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Comparing FRACHEM and SHEMAT for the modelling of brine-rock interactions in Enhanced Geothermal Systems.

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ABSTRACT

Coupled numerical simulations of heat transfer, fluid flow and chemical reactions in geothermal systems are complex because of the highly heterogeneous geology, high temperatures, elevated pressures and often high salinity of the formation fluids. Codes such as FRACHEM and SHEMAT have been developed to forecast the long-term evolution of exploited geothermal reservoirs in order to determine how fluid circulation within geothermal reservoirs can modify the rock properties.

FRACHEM is a thermo-hydraulic-chemical coupled program developed from the combination of two existing codes: FRACTure, a 3-D finite element code for modelling hydraulic, fluid and heat transport and elastic processes, that was developed originally for the study of flow-driven interactions in fractured rock; and CHEMTOUGH2, a modified version of the TOUGH2 simulator able to simulate the coupled transport of water, vapour, non-condensable gas and heat in porous and fractured media. FRACHEM has been developed especially to simulate the behaviour of the fractured granitic EGS reservoir at Soultz-sous-Forêts (Alsace). Consequently, it contains specific implementations, such as the Pitzer formalism used to determine activity coefficients. The precipitation/ dissolution reaction rates of carbonates (calcite, dolomite), quartz, amorphous silica, pyrite and some alumosilicates (K-feldspar, albite, illite) are computed according to kinetic expressions deduced from published experimental data for high-temperature NaCl brines. FRACHEM also allows the coupling of porosity and permeability to chemical processes occurring within the reservoir.

SHEMAT, the "Simulator for HEat and MAss Transport", has been developed in several phases and is today a general purpose reactive transport code for a wide variety of thermal and hydrogeological problems in two and three dimensions. SHEMAT solves coupled problems involving fluid flow, heat transfer, species transport and chemical water-rock interaction. It is a finite difference code that solves the flow and transport equations on a Cartesian grid. The chemical modules for calculating the activity-concentration relationships underlying the mineral reaction processes are based on the one hand on Pitzer's equations and on the other hand on Debye-Hückel's theory. SHEMAT is particularly well suited to quantify the effect on flow and transport of chemically induced changes in the pore space of deep sandstone aquifers and was successfully employed for the prediction of the 30-year behaviour of geothermal fluid production systems.

The Soultz-sous-Forêts Enhanced Geothermal System (EGS), established in the Rhine Graben, North of Strasbourg (France), has been investigated since the mid 1980's. The final goal of this project is to extract energy from a forced fluid circulation between injection and production boreholes within a granitic basement rock. The two codes have been applied to simulate fluid circulation in the enhanced geothermal system of Soultz-sous-Forêts. The same geometrical model and identical thermodynamic and kinetic input data have been used. The specific features of each code concerning calculation schemes and coupling mechanisms are presented. Such differences could typically lead to differences in numerical simulation results. Focus has been on the evolution of reservoir temperature, calcite and quartz reaction rates and porosity evolution.

1. INTRODUCTION

A major concern in EGS reservoirs is maintaining adequate injectivity, while avoiding the development of preferential short-circuiting flow paths. Past analyses have focused primarily on the coupling between fluid flow, heat transfer and rock mechanics. Recent studies suggest that chemical interactions between rocks and fluids and associated mineral dissolution and precipitation effects, could have a major impact on the performance of EGS.

Prediction of long-term evolution of geothermal reservoirs is of primary interest, in particular for maintaining optimised injectivity and productivity. However, modelling of fluid flow and reactive transport in geothermal systems is challenging because of reservoir conditions such as high temperatures, elevated pressures and sometimes high salinities of the formation fluids. Reactive transport codes coupling thermal, hydrological, and chemical (THC) processes have been developed and used in Enhanced Geothermal Systems to predict permeability evolution by modelling the behaviour of hot, hypersaline brines and their interactions with reservoir minerals.

In this study, two THC simulators were applied using identical thermodynamic and kinetic input data to forecast geothermal reservoir evolution: FRACHEM, a multi-component reactive transport code (Durst, 2002; Bächler, 2003), designed to use the Pitzer activity coefficient model and SHEMAT (Simulator for HEat and MAss Transport), a multi-component reactive transport code for the simulation of the stationary and transient processes in geothermal reservoirs in two and three dimensions, which allows to use the Pitzer activity coefficient model (Clauser, 2003).

2. PROBLEM SETUP

A great deal of specific and detailed information is required to assess the chemical impact of an injection operation. The present study is intended to represent the granitic reservoir of Soultz-sous-Forêts. Consequently, well configuration data as well as chemical and mineralogical composition were taken from the European Enhanced Geothermal System at Soultz-sous-Forêts (Jacquot, 2000; Durst, 2002; Bächler, 2003).

The Soultz-sous-Forêts EGS is located in Alsace, about 50 km north of Strasbourg (France). The Soultz area was selected as the European EGS pilot site because of its high temperature gradient in the sedimentary cover (up to 100 °C km^{-1}) and its high heat flow, locally up to 0.15 W m^{-2} (Kohl and Rybach, 2001). The geology of the Soultz region is characterized by a graben structure affected by several N-S striking faults. The crystalline basement, covered by 1400 m of Triassic and Tertiary sediments, is composed of three facies in granitic rocks: (1) an unaltered granite; (2) a hydrothermally altered granite facies and (3) altered veins within the hydrothermally altered granite (Jacquot, 2000). The hydrothermally altered granite is the most porous facies (Genter et al., 1997) and altered veins are highly fractured. Natural circulation of formation fluid and fluid-rock interaction processes take place mainly within the hydrothermally altered granite and to a lesser extent within altered veins. Flow in the unaltered granite is essentially nil. To extract the heat from the Soultz reservoir, three deviated wells have been installed to a depth of 5,000 m, with lower ends separated by 600 m. The reservoir temperature at this depth is initially 200 °C. One well (GPK3) will be dedicated to the injection of cold water in the granitic reservoir at a rate of about ~50 L.s^{-1}, whereas the two other wells (GPK2 and GPK4), located on both sides of the injector, will be used to produce ~25 L.s^{-1} of the formation fluid each. At Soultz, the injection–production system has been designed as a closed loop. The fluid used in this loop is the formation fluid abundant in the altered granite, namely a brine with total dissolved solids of around 100,000 ppm. Injection of cooled brine disturbs the equilibrium between the formation fluid and reactive minerals. The resulting change in temperature and pressure in the reservoir and the forced circulation in fractured granite will drive geochemical reactions able to affect the physical properties of the reservoir through mineral precipitation and dissolution. The main task of the research on THC coupled modelling for this site has been to forecast the evolution of reservoir porosity and permeability.

However, the highly heterogeneous and complicated structure of the Soultz reservoir has been simplified to the following concept.

2.1 Conceptual model and hydraulic parameters

Benchmark simulations described below were performed with the same simplified, horizontal, confined 2D model with a geometry that is close to that of the Soultz system. Injection and production wells are linked by 650 m long fractured zones in the granite rock mass. If we consider that the granitic Soultz reservoir can be represented by a series of alternating fractured and impermeable matrix zones (Dezayes et al., 2005) only one of these fractured zones needs to be modelled; it would be 10 cm thick, have a horizontal width of 10 m (Fig. 1a) and a mean porosity of 10 %. The fractured zones are separated by 100-m thick rock matrix zones, this being the distance required to assume a semi-infinite matrix for heat transfer purposes.

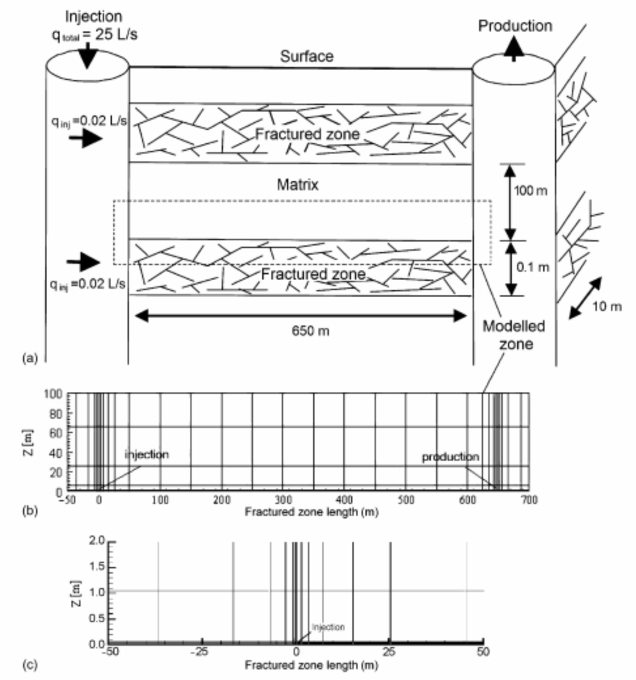

Figure 1: (a) Simplified, vertical 2D model of the Soultz system (dimensions are not shown to scale); (b) spatial discretization of the model; (c) finer mesh discretization near the injection zone. The black bar near the bottom corresponds to the fractured zone.

We consider that the fluid exchange between fractured zones and the surrounding low-permeability matrix is insignificant and thus can be neglected. Only heat transfer between the matrix and the fractured zones is allowed, following the model of Sauty (1981). Because of symmetry, only half (the upper part) of a fractured zone and of the adjacent porous matrix is modelled, by subdividing them into 222 elements (Fig. 1b). The size of the elements ranges from a minimum of 0.5 m × 0.05 m near the injection and the production wells to a maximum of 50 m × 35 m. The fractured zone is located between 0 and 650 m; injection is made at 0 m and production occurs at point 650m (Fig. 1c).

The initial temperature throughout the modelled area was set to 200 °C, the natural-state reservoir temperature. During the simulations, the fluid was injected into the modelled fractured zone at a constant temperature of 65 °C. In FRACHEM hydrostatic pressure distribution was assumed in the production well, while a constant overpressure of 8 MPa was set at the injection well. The pressure gradient between the two wells does not change during the injection period, resulting in an initial flow of 0.02 L s^{-1} into the modelled fractured zone. In SHEMAT the injection well was recharged with 0.02 L s^{-1} and at the production well the same amount of fluid was produced throughout the simulation. Mineral dissolution and precipitation bring about changes in the porosity and permeability of the modelled fractured zone affecting the flow rates through the mesh elements. Therefore the hydraulic rock properties were updated/recalculated after each time step. Dirichlet boundary conditions (i.e. constant temperature and pressure conditions) were applied to the upper, left and right boundaries of the modelled zone. The values of the thermo-hydraulic parameters considered in the simulations are listed in Table 1.

Table 1: Values of the thermo-hydraulic parameters used in benchmark simulations.

Parameter	Fracture	Matrix	Fluid
Hydraulic conductivity ($m\ s^{-1}$)	$7.03.10^{-4}$	$9.5.10^{-12}$	-
Thermal conductivity ($W\ m^{-1}\ K^{-1}$)	2.9	3	0.6
Density ($kg\ m^{-3}$)	-	2650	1000
Heat capacity ($J\ kg^{-1}\ K^{-1}$)	-	1000	4200
Porosity (%)	10	0	-

2.2 Initial mineralogical composition

The geothermal reservoir at Soultz is made up of three types of granite (Jacquot, 2000; Hooijkaas et al., André et al., 2006) (Table 2). The first is non-altered (fresh) granite that is characterized by a predominance of feldspar, plagioclase and quartz, and by an extremely low fracture density. Consequently, its porosity is close to zero and does not contain significant amounts of water. The properties of this granite are that of the impermeable rock matrix. Fluid exchange, by advection or diffusion processes, will be disregarded for this granite; it will only act as a good heat conductor.

The second rock facies is a fractured, hydrothermally altered granite with quartz as the major mineral component; because of alteration the amount of feldspar decreases and some secondary minerals such as galena, pyrite, smectite or illite are present. This facies is the most porous (porosity ranging from 5 to 10 %) and contains most of the formation fluid. The third rock facies is the most altered; it corresponds to alteration veins that contain minerals such as illite, smectite and quartz. Precipitated secondary minerals (clays, carbonates) fully cement the fractures, resulting in a decrease of porosity and permeability. As a consequence, fluid circulation within the rock mass takes place through the second facies only (Genter et al., 1998).

Table 2: Mean composition (in %) of the different types of granite in the Soultz reservoir (Jacquot, 2000).

	Fresh granite	Hydrothermally altered granite	Alteration veins
Quartz	24.2	40.9	43.9
K-feldspar	23.6	13.9	
Plagioclase	42.5		
Illite		24.6	40.2
Smectite		9.7	9.6
Mica	9.4		
Calcite	0.3	3.3	4.3
Dolomite		0.8	0.7
Pyrite		0.7	1.0
Galena		1.3	0.3
Chlorite		4.8	

2.3 Water chemistry

The formation fluid circulating through the fracture network is a sodium-chloride brine with total mineralization close to 100 g L^{-1}. Its pH is approximately 4.9. The water is in thermal equilibrium (200 °C) with the rock at 5000 m depth. The composition of the formation brine extracted during a 1999 production test is given in Table 3. The chemistry of the deep fluid is similar to that of the fluid produced from the shallower reservoir at 3000 m depth (Durst, 2002). Its silica and carbon concentrations are higher because of the elevated temperatures and CO_2 partial pressures, respectively.

Table 3: Representative chemical analysis of the fluid sampled at the wellhead of GPK2 after being deepened to 5000 m in 1999 (Durst, 2002)

Species	Concentration (mmol/kg)
Na^+	1148.00
K^+	73.40
Ca^{2+}	169.50
Mg^{2+}	3.21
Cl^-	1648.00
S	1.77
C	42.76
Fe^{2+}	2.61
SiO_2	6.06
Al^{3+}	$3.7.10^{-3}$

3. NUMERICAL SIMULATORS

This description of the codes is a brief overview of the computation capabilities of the two simulators. For more details, the reader can consult the SHEMAT User's Guide (Clauser, 2003), as well as the different FRACHEM studies on the Soultz system (Durst, 2002; Bächler et al., 2005; André et al., 2006).

The methods for calculating activity coefficients are described for each code below. A Pitzer ionic interaction model has been introduced into both codes for solving non-isothermal reactive transport problems under conditions of high ionic strength, as encountered in typical EGS systems.

Applied thermodynamic data and equilibrium constants have been chosen to be consistent for both codes.

3.1 FRACHEM code

Different researchers (Durst, 2002, Bächler, 2003, Rabemanana et al. 2003, André et al., 2006) have incrementally built a reactive transport simulator, FRACHEM, able to simulate the main characteristics of the Soultz reservoir at 5 km below the surface, 200 °C, 500 bar, and a fluid salinity of around 100,000 ppm.

FRACHEM is a THC simulator issued from the combination of two existing codes: FRACTure and CHEMTOUGH2. FRACTure is a 3D finite-element code for modelling hydrological, transport and elastic processes. It was developed originally for the study of flow-driven interactions in fractured rock (Kohl & Hopkirk, 1995). CHEMTOUGH2 (White, 1995) is a THC code developed based on the TOUGH2 simulator (Pruess, 1991), a 3D numerical model for simulating the coupled transport of water, vapour, non-condensable gas, and heat in porous and fractured media. CHEMTOUGH2 represents the possibility to transport chemical species and to model the chemical water-rock interactions as well as the chemical reactions driven by pressure and temperature changes. Transport and reactions are coupled in a one-step approach. FRACHEM has been built by introducing geochemical subroutines from CHEMTOUGH2 (White, 1995) into the framework of the code FRACTure (Bächler, 2003; Bächler and Kohl, 2005). After an initialization phase, FRACTure calculates, over each time step, the thermal and hydrological conditions within each element volume and determines the advective flow between each of them. Resulting thermal and hydrological variables are stored in arrays common to FRACTure and the geochemical modules. At this point, the program calculates the chemical reactions using a mass balance/mass action approach, the advective transport of chemical species, and the variations of porosity and permeability. Once this calculation is performed, porosity and permeability are updated and fed into the FRACTure part of the code. The program then returns to the start of the loop until the end of the simulation time (sequential non-iterative approach, SNIA).

FRACHEM has been developed especially for the granitic reservoir of Soultz-sous-Forêts and consequently, specific implementations have been added to the chemical part of this code. Considering the high salinity of the fluid, the Debye-Hückel model, initially implemented in the CHEMTOUGH2 routines to determine the activity coefficients, has been replaced by a Pitzer activity model. It should be mentioned here that the activity coefficient calculations are carried out indirectly using the code TEQUIL for the Na-K-H-Ca-Cl-SO_4-HCO_3-CO_3-CO_2-H_2 system from 0 to 250 °C (Moller et al., 1998). Using this model, total concentrations obtained from chemical analyses (Table 3) are used in TEQUIL to compute speciation and corresponding activity coefficients. Presently, a limited number of minerals are considered, which correspond to the minerals constituting the Soultz granite. The precipitation/dissolution reactions of carbonates (calcite, dolomite), quartz, amorphous silica, pyrite, and some aluminosilicates (K-feldspar, albite, illite) can be modelled under kinetic constraints. Rate laws follow the transition state theory (e.g., Lasaga et al., 1994). The implemented kinetic rate laws are specific to each mineral and taken from published experiments conducted at high temperature in NaCl brines.

Thermodynamic data (equilibrium constants) are taken mostly from SUPCRT92 (Johnson et al., 1992) and Helgeson et al. (1978) and are functions of temperature and pressure. The effect of pressure on equilibrium constants is explicitly taken into account with regard to the mineral reactions.

Finally, a supplementary module allows the determination of porosity and permeability variations linked with chemical processes occurring in the reservoir. Considering the alteration of the Soultz granite, the flow is assumed to circulate in a medium composed of fractures and grains. Therefore, a combination of a fracture model (Norton and Knapp, 1977; Steefel and Lasaga, 1994) and a grain model (Bolton et al., 1996) is used to determine the permeability evolution.

3.2 SHEMAT code

The Simulator for HEat and MAss Transport (SHEMAT, Bartels et al., 2003) is in combination with its graphical user interface "Processing SHEMAT" (Kühn and Chiang, 2003) an easy-to-use, general purpose reactive transport code for a wide variety of thermal and hydrogeological problems in two and three dimensions. SHEMAT solves coupled problems involving fluid flow, heat transfer, species transport and chemical water-rock interaction. It is a finite difference code that solves the flow and transport equations on a Cartesian grid. The "IAPWS Industrial Formulation" (Wagner et al. 2000) is the equation of state used for water. In SHEMAT, the different flow, transport and reaction processes can be selectively coupled. Flow and heat transport are coupled in that the fluid parameters density, viscosity, compressibility, thermal conductivity and thermal capacity are functions of temperature and pressure. Flow and salt transport are coupled via fluid density implemented by a linear approximation.

The current version of SHEMAT offers the user two choices for calculating the activity-concentration relationships underlying the mineral reaction processes: (1) Pitzer's equations (best suited for concentrated brines) or (2) Debye-Hückel's theory (useful for more dilute solutions).

SHEMAT's first chemical speciation module CHEMEQ is a modification of the geochemical modeling code, PHRQPITZ (Plummer et al. 1988). It permits calculations of geochemical reactions in brines and other highly concentrated electrolyte solutions using the Pitzer virial-coefficient approach for activity-coefficient corrections. Reaction-modeling capabilities include calculation of aqueous speciation and mineral-saturation as well as mineral solubility.

To extend the applicability of SHEMAT with a second chemical speciation module, for example to enable re-engineering ore deposits or simulate permeable reactive barriers, the program has now been interfaced additionally to the chemical code PHREEQC (Parkhurst and Appelo 1999). PHREEQC is based on the Debye Hückel ion association approach. Compared to PHRQPITZ and due to the considerably larger thermodynamic data set for the chemistry of dilute aqueous solutions, it allows to study chemical reactions between much more elements.

4. RESULTS AND DISCUSSION

The two codes were applied to a geometrical model representing the granitic reservoir at Soultz. We assume that major circulation occurs in the hydrothermally altered granite. Injected cooled brine mainly interacts with carbonates and quartz. Secondary precipitation of amorphous silica was considered.

FRACHEM and SHEMAT simulations have been compared in order to determine how fluid circulation within fractured granitic rock modifies fracture porosity. Total simulations time lasted 1800 days.

4.1 Reservoir temperature

The circulation of cooled fluid in the porous zone affects the temperature of the reservoir. But considering the flow rate (about 0.02 $L.s^{-1}$ during five years), the temperature decrease is only effective in the first 100 m of the porous zone. Obviously, the most important decrease concerns the near vicinity around the injection well with a temperature of about 65 °C. The predicted general trend of temperature with distance from injection well after roughly 5 years of fluid circulation is similar for the two codes. These results show that model conceptualizations regarding heat transport are almost identical (Fig. 2).

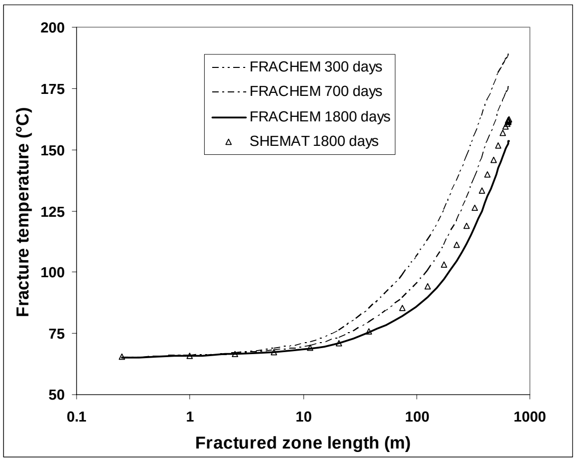

Figure 2: Temperature evolution along the fractured zone at different times.

4.2 Mineral-brine interactions

Results of numerical simulations for a long-term circulation confirm the major role of the carbonates on the evolution of reservoir porosity. Due to their fast reaction rates, carbonate minerals are responsible for most of the evolution. Silicates and pyrite behaviour is also simulated between the two wells, but their influence is minor.

The reservoir water has a ionic strength of about 1.8. The Debye-Hückel model does not account for any ionic interaction terms and generally is only applicable to solutions with I < 1. At high ionic strength and temperature, γCa^{2+} calculated from the Pitzer model is much larger than from Debye-Hückel. This means a lower Ca^{2+} concentration is needed to maintain calcite equilibrium or calcite is less soluble. The effect of increased Ca^{2+} activity coefficients on calcite solubility in this case is similar to the "salting out" effects for dissolution of non-condensible gases such as CO_2.

In both FRACHEM and SHEMAT models, the 65°C injection water is under-saturated with respect to calcite because calcite solubility increases with decreasing temperature. Calcite then dissolves close to the injection point. As temperature increases away from the injection point, calcite precipitation occurs (Fig. 3). Figure 4 shows that dolomite dissolves within the first ten meters from the injection well. The general dissolution and precipitation behaviour of dolomite is similar to calcite. Among silicates, quartz and K-feldspar are major minerals in granite. Contrary to calcite, the solubility of these minerals improves with decreasing temperature. As a consequence, these minerals precipitate near the injection well, but less so further away where temperature increases. Thus, quartz precipitates close to the injection point, and as temperature increases away from the injection point, quartz dissolution occurs (Fig. 5). Amorphous silica precipitates near the injection well at a maximum rate of 4.10^{-5} mol.m^{-3}.s^{-1} (Fig. 6). After 25–30 m from the injection well, towards the production well and along the fracture, the reactions between the fluid and the minerals fade away because the injected brine comes close to thermodynamic equilibrium with regard to these minerals.

With FRACHEM, the observation of the mineral behaviour shows that all the reactions occur in the first 20 m of the injection zone. Calcite, a secondary mineral present within granite fractures in relatively small proportions, shows the highest reactivity. In the vicinity of the injection well, calcite dissolves, whereas it precipitates from about 2 to 20 m, because of the retrograde solubility of calcite (solubility decrease with temperature increase). At the onset of fluid circulation within the reservoir, calcite dissolves mainly within the first two meters of the injection well. This dissolution releases calcium in solution, which is then available for calcite precipitation further away from the injection well, where the temperature increases. With increasing simulation time and decreasing rock temperatures the calcite dissolution zone moves towards the production well and stops as soon as the mineral has been consumed completely in a specific area around the injection well.

Although the two codes yield similar results, in a qualitative sense, quantitative results differ significantly. These differences are primarily caused by differences in implemented kinetic models. Concerning the mineral reaction rates, significant differences were observed for calcite, dolomite and quartz. The largest differences in reaction rates were observed for calcite and dolomite.

With SHEMAT, after 1800 days of fluid circulation, calcite dissolves near the injection point at a maximum rate of two order of magnitude less than with FRACHEM (5.10^{-7} mol.m^{-3}.s^{-1} compared to 5.10^{-5} mol.m^{-3}.s^{-1}), and then precipitates further in the fracture at a rate smaller than with FRACHEM (Fig. 3).

With FRACHEM, dissolution and precipitation of dolomite and quartz are about one order of magnitude smaller than calcite. In contrary, with SHEMAT, reaction rates of quartz and dolomite are one order of magnitude higher than calcite. Dolomite, a secondary mineral present within granite fractures in relatively small proportions, shows the highest reactivity (Fig. 4).

The diverging amount of dissolved and precipitated calcite has to be traced back to different chemical kinetic calculations in FRACHEM and SHEMAT. The equilibrium constants for minerals and activity coefficients of solutes used with FRACHEM and SHEMAT have been mostly issued from the same sources. But, kinetic rate laws do not take exactly the same form in both codes. The rate laws and parameters implemented into FRACHEM were specifically developed for each mineral and specifically established for high-salinity and/or high-temperature fluids most relevant to the reservoir conditions at Soultz. In SHEMAT, one generic equation is used for all minerals using varying initial reaction rates, activation energies and initial surface reaction areas to differentiate between the minerals. For calcite, the spread between models can reach 5 orders of magnitude, for dissolution and precipitation, respectively, regardless of the type of calcite considered (hydrothermal or sedimentary).

4.3 Effects on porosity

Evolution of the reservoir porosity is determined by the mineral reactions occuring in the fractured zone. With SHEMAT, as with FRACHEM, the porosity is enhanced in the first 10 meters from the injection well, due to the dissolution of carbonates (Fig. 7). Carbonates then precipitate between about 10 and 100 meters, yielding a maximum porosity decrease in this zone.

The two codes give generally similar trends. Consequently, the porosity-permeability models implemented in FRACHEM and SHEMAT result in similar porosities.

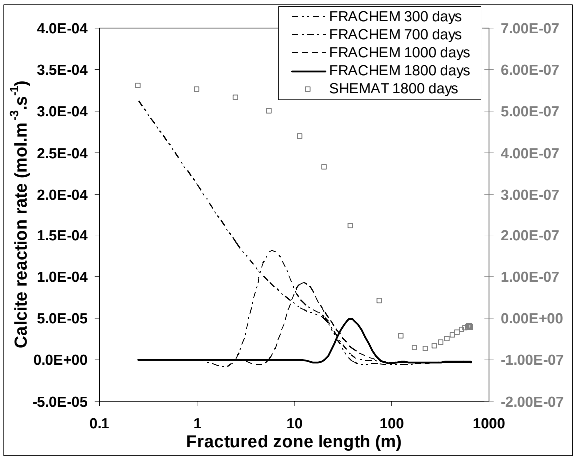

Figure 3: Calcite reaction rate along the fractured zone at different times (positive values indicate dissolution). Left and right y-axis correspond to FRACHEM and SHEMAT plots respectively.

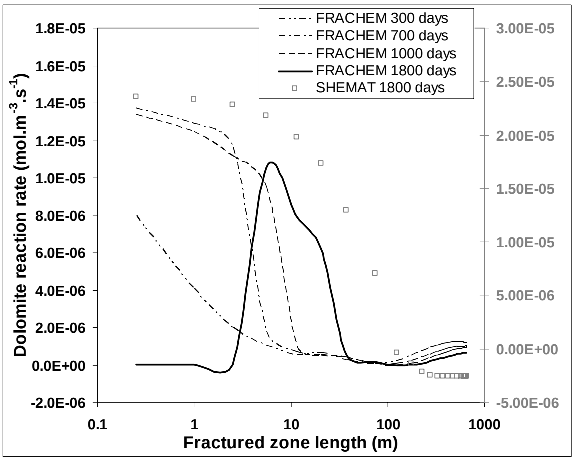

Figure 4: Dolomite reaction rate along the fractured zone at different times (positive values indicate dissolution).

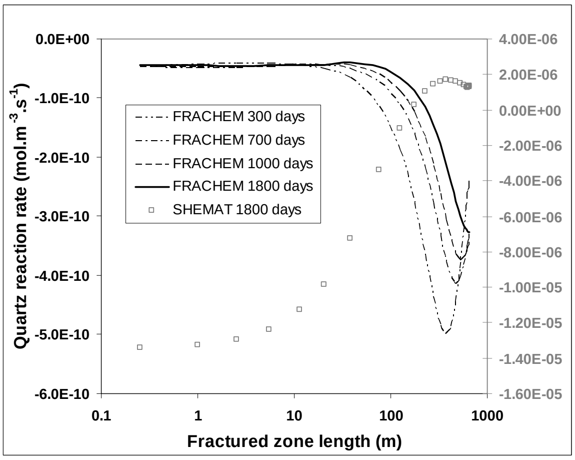

Figure 5: Quartz reaction rate along the fractured zone at different times (positive values indicate dissolution).

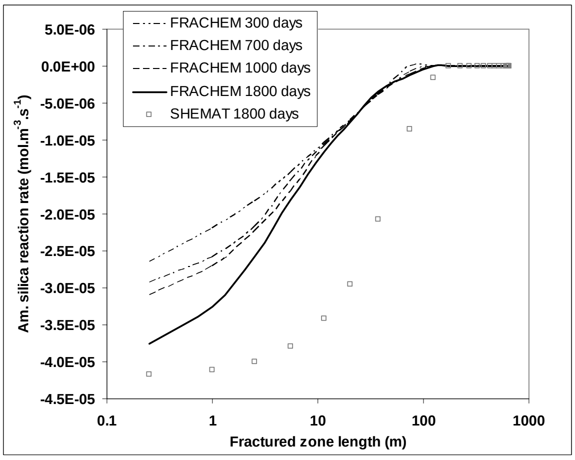

Figure 6: Amorphous silica reaction rate along the fractured zone at different times.

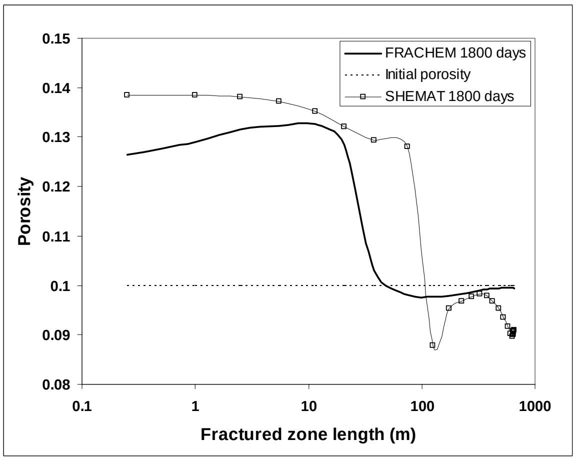

Figure 7: Porosity evolution for the two models along the fractured zone after five years of forced fluid circulation.

5. CONCLUSIONS

The goals of this work were to compare two geochemical transport codes, FRACHEM and SHEMAT (with similar databases), and to model complex systems like Enhanced Geothermal systems.

The two codes were applied to simulate reactive transport processes in the Soultz reservoir, using essentially identical conceptual model and input chemical and hydraulic data. Three main processes were investigated for a forced fluid circulation of 5 years: the evolution of reservoir temperature, mineral precipitation/dissolution behaviour and the evolution of reservoir porosity. Significant differences in models results were found, primarily due to differences in the kinetic models and their parameters. This study highlights the importance of these models in reactive transport simulations, in particular for systems involving brines.

Nevertheless, it can be seen from the porosity evolution that the results of FRACHEM and SHEMAT are very similar. Even though the simulators show significant differences with regard to the quantities of minerals precipitated and dissolved it is determined that changes of the hydraulic system are equally well described by both models. The fact that both models yield similar results is of great importance, since no reliable measured data nor adequate laboratory experiments are available for comparison. FRACHEM and SHEMAT calculate the same temperature development and fluid velocities as well as resulting porosities from the mineral reactions. Thermodynamic equilibrium modelling resulted in comparable species and mineral concentrations in both models (applied activity coefficients and equilibrium constants have been chosen to be consistent for both codes). Thus, the Pitzer approach is well implemented. Finally, assuming an adequate calcite reaction rate in the SHEMAT code should result in a better fit of calcite amounts precipitated and dissolved.

6. ACKNOWLEDGEMENTS

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