\,\xi_L^I - z^I \\ \xi_G^I \phi_G^I(\mathbf{x}_G, T) - \xi_L^I \phi_L^I(\mathbf{x}_L, T) \\ \xi_G^{II} \phi_G^{II}(\mathbf{x}_G, T) - \xi_L^{II} \phi_L^{II}(\mathbf{x}_L, T) \\ V h_G(\mathbf{x}_G, T) + (1-V)\, h_L(\mathbf{x}_L, T) - H \end{bmatrix}, \; G(\mathbf{Y}) = \begin{bmatrix} V \\ 1-V \end{bmatrix}, \; H(\mathbf{Y}) = \begin{bmatrix} 1-\xi_G^I - \xi_G^{II} \\ 1-\xi_L^I - \xi_L^{II} \end{bmatrix} \tag{2}$$

where the solution $\mathbf{Y} = \left\{V, \xi_G^I, \xi_G^{II}, \xi_L^I, \xi_L^{II}, T\right\}$ compiles the vapor fraction V, the extended partial fractions $\left\{\xi_G^I, \xi_G^{II}, \xi_L^I, \xi_L^{II}\right\}$ and the temperature T. The extended fractions are related to the partial (physical) fractions $\{\mathbf{x}_G, \mathbf{x}_L\}$ as $x_\alpha^i = \frac{\xi_\alpha^i}{\sum_\alpha \xi_\alpha^i}$ with $\alpha \in \{G, L\}$ and $i = \{I, II\}$. The vector $\mathbf{z} = \left\{z^I, z^{II}\right\}$ is the overall molar composition. The fugacity coefficients $\left\{\phi_G^I, \phi_G^{II}, \phi_L^I, \phi_L^{II}\right\}$ are defined using the Peng-Robinson cubic equation of state for a mixture of any number of components (Peng and Robinson, 1976). To assure that while solving the Peng-Robison equation of state the compressibility factors are correctly identified, we incorporate the labeling procedure by Vu et al. (2021). Finally the full expression of the total enthalpy $H_t := V h_G(\mathbf{x}_G, T) + (1-V)\, h_L(\mathbf{x}_L, T)$ and phase enthalpies are presented by Zhu and Okuno (2014). The equilibrium problem amounts to solving eq. 1 while $\{P, H, \mathbf{z}\}$ are given.

Numerical solution of the equilibrium problem

For the numerical solution of the equilibrium problem, we adopt the nonparametric interior point algorithm presented by Vu et al. (2021). For completeness, we introduce some details about the numerical solution. Let's expand the solution vector $\mathbf{Y} = \left\{V, \xi_G^I, \xi_G^{II}, \xi_L^I, \xi_L^{II}, T, v_G, v_L, w_G, w_L, \nu\right\}$ with additional unknowns $\{v_G, v_L, w_G, w_L\}$, so-called slack variables, and ν, the interior parameter. With this modification the equilibrium problem is:

Given $\{P, H, \mathbf{z}\}$ find $\mathbf{Y}$ such that

$$\mathbf{F}(\mathbf{Y}) = 0, \text{ with } \mathbf{F}(\mathbf{Y}) = \begin{bmatrix} \Lambda(\mathbf{Y}) \\ G(\mathbf{Y}) - \mathbf{v} \\ H(\mathbf{Y}) - \mathbf{w} \\ \mathbf{v} \odot \mathbf{w} - \nu \mathbf{1} \\ f(\mathbf{Y}, \nu) \end{bmatrix}, \tag{3}$$

where $\mathbf{v} = \{v_G, v_L\}$, $\mathbf{w} = \{w_G, w_L\}$ and $\odot$ denotes the Hadamard's component-wise product. The function $f(\mathbf{Y}, \nu)$ is defined as

$$f(\mathbf{Y}, \nu) := \frac{1}{2}\left(\sum_\alpha \min(v_\alpha, 0)^2 + \sum_\alpha \min(w_\alpha, 0)^2\right) + \frac{\mu}{2\, m^2} \max(\mathbf{v} \cdot \mathbf{w}, 0)^2 + \eta\ \nu + \nu^2 \tag{4}$$

Remark: The variable ν is 0 at the minima of eq. 3, wich gives the same solution of the original problem, eq. 1.

The solution procedure relies on an iterative quasi-Newton method with an Armijo line search (Vu et al., 2021).

Example of constitutive modelling

As an example, we set up a narrow-boiling situation similar to the one described by Zhu and Okuno (2014, 2016), in order to demonstrate the effectiveness of the numerical method presented in the preceding section.

The majority of geothermal fluids contain non-condensable gases (NCG). Typically, carbon dioxide (CO2) accounts for more than 95 percent of the total NCG content (Bonafin and Bonzanini, 2021). Therefore, it is natural to use a binary mixture with composition $\mathbf{z} = \{0.99, 0.01\}$ (99.0 % water (H2O) and 1.0% carbon-dioxide (CO2)) as an example. The pure substance properties can be found in (Zhu and

Okuno, 2014, 2016). Figure 1 shows the phase envelope in P-H space, for an example of validation, we computed the isotherms with an thermodynamic package (https://github.com/CalebBell/thermo) rather than using an isothermal unified formulation. The red circle represents the critical point of water (22.064 MPa and 647 K). Path A (black line) represents a narrow boiling condition, while path B (red line) represents a condition far from the critical point. Both paths are computed using the isenthalpic unified formulation, and no convergence failure was found. Figure 2 shows that path B has fewer iterations than path A. Since path A was deliberately traced near the critical point, narrow-boiling conditions results in more iterations.

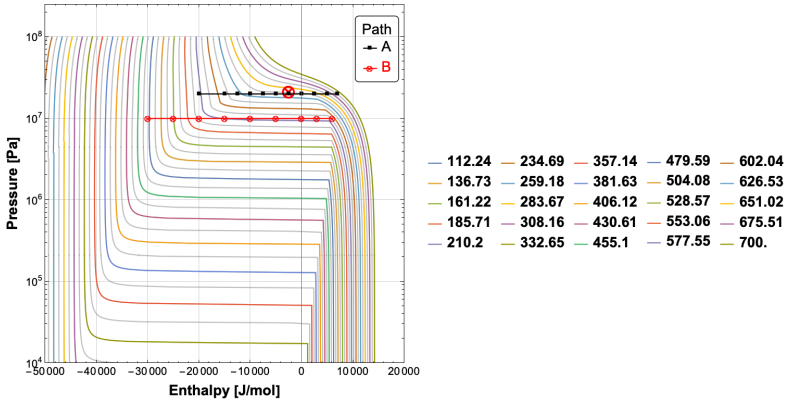

Figure 1 *PH-diagram for binary mixture with composition* $\mathbf{z} = \{0.99, 0.01\}$ *(99.0 % water (H2O) and 1.0% carbon-dioxide (CO2)). Path A (black line) represents a narrow boiling condition, while path B (red line) represents a condition far from the critical point.*

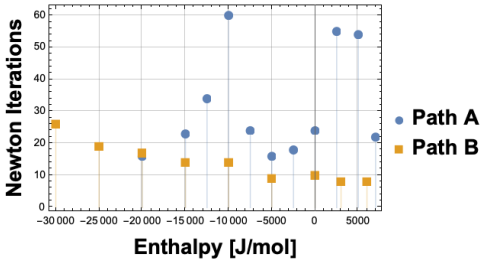

Figure 2 *Iteration number vs enthalpy for path A and B.*

Another important characteristic of narrow boiling is that the equations are near degenerate towards one degree of freedom (edges of compositional space) (Zhu and Okuno, 2014, 2016). Using path A, we decrease CO2 composition until it reaches machine precision $z^{II} \in \{0.01, 10^{-5}, 10^{-15}\}$ and demonstrate the capabilities of the proposed approach in simulating one degree of freedom fluids. Figure 3 shows that V and the enthalpy H are sensitive with respect to temperature in the two-phase region and both vary rapidly in the range of 629.38 K to 642.45 K for $z = \{0.99, 0.01\}$ and 639.57 K to 642.45 K for $\mathbf{z} = \{1.0 - 10^{-15}, 10^{-15}\}$. The phase disappearing and reappearing at the critical points occurs within a few Kelvin degrees. Therefore, those conditions must be checked to obtain a robust numerical solution.

Connection with geothermal modeling

To connect the unified formulation with equations for mass and energy conservation for a geothermal system, we employ the overall molar composition formulation with the $\mathbf{X} = \{p, H, \mathbf{z}\}$ and the fully discrete scheme is a combination of Euler time-stepping and a multi-point finite volume discretization. Simulations using this new approach are currently in the development phase. With some abuse of notation $\tilde{\cdot}$ denotes the discrete unknowns and $(t^n)_{0 \leq n \leq N}$ is the discrete time nodes with $t^0 := 0$ and $t^N := t_f$. The discrete set of PDEs compiles mass and energy balance, initial and boundary conditions. We close the discrete set of PDEs $\tilde{\mathbf{D}}\left(\tilde{\mathbf{X}}(t^n), \tilde{\mathbf{Y}}(t^n)\right)$ with the set of local isenthalpic equilibrium problems $\tilde{\mathbf{F}}\left(\tilde{\mathbf{X}}(t^n), \tilde{\mathbf{Y}}(t^n)\right)$. The global discrete problem is to find $\left\{\tilde{p}(t^n), \tilde{H}(t^n), \tilde{\mathbf{z}}(t^n)\right\} \forall\, n \in \{1, \ldots N\}$ such

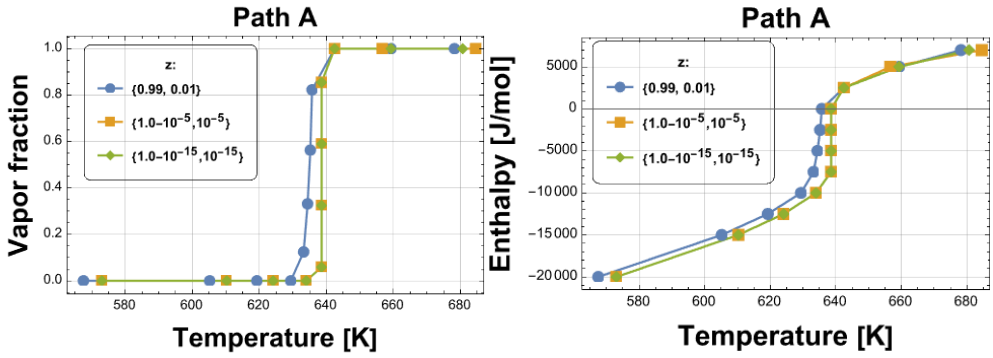

Figure 3 *Vapor fraction and the total enthalpy vs temperature. The properties used for the components are given in Table 1. Two phases are present from 629.38 K to 642.45 K for* $\mathbf{z} = \{0.99, 0.01\}$. *Overall compositions for each case* $\mathbf{z} \in \left\{\{0.99, 0.01\}, \left\{1.0 - 10^{-5}, 10^{-5}\right\}, \left\{1.0 - 10^{-15}, 10^{-15}\right\}\right\}$.

that

$$\begin{bmatrix} \mathbf{D}\left(\tilde{\mathbf{X}}\left(t^n\right), \tilde{\mathbf{Y}}\left(t^n\right)\right) \\ \mathbf{F}\left(\tilde{\mathbf{X}}\left(t^n\right), \tilde{\mathbf{Y}}\left(t^n\right)\right) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{5}$$

At a particular time node t^n, the Jacobian matrix $J\left(\tilde{\mathbf{X}}\left(t^n\right), \tilde{\mathbf{Y}}\left(t^n\right)\right)$ takes the algebraic and reduced algebraic form

$$\mathbf{J} = \begin{bmatrix} \tilde{\mathbf{A}} & \tilde{\mathbf{B}} \\ \tilde{\mathbf{C}} & \tilde{\mathbf{E}} \end{bmatrix}, \ \mathbf{J}_r = \tilde{\mathbf{A}} - \tilde{\mathbf{B}}\tilde{\mathbf{E}}^{-1}\tilde{\mathbf{C}}. \tag{6}$$

If we adopt the formulation of an overall composition with enthalpy as the variable, the structure of $\tilde{\mathbf{E}}$ is block diagonal. In this case, the Schur complement technique is applied to reduce the global problem only in terms of $\tilde{\mathbf{X}}\left(t^n\right)$. Furthermore, the evaluation of $\mathbf{F}\left(\tilde{\mathbf{X}}\left(t^n\right), \tilde{Y}\left(t^n\right)\right)$ can be trivially parallelized.

Conclusions

The equilibrium problem of compositional multiphase mixtures has been presented using an isenthalpic unified formulation. It is robust to narrow boiling conditions, capable of addressing phase change phenomena naturally, and can be used for thermal simulations with the overall composition formulation. An interior point method with line search is employed to solve the problem numerically, which avoids solving complementary conditions in their natural form. Using the unified formulation, we model the constitutive behavior of a binary mixture of water and carbon dioxide and tie the unified formulation to equations for mass and energy conservation in a geothermal system. Currently, simulations of mass and heat transfer in a geothermal reservoir are being conducted as part of this research.

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