A Numerical Simulation of a Boiling Front Moving through Porous Medium

Larus Thorvaldsson*, Halldor Palsson

University of Iceland, Sæmundargötu 2, 101 Reykjavík; *lth31@hi.is

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Abstract. A boiling front of water moving through porous medium is simulated using a numerical finite volume method (FVM) which is then compared to an analytical solution. The FVM is constructed on top of the OpenFOAM framework, which is a highly customizable set of C++ libraries and tools for the solution of problems in continuum mechanics. The solution is stabilized using Fréchet derivatives which enables the use of appropriately sized time steps. The physical properties of the water are determined from the IAPWS-IF97 thermodynamic formulation. The results show that the numerical model is able to simulate the overall behavior of the boiling front sufficiently well. This increases the confidence in the numerical solutions outside the limits of the analytical solution.

Introduction

Numerical simulation of hydrothermal systems has played an important role in their modeling for the past decades. For researchers it has been used to test competing hypothesis in these complex environments, where data is often scarce, and in industry numerical simulation has become standard practice in the planning and management of the development of geothermal fields [9].

The earliest efforts to apply numerical models to geothermal reservoirs were made in the early 1970's, but the usefulness of numerical modelling did not begin to gain acceptance by the geothermal industry until after the 1980 Code Comparison Study [14]. Since that study was performed, the experiences gained in carrying out site-specific studies as well as generic reservoir modelling studies have led to a constant improvement in the capabilities of numerical reservoir models.

Numerical modeling of hydrothermal systems is often defined by which components of the system are taken into account. Traditionally they have been divided into hydrological (H), thermal (T), mechanical (M) and chemical (C) components. Those components are coupled together in a way that is inherently multiscale in nature, such that their temporal and spatial scales vary be several orders of magnitude [4]. Because of the complex nature of those couplings, models involving all four components are rare.

The equations that describe hydrothermal systems are relatively complex but they can nevertheless be solved analytically for a highly idealized set of initial and boundary conditions. Such cases usually only involve one of the four (HTMC) components, where the Theis problem is an example thereof [15]. Some analytical solutions also exists for two components, such as the description of a boiling front moving through a porous medium [13] and the advance of a diffused salt water wedge in a confined aquifer [2]. These analytical solutions are very important in validating numerical models that are supposed to handle more complicated problems.

The current generation of numerical simulators is in most cases able to account for multiphase, multicomponent flow. The most versatile ones are software packages such as Finite Element Heat and Mass Transfer (FEHM) [6] and the Transport of Unsaturated Groundwater. and Heat (TOUGH) family of codes [12]. These solvers have been applied to a wide variety of problems, such as CO2 sequestration, geothermal studies and other environmental issues [4].

Other solvers are more specialized, such as the Complex Systems Modeling Platform (CSMP++) [8] and Fully Implicit Seafloor Hydrothermal Event Simulator (FISHES) [7]. They have been developed specifically to allow simulation of high-temperature multiphase flow of NaCl-H2O fluids. Other codes such as FALCON [10], developed at Idaho National Labs have

focused on the tightly coupled process of fluid rock interaction.

In this paper the applicability of using a free and open source package named OpenFOAM for modeling hydrothermal systems is examined. Open- FOAM is a highly customizable set of C++ libraries and tools for the solution of problems in continuum mechanics. It is also gaining considerable popularity in academic research and among industrial users, both as a research platform and a black-box CFD and structural analysis solver [5].

The object orientation and operator overloading of C++ has enabled the developers of OpenFOAM to build a framework for computational fluid dynamics that enables modelers to work at a very high level of abstraction [17]. This makes it possible to manipulate the set of partialdifferential equations that describe the problem and customize the solver itself for each class of cases that need to be solved. This will enable researchers with sufficient knowledge about the relevant dynamics of each problem to construct efficient and accurate solvers for it. This is the main motivation for using OpenFOAM, rather than currently existing models.

As well as showing how easily an equation of state can be implemented in the previously existing framework, this paper also shows how the underlying equations can be modified in an easy way. This is demonstrated by linearizing the partial differential equations describing the hydrology of the problem using Fréchet derivatives. In this manner it is possible to stabilize the solution for superheated steam, which makes it possible to treat the pressure equation as steady state, allowing for a more computationally efficient solution.

1 Methods and Materials

1.1 Governing equations

For mass conservation the continuity equation must be satisfied

$$\frac{\partial \phi \rho}{\partial t} + \nabla \cdot (\phi \vec{u}) = 0 \tag{1}$$

where ϕ is porosity and ρ is density. In this equation $\vec{u}$ denotes the superficial velocity, which is a hypothetical velocity calculated as if the fluid were the only thin present in a given cross sectional area. For pressure-velocity coupling, Darcy's law can be applied

$$\vec{u} = -\frac{\kappa}{\mu}(\nabla p - \rho \vec{g}) \tag{2}$$

where κ is permeability, μ is viscosity and $\vec{(}g)$ is gravitational acceleration.
This gives following equation for groundwater flow

$$\frac{\partial \phi \rho}{\partial t} - \nabla \cdot \left(\frac{\rho \kappa}{\mu} \nabla p \right) + \nabla \cdot \left(\frac{\rho^2 \kappa}{\mu} \vec{g} \right) = 0 \tag{3}$$

The energy equation includes both effects from the fluid and the soil, and is given as

$$\frac{\partial}{\partial t} (\phi \rho h + (1-\phi) \rho_s c_s T) + \nabla (\rho \vec{u} h) = \nabla (\Gamma \nabla T) \tag{4}$$

where ϕ is porosity, ρ_s is the density of rock, $c_s$is the heat capacity of soil and Γ is the combined conductivity of fluid and soil.If the properties of the soil are assumed to be constant the laplacian of temperature can be broken up in terms of enthalpy and pressure. In this case, conduction effects in the water are also neglected, which gives the following equation for energy

$$\begin{aligned} \phi \frac{\partial \rho h}{\partial t} + (1-\phi) \rho_s c_s \left(\frac{\partial T}{\partial h} \frac{\partial h}{\partial t} + \frac{\partial T}{\partial p} \frac{\partial p}{\partial t} \right) \\ + \nabla \cdot (\rho \vec{u} h) = 0 \end{aligned} \tag{5}$$

Since the density is a strong function of pressure in the liquid-vapor phase, it can be accounted for in the time derivative by using a first order Taylor expansion. If it is also assumed that the porosity is not a function of time, the Taylor expansion of the time derivative becomes

$$\frac{\partial \phi \rho}{\partial t} = \phi \frac{\partial \rho}{\partial t} + \phi \frac{\partial}{\partial t} \frac{\partial \rho}{\partial p} \bigg|_{p=p_0} (p - p_0) \tag{6}$$

The stability of the pressure equation can be increased by linearizing the Laplacian term. This is possible by applying a Fréchet derivative operator on the term, such that

$$\begin{aligned} \frac{\delta F}{\delta p} &= \frac{\delta}{\delta p} \nabla \cdot \left(\frac{\rho \kappa}{\mu} \nabla p \right) \\ &= \nabla \cdot \left(\frac{\kappa}{\mu} \frac{\partial \rho}{\partial p} \nabla p \right) + \nabla \left(\frac{\kappa}{\mu} \rho \nabla \right) \end{aligned} \tag{7}$$

this can then be applied to a first order Taylor expansion of the function

$$\begin{aligned} p &= p_0 + \frac{\delta F}{\delta p} \bigg|_{p=p0} (p - p_0) \\ &= \nabla \cdot \left(\frac{\kappa}{\mu} \rho \nabla p \right) + (p - p_0) \nabla \cdot \left(\frac{\kappa}{\mu} \frac{\partial \rho}{\partial p} \nabla p_0 \right) \end{aligned} \tag{8}$$

Having applied both the Taylor expansion of the time derivative and the linearization of the laplacian term, the pressure equation finally becomes

$$\phi\frac{\partial\rho}{\partial t}+\phi\frac{\partial}{\partial t}\frac{\partial\rho}{\partial p}\bigg|_{p=p_0}(p-p_0)-\nabla\cdot\left(\frac{\kappa}{\mu}\rho\nabla p\right)- \\ -(p-p_0)\nabla\cdot\left(\frac{\kappa}{\mu}\frac{\partial\rho}{\partial p}\nabla p_0\right)+\nabla\cdot\left(\frac{\rho^2\kappa}{mu}\vec{g}\right)=0 \tag{9}$$

The equation of state is implemented from the IAPWS-IF97 thermodynamic formulation [3]. The primary variables for the equation of state are taken to be pressure and enthalpy, since pressure-temperature formulation has been shown to have more difficulties close to the critical point [4]. Given those two state variables the algorithm returns the steam quality x, the density ρ, the temperature T and the partial derivatives of all those variables both with respect to pressure and enthalpy. Those values are then used in the system equation, which makes it possible to solve for each timestep.

1.2 Analytical solution

The problem which Pruess derived an analytical solution to [13] concerns cold water injection into a reservoir initially filled with superheated steam.If the reservoir is assumed to be infinite and the initial conditions to be uniform, this problem can be shown only to depend on the similarity variable $\eta = r^2/t$, where r is the radial distance from the well, and t is the time. Therefore the boiling front must occur at a fixed value $\eta = \eta_f$ and by extension, the front temperature and pressure must be time-independent.

Pruess gives the solution in terms of pressure at the front p_f and the boiling fraction $b = q_v f/q_l$, where q_l is the mass flow rate of liquid water into the vapor zone and $q_v f$ is the mass flow rate of vapor at the boiling front. For the vapor flow Pruess applies mass balance, Darcy's law and the real gas law, which gives the pressure at the front in the following terms [13]

$$p_f^2 = p_0^2 - \frac{ZR_sT_0\mu_v q_{vf}}{2\pi\kappa H}exp\left(\frac{r_f^2}{4\alpha t}\right)Ei\left(\frac{-r_f^2}{4\alpha t}\right) \tag{10}$$

where Ei is the exponential integral and H is the depth of the reservoir. The crompressibility factor Z is evaluated at the initial steam temperature T_0 and the front pressure p_f. The viscosity μ_v is also evaluated at T_0 but an average pressure between the initial and front pressure is used, such that

$$\bar{p} = \frac{1}{2}(p_f + p_0). \tag{11}$$

The diffusivity parameter α in equation 10 is given as

$$\alpha = \frac{\bar{p}\kappa}{\phi\mu_v}. \tag{12}$$

Using mass conservation it is possible to derive a relation for the location of the front in terms of the similarity variable $\eta_f = r_f^2/t$. Looking at the total liquid mass present in the injection plume gives the following

$$M_l(t) = (q_l - q_v f)t = \pi r_f^2 H\phi\bar{\rho}_l \tag{13}$$

$$\Rightarrow \eta_f = \frac{r_f^2}{t} = \frac{(1-b)q_l}{\pi H\phi\bar{\rho}_l} \tag{14}$$

where $\bar{\rho}_l$ is the average liquid density in the single phase liquid plume. Neglecting small pressure effects it is given as follows

$$\bar{\rho}_l = \omega\rho_l(T_{inj}) + (1-\omega)\rho_l(T_f) \tag{15}$$

where ω is the retardation factor which is the ratio of cold volume to total swept volume. The relation for the retardation factor is given by [1] as follows

$$\omega = \frac{\phi c_{l,h}\rho_l, h}{(1-\phi)\rho_s c_s + \phi c_{l,h}\rho_{l,h}} \tag{16}$$

There $c_{l,h}$ and $\rho_{l,h}$ are respectively the heat capacity and density of the liquid water that has been heated by the superheated steam. Pruess then applies heat balance at the front, which is derived from the fact that temperature and pressure at the front must be related by the vapor pressure relationship for water

$$p_f = p_{sat}(T_f) = p_{sat}\left(T_0 - \frac{h_{vl}\phi\bar{\rho}_l}{(1-\phi)\rho_s c_s(b^{-1}-1)})\right). \tag{17}$$

This set of non-linear equations can be solved in various ways, Pruess uses a Newton-Raphson method, while this paper applies a trust region dogleg method [11]. In order for the solution method to function robustly, the front pressure (pf) has to be scaled, such that it is on the same order of magnitude as the boiling fraction b. This is done by defining the non-dimensional pressure in the following way

$$p_{nd} = \frac{p_f - p_0}{p_{max} - p_0} \tag{18}$$

There p_{max} is an estimation of the maximum pressure in the reservoir.

The physical properties are retrieved from a C++ implementation of the IAPWS-IF97 thermodynamic formulation [IAPWS, 2007]. The primary variables are taken to be pressure and temperature which return saturation pressure $p_{sat}(T)$, density ρ, heat capacity c, viscosity μ_v and the compressibility factor Z.

1.3 Discretization and boundary conditions

The numerical solution is calculated on a axisymmetrical grid with logarithmically spaced cells, with the boundaries of the domain at r_0 and r_N. The logarithmic spacing is constructed by making an equally spaced vector which then gives a logarithmically spaced r_i vector

$$r_i = 10^{x_i}, i = 0, ..., N. \tag{19}$$

$$x_i = log_{10}(r_0) + \frac{i}{N}(log_{10}(r_N) - log_{10}(r_0)) \qquad i = 0, ..., N \tag{20}$$

In the numerical solution, the injection well has to have

param	value
κ	$5 \cdot 10^{-14} m^2$
H	$200m$
r_0	$1m$
r_N	$2500m$
ρ_s	$2600kg/m^3$
c_s	$920J/kg/K$
Γ	$5W/m/K$
h_{vl}	$2260kJ/kg$
q_l	$27.8kg/s$
ϕ	8%
p_0	$600kPa$

Table 1: Numerical values for problem parameters.

some finite radius, r_0. If the injection rate is given as the mass flow rate q_l the appropriate Neumann pressure boundary condition can be found from Darcy's law, such that

$$r_i = 10^{x_i}, i = 0, ..., N. \tag{21}$$

$$r_i = 10^{x_i}, i = 0, ..., N. \tag{22}$$

$$r_i = 10^{x_i}, i = 0, ..., N. \tag{23}$$

$$r_i = 10^{x_i}, i = 0, ..., N. \tag{24}$$

In order to be able to compare the numerical solution to the analytical one, the outer radius is made sufficiently large, as to approximate boundary conditions at infinity. A Dirichlet boundary condition for pressure is applied there with $p = p_0$. Dirichlet boundary conditions are assumed at both sides for the enthalpy, where a temperature of $T_{inj} = 302.55K$ at the well gives $h_{inj} = 1.258 \cdot 10^2 kJ/kg$, At the boundary the temperature is $T_0 = 513.15K$ which corresponds to enthalpy of $h_0 = 2.937 \cdot 10^3 kJ/kg$.

2 Results

In order to validate the OpenFOAM model, a case where cold water was injected into a reservoir with superheated steam, was set up and then compared to the analytical solution. The parameters which were chosen for the problem are given in Table 1.

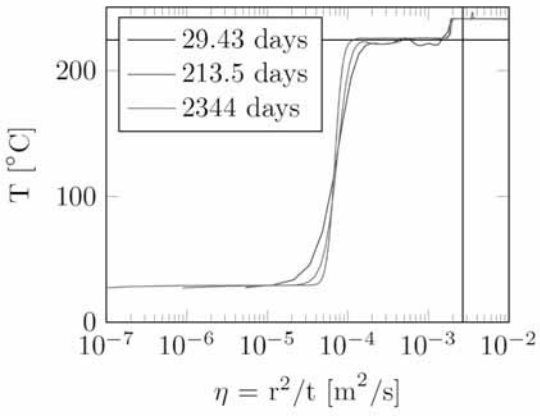

Figure 1: Temperature as a function of the similarity variable $\eta = r^2/t$, along with the analytical solution for the boiling front.

Figure 1 shows the temperature of the reservoir as a function of the similarity variable $\eta = r^2/t$. The figure shows the temperature profile after approximately 29.5 days, 213.5 days and 2344 days. The cross shows the location of the analytical solution as given by equations 10 and 17.

The numerical solution confirms that the location of the front in terms of the similarity variable $\eta_f = r_f^2/t$ is in fact constant. Even though that the time differs by a factor of 10, η_f stays approximately the same. Even though that conduction effects are not taken into account in the numerical solution, it shows some clear signs of numerical diffusion at the interface between hot

and cold single phase liquid. How ever it seems to get sharper as time progresses, probably due to the fact the the width of the interface stays constant in terms of r.

The analytical solution gives the location of the front at $\eta_f = 2.663 \cdot 10^{-3} m2/s$ with temperature of $T_f = 224.1°C$. When compared to the numerical solution at at time $t = 2344$ days the temperature of the front is approximately $T_f = 225.6°C$, which gives a $\Delta T_f = 1.5°C$. For the location of the front there is slightly more difference, where the numerical solution at the same time gives $\eta_f = 1.953 \cdot 10^{-3} m2/s$ which results in a difference of $\eta_f = 7.1 \cdot 10^{-4} m2/s$. This could be due to the fact that in the analytical case, the injection well is infinitely small and the reservoir infinitely large. Numerical constraints result in a finite value for both those quantities, which might result in some small inaccuracies when comparing them to the analytical solution.

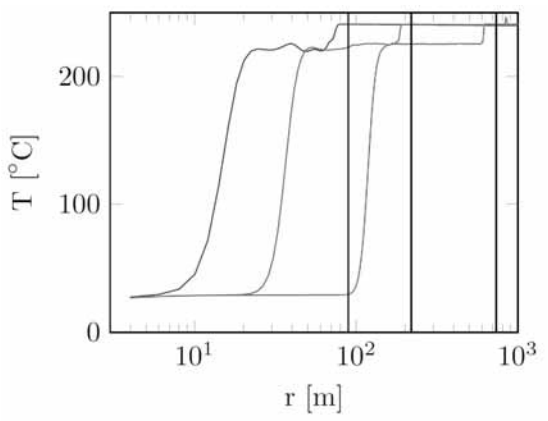

Figure 2: The temperature of the reservoir as a function of distance from the injection well. The temperature profile is given at three different times, after 29.43 days, 213.5 days and 2344 days.

Figure 2 gives a more physical representation of the solution by plotting it as a function of radial distance from the well. In that case it can clearly be seen how the front propagates in time. The vertical lines show the location of the analytical solution for each respective time and seem to show a rather good agreement between the analytical solution and the numerical one.

Figure 3 gives again a more physical representation of Figure 1, but now in terms of time. The phase change from superheated steam to liquid water occurs after 12, 23 and 58 days for the respective distances from the well. After that the hot water slowly cools down as the injection into the well is continued and finally reaches the injection temperature of $29.4°C$.

3 Discussion

This paper has described the applicability of the OpenFOAM framework to take on problems involving phase change in hydrothermal systems. In particular the results show that the numerical model is able to simulate the overall behavior of the benchmark problem of a boiling front, propagating through porous medium, sufficiently well. This is confirmed by comparing the numerical solution $(\eta_f, T_f)_{num} = (1.953 \cdot 10^{-3} m^2/s, 225.6°C)$ to an analytical solution $(\eta_f, T_f)_{an} = (2.663 \cdot 10^{-3} m^2/s, 224.1°C)$, which seem to be in rather good agreement.

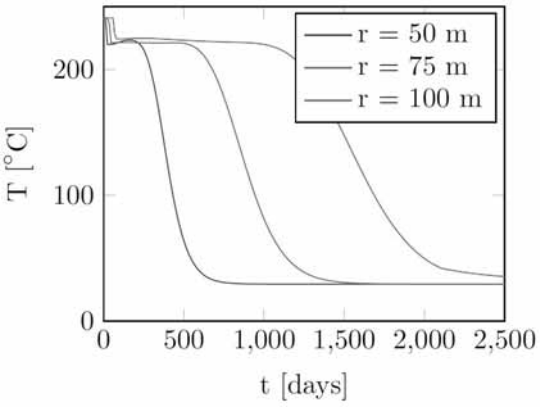

Figure 3: The temperature of the reservoir as a function of time for three different distances from the well.

However both the numerical and analytical solution provided in this paper seems to differ from the solution provided in [13] which uses the same parameters. One explanation for that difference could be that the papers use different thermodynamic formulations for the physical properties. While this paper uses IAPWSIF97 for the physical properties of steam and water, [13] uses the IFC-67 standard.

The ability of the OpenFOAM solver to handle phase change in porous media has also been demonstrated. Phase change can often result in numerical instabilities as displayed by [16]. These instabilities however do not seem to pose a problem in this paper. This is largely due to the fact that by applying Fréchet derivatives a more stable solution can be reached in the two phase region, and in the single phase region an unconditionally stable solution is made possible.

4 Conclusion

This paper has described the applicability of the OpenFOAM framework to take on problems involving phase change in hydrothermal systems. A benchmark case involving a boiling front moving through porous medium, which there exists an analytical solution of, was used to validate the results. The numerical model was also able to simulate the overall behavior of the boiling front sufficiently well. This increases our confidence in the numerical solver outside the limits of the analytical solution, and encourages continued usage of the OpenFOAM framework in geothermal reservoir modeling.

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