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***porousMedia4Foam*: An open-source multiphase reactive transport platform based on OpenFOAM for geothermal applications**

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ABSTRACT

Geothermal energy is an abundantly available renewable energy source that has not yet been exploited to its full potential citing issues related to longevity of geothermal wells. Precipitation of salts within the wells pose a major threat to premature closure of many geothermal wells. A priori knowledge of the minerals that may precipitate within the well is crucial to develop solutions to avoid scaling beforehand. In this regard, *porousMedia4Foam* is used to investigate hydro-geochemistry within geothermal wells. Based on the composition, pressure and temperature conditions of the solution injected through the feedzone, we were able to characterize the potential scaling within the wells. We further analyse high-resolution (Navier-Stokes-based) simulations to probe the scaling formation at the junction between two expanding cross-sections of the well of different diameters.

1. INTRODUCTION

Renewable sources of energy are seen to play a vital role in the foreseeable future to address concerns regarding the emissions of contaminant gases and to further reduce extensive dependence on fossil fuels. World Energy Resources (2013) has reported that there is a rising trend in tapping geothermal energy over the past few decades. However, geothermal energy has not been exploited to its full potential yet (Payam, 2020). A major concern for geothermal wells is their longevity. On the one hand, maintaining the wells integrity at high temperatures and pressures is a challenge (Kiran et al., 2017). On the other hand, scaling within the geothermal

wells (Jamero et al., 2018) has been a cause for the premature closure of many wells before exploiting their full potential.

A priori knowledge of the potential minerals that precipitate within the wells is key to explore solutions to avoid clogging the wells during the operating cycles. In that regard, numerical simulators with hydro-geochemical modelling capabilities come in handy. Though there exist many studies related to scaling in geothermal reservoirs (Wagner et al., 2005) and many studies analysing fluid flow in geothermal wells without considering effects of scaling (Bjornsson, 1987), there is limited literature where scaling is studied exclusively in a geothermal well.

In this work, *porousMedia4Foam* is used to investigate the minerals that may precipitate within geothermal wells inspired from different studies. We compute the saturation indices of several minerals according to the solution injected through the feedzone. Two sets of simulations are considered. First, the saturation index is computed in a one-dimensional (1D) well using a cross-section-averaged formulation (Darcy-like). Second, we use high-resolution modelling using Navier-Stokes-based Direct Numerical Simulations (DNS) to investigate the impact of turbulent flow mechanisms on the scaling formation at the junction of two well segments of different diameters.

In the following (Section 2), we describe briefly the hydro-geochemical coupling used to model the scaling formation in geothermal wells. In Section 3, we discuss the large and fine-scales results. Finally, we end with conclusions and future outlook.

2. HYDRO-GEOCHEMICAL COUPLING STRATEGY

Simulations of scaling formation are run with *porousMedia4Foam* – a multi-scale open-source hydro-geochemical simulation platform developed by the authors to model reactive transport phenomena at multiple scales i.e. at the pore-, hybrid- and Darcy-scales (Soulaine et al., 2021). *porousMedia4Foam* is built on the skeletal framework of OpenFOAM (<https://www.openfoam.org>) for solving for flow and transport and has been successfully coupled with PHREEQC to account for geochemistry (<https://www.usgs.gov/software/phreeqc-version-3>). The code is available at <https://github.com/csoulain/porousMedia4Foam>.

2.1. Flow and transport mathematical model

The package comprises of several flow solvers such as the ‘constantVelocityFoam’ – assigns a constant velocity field within the flow domain, ‘dbsFoam’ – solves the Darcy-Brinkman-Stokes equation and ‘darcyFoam’ – solves the Darcy's equations. *porousMedia4Foam* also includes an extensive set of models that describes the evolution of porous media and fluid properties.

In this study, we investigate flow and scaling formation, first at the scale of the well using a 1D approach, and then, using high-resolution 3D simulations to interrogate emerging processes at the junction between two segment of different diameters.

In the first case, governing equations are cross-section-averaged. The resulting equations form a Darcy-like system that is solved using *darcyFoam* solver. For an incompressible fluid, the mass balance equation in a well comprising of varying cross-sections (A_c) is given by,

$$\frac{\partial}{\partial z}(A_c v_f) = 0 \quad [1]$$

where v_f refers to the fluid velocity defined by cross-section averaged momentum that looks like Darcy's law,

$$v_f = \frac{-k}{\mu} \left(\frac{\partial p}{\partial z} - \rho g_z \right) \quad [2]$$

k is a friction factor that depends on the well diameter and flow rates, μ is the fluid viscosity and $\partial p / \partial z$ is the pressure gradient. The friction factor is computed by a Colebrook-White model. Though we are interested in 1D analysis, the cross-sectional area A_c is integrated into the mass balance equation (Eq. 1) to account for change in cross-sectional areas. Substituting Eq. 1 in Eq. 2 results in a Laplacian equation to be solved for the pressure. Once the pressure is computed, the

velocity is calculated following Eq. 2, and transport equations for species are computed to update the concentration profile.

In the second case, we use Navier-Stokes-based simulations to investigate the saturation index at the vicinity of the corners of the expanding cross-section of the well. The simulation is performed in two consecutive steps. First, a steady-state Reynolds Average Navier-Stokes (RANS) simulation based on k-Epsilon model is run with *simpleFoam*. Then, resulting velocity profile is used in *porousMedia4Foam* (using *constantVelocityFoam*) to transport chemical species and compute geochemistry.

2.2 Coupling of OpenFOAM with PHREEQC

In this work, we use the *phreeqcRM* geochemical package that acts as an interface between OpenFOAM and PHREEQC. The coupling between the packages relies on an operator splitting strategy. We use the Strangs algorithm in which advection-dispersion of chemical species is solved for half a time-step initially, the geochemistry for a full time-step, and the transport equation is computed for the remaining half time-step.

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (v_f c_i) - \nabla \cdot (D_i \cdot \nabla c_i) = 0 \quad [3]$$

In the transport equation, C_i is the species concentration, D_i is the effective dispersion tensor that accounts for molecular diffusion and hydrodynamic dispersions. The geochemical time step is run by PHREEQC. The sequential order of steps followed in *porousMedia4Foam* is illustrated in the form of a flowchart shown in Fig. 1.

The hydro-geochemical coupling strategy implemented in *porousMedia4Foam* has been extensively benchmarked against state-of-the-art reactive transport packages for well established cases (Pavuluri et al., 2022).

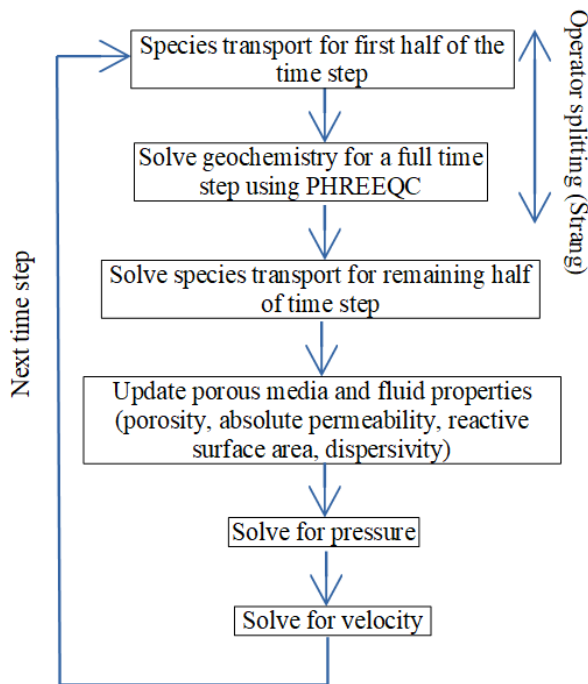


Fig. 1: Sequential steps followed during solving a hydro-geochemical time step in porousMedia4Foam.

3. HYDRO-GEOCHEMICAL INVESTIGATION OF GEOTHERMAL WELLS

In this section, we discuss specifics of two geothermal wells, well #1 that is straight and well #2 with three subsections of different diameters. Both the hydraulic conditions and the chemical reactivity of the pumped solutions are investigated.

3.1 Geothermal well #1

Well #1 is straight with a constant diameter of 0.244 m and a length of 2,600 m. The reservoir temperature is about 120°C whereas pressure is 250 bar. Wellhead pressure is 10 bar and temperature is 104°C. According to temperature and pressure conditions at the boundaries of the well, the fluid is supposed to remain under liquid phase (no degassing). We consider a linear temperature gradient in the well between the feedzone and the wellhead.

The geometry of the well allows testing the code on a simple application case. First, the fluid velocity is estimated to about 0.40 m.s⁻¹. It is constant all along the well and the impact of fluid density variations is negligible.

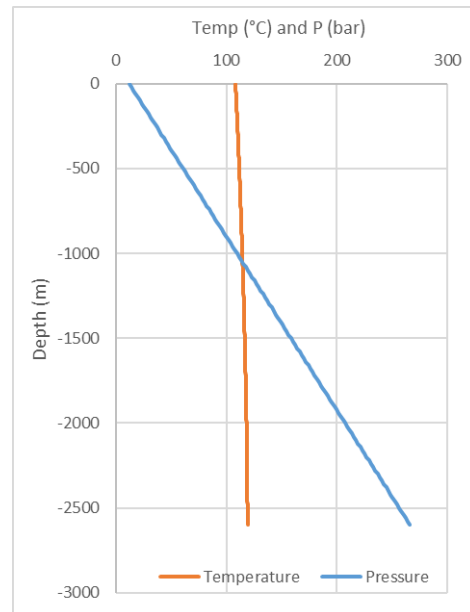


Fig. 2: The temperature (in red) and pressure (in blue) profiles in the geothermal well #1.

Then, we perform reactive transport calculations by considering the chemical composition of the geothermal fluid. The fluid pumped in the reservoir is undersaturated with respect to main minerals such as calcite and quartz but at equilibrium with respect to barite (Fig. 3).

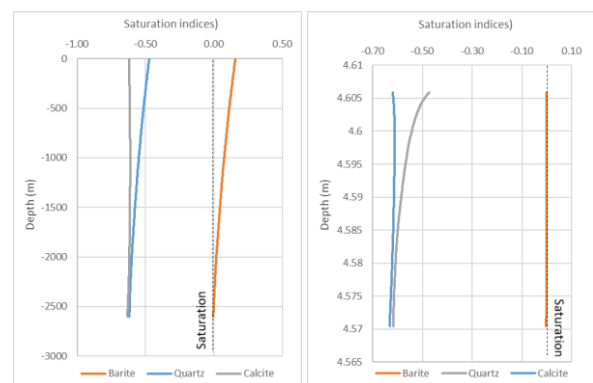


Fig. 3: Saturation indices of quartz, calcite and barite in the well without (left) and with chemical reactivity (right)

A first simulation allows studying the evolution of the saturation indices along the well. By decreasing temperature, saturation indices of quartz and barite

increases (Fig.3 left). If quartz remains undersaturated in the solution, barite is oversaturated (Fig. 3 - left). A second simulation is then proceeded by activating precipitation of minerals (Fig. 3 - right). Since barite is oversaturated, this mineral precipitates along the well and the deposited amounts of mineral can be estimated.

3.2 Geothermal well #2

The geothermal well is 540 meters deep and it is made of three segments of different cross-sections whose dimension is shown in Table 1 (Baba et al., 2009).

Table 1: Geometrical dimensions of the geothermal well. The feedzone of the well is located at 540 m and well head is at 0m.

Well Interval	Length [m]	Cross-section diameter [m]
0 m – 49 m	49	0.50
49 m – 220 m	171	0.35
220 m – 540 m	320	0.25

The fluid viscosity and density are $\mu = 0.001 \text{ kg/m.s}$ and $\rho = 1000 \text{ kg/m}^3$, respectively.

The aqueous solution that enters through the feedzone comprises of carbon (C), calcium (Ca), magnesium (Mg), barium (Ba), sulfate (SO_4) and silica (Si). The pH of the solution is 5.34. At this stage, a simplified composition of fluid is used. For the specified solution composition, there exists potential to precipitate calcite (CaCO_3), dolomite ($\text{CaMg}(\text{CO}_3)_2$) and chalcedony (SiO_2) within the well. The chemical reactivity of barite is also followed during the simulations.

3.2.1 1D simulation in geothermal well #2

The well is discretized by 540 cells along the length of the channel ($\Delta y = 1 \text{ m}$). The three different cross-sectional areas of the well have been assigned to the setup according to the data provided in Table 1. The friction coefficient is computed through the cross-section diameter and the flow rate using the Colebrook-White formula.

According to the available field data, the feedzone is set a Dirichlet boundary condition for pressure $p_{\text{feedzone}} = 50 \text{ atm}$ and $p_{\text{wellhead}} = 3 \text{ atm}$. The velocity at the boundaries is a zero gradient Neumann boundary. The temperature at the feedzone is $T_{\text{feedzone}} = 180^\circ\text{C}$ and $T_{\text{wellhead}} = 130^\circ\text{C}$.

Fig. 4 shows the pressure and temperature profiles in the geothermal well #2. The pressure drop is more pronounced in the thinner cross-section of the well due

to larger viscous dissipation. On the other hand, the thicker cross-section of the well shows a lower pressure drop due to lesser viscous dissipations. The impact of degassing in the well can be observed on the temperature profile: temperature suddenly decreases at 100 m depth because of phase change.

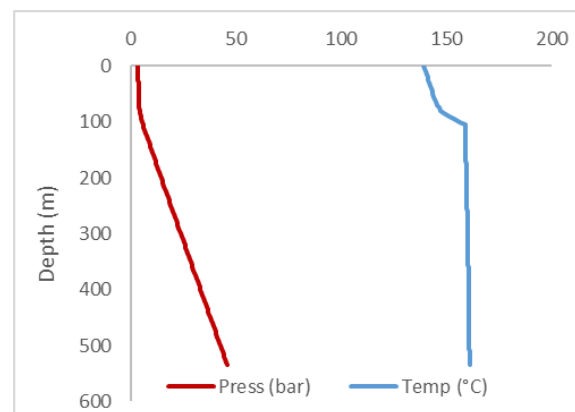


Fig. 4: The pressure (in red) and temperature (in blue) profiles in the geothermal well #2.

The saturation index of calcite and chalcedony is shown in Fig. 5.

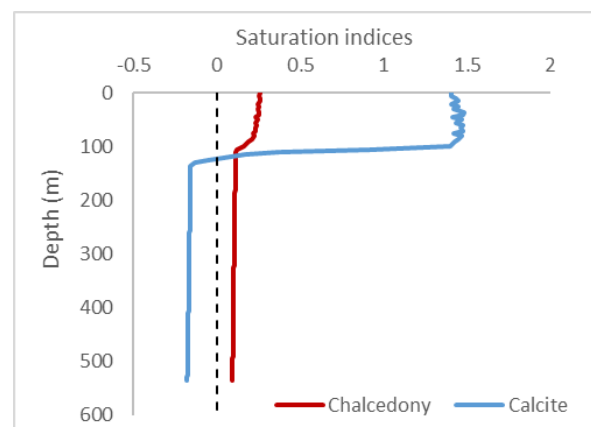


Fig. 5: The saturation index profile for minerals – calcite (in blue) and chalcedony (in red) in the geothermal well #2. The dashed black line indicates equilibrium (saturation index of 0) for reference.

The saturation index of calcite (shown in continuous blue line) increases towards the wellhead. First undersaturated in the lower part of the well, it becomes positive at 100 m depth indicating that calcite is oversaturated and ready to precipitate within the well (due to the fluid composition initially selected). This sudden increase is mainly due to the degassing. CO_2 is exsolved and pH increases involving the oversaturation of calcite and the risk of calcite precipitation. On the other hand, chalcedony is more soluble at high temperatures. Hence, the saturation index of

chalcedony (shown in continuous red line) rises towards the wellhead. Close to the feedzone, the saturation index of chalcedony is close to zero. Moving towards the wellhead, the saturation index of chalcedony increases indicating oversaturation of this mineral in the well and a potential precipitation, mainly in the upper part of the well.

3.2.2 High-resolution simulations observations

The impact of hydrodynamics on the scaling formation at the change of cross-section has received little attention so far. We use Navier-Stokes-based simulations to interrogate emerging processes in this area of the well.

The geometry consists in a 2m long subset of the geothermal well #2 centered on the change of diameter from 0.5 to 0.35 m. It is described by a 2D axisymmetric domain meshed with 9800 hexahedral cells with refinement near the walls. A constant velocity of $0.44 \text{ m}\cdot\text{s}^{-1}$ is applied at the bottom boundary. The top boundary has a fixed pressure value (0 Pa). No-slip conditions is used on the walls. We use the k-Epsilon model to compute turbulent flow in the well. The resulting steady-state velocity profile is then used in our coupled hydrogeochemical package to compute the geochemistry.

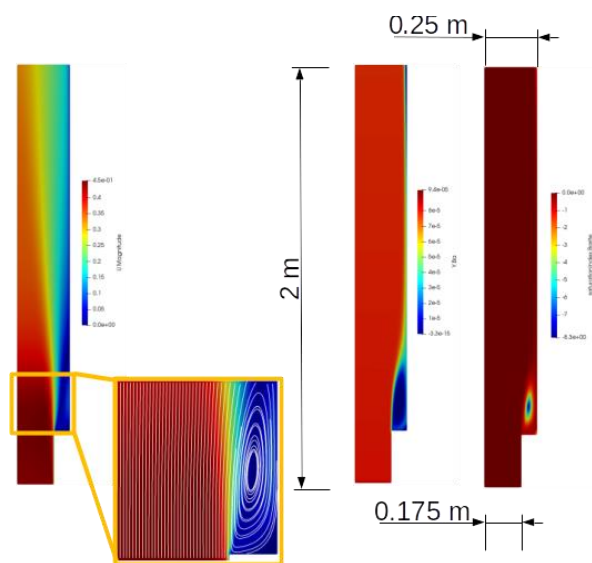


Fig. 6: Left: flow profile in the well where the cross-section expands with vortices developed at the corners of the expanding cross-section of the well. Right: Barium concentration profile and barite saturation index

Typical results are shown in Fig. 6. As expected, we observe a fluid recirculation at the corners of the expanding cross section of the well. These corner zones act as mixing zones for the chemical species. Recirculation could modify chemical concentrations in the fluid and impact the saturation indices of precipitable minerals (we only show barite saturation index in Fig 6). The corner zones are therefore a favourable location for the creation of seeds that move inside the well, eventually. These disseminated seeds can then become ideal precursors for larger precipitations.

4. CONCLUSIONS

A novel hydro-geochemical simulation platform *porousMedia4Foam* has been used to address questions related to minerals that may precipitate within the geothermal well. *porousMedia4Foam* benefits from the coupling of OpenFOAM with PHREEQC where the flow physics is solved using OpenFOAM whereas the geochemistry is solved using PHREEQC.

The code was applied to different geometries of geothermal wells, with various pressure and temperature conditions. It allows calculating the pressure and temperature profiles in the well, fluid velocities and predicting the degassing. The coupling between transport and chemistry allows estimating the reactivity of geothermal fluids in the well and the potential precipitation of minerals due to temperature changes or phase changes.

High-resolution simulations (Navier-Stokes-based) have been run to account for bridging of scales. This high-resolution simulation of hydrochemical processes is the first attempt to model the scale formation in geothermal well. We noticed mixing zones as consequence of vortices developed at expanding cross-sections of the well that are favorable for the development of precipitable minerals. The coupled hydrogeochemical OpenFOAM-PHREEQC platform introduced in this paper has all the capabilities to investigate these specific locations in detail in future studies.

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