Coupled thermal–hydraulic–chemical modelling of enhanced geothermal systems

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SUMMARY

The study investigates thermal-, hydraulic- and chemically coupled processes of enhanced geothermal systems (EGS). On the basis of the two existing numerical codes, the finite element program FRACTURE and the geochemical module of CHEMTOUGH, FRACHEM was developed, to simulate coupled thermal–hydraulic–chemical (THC) processes, accounting for the Soultz specific conditions such as the high salinity of the reservoir fluid and the high temperatures. The finite element part calculates the thermal and hydraulic field and the geochemical module the chemical processes. According to the characteristics of the Soultz EGS reservoir, the geochemical module was modified.

(i) The Debye–Huckel approach was replaced by the Pitzer formalism.
(ii) New kinetic laws for calcite, dolomite, quartz and pyrite were implemented.
(iii) The porosity–permeability relation was replaced by a new relation for fractured rock.
(iv) The possibility of re-injecting the produced fluid was implemented.

The sequential non-iterative approach (SNIA) was used to couple transport and reactions. Sensitivity analyses proved the proper functionality of FRACHEM, but highlighted the sensitivity of the SNIA approach to time steps. To quantify the FRACHEM results, a comparative simulation with the code SHEMAT was conducted, which validated FRACHEM. Coupled THC processes in a fractured zone in the Soultz reservoir at 3 500 m ($T_0 = 165\, ^\circ\text{C}$), which occur as a result of the injection of fluid ($T_{\text{inj}} = 65\, ^\circ\text{C}$) at one end of the zone and the production at the other end, were modelled for 2 yr. Calcite is the most reactive mineral and therefore the porosity and permeability evolution results from the calcite reactions: near the injection point, porosity and permeability increase and near the production well they decrease. After 2 yr, the system seems to be very close to steady-state. Therefore, mineral dissolution and precipitation during the circulation of the fluid in the reservoir do not represent a limiting factor on the EGS reservoir (at 3 500 m depth) performance at the Soultz site. Finally, the numerical transmissivity was compared to the transmissivity of the 1997 circulation test. The fact that the transmissivity decreases during the circulation test, when thermomechanical effects are factored out, points to geochemical processes in the reservoir such as the precipitation of calcite. These findings highlight the importance of THC coupled EGS reservoir models. The integration of geochemical considerations is therefore indispensable for integrated simulations of EGS systems and predictions of its performance.

Key words: EGS, thermal–hydraulic–chemical coupled reservoir modelling, Soultz-sous-Forêts (France), THC code.

1 INTRODUCTION

The European enhanced geothermal system (EGS) research site at Soultz-sous-Forêts is located in France approximately 50 km north of Strasbourg in the NNE–SSW striking Rhine graben between the Vosges and Black Forest mountains to the East and West, respectively (Fig. 1). The site was selected because high heat flow was observed during former oil exploration in this region (Gérard & Kappelmeyer 1989). Since the beginning of the EGS project in 1987, three deep boreholes GPK1 (3590 m), GPK2 (5084 m) and GPK3 (5100 m) were drilled. A fourth borehole (GPK4) is under construction. The future EGS pilot plant module will be a three-well system.
results show that the interaction of the formation fluid with altered granite leads to granite dissolution and porosity increase. Thermodynamic equilibrium calculations set limits in possible processes and, therefore, kinetics is needed to determine if reactions actually happen in a reasonable time. In addition, the Debye–Hückel approach is not adequate to model the Soultz reservoir regarding the high salinity of the formation fluid (Durst & Vuataz 2001). An approach more suited to calculate the activity coefficients for ions for saline solutions with ionic strengths >0.8 are the Pitzer equations (Pitzer 1973, 1975). The application of the Pitzer theory for the Soultz system was first studied by Azaroual (1992). He highlighted the need for this approach but also stressed its difficulties. Yet in his studies, he simulated interaction of unaltered granite with distilled water and compared these results to experimental findings. Consequently, the model is not representative for the Soultz reservoir. Jacquot (2000) carried out kinetic simulations of the interaction between altered granite and the formation fluid. The models contained the main minerals of the altered Soultz granite except sulphides and sulphates, but including clay minerals. In his results, he shows that the carbonates are the most reactive minerals in the Soultz EGS system. However, these models are still based on the Debye–Hückel formalism.

The previous works were helpful in understanding the system but were not directly applicable for the intended coupled modelling. None of these models was able to simulate the thermal–hydraulic–chemical (THC) coupled processes for the conditions at the Soultz EGS system.

To perform representative simulations, a computer program that allows the simultaneous modelling of THC coupled processes for temperatures up to 200 °C and high-saline fluids has to be used. Geochemical kinetic modelling of hot brines is rarely done, especially when coupled with thermal and hydraulic processes. THC coupled codes exist only for either hot diluted fluids or cold brines: on the basis of Tough (Pruess 1991), CHEMTOUGH (White 1995) and TOUGHREACT (Xu & Pruess 1998) were developed. Both apply the Debye–Hückel approach to calculate the activity coefficients. SHEMAT (Clauser 2003) in contrast uses the Pitzer equations, but is generally valid for temperatures up to 90 °C. Other codes such as CSP (Geiger et al. 2001) integrate the Pitzer equations and are valid up to high temperatures but do not account for chemical kinetics. Thus, none of these codes entirely fulfils the claims for Soultz conditions.

This study aims at predicting the long-term behaviour of the EGS reservoir at Soultz by investigating the THC coupled processes. In the following, the geology at Soultz is described and a new code FRACHEM to simulate THC coupled processes according the Soultz conditions is presented. To test the capability of the code, sensitivity studies are carried out and a benchmark with SHEMAT is undertaken. FRACHEM is then applied to simulate the long-term behaviour of the Soultz EGS reservoir and the results are compared to field data.

2 GEOLOGY

The Rhine graben forms the central part of the great Western European rift zone from the Mediterranean to the North sea and Scandinavia. Its tectonic structure is characterized by prominent north–south striking faults and kilometre wide horsts and grabens. The Soultz site corresponds to a local horst structure (Genter & Traineau 1996) with a lateral elevation of ~500 m. The topmost part of the horst and its cover are traversed by several large fault systems parallel to the graben shoulder, which are well known from oil exploration wells and are even partly visible on the surface morphology.
2.1 Granitic host rock

The granitic host rock (∼350 Ma) at Soultz has been intensively investigated since the drilling of GPK2 (Genter 1990; Traineau et al. 1991; Azaroual 1992; Jacquot 1998). The top is at 1400 m depth (Gérard & Kappelmeyer 1991) and is directly overlain by Buntsandstein sandstone, Muschelkalk limestone and a thick pile of less permeable sediments (Keuper, Jurassic, Oligocene). The granite underwent an early pervasive alteration stage, which is widespread in the massif. Transformation of primary minerals (biotite, hornblende, plagioclase) has given way to the secondary assemblages, where chlorite is the most common phase. Later vein alteration related to fluid–rock interactions developed in the fracture system. Three different granitic host rock facies were distinguished via synthetic calculations by Jacquot (1998): unaltered granite, hydrothermalized granite and vein alteration. The term hydrothermalized refers to hydrothermal alteration in general (result of several phases). The reservoir fluid is not in contact with fresh granite, because of its low fracture density, but with the hydrothermalized granite and the vein alteration. The mineral assemblage of the hydrothermalized granite, which will be used for the subsequent models, consists after Jacquot (1998) of illite (27.7 per cent), quartz (24.8 per cent), k-feldspar (12.6 per cent), montmorillonite (10.0 per cent), calcite (1.6 per cent), pyrite (1.4 per cent), galena (0.8 per cent), chlorite (0.4 per cent) and dolomite (0.3 per cent).

2.2 Composition of reservoir fluid

The reservoir fluids originate from brines within Triassic sediments on the border of the Rhine graben. They became diluted by meteoric water, which dissolved micas and sulphates in the Triassic Buntsandstein and in the granitic basement (Pauwels et al. 2000). As a result of percolation of the fluid into the fractured granitic basement, plagioclases were dissolved and secondary minerals, such as quartz, illite, montmorillonite, calcite, dolomite and pyrite, were precipitated in fractures.

During past circulation and production tests, several fluid samples were taken. In this study, we use the data from analyses of fluid samples from GPK2 collected throughout the 1997 production test and assume that the production fluid samples represent the 3500-m-deep reservoir fluids. The fluid sample we are referring to is KP3-97-600 and was collected at the surface of the production site on 1997 November 16. The laboratory measurements were done by the Centre de Géochimie de la Surface (CGS) in Strasbourg (for details see Jacquot 2000). After Durst (2002), the main fluid components at pH = 5 are: Cl⁻ (1.61 mol kg⁻¹), Na⁺ (1.10 mol kg⁻¹), Ca²⁺ (1.67 × 10⁻¹ mol kg⁻¹), K⁺ (8.67 × 10⁻² mol kg⁻¹), Mg²⁺ (4.96 × 10⁻³ mol kg⁻¹), Fe²⁺ (4.14 × 10⁻³ mol kg⁻¹), SiO₂ (2.36 × 10⁻³ mol kg⁻¹) and SO₄²⁻ (2.30 × 10⁻³ mol kg⁻¹). The total amount of dissolved solids (TDS) is greater than 100 g/l. This means that the reservoir fluids are brines with an ionic force of 1.6.

3 FRACHEM

Because none of the existing codes entirely fulfilled the claims for Soultz conditions, a new THC coupled code called FRACHEM was created from two existing codes, FRACTURE (Kohl & Hopkirk 1995) and CHEMTOUGH (White 1995). FRACTURE was chosen because it was developed especially to model the long-term behaviour of EGS reservoirs (Kohl et al. 1995). FRACHEM was developed in close cooperation with the University of Neuchâtel in Switzerland.

3.1 Code development

3.1.1 Modifying CHEMTOUGH to the geochemical module of FRACHEM

The characteristics of the Soultz system, such as the high salinity of the fluids and the re-injection of the fluid after production, preclude the use of the original geochemical model implemented in CHEMTOUGH. Therefore, Durst (2002) had to make several modifications.

(i) As a result of the high salinity of the fluids, the Pitzer formalism was implemented to calculate the activity coefficients.

(ii) CHEMTOUGH contained simple kinetics for most mineral reactions. Some mineral reactions like carbonate minerals were not included. However, the use of the Pitzer approach raises new problems such as the lack of parameters for aluminum, and Mg²⁺ and Fe²⁺ at higher temperatures. Other minerals like feldspar and galena are intended to be incorporated in the model at a later stage. The kinetic modelling of clays has also to be postponed as a result of the lack of available data and the complexity of the model including variable composition minerals. Thus, only calcite, dolomite, pyrite and quartz could be integrated into the model. New kinetic laws for these minerals were implemented (see Appendix).

(iii) The empirical equations to calculate the effect of porosity changes on permeability were replaced. Because the fluid circulation in the Soultz system occurs in clusters of fractures and highly altered granite, a combination of Northon & Kapp’s (1977) fracture-type model and the grain-type porosity model after Bolton et al. (1996) was implemented.

(iv) Modifications were made so that re-injection of produced fluids is now possible with CHEMTOUGH.

3.1.2 Coupling FRACTURE and CHEMTOUGH to FRACHEM

To couple thermal, hydraulic and chemical processes, different methods come into consideration: one-step (global implicit), sequential non-iterative (explicit) and the sequential iterative (explicit/implicit) approach (Steefel & MacQuarrie 1996). FRACHEM adopts a sequential non-iterative approach (SNIA) (Durst 2002; Bächler 2003). By this method, first the reaction equations are solved, then the fluid flow between the elements is calculated and finally the chemical species are transported from element to element. The method can lead to numerical instabilities, because reaction rates calculated at time t are supposed to stay constant until t + Δt without considering further chemical reactions resulting from changes in fluid composition and temperature during the interval Δt. To reduce such instabilities, time steps have to be small (see Section 3.3).

FRACHEM consists of a set of modified FRACTURE and CHEMTOUGH routines. The coupling sequence is illustrated in Fig. 2. First, FRACTURE calculates thermal and hydraulic processes resulting temperature T and pressure P distributions as well as fluid velocities. The transient heat transport equation (Sauty 1981) is

\[
\frac{\partial}{\partial t}[(\rho_m \times c_m) \times T] = -\nabla[(\Phi \times \rho_f \times c_p_f \times v_f) \times T] \\
- (\lambda_m \times \nabla T) + q_H. \tag{1}
\]

\(\Phi\) is the porosity, \(\rho_f\) the fluid density, \(c_m\) the matrix density, \(c_p_f\) the fluid heat capacity, \(c_m\) the matrix heat capacity, \(v_f\) the fluid particle velocity, \(\lambda_m\) the matrix thermal conductivity and \(q_H\) a heat source.
The transient hydraulic equation (Bear 1979) is

\[
\frac{\partial}{\partial t} \left( \frac{S_i}{P} \right) = -\nabla \left[ K \times \left( \nabla P + \rho_0 \times g \times \nabla z \right) \right]
- (\rho_0 \times g \times \nabla z \times \beta_f \times \Delta T)).
\] (2)

\(S_i\) is the storativity, \(K\) hydraulic conductivity, \(\rho_0\) initial fluid density, \(g\) gravity, \(z\) depth and \(\beta_f\) thermal expansion coefficient.

Because FRACTURE is a finite element code and CHEMTOUGH a finite volume code, an interface was written to unify the different geometrical information required by both codes. The interface also calculates the volume of fluid transported from element to element based on the fluid velocities from FRACTURE. Then, CHEMTOUGH routines calculate the chemistry subject to temperature, pressure and transported fluid amount (Steefel & MacQuarrie 1996):

\[
\frac{\partial}{\partial t} (\Phi \times C_i) = -\nabla [(v \times C_i) - (\Phi \times \tau \times D_i \times \nabla C_i)] + q_i.
\] (3)

\(C_i\) is the concentration of a species \(i\), \(v\) particle velocity, \(\tau\) tortuosity of the medium, \(D_i\) diffusion coefficient and \(q_i\) a chemical source.

It is assumed that mechanical dispersion can be neglected because a simple fracture system is treated. \(C_i\) is calculated by chemical kinetics where the most general form is (Krauskopf & Bird 1995):

\[
\frac{d[C_i]}{dt} = r(T) \times s \times (SI^{m-1})^n
\] (4)

\(r\) is the reaction rate, \(s\) is the mineral surface, \(SI\) is the saturation index and \(m, n\) are empirical constants. The specific reaction laws for each mineral are listed in the Appendix.

Finally, the effect of the fluid–rock interaction on \(\Phi\) and \(K\) is calculated (Durst 2002), the updated \(\Phi\) and \(K\) values are returned to the FRACTURE routines and the cycle restarts.

In the following, sensitivity analyses are conducted to test the numerical behaviour of FRACHEM.

### 3.2 Numerical model

Fig. 3 sketches a simplified physical model of the Soultz reservoir: the injection and the production well are connected through fractured zones surrounded by a granitic matrix. The zones are 0.1 m wide, 200 m deep and \(\Phi = 10\) per cent. Each zone consists of several fractures. One of these fractured zones is modelled. All following simulations were performed with the same model geometry (Fig. 4). Near the injection (at \(x = 50\) m) and the production point (at \(x = 500\) m), the discretization of the mesh is finer than elsewhere. Fig. 4(a) illustrates the refined area around the injection point and the fracture (black). The area around the production well has the same geometry. Fig. 4(b) represents the entire model. The roughest mesh has 198 rectangular quadrilateral elements consisting of 238 nodes. Because the model is symmetric to the \(x\)-axis, only the upper part of the model (\(y > 0\)) was simulated to save calculation time.

The initial temperature was set to \(T_0 = 165\) °C (reservoir temperature at 3500 m depth) and Dirichlet boundary conditions were applied to the upper, left and right model boundary. A constant overpressure of 2 MPa was assumed at the injection well and hydrostatic conditions at the production. In each of the fractured zones fluid was injected at \(q_{inj} = 0.2\) l/s and \(T_{inj} = 65\) °C. The injection rate for each fracture was \(q_i = 2 \times 10^{-3}\) l/s. This is based on the fluid production rate \(q_{tot} = 25\) l/s (1997 circulation test) and assuming 125 fractured zones (\(q_{tot}/q_{inj} = 125\) fractured zones) consisting of 100 fractures. The hydraulic model parameters are calculated following empirical laws from laboratory experiments that measured flow rates through fractures as a function of the pressure gradient (Bear 1979). The thermal model parameters are calculated using the equations from Pribnow (1994) to calculate the arithmetic means. Table 1 lists the resulting parameter values for the matrix, fracture

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and fluid. The chemical composition of the matrix and the reservoir fluid at $T_0 = 165$ °C is given in Table 2. The composition of the fluid was recalculated from the chemical analyses of Jacquot (1998) assuming that the fluids are in equilibrium with the host rock. The results were obtained using codes based on the Pitzer concept such as TEQUIL (Duan et al. 1996) and EQ3NR (Wolery 1992).

### 3.3 Sensitivity analyses

To investigate the numerical behaviour of FRACHEM, the sensitivity to time steps and mesh discretization was tested. The primary focus is to evaluate the capacity of the code and the model sensitivity. Details of the simulation results are of secondary importance. A discussion of the results is given with the long-term model.

Because the SNIA method is very sensitive to time steps, the effect of different time steps is investigated. Empirical formulae indicate that for 1-D models numerical instabilities are in an acceptable range for Courant numbers $Cr < 1$. Knowing that $Cr = (v \times \Delta t)/element$ length, for resulting fluid velocities of $3.7 \times 10^{-4}$ m s$^{-1}$ and (smallest) element lengths of 0.5 m, the largest time step $\Delta T_{max}$ (for $Cr < 1$) is $10^3$ s. Our sensitivity analyses show that, for the present 2-D model, $\Delta T_{max} = 10^2$ s. This is shown in Fig. 5

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Fracture</th>
<th>Matrix</th>
<th>Fluid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydraulic conductivity $K_0$ (m$^2$ Pa s$^{-1}$)</td>
<td>$8.5 \times 10^{-8}$</td>
<td>$10^{-15}$</td>
<td>—</td>
</tr>
<tr>
<td>Porosity $\Phi_0$ (per cent)</td>
<td>10</td>
<td>0</td>
<td>—</td>
</tr>
<tr>
<td>Thermal conductivity $\lambda$ (W m K$^{-1}$)</td>
<td>2.9</td>
<td>3</td>
<td>0.6</td>
</tr>
<tr>
<td>Density $\rho$ (kg m$^{-3}$)</td>
<td>—</td>
<td>2650</td>
<td>995</td>
</tr>
<tr>
<td>Heat capacity $c_p$ (J kg$^{-1}$ K$^{-1}$)</td>
<td>—</td>
<td>1000</td>
<td>4200</td>
</tr>
<tr>
<td>$\rho c_p$ (J K$^{-1}$ m$^{-3}$)</td>
<td>$2.73 \times 10^6$</td>
<td>$2.65 \times 10^6$</td>
<td>$4.2 \times 10^6$</td>
</tr>
<tr>
<td>Storativity $S_0$ (1/Pa)</td>
<td>$10^{-10}$</td>
<td>$10^{-10}$</td>
<td>—</td>
</tr>
</tbody>
</table>

### Table 2. Chemical model components and initial concentrations.

<table>
<thead>
<tr>
<th>Component</th>
<th>Concentration (mol kg$^{-1}$)</th>
<th>Component</th>
<th>Concentration (mol kg$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$O</td>
<td>$5.55 \times 10^{-1}$</td>
<td>HS$^-$</td>
<td>$7.20 \times 10^{-4}$</td>
</tr>
<tr>
<td>Na$^+$</td>
<td>$9.93 \times 10^{-1}$</td>
<td>CO$_2^-$</td>
<td>$2.41 \times 10^{-7}$</td>
</tr>
<tr>
<td>K$^+$</td>
<td>$8.08 \times 10^{-2}$</td>
<td>OH$^-$</td>
<td>$8.07 \times 10^{-7}$</td>
</tr>
<tr>
<td>Ca$^{2+}$</td>
<td>$1.60 \times 10^{-1}$</td>
<td>Ca(HCO$_3$)$^+$</td>
<td>$2.65 \times 10^{-4}$</td>
</tr>
<tr>
<td>H$^+$</td>
<td>$2.08 \times 10^{-5}$</td>
<td>HCO$_3^-$</td>
<td>$1.96 \times 10^{-3}$</td>
</tr>
<tr>
<td>Cl$^-$</td>
<td>1.46</td>
<td>CaCO$_3$(aq)</td>
<td>$2.81 \times 10^{-6}$</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>$3.80 \times 10^{-2}$</td>
<td>CaSO$_4$(aq)</td>
<td>$3.12 \times 10^{-4}$</td>
</tr>
<tr>
<td>SO$_4^{2-}$</td>
<td>1.16 $\times 10^{-3}$</td>
<td>Quartz</td>
<td>$1.67 \times 10^{-2}$</td>
</tr>
<tr>
<td>H$_2$SiO$_4$</td>
<td>2.17 $\times 10^{-3}$</td>
<td>Calcite</td>
<td>$1.21 \times 10^{+1}$</td>
</tr>
<tr>
<td>Fe$^{2+}$</td>
<td>5.01 $\times 10^{-4}$</td>
<td>Dolomite</td>
<td>1.63</td>
</tr>
<tr>
<td>Mg$^{2+}$</td>
<td>5.43 $\times 10^{-3}$</td>
<td>Pyrite</td>
<td>$8.30 \times 10^{-1}$</td>
</tr>
</tbody>
</table>
that illustrates the calcite reaction rate in the fractured zone (at $x = 300$ m) for five different time steps: the temporal evolution of the reaction rate is the same for time steps of $10$ and $10^2$ s, whereas for all other time steps the reaction rates differ.

The model was refined to test if the mesh discretization has an impact on the results. The results do not differ significantly from the previous findings and, therefore, it can be stated that the mesh discretization does not influence the model results.

4 BENCHMARK WITH SHEMAT

Because no reliable measured data are available, a comparative simulation with the code SHEMAT (Clauser 2003) was conducted to validate the FRACHEM results. SHEMAT is a tool for simulating coupled flow, heat transfer, multicomponent transport and chemical reactions in porous media similar to FRACHEM. It was intensively tested and a laboratory experiment was successfully simulated.

Using the Pitzer approach to determine the activity coefficients, SHEMAT calculates the precipitated or dissolved amount of minerals species of the system Na–K–Mg–Ca–H–Cl–SO₄–OH–(HCO₃–CO₃–CO₂)–H₂O for high salinity and temperatures from 0 to $90\,^{\circ}\,C$. The database. Dolomite was left out, to avoid interactions between calcite and dolomite and to keep the model simple.

For an ideal comparison both the FRACHEM and the SHEMAT models are set up gradually. In a first step, the temperature and the pressure field were simulated. Then, the thermodynamic equilibrium at temperatures of 65 and $90\,^{\circ}\,C$ was calculated. Finally, fully coupled models including kinetics were calculated.

4.1 Temperature and pressure field

The aim of the first model run was to obtain the same temperature and pressure field in the FRACHEM and the SHEMAT model in order to have the same basis for the chemical model. SHEMAT calculates the species concentrations by neutralizing the charge

4.2 Equilibrium calculations

The initial model temperature of $T_0 = 90\,^{\circ}\,C$ required re-equilibration of species and mineral concentrations from Table 2. To compare the thermodynamic modules of FRACHEM and SHEMAT and to check if the Pitzer approach yields the same results, equilibrium concentrations were calculated for a temperature of $T_0 = 90\,^{\circ}\,C$ with SHEMAT.

Table 3 lists all concentrations. In contrast to FRACHEM, SHEMAT calculates the species concentrations by neutralizing the charge
balance of the fluid (Clauser 2003), leading to slightly higher Na⁺ concentrations. Because Na⁺ is not a component of calcite or quartz and does not actively take part in the reactions, this difference has no impact. All other concentrations are in good agreement. Additional equilibrium simulations prove that also at $T_0 = 65$ °C the results for FRACHEM and SHEMAT are similar (Table 3).

### 4.3 Kinetics

With the calculated equilibrium concentrations at $T_0 = 90$ °C as initial parameters, chemical kinetic models were calculated for 6 months simulation time. Based on the resulting reaction rates from the FRACHEM simulation, in the SHEMAT model the initial reaction rates were set for calcite ($10^{-4}$ mol m$^{-2}$ s$^{-1}$) and quartz ($10^{-11}$ mol m$^{-3}$ s). The activation energy for calcite was assumed to be $4 \times 10^{-21}$ J (Sjoberg & Rickard 1984) and for quartz $2.5 \times 10^{-18}$ J (Rimstidt & Barnes 1980). The initial reactive surface of minerals was set to 1 m² per total mineral volume present in each element. The Kozeny–Carman porosity–permeability model was used with the fractal coefficients 1, 2 and 10 for the porosity ranges 0–1, 1–10 and 10–100 per cent, respectively. Sensitivity analyses with SHEMAT showed that refining the mesh does not influence the results. Further sensitivity analyses highlighted that in SHEMAT the maximum time step had to be set to $10^5$ s, as in the FRACHEM model.

Comparing the resulting calcite and quartz concentrations shows that there is no difference in the behaviour of quartz. It neither dissolves nor precipitates in both models. The behaviour of calcite differs, being more reactive in the FRACHEM model than in SHEMAT. The maximum difference occurs near the injection well with 8 per cent more dissolved calcite after 6 months. In the middle of the fracture and near the production well, the difference is smaller. The trend is the same in both models: at the injection point calcite is dissolved and towards the production well it is precipitated. Because both models yield similar equilibrium concentrations at $T_0 = 90$ and $T_0 = 65$ °C, the diverging amount of dissolved and precipitated calcite has to be attributed to different chemical kinetic calculations in FRACHEM (Bächler 2003) and SHEMAT (Clauser 2003). Several factors may contribute: (i) the kinetic laws for the mineral reactions, (ii) the size of the assumed activation energy, (iii) the reaction surface area and (iv) the size of the initial reaction rate.

Sensitivity analyses with SHEMAT showed that varying the activation energy and the initial surface reaction area did not influence the results much. However, varying the initial calcite reaction rate two orders of magnitude to $10^{-2}$ mol m$^{-3}$ s results in concentrations of the same range in the FRACHEM model. Fig. 6 illustrates the results. Maximum concentration differences located again near the injection well are approximately 0.15 mol kg$^{-1}$ (~1 per cent of the initial concentration). The differences in the middle of the fracture and near the production well are approximately 0.05 mol kg$^{-1}$ (~0.5 per cent of the initial concentration).

Unfortunately, SHEMAT does not allow controlling the actual reaction rates but calculates directly the resulting amount of mineral dissolution or precipitation. Therewith, no comparison between the calculated reaction rates of FRACHEM and SHEMAT is possible. It may be assumed that initial SHEMAT calcite reaction rates of $10^{-2}$ mol m$^{-2}$ s result in actual reaction rates of $10^{-3}$ mol m$^{-3}$ s, because all other parameters are nearly identical.

The porosity–permeability models implemented in FRACHEM (model for fractured rocks) and SHEMAT (Kozeny–Carman model) imply different porosities. As a result of the dissolution of calcite, the porosity is increased near the injection well, whereas in the middle of the fracture and near the production well they are decreased, because calcite is precipitated. The 1 per cent excess of calcite that is dissolved in FRACHEM near the injection results in 3.5 per cent (compared with the initial porosity) increased porosity compared with SHEMAT results. The 0.5 per cent of calcite that is precipitated more in the FRACHEM model leads to 0.5 per cent decreased porosity. Different models with varying fractal exponents were tested without achieving major changes in the results.

### 4.4 Conclusion

The comparative modelling validated FRACHEM: the FRACHEM and the SHEMAT model calculate the same temperature development and fluid velocities. Thermodynamic equilibrium modelling at $T_0 = 65$ °C and $T_0 = 90$ °C resulted in comparable species and mineral concentrations for both models. Thus, the Pitzer approach is correctly implemented. Assuming $10^{-2}$ mol m$^{-3}$ s for the initial calcite reaction rate in the SHEMAT model results in a good fit of calcite concentrations. The only major differences between the two codes are the porosity and the permeability distributions resulting from the different porosity–permeability models implemented.

The fact that both models yield sensible results is of great importance, because neither reliable field data nor adequate laboratory experiments are available for comparison. Currently, FRACHEM seems to be better suited than SHEMAT to simulate the long-term behaviour of a fractured EGS reservoir under Soultz conditions because of several factors.

- The chemical thermodynamics are limited to $T = 90$ °C for carbonate minerals in SHEMAT. In FRACHEM these can be calculated

<table>
<thead>
<tr>
<th>Species</th>
<th>$90$ °C FRACHEM (mol kg$^{-1}$)</th>
<th>$90$ °C SHEMAT (mol kg$^{-1}$)</th>
<th>$65$ °C FRACHEM (mol kg$^{-1}$)</th>
<th>$65$ °C SHEMAT (mol kg$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca</td>
<td>$1.6361 \times 10^{-1}$</td>
<td>$1.6283 \times 10^{-1}$</td>
<td>$1.6547 \times 10^{-1}$</td>
<td>$1.6350 \times 10^{-1}$</td>
</tr>
<tr>
<td>Mg</td>
<td>$5.4274 \times 10^{-3}$</td>
<td>$5.4206 \times 10^{-3}$</td>
<td>$5.4274 \times 10^{-3}$</td>
<td>$5.4205 \times 10^{-3}$</td>
</tr>
<tr>
<td>Na</td>
<td>$9.9300 \times 10^{-1}$</td>
<td>$1.0534$</td>
<td>$9.9300 \times 10^{-1}$</td>
<td>$1.0536$</td>
</tr>
<tr>
<td>K</td>
<td>$8.0800 \times 10^{-2}$</td>
<td>$8.0746 \times 10^{-2}$</td>
<td>$8.0800 \times 10^{-2}$</td>
<td>$8.0757 \times 10^{-2}$</td>
</tr>
<tr>
<td>Si</td>
<td>$5.5910 \times 10^{-4}$</td>
<td>$3.6654 \times 10^{-4}$</td>
<td>$3.0643 \times 10^{-4}$</td>
<td>$1.9813 \times 10^{-4}$</td>
</tr>
<tr>
<td>Cl</td>
<td>$1.4600$</td>
<td>$1.4590$</td>
<td>$1.4600$</td>
<td>$1.4592$</td>
</tr>
<tr>
<td>C</td>
<td>$4.3740 \times 10^{-2}$</td>
<td>$4.3039 \times 10^{-2}$</td>
<td>$4.5602 \times 10^{-2}$</td>
<td>$4.3680 \times 10^{-2}$</td>
</tr>
<tr>
<td>S</td>
<td>$2.1904 \times 10^{-3}$</td>
<td>$2.1853 \times 10^{-3}$</td>
<td>$2.1904 \times 10^{-3}$</td>
<td>$2.1857 \times 10^{-3}$</td>
</tr>
<tr>
<td>Calcite</td>
<td>$12.0964$</td>
<td>$12.0729$</td>
<td>$12.0946$</td>
<td>$12.0673$</td>
</tr>
<tr>
<td>Quartz</td>
<td>$167.0016$</td>
<td>$167.0467$</td>
<td>$167.0018$</td>
<td>$167.0561$</td>
</tr>
<tr>
<td>pH</td>
<td>$5.0$</td>
<td>$5.2$</td>
<td>$5.13$</td>
<td>$5.28$</td>
</tr>
</tbody>
</table>

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at least to $T = 200 \, ^\circ C$, which is the reservoir temperature at 5000 m depth.

(ii) The kinetic laws in FRACHEM are especially developed for the Soultz conditions, whereas in SHEMAT one general kinetic law for all minerals is implemented.

(iii) The Kozeny–Carman porosity–permeability model of SHEMAT was derived for porous media. In Soultz however, the target host rock is highly fractured granite and, therefore, the porosity–permeability model implemented in FRACHEM that was developed to simulate fractured media is more suited. In contrast, SHEMAT is clearly better applicable for porous media simulations.

5 LONG-TERM MODEL

The present model was set up to simulate the 1997 circulation test (Kohl 1998). The same geometry as in the previous models was used (Fig. 4). All initial and boundary conditions were the same as before, except the 6-MPa injection pressure above hydrostatic used at the 1997 circulation test. The model parameters were the same as listed in Table 1; only hydraulic conductivity of the fracture was changed to $K_0 = 4.2 \times 10^{-3} \, m^2 \, Pa^{-1} \, s^{-1}$ to account for the modified pressure conditions. Also, the initial chemical composition of the matrix and the fluid at $T_0 = 165 \, ^\circ C$ were the same (Table 2). The injected fluid was of the same chemical composition as the produced fluid. Note that the injected fluid was not equilibrated with respect to $T_{inj} = 65 \, ^\circ C$. The simulation time was 2 yr.

5.1 Temperature evolution

The fluid temperature evolution along the axis of the fractured zone is illustrated in Fig. 7. The injection of fluid at $T_{inj} = 65 \, ^\circ C$ leads to a temperature decrease around the injection point. On its way through the fractured zone towards the production point, the fluid is reheated up to a maximum of $T_0 = 165 \, ^\circ C$ at the production point by the surrounding granitic rock matrix. With increasing simulation time, the temperature in the fractured zone decreases. After 2 yr, a temperature of 155 $^\circ C$ is reached at the production well.

5.2 Chemical processes

The reservoir fluid is assumed to be in equilibrium with the surrounding rock matrix at $T_0 = 165 \, ^\circ C$. Injecting fluid at $T_{inj} = 65 \, ^\circ C$ causes the fluid to become disequilibrated leading to either the dissolution or precipitation of minerals. Instead of the concentrations, the reaction rates of the different minerals will be presented below, because mineral behaviour is best illustrated by the reaction rate. The resulting total amount of dissolved or precipitated minerals is discussed later. Note that negative reaction rates represent mineral precipitation and positive rates dissolution.

5.2.1 Carbonate dissolution and precipitation

Injecting fluid at $T_{inj} = 65 \, ^\circ C$ causes the fluid in the fracture to be undersaturated in calcite and, therefore, calcite dissolves. At the beginning of the simulation, calcite dissolution occurs at the injection point at a rate of $4 \times 10^{-4} \, mol \, m^{-3} \, s^{-1}$. With increasing simulation time, the dissolution zone moves towards the production point (Fig. 8). The maximum dissolution rate of $5.4 \times 10^{-2} \, mol \, m^{-3} \, s^{-1}$ is reached at 27 hr and decreases afterwards. As a result of the dissolution of calcite near the injection well, the fluid is enriched in Ca$^{+2}$. Thus, calcite starts to precipitate with increasing temperature towards the production point. The maximum precipitation rate is reached after 1 yr ($6.8 \times 10^{-4} \, mol \, m^{-3} \, s^{-1}$). From this time onwards, the precipitation rate decreases towards zero, which is the rate at thermodynamic equilibrium.

Fig. 9 illustrates the dolomite reaction rate. Its behaviour is similar to the calcite rate: at the beginning of the simulation dolomite dissolves at $r = 10^{-3} \, mol \, m^{-3} \, s$ (not shown in figure) at the injection point as a result of the injection of fluid at $T_{inj} = 65 \, ^\circ C$. With increasing simulation time, the dissolution zone moves towards the production point. The maximum dissolution rate of $1.85 \times 10^{-5} \, mol \, m^{-3} \, s^{-1}$ is reached after 1 yr ($6.8 \times 10^{-4} \, mol \, m^{-3} \, s^{-1}$). From this time onwards, the precipitation rate decreases towards zero, which is the rate at thermodynamic equilibrium.

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m$^{-3}$s is reached at 0.3 yr and decreases afterwards. Dolomite never precipitates because the calcite precipitation rate is higher than that of dolomite. Therefore, the calcite precipitation consumes all the Ca$^{2+}$ and the CO$_2$ before dolomite is precipitated. The results are in good agreement with the estimated behaviour of the carbonates from the theoretical kinetic model of the Soultz system by Durst (2002).

5.2.2 Quartz precipitation
Quartz precipitates near the injection well as a result of the injection of cold fluid. With increasing simulation time, the temperature in the fracture decreases (Fig. 10) and therefore the range in the fracture where quartz is precipitated broadens and moves towards the production well. The maximum precipitation rate is $1.6 \times 10^{-8}$ mol m$^{-3}$s, which is 1 order of magnitude lower than the reaction rates found by Durst (2002). This might be related to the different model geometry, hydraulic conductivity or pressure boundary conditions.

5.2.3 Pyrite precipitation
Pyrite precipitates as a result of the oversaturation resulting from the fluid injection at $T_{\text{inj}} = 65$ °C (Fig. 11). Maximum precipitation occurs around 135 °C (compare Fig. 7). According to the temperature
Figure 9. Temporal evolution of the dolomite reaction rate in the fracture.

Figure 10. Temporal evolution of the quartz reaction rate in the fracture.

evolution, the area of maximum precipitation moves towards the production point. The maximum precipitation rate of $3.7 \times 10^{-12}$ mol m$^{-3}$ s is in good agreement with the rate from Durst (2002).

5.3 Amount of dissolved and precipitated minerals

Based on the reaction rates, the amount of dissolved and precipitated minerals per element was calculated:

$$M_{i,E} = MW_i \times V_E \times \sum_{n=0}^{n_{max}} (r_{i,n} \times \Delta t).$$

(5)

$M_{i,E}$ is the amount of dissolved or precipitated mineral $i$ in element $E$, $MW$ is the molecular weight of mineral $i$, $V_E$ the volume of element $E$, $T_0$ the initial time, $T_{tot}$ the total simulation time, $r_{i,n}$ the reaction rate of mineral $i$ at time $n$ and $\Delta t$ the time interval. Positive $M_{i,E}$ values indicate the dissolved and negative values the precipitated amount of minerals.

Table 4 lists the total amount of initial minerals, the total amount of dissolved and precipitated minerals as well as the percentage of the initial amount for one fractured zone. This table clearly shows that the biggest amount of dissolved and precipitated minerals is calcite. Thus, porosity and permeability changes are the result of calcite reaction. The impact of the other minerals is negligible.

5.4 Evolution of porosity and permeability

The dissolution of calcite and dolomite near the injection well causes the porosity to increase. The calcite precipitation towards the production well leads to a porosity decrease. Because the precipitated
Table 4. Total initial and dissolved or precipitated amount of minerals in one fractured zone during 2 yr.

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Total amount (kg)</th>
<th>Dissolved amount (kg)</th>
<th>Precipitated amount (kg)</th>
<th>Dissolved percentage (per cent)</th>
<th>Precipitated percentage (per cent)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calcite</td>
<td>27 225</td>
<td>990</td>
<td>1180</td>
<td>3.6</td>
<td>4.3</td>
</tr>
<tr>
<td>Dolomite</td>
<td>6748</td>
<td>100</td>
<td>—</td>
<td>1.5</td>
<td>—</td>
</tr>
<tr>
<td>Quartz</td>
<td>225 450</td>
<td>—</td>
<td>0.05</td>
<td>2 × 10⁻⁵</td>
<td>5 × 10⁻⁴</td>
</tr>
<tr>
<td>Pyrite</td>
<td>2241</td>
<td>—</td>
<td>0.01</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

The amount of quartz and pyrite is orders of magnitudes smaller than the amount of precipitated calcite, the effect of quartz and pyrite is negligible. According to the evolution of the calcite reaction rate that decreases after 1 yr, the increase of the porosity near the injection well (and the decrease towards the production well, respectively) from 1 to 2 yr is smaller than in the first year. At the end of the simulation, the maximum porosity is 14.8 per cent and the minimum is 6.8 per cent, from initially 10 per cent. These results are in good agreement with the data from Durst (2002).

The evolution of the permeability (Fig. 12) is similar to the porosity: near the injection point, permeability increases with simulation time as a result of calcite and dolomite dissolution. Towards the production point, permeability is decreased because of calcite precipitation. Like the porosity evolution, the permeability increase near the injection well (and towards the production well) within the first year is four times as large as between 1 and 2 yr. The maximum permeability after 2 yr is 2.1 × 10⁻¹¹ m² and the minimum is 3 × 10⁻¹² m², down from initially 6.8 × 10⁻¹² m².

Note that the evolution of porosity and permeability not only depends on the mineral reaction rates, but is also very much...
influenced by the porosity–permeability relation implemented in FRACHEM.

The initial fluid velocity of $3.8 \times 10^{-4}$ m s$^{-1}$ decreases with time, because of the permeability decrease near the production well. After 2 yr, the fluid velocity is decreased to $1.5 \times 10^{-4}$ m s$^{-1}$. Accordingly, the initial amount of injected fluid of 0.02 l/s decreases to 0.012 l/s after 2 yr.

6 SIMULATION OF 1997 SOULTZ CIRCULATION DATA

The 1997 Soultz circulation test has proven that this reservoir seems to be well suited for a long-term EGS operation. However, the fact that the uniform flow rate generated strong downhole pressure variations at injection and production borehole gave a hint on the complex interaction of physical–chemical processes in the subsurface. It was intended to simulate the system behaviour during the whole 4-month circulation period by the model used in the previous section. Because the numerical model used fixed pressure at injection and production, it is suitable to compare the measured and modelled transmissivity evolution instead of pressure variation.

Fig. 13 shows the pressure evolution at GPK1 (injection well) and GPK2 (production well) during the circulation test (from day 30 to 110) as well as the fluid injection rate. The pressure evolution at GPK1 is strongly influenced by the injection activities: sudden pressure drops are caused by shut-in stops during injection. This is clearly seen when comparing the injection rate with the pressure at GPK1. The pressure drop after 80 days is the result of the injection stop of anti-scaling agent. The pressure decrease after each shut-in is assumed to be related to thermoelastic processes such as tensile stresses developing as a result of the injection of cold fluid. The occurrence of thermoelastic tensile stress at the injection well is a well-known effect during heat extraction from fractured rock (Kohl 1992). Because no thermoelastic processes will be considered herein, obvious effects from these processes have to be properly treated and measured data were corrected in order to perform a comparison with the coupled geochemical numerical approach. The most obvious hydraulic events occurred after 50 and 70 days with a sudden pressure change of $10^5$ Pa and $2 \times 10^5$ Pa (see fine arrows in Fig. 13) at injection. It is believed that these events are related to brittle processes in the rock matrix that have little impact on the herein treated processes. To compensate these effects, uniform pressure steps were added to the measured pressure curve. A further effect rose from the injection stop of anti-scaling agent after 85 days and a similar correction was performed. Under these premises a nearly constant injection pressure at GKP1 of 4 MPa resulted.

At GPK2 the pressure increased during the circulation test. Note that the pressure evolution at production wells is plotted as drawdown pressure in Fig. 13 on the same axis like the injection pressure at GPK1. The distance of 450 m from GPK2 production well to GPK1 is big enough that injection activities have no impact on the pressure evolution. The sudden pressure drops occurring at GPK1 have no impact on the GPK2 pressure history. In addition, because the temperature of the produced fluid is near the reservoir temperature (see Fig. 7), no thermoelastic effects are expected to occur.

The evolution of transmissivity, $T_r$, can be calculated from the pressure history by (Bear 1979):

$$T_r = \frac{q_{\text{tot}}}{L \times \nabla P} \quad (6)$$

$q_{\text{tot}}$ is the fluid circulation rate, $L$ the depth of the fracture and $\nabla P$ the pressure gradient. Given a 1-D flow with fixed injection rate, temperature dependent density and viscosity effects are of second order.

As a result of constant circulation rate, the measured transmissivity variation is the result of the $\nabla P(t)$ history. For the FRACHEM

![Figure 13. Fluid injection rate and pressure evolution during the 1997 circulation test. Time is days since July 9, when the test started. The fine arrows show the zones where the pressure at GPK1 was changed to neglect thermoelastic effects.](https://academic.oup.com/gji/article-abstract/161/2/533/1995665)
model, transmissivity variation is only the result of \( q_{\text{tot}}(t) \) because \( L = 200 \text{ m} \) and \( \nabla P \) is constant, because the pressure was fixed at the injection and the production point. \( q_{\text{tot}} \) history is calculated by

\[
q_{\text{tot}}(t) = v_f(t) \times A_i \times \Phi_1(t),
\]

(7)

\( v_f \) is the fluid velocity, \( A_i \) the area of the element interfaces and \( \Phi \) the porosity.

In the FRACHEM model, the transmissivity evolution during the circulation test is calculated for a single fractured zone. Therefore, the fluid injection rate is divided by the total number of assumed fractured zones.

The measurements indicate a transmissivity drop from \( 1.9 \times 10^{-10} \) to \( 1.7 \times 10^{-10} \text{ m}^3 \text{ Pa}^{-1} \). As a result of different initial pressure conditions, the simulated transmissivity is higher than the measured values. However, when plotting the transmissivity evolution as a percentage of the initial value (Fig. 14), it is clearly seen that the general trend shows a nearly identical, gradual transmissivity decrease with time. The numerical results fit the circulation test very well. The outliers in Fig. 14 are the result of the stop and shut-in activities.

The fact that the transmissivity in the circulation test decreases with time, when thermoelastic effects are factored out, points to geochemical processes in the reservoir, such as the precipitation of calcite. The good fit between the transmissivity evolution of the numerical model and the 1997 circulation test confirms this assumption. The pressure evolution in the reservoir seems to be the result of interactions between elastic and geochemical processes.

7 CONCLUSION

The presented work investigated the characteristics of the Soultz EGS reservoir and yielded important results towards understanding fluid–rock interactions as well as coupled thermal, hydraulic and chemical processes.

The code FRACHEM was developed to simulate coupled thermal, hydraulic and chemical processes (including chemical kinetics) accounting for the specific Soultz conditions such as the high salinity of the reservoir fluid and the high temperatures. To our knowledge, there is at present only the SHEMA code available with similar treatment of geochemical interactions. As a result of its special adaptation to the Soultz conditions, which are mainly the implemented kinetic laws and the porosity–permeability relation for fractured rock, FRACHEM is suitable to simulate conditions of the Soultz EGS reservoir. Sensitivity analyses and a benchmark tests have proven its reliability. Future FRACHEM versions should extend the range of possible applications.

The long-term model of the EGS reservoir confirms the theoretical results of Durst (2002) that predicted calcite to be the most reactive mineral. The changes in porosity and permeability are therefore the result of the dissolution and precipitation of calcite. The impact of other minerals can be neglected. After 1 yr, the decrease of calcite reaction rate leads to a less distinct porosity and permeability change compared with the early evolution. The system seems to be close to steady-state. Thus, it may be assumed that no major changes in the porosity and the permeability will occur for longer simulation periods. The geochemical processes are not expected to be a limiting factor for the successful operation of the EGS concept at Soultz.

The comparison of the numerical results with the 1997 circulation test reveals that the geochemistry may have an impact on the transmissivity evolution. At the beginning of the circulation, the transmissivity decrease is more rapid (\( \sim 5 \) per cent in 20 days, see Fig. 14) and slows down at longer times (\( \sim 10 \) per cent in 100 days). It seems to asymptotically converge to a constant value. This agrees with the decrease of the calcite reaction rate with time (see Fig. 8). It may be suspected that transmissivity will not decrease more during longer circulation periods.

The fact that geochemical effects are observed in the data of the 1997 circulation test highlights the importance of thermal, hydraulic and chemically coupled reservoir models. The integration of
geochemical considerations is therefore indispensable for integrated simulations of EGS systems and predictions of its performance.

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REFERENCES


Appendix A: Kinetic Equations for Calcite, Dolomite, Pyrite and Quartz Dissolution and Precipitation in the Soultz Reservoir

For the Soultz system, calcite, dolomite, pyrite and quartz are integrated in the geochemical model. Durst (2002) assumed one kinetic law for each mineral dissolution and precipitation reaction. The laws derived from published experiments conducted in NaCl brines are briefly outlined below. Detailed information on the derivation of the reaction rate laws can be found in Durst (2002).

A1 Calcite dissolution and precipitation

Far from the equilibrium, the calcite dissolution rate is controlled by two processes, the surface reaction and the diffusion of H⁺ to the mineral surface (Sjöberg & Rickard 1984). In the Soultz system both of the processes co-exist with a predominance of surface reaction. Eq. (A1) defines the calcite dissolution law accounting for the temperature, pH, surface reaction and dependency of the H⁺ activity, aH⁺. S is the reaction surface area, T the temperature, Q the ion activity product and K the equilibrium constant.

\[
r_d^{\text{calcite}} = \left[\frac{(1.643 \times 10^{-1} \times a_{\text{H}^+}) + (1.11 \times 10^{-5})}{\exp\left(\frac{T - 321.15}{321.15}\right)}\right] \times S \times \frac{T}{\exp\left(\frac{2.36}{\ln K}\right)} \times \left(1 - \frac{Q}{K}\right).
\]

(A1)

The calcite precipitation law is based on the study from Shiraki & Brantley (1995) on near equilibrium kinetics at 100 °C. Precipitation is dominated by spiral growth for Q/K < 1.72 and by nucleation at higher oversaturation. The inhibitor effect of magnesium on calcite precipitation (Zhang & Dawe 2000) is not significant for the Ca²⁺/Mg²⁺ ratio of the Soultz fluid. Eq. (A2) defines the calcite precipitation rate. R is the ideal gas constant.

\[
r_p^{\text{calcite}} = 1.93 \times 10^{-2} \times T \times \exp\left(\frac{-41840}{R \times T}\right) \times S \times \left(\frac{Q}{K} - 1\right)^{1.93} \quad \text{for } \frac{Q}{K} < 1.72,
\]

\[
r_p^{\text{calcite}} = 1.011 \times T \times \exp\left(\frac{-41840}{R \times T}\right) \times S \times \exp\left(\frac{2.36}{\ln K}\right) \quad \text{for } \frac{Q}{K} > 1.72.
\]

(A2)

A2 Dolomite dissolution and precipitation

The dissolution law is based on the work of Gautelier et al. (1999). The temperature and pH-dependent dolomite dissolution rate is

\[
r_d^{\text{dolomite}} = \left[10^{(1(-0.0436 \times pH^2) - 0.5948 \times pH - 2.0591)} \times 2.104 \times 10^7\right] \times \exp\left(-2.754 \times pH\right) \times \exp\left(\frac{972 \times pH - 5951}{R \times T}\right) \times \left(1 - \frac{Q}{K}\right).
\]

(A3)

The dolomite precipitation law is derived from Arvidson & Mackenzie (1999):

\[
r_p^{\text{dolomite}} = 1.122 \times 10^5 \times S \times \exp\left(-\frac{16060}{T}\right) \times \left(\frac{Q}{K} - 1\right)^{2.26}.
\]

(A4)

A3 Quartz dissolution and precipitation

Dove (1994) derived a quartz dissolution equation depending on temperature and the pH:

\[
r_d^{\text{quartz}} = \exp\left[-0.7 \times T \times \exp\left(\frac{-66}{10^7 \times R \times T}\right) \times \theta_{\text{Si} \text{OH}^-} + \exp^4.7\right] \times T \times \exp\left(\frac{-82.7}{10^7 \times R \times T}\right) \times \left(\theta_{\text{Si} \text{OH}^-}\right)^{1.1} \times S \times \left(1 - \frac{Q}{K}\right).
\]

(A5)
The quartz precipitation equation comes from Rimstidt & Barnes (1980):

\[ r_p = \left\{ a_{H_2O}^2 \times \exp \left[ \left( (1.174 - 2.028) \times 10^{-3} \times \left( T - \frac{4158}{T} \right) \right) \ln 10 \right] \right\} \times s \times \left( \frac{Q}{K} - 1 \right). \]  

(A6)

\( \theta_{>SiOH} \) is the fraction of the total surface sites occupied by hydrogen ions as >SiOH and \( \theta_{>SiOtot} \) is the sum of the fraction of the total sites existing as a deprotonated >SiO⁻ site and as a complex with a sodium ion as >SiO-Na⁺.

A4 Pyrite dissolution and precipitation

The pyrite dissolution equation is derived from the studies by Williamson & Rimstidt (1994):

\[ r_d = 250 \times s \times \exp \left( \frac{-6500}{R \times T} \right) \times \left( 1 - \frac{Q}{K} \right). \]  

(A7)

The pyrite precipitation law is derived from studies by Rickard (1997) and Rickard & Luther (1997):

\[ r_p = 0.125 \times \frac{a_{HS^-} \times a_{Fe^{2+}} \times \sum S^{2-}}{K_{FeS} \times [3 \times KH_2S] + a_{H^+}} \times V \times \exp \left( \frac{-3500}{R \times T} \right). \]  

(A8)

\( V \) is the volume.