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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 priory knowledge regarding the potential minerals that may precipitate within the well may result in finding solutions to avoid scaling beforehand. In this regard, *porousMedia4Foam* is used to investigate hydro-geochemistry within a geothermal well. For the solution that is injected through the feedzone, we noticed that the system is oversaturated with respect to some minerals, which indicate potential scaling within the well. We further analyse high-resolution (Navier-Stokes-based) simulations for the well where we realise potential mixing zones caused due to the vortices that developed at the corners of the expanding cross-sections of the well.

1. INTRODUCTION

The 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 the fossil fuels. World Energy Resources (2013) has reported that there has been a rising trend in tapping the geothermal energy over the past few decades. However, geothermal energy has not yet been exploited to its full potential (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 wells (Jamero et al., 2018) has been a cause for the closure of many wells before exploiting the full potential of the renewable source of energy.

A priory knowledge regarding the potential minerals that may precipitate within the wells may provide possibilities to explore for solutions to avoid clogging of the wells during the operation cycles. In this 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 analysing the fluid flow in the geothermal well without considering effects of scaling (Bjornsson, 1987), there is limited literature where scaling is studied exclusively in a geothermal well.

The authors have developed *porousMedia4Foam* - an open-source hydro-geochemical simulation platform that can model reactive transport phenomenon at multiple scales i.e. at the pore-, hybrid- and Darcy-scales (Soullaine et al., 2021). *porousMedia4Foam* is built on the skeletal framework of OpenFOAM (<https://www.openfoam.com>) and has been successfully coupled with PHREEQC (<https://www.usgs.gov/software/phreeqc-version-3>). OpenFOAM is used to solve for the hydrology, whereas PHREEQC is used to solve for the geochemistry.

In this work, *porousMedia4Foam* is used to investigate the potential minerals that may precipitate within a geothermal well inspired from Baba et al. (2009). We compute the saturation indices of several minerals according to the solution that is being injected through the feedzone. The investigation has been performed considering a one dimensional well with a Darcy-like formulation. We noticed that the saturation index for

several minerals is over unity i.e. these minerals are oversaturated and ready to precipitate in the well whereas, there also exist minerals that remain undersaturated i.e. these minerals require more concentration of specific species to commence precipitation. We also investigated the flow phenomena in the geothermal well at high-resolution using Navier-Stokes-based Direct Numerical Simulations (DNS). In fact where the cross-section of the well increases, we noticed vortices being generated at the corners of the well.

In the next section, the mathematical expressions used to model the case and the hydro-geochemical coupling strategy is briefly explained. In Section 3, we discuss the case setup and the results. Finally, we end with conclusions and future outlook.

2. POROUSMEDIA4FOAM

The multi-scale open-source hydro-geochemical code – *porousMedia4Foam* is available at <https://github.com/esoulain/porousMedia4Foam>.

porousMedia4Foam comprises of several 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 comprises of an extensive set of models that describes the evolution of porous media and fluid properties. *porousMedia4Foam* has also been extensively benchmarked against state-of-the-art reactive transport packages for well established cases (Pavuluri et al., 2022).

2.1. Mathematical model

We investigate the flow physics solving a one dimensional system arising from the cross-section averaging of Navier-Stokes equations.

For an incompressible fluid, the mass balance equation in a well comprising of varying cross-sections (A_c) is given by,

$$\nabla \cdot (A_c \cdot v_f) = 0 \quad [1]$$

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

$$v_f = -\frac{k}{\mu} \nabla p \quad [2]$$

k is a friction factor that depends on the well diameter (it is equivalent to the absolute permeability by analogy with porous media), μ is the fluid viscosity and ∇p is the pressure gradient. Note that in Eq. 2, the gravity has been neglected for simplicity. 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 the flow physics occurring in a well having different 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.

The chemical species present within the system are transported according to the following equation,

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

Where ϵ is the porosity of the medium, C_i is the concentration for the chemical species and D_i^* is the effective diffusion tensor that accounts for tortuosity and hydrodynamic dispersion effects.

2.2 Coupling of OpenFOAM with PHREEQC

In the *porousMedia4Foam* toolbox there exist several geochemical packages such as ‘phreeqcRM’ – geochemistry solved using PHREEQC, ‘simpleFirstOrderKineticMole’ – solves first order kinetics, ‘transportOnly’ – solves transport of species (Eq. 3) and ‘flowOnly’ – solves the fluid flow only.

For this work, we use the phreeqcRM geochemical package. The phreeqcRM library acts as a communication link between the OpenFOAM and PHREEQC packages. The coupling between the packages relies on the operator splitting strategy. We use the Strang’s algorithm in which transport of chemical species (Eq. 3) is solved for half a time step initially. This is followed by a full geochemical time step run by PHREEQC. Finally, the remaining half time step for the transport of species is performed. The sequential order of steps followed in *porousMedia4Foam* is illustrated in the form of a flowchart shown in Fig. 1.

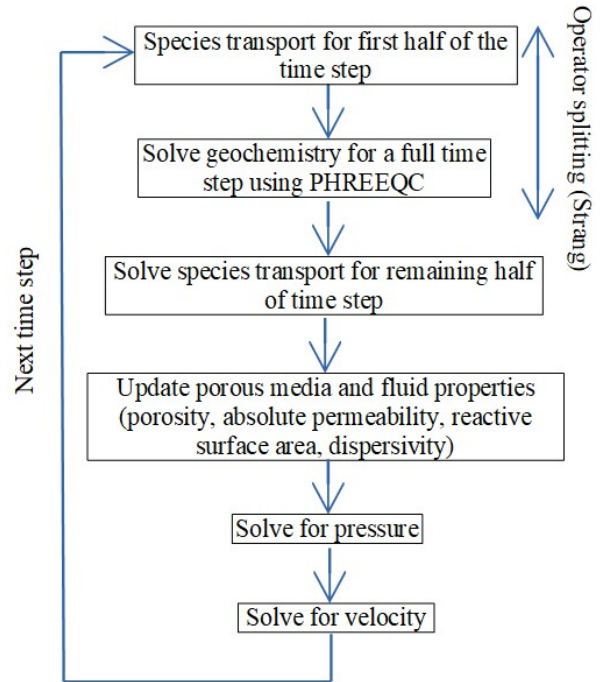


Fig. 1: Sequential steps followed during solving a hydro-geochemical time step in *porousMedia4Foam*.

3. HYDRO-GEOCHEMICAL INVESTIGATION OF A GEOTHERMAL WELL

In this section, we discuss specifics of a geothermal well, aqueous solution composition that is injected through the feedzone, parameters used for modelling the case and our observations.

3.1 Specifics of the geothermal well

The geometrical dimensions of the geothermal well is shown in Table 1.

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]
0m – 49m	49	0.50
49m – 220m	171	0.35
220m – 540m	320	0.25

The aqueous solution that enter through the feedzone comprises of carbon (C), calcium (Ca), magnesium (Mg) 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 quartz (SiO_2) within the well.

3.2 Case setup for numerical investigations

The well has been 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 values that are required in the cross-section averaged momentum equation (Eq. 2) are obtained through the 2D Navier-Stokes simulations. From these simulations, the pressure drop and average velocity data are computed that are used as input parameters in Eq. 2 to determine the friction coefficient. The fluid viscosity is set to $\mu = 0.001 \text{ kg/m.s}$. The friction coefficient in the thinner cross-section of the well is $k_0 = 2.6 \times 10^{-9} \text{ m}^2$, $k_1 = 5.1 \times 10^{-9} \text{ m}^2$ in the intermediate cross-section, and $k_2 = 1.03 \times 10^{-8} \text{ m}$ in thicker cross-section of the well.

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 $T_{\text{wellhead}} = 100^\circ\text{C}$.

3.3 Results

Fig. 2 shows the pressure and velocity profiles in the geothermal wells for the setup discussed in Section 3.2.

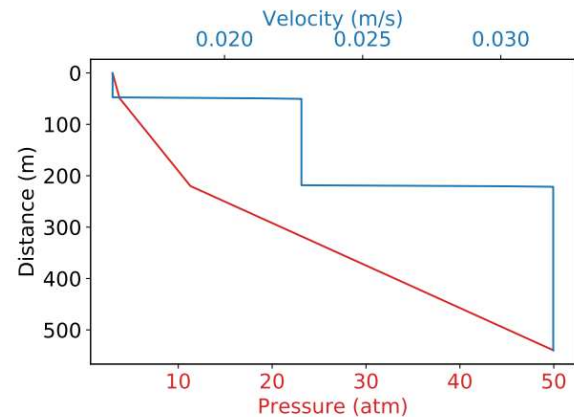


Fig. 2: The pressure (in red) and velocity (in blue) profiles in the geothermal well.

As observed in Fig. 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 varying cross-sections of the well can be observed in the velocity profile where larger velocities exist in the thinner cross-section of the well. As the well diameter increases, the average velocity within the section decreases to balance the mass (Eq. 1).

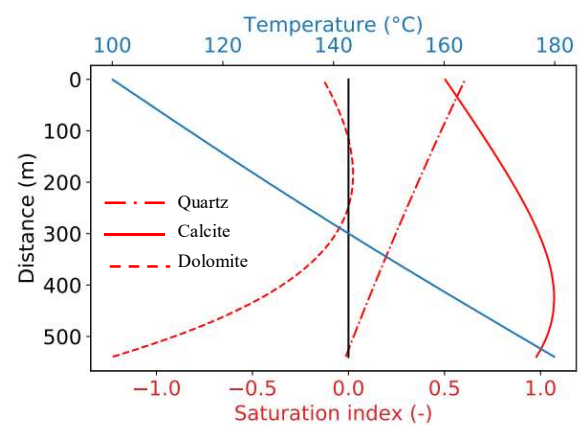


Fig. 3: The saturation index profile for minerals – calcite, dolomite and quartz in the geothermal well. The continuous black line indicates equilibrium (saturation index of 0) for reference and the blue line indicates the temperature.

The saturation index of calcite, dolomite and quartz is shown in Fig. 3. Note that the temperature at the feedzone is 180°C and at the wellhead the temperature is 100°C .

Calcite is more soluble at low temperatures. Hence the saturation index of calcite (shown in continuous red line) reduces towards the wellhead. However, at all times the saturation index of calcite is over unity indicating that calcite is oversaturated and ready to precipitate within the well (due to the fluid composition initially selected). On the other hand, quartz is more soluble at high temperatures. Hence, the saturation index of quartz (shown in dash-dotted red line) rises towards the wellhead. Only at the feedzone, the saturation index of quartz is equal to zero. Moving towards the wellhead, the saturation index of quartz is above unity indicating oversaturation of the mineral in the well. Finally, the saturation index of dolomite (shown in dashed red line) largely remains undersaturated. At a distance between 140 m – 280 m, the saturation index of dolomite is equal to 0 or slightly oversaturated.

3.4 High-resolution simulations observations

In future works, to better predict the hydro-geochemical interactions occurring within the geothermal wells using cross-section averaged models, it is essential to investigate the flow physics at higher resolution using Navier-Stokes simulations. Any vital observations at that degree of refinement will be included into the 1D cross-section averaged model (Eq. 2).

For the Navier-Stokes-based simulation, we consider a 2D setup as shown in Fig. 4 which comprises of 3.5 million cartesian cells ($\Delta x = \Delta y = 5 \text{ mm}$). The Navier-Stokes equations are solved until steady-state conditions are reached.

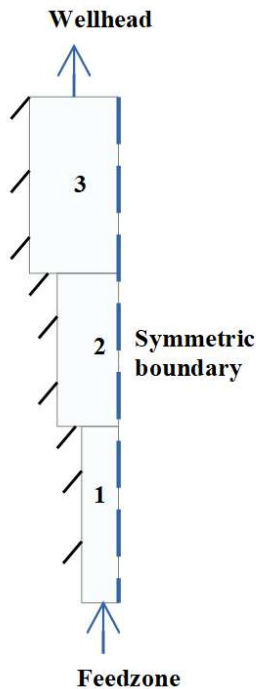


Fig. 4: Case setup for the 2D simulation. 1, 2 and 3 refer to the three cross-sections of the geothermal well indicated in the Table 1.

The pressure at the feedzone is $p_{feedzone} = 50 \text{ atm}$ and at the wellhead is $p_{wellhead} = 3 \text{ atm}$. The velocity at the boundaries is set to a zero gradient boundary condition.

For the setup, we observe an interesting flow pattern that occur at the corners of the expanding cross-section of the well as shown in Fig. 5.

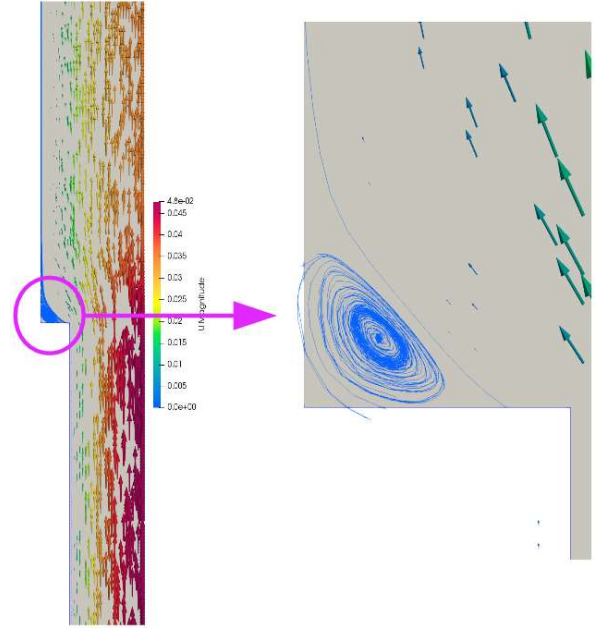


Fig. 5: Left: flow profile in the well where the cross-section expands. Right: vortices developed at the corners of the expanding cross-section of the well.

According to the boundary conditions used in the setup (no-slip on the wall), we notice a parabolic flow profile along the horizontal axis within all the sections of the well as seen in Fig. 5 (left). As the cross-section of the well increases, the flow velocity decreases to conserve mass as seen in Fig. 5 (left). An interesting observation was that of vortices developed at the corners of the expanding cross-sections of the well as shown by the streamlines in Fig. 5 (right). These corner zones may act as potential mixing zones for the chemical species. Re-circulation could modify chemical concentrations in the fluid and potentially impact the saturation indices of precipitable minerals. This corner zones can be a favourable location for the creation of seeds that can then move inside the well. 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 potential 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. For the chemical composition of the solution that is fed into the geothermal well, we noticed that the saturation index of

calcite and quartz are above unity and hence oversaturated that indicate potential scaling within the well. However, we noticed that dolomite largely stays undersaturated which indicated minimal chance for recipitation within the geothermal well. High-resolution simulations using Navier-Stokes equations have also been run to account for bridging of scales for future studies. We noticed mixing zones a consequence of vortices developed at expanding cross-sections of the well. These specific location must be investigated in detail since they can be at the origin of potential precipitations of minerals.

World Energy Resources: Geothermal: World Energy Council, 2013.

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