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TOUGHREACT Code Applications to Problems of Reactive Chemistry in Geothermal Production-injection Wells. First Exploratory Model for Ahuachapán and Berlín Geothermal Fields.

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ABSTRACT

The first preliminary simulations to study calcite and silica scaling problems at two geothermal fields in El Salvador have been performed using a non-isothermal multiphase reactive geochemical transport code TOUGHREACT. This code was developed by Earth Sciences Division at Lawrence Berkeley Laboratory introducing reactive chemistry into the code TOUGH2. Production well AH-33B at Ahuachapan geothermal field was used for calcite scaling problem. For the calcite scaling in the well AH-33B, simulation results agree well with the observation data collected at depth in the borehole. Increases in calcite volume fraction over time were obtained close to the wellbore, due to high concentrations of Ca^{+2} and HCO_3^-. Injection well TR-1A at Berlin field was used for studying silica scaling. The silica scaling simulation reproduces in same way the decline in injectivity in the well TR-1A. Amorphous silica and quartz precipitation was obtained in the simulation. Results indicate that the kinetics of silica deposition is very important for predicting the future injectivity decline in the permeable zone of injection wells under different geological and thermodynamic conditions. The reactive transport simulations could be helpful for understanding the physical and chemical processes occurring in geothermal reservoirs and the potential risk of calcite and silica scaling problems in new geothermal developments. The mineral dissolution/precipitation application (production/injection well scaling) was used as a baseline and first approach of the geochemical-hydrological model.

1. INTRODUCTION

A comprehensive non-isothermal multi-component reactive fluid flow and geochemical transport simulator, TOUGHREACT, has been developed initially by Xu and Pruess (1998), by introducing reactive geochemistry into the framework of the existing multi-phase fluid and heat flow code TOUGH2 (Pruess, 1991).

A wide range of subsurface thermo-physical-chemical processes is considered under various thermohydrological and geochemical conditions of pressure, temperature, water saturation, and ionic strength. The program can be applied to one-, two- or three-dimensional porous and fractured media with physical and chemical heterogeneity. The model can accommodate any number of chemical species present in liquid, gas and solid phases. A variety of equilibrium chemical reactions are considered, such as aqueous complexation, gas dissolution/exsolution, and cation exchange. Mineral dissolution/precipitation can proceed either subject to local equilibrium or kinetic conditions. Temporal changes in porosity and permeability due to mineral dissolution and precipitation processes can modify fluid flow. This feedback between transport and chemistry can be important (Raffensperger, 1996), and can be considered in our model. Changes in porosity during the simulation are calculated from changes in mineral volume fractions. The porosity-permeability correlation in geologic media is very complex, depending on an interplay of many factors, such as pore size distribution, pore shapes, and connectivity (Verma and Pruess, 1988).

2. COMPUTER MODELING

Calcite and silica saturation conditions can be modeled using computer programs containing thermodynamic equilibrium data for all the key constituents which control solution pH.

The speciation program used TOUGHREACT can be applied to a wide range of subsurface conditions. Temperature ranges from 0 ^{0}C to 300 ^{0}C, because the present most available geochemical database is up to 300 ^{0}C such as EQ3/6 (Wolery, 1992). Pressure can be from 1 bar (atmospheric pressure) to several hundred bars (at several thousand meter depth). Water saturation can range from 0 to 1 (or from completely dry to fully water saturated). The model can deal with ionic strength from diluted to highly saline water (up to 6 mol/kg H_2O for NaCl dominant solution). TOUGHREACT can be applied also to model saturation changes that occur when water flows up a well, flashes and loses gas.

This code contains component species data, reaction stoichiometries and log (K) data entries that must have the same format as the entries for aqueous species, gases, and minerals in the TOUGHREACT thermodynamic database, including the same structure as the thermodynamic database with a top record specifying temperature values for the log (K) data, then component (basis) species, derived species, minerals, and gases.

The chemical data base also have been updated including more minerals for different applications and geological conditions. For instances using log (K) values given by Gunnarsson and Arnorsson (2000) or values given by Arnorsson and Stefansson (1999) depending of the specific problem evaluated.

In the data files the log (K) grids for gases, minerals, and aqueous species have been extended up to 300°C. In addition,the log (K) values for the dissolution reactions of SiO_2 containing minerals have been updated/recalculated with the most recent thermodynamic data for aqueous silica (Stefansson, 2001) which is the basis for the WATCH program.

2.1 Numerical Model

To simulate the production and injection flow a numerical model with simple radial 1-D geometry was used for both cases (Ahuachapan and Berlin) due to the fact that the main task is to simulate the chemical scaling near the well bore.

The main differences between both models are the INCON (initial conditions input) and related thermodynamic and chemical data.

The model consists of 70 elements in a single layer of 100 m thick. The first element is the well bore itself (0.3 m) and 29 elements with constant increment of 100 m radius and the rest of the elements increase logarithmically until 10000 m (Fig. 1).

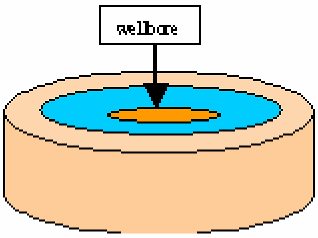

Figure 1. Reservoir model concentrically to the well showing the well bore and the nearest elements.

The first step in the modeling is to get a fluid and heat flow model from TOUGH2 as a basis for further modeling for the geochemical transport simulator, TOUGHREACT.

The input files mainly includes rock properties, time-stepping information, geometric grid information, initial and boundary conditions, and data related to multi-phase fluid and heat flow simulation. The flow input is the same as the original TOUGH2 V2 (see the manual; Pruess et al, 1999), with an additional data block REACT. Including the input parameters for calculations of reactive transport, such as diffusion coefficients, tolerance limits for convergence of transport and chemical iterations, mineral and aqueous species, and the configuration of model zones with different chemical composition, the geochemical system (i.e. the type and number of aqueous component species, minerals, gases, and sorbed species considered in the simulation). It also includes the initial compositions of water, mineral, and gas zones configured and kinetic data for minerals (rate constants, surface areas, etc.). In addition the program needs a thermodynamic database file. This file contains reaction stoichiometries, dissociation constants (log (K)), and regression coefficients of log (K) as a function of temperature.

One of the output files is identical to the original TOUGH2, including data on temperature, pressure, liquid saturation, mass flux, and phase velocities for all grid blocks of the model. Other output files including all transport parameters, chemical zone configuration, and other run-specific parameters, chemical database, including initial water, rock, and gas compositions, equilibrium constants and stoichiometries of chemical reactions, kinetic data, results of geochemical speciation calculations for each initial water composition, chemical mass balances (total mass balance and aqueous species mass balance).

The main features and data that will be necessary to include in the code are the following: chemical composition of initial and injection waters, initial mineral composition, temperature and pressure reservoir data, water injection

This would lay the groundwork in terms of reservoir conditions and parameters for reactive chemistry modeling.

3. THE AHUACHAPAN GEOTHERMAL FIELD. CALCITE CASE.

At present the Ahuachapán geothermal field has 16 production wells but as a regular base only 12 are in continuous production generating around 60 MWe that represent 22 % of the total electricity consumption in the country. Production wells AH-33B and AH-35A located in the SSE part of the field, needs antiscalent chemical dosing system to prevent calcite scaling. The Ahuachapan waters are medium to high salinity waters (10,000-18,000 mg/lt), similar to those found at many other geothermal fields. Waters of this salinity are characterized by near-neutral pH's, high calcium concentrations and relatively low bicarbonate concentrations

Well AH33B, was initially discharged partially from October 1997 to May 1998. Commercial production discharge from August to October 2001 was undertaken without calcite inhibition and resulted in the development of extensive well bore deposition of calcite at 790 to 841 m depth and a large run down in wellhead pressure and mass flow. The blockage was found to be 100% calcite. Continued production from this well from February 2002 until the present time after it had been worked over and a calcite antiscalent chemical dosing system installed indicate that under the present discharge conditions, well AH33B is not depositing calcite scale, either in the well bore or in the formation. Temperature and pressure measurements show the well to have two main production zones with a 225°C liquid feed at 1100 m depth and a 240°C liquid feed at 1300m depth. The average well parameters show a total flow rate of about 60 kg/s at 94 psig separated at 78 psig generating around 3.4 Mwe. The flash point under the production conditions was located from 780 to 825 m which is where the calcite deposition occurred and the inhibition chamber was located around 975 m depth (Fig. 2).

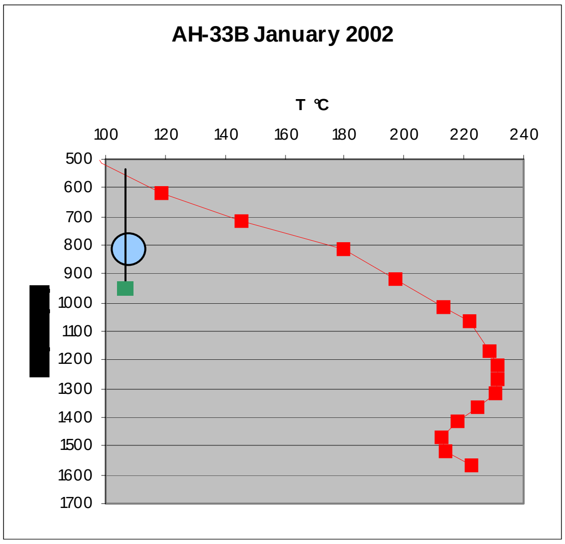

Figure 2. Temperature profile for well AH-33B and antiscalent chemical dosing system location

This is a classic case of well bore calcite scaling in a flashing liquid well column where:

rapid loss of CO_2 from the boiling liquid into the developing steam phase promotes the rapid deposition of calcite in the form of an “hour glass” shaped deposit in the well bore, distributed over several tens of meters of the bore hole at the flash point. The reduction in well head pressure and mass flow from the well occurs quite quickly as the cross sectional area of the remaining opening in the deposit in the well bore declines in proportion to the square of the radius (SKM, 2003).

The well was mechanically worked over and acidized in 2002 and put back into service with downhole injection of calcite inhibitors at 975m depth – i.e. at a depth above the location of the upper feed zone, but below the flash point, and was found to provide good antiscalant inhibition .

For the definition of the geochemical system the information on the aqueous species, minerals, gases and exchangeable cations involved in the system is needed. The following tables showing water composition and mineral assemblages that have been used as a initial conditions for running TOUGHREACT:

Well
AH33B

Date	**SamplingPoint**	**Na**	**K**	**Ca**	**Mg**
29-30.10.97	Well head	0.176600288	0.014431574	0.005576347	6.24018E-05
Cl	**SO_4**	**HCO_3**	**SiO_2**	**pH**	**CO_2**
0.18593631	0.00059938	0.000457577	0.007626784	7.1675	0.088406

Table 1. Chemical content for well AH-33B. Aqueous species in mol/l and gas CO_2 in mol/kg H2O

Mineral Composition	%
Calcite - $CaCO_3$	2-32
Clorite -$(Mg,Fe)_3(Si,Al)_4O_{10}(OH)_2(Mg,Fe)_3(OH)_6$	1-15
Epidote- $Ca_2(Al,Fe)Al_2O(SiO_4)(Si_2O_7)(OH)$	10-40
Cuarzo - SiO_2	10-50
Hematite - Fe_2O_3	1-10
Wairakite- $CaAl_2Si_4O_{12}.2H_2O$	1-7
Anhidrita - $CaSO_4$	3-7

Table 2. Mineral composition for phyllitic-propyllytic facies at 900-1500 m depth in wells AH-33B

The mineral percentages used as an input (initial mineral zone in chemical.inp) in terms of volume fraction are estimated. For the case of calcium was considered only calcite, and instead hematite has been considered pyrite.

3.1 Simulation Results

The results obtained from the first exploratory chemical model for well AH-33B are shown in the following graphics:

The Fig. 3 shows the results for pressure and temperature against the distance for the radial model using the TOUGH2 code. It is clear a drop in reservoir pressure near the wellbore that could be related a more extensive boiling inside the well (flashing level) were the calcite deposition occurred. Meantime the reservoir temperature remains constant (Fig.4).

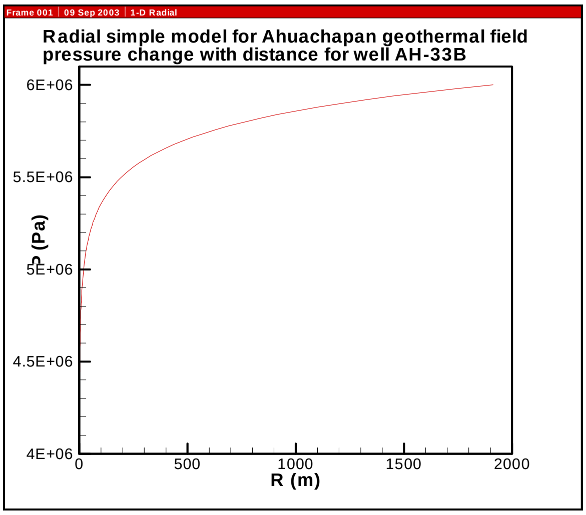

Figure 3. Pressure change with distance from (TOUGH2)

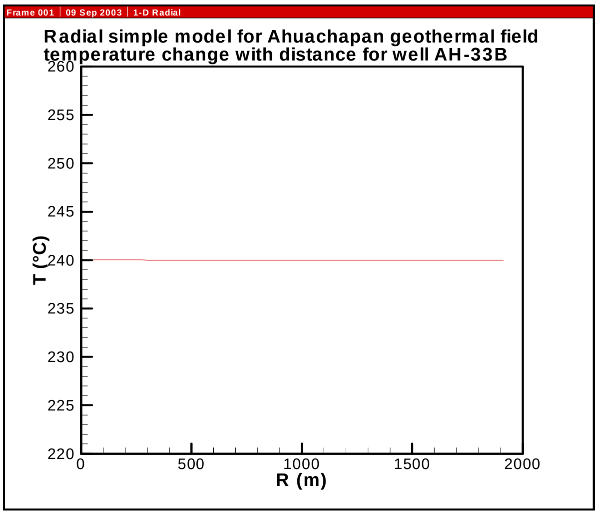

Figure 4 Temperature profile with distance from (TOUGH2)

The Fig. 5 and 6 shows the dissolution of calcium + bicarbonate from the minerals and calcite oversaturation against the time. As an example is also plotted the chlorite mineral showing in this case equilibrium. Others results also shows the dissolution of others species like chloride, silica and changes in pH.

In Fig. 7 are plotted the saturation conditions for other minerals like quartz and pyrite showing oversaturation , epidote undersaturation and wairakite in equilibrium in Fig. 8 .

The Fig. 9 shows temperature change with distance in agreement with the pressure drop, but not change is observed for the permeability. In this case was not possible reproduce the decrease in permeability due to the scaling in the wellbore. Should be adjusted in further simulations. In Fig. 10 the calcite drop in saturation is very clear inside the well.

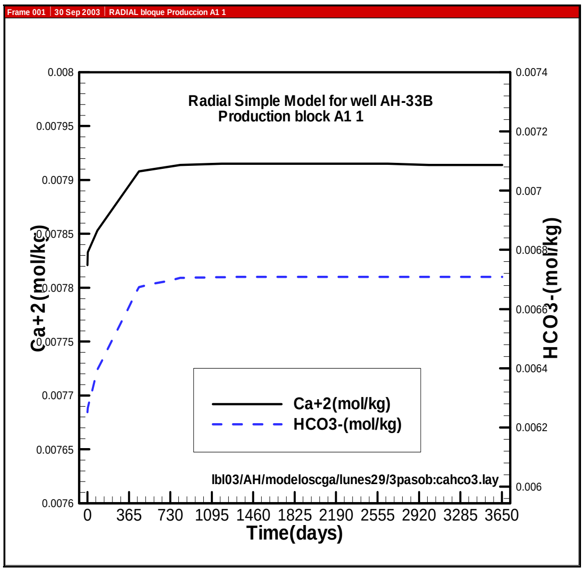

Figure 5 Chemical changes for calcium and bicarbonate

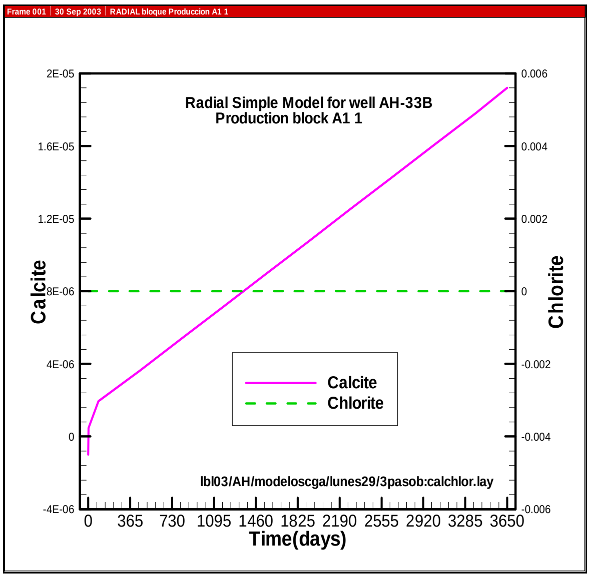

Figure 6 Calcite saturation with time

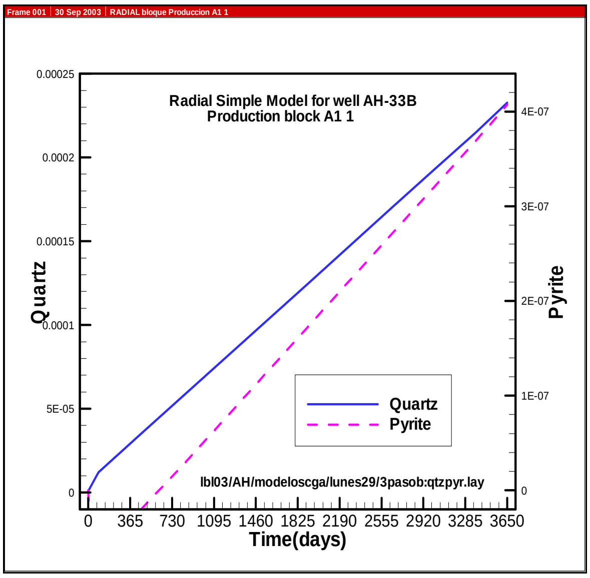

Figure 7 quartz and pyrite showing oversaturation

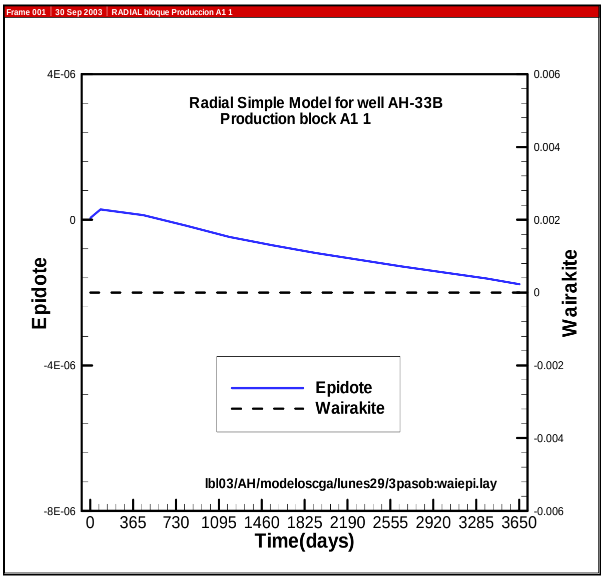

Figure 8 epidote and wairakite in equilibrium

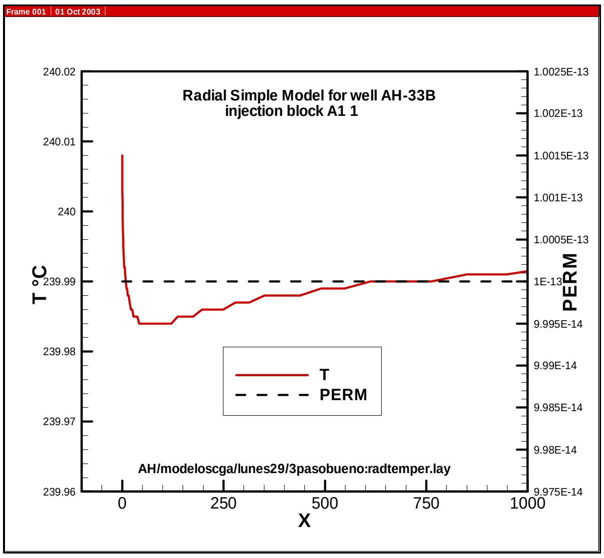

Figure 9 Temperature and permeability with distance

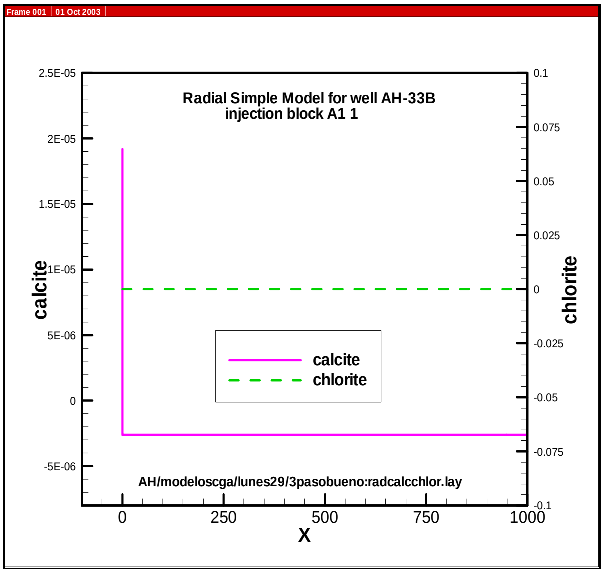

Figure 10 calcite saturation with distance

4. THE BERLIN GEOTHERMAL FIELD. SILICA CASE

At present the water flow rate discharged from the production wells is about 318 kg/s, where 280 kg/s is reinjected as a hot fluid injection (88 %), meantime 28 kg/s is cold injection in well TR-11A (data from July 2003). So the total reinjection at Berlin field is about 97 %. The rest of the waste water is discharged to a couple of ponds.

For purpose of simulation we select the chemical composition and mineral assemblages for the wells TR-2&TR-9 and TR-1A. The injection well TR-1A, is operated at separation pressure of 9.9 barg, and starts with a stable absorption capacity around 30 kg/sec with WHP= 26.3 barg. The wells has a main permeable zone below 2000 m depth (Fig 11). At 2300 depth was collected sample of SiO2 amf. After more than 2 years of injection, the absorption capacity declined drastically to around 20 kg/s. After an acid stimulation job in October 2001 the well improve permeability (Fig. 12).

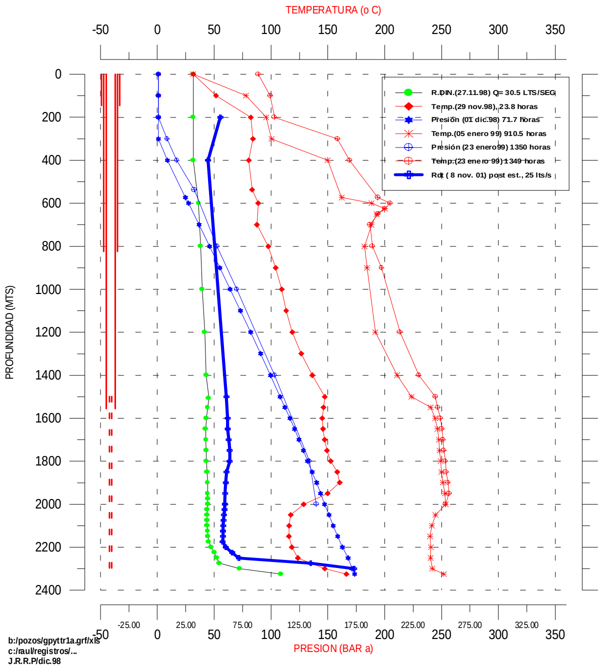

Fig. 11 Temperaure recovery curves for well TR-1A

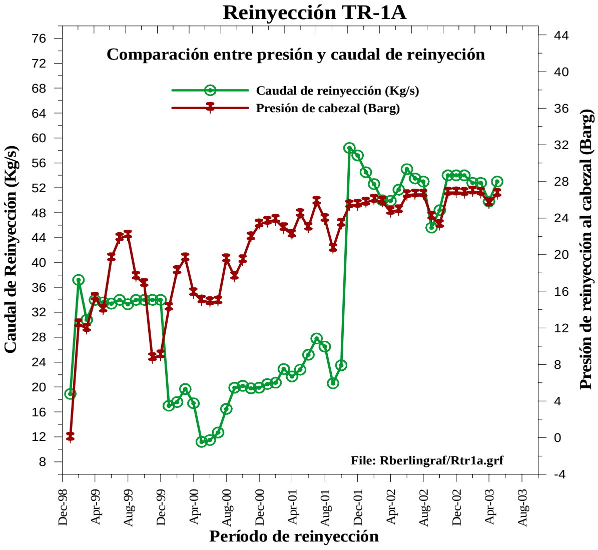

Fig. 12 Water injection changes due to loss in absorption capacity for well TR-1A

For the definition of the geochemical system the information on the aqueous species, minerals, gases and exchangeable cations involved in the system is needed. The names must be written according to those labeled in the thermodynamic database file. The following tables showing water composition and mineral assemblages that have been used as a initial conditions for running TOUGHREACT:

Date	SamplingPoint	Na	K	Ca	Mg
Average 2001	well head	0.206987717	0.023781597	0.003389371	1.89015E-06
	Cl	SO_4	HCO_3	SiO_2	pH
	0.239003751	9.64005E-05	6.29532E-05	0.016357684	6.896

Table 3. Chemical content for well TR-2&TR-9 (in mol/l)

Date	SamplingPoint	Na	K	Ca	Mg
Average 2001	well head	0.161647985	0.020282851	0.002288548	1.93993E-06
	Cl	SO_4	HCO_3	SiO_2	pH
	0.189321073	0.000140541	0.000319473	0.014996846	6.7225

Table 4. Chemical content for well TR-1A (in mol/l)

Mineral Composition	%
Calcita - CaCO3	7-20
Clorita -(Mg,Fe)3(Si,Al)4O10(OH)2(Mg,Fe)3(OH)6	3-50
Sericita/Illita- K0.5(Al, Fe, Mg)3(Si,Al)4 O10(OH)2	5-25
Epidota- Ca2(Al,Fe)Al2O(SiO4)(Si2O7)(OH)	1-30
Cuarzo - SiO2	2-30
Actinolita - Ca2(Mg,Fe)5Si8O22(OH)2	1-7
Wairakita- CaAl2Si4O12.2H2O	30
Prehnita - Ca2Al(AlSi3O10)(OH)2	1-7
Prehnita - Ca2Al(AlSi3O10)(OH)2	1-7

Mineral Composition	%
Calcita - CaCO3	2-25
Clorita -(Mg,Fe)3(Si,Al)4O10(OH)2(Mg,Fe)3(OH)6	1-15
Sericita/Illita- K0.5(Al, Fe, Mg)3(Si,Al)4 O10(OH)2	1-12
Epidota- Ca2(Al,Fe)Al2O(SiO4)(Si2O7)(OH)	10-35
Cuarzo - SiO2	10-70
Minerales opacos (pirita) - FeS	1-15
Wairakita- CaAl2Si4O12.2H2O	< 1
Prehnita - Ca2Al(AlSi3O10)(OH)2	3
Minerales de oxidos	12

Table 5. Mineral composition for phyllitic-propyllytic facies to propyllitic at 1500-2000 m depth in production wells TR-2 & TR-9 and TR-1A

4.1 Simulation Results

The results obtained from the first exploratory chemical model for well TR-1A are shown in the following graphics:

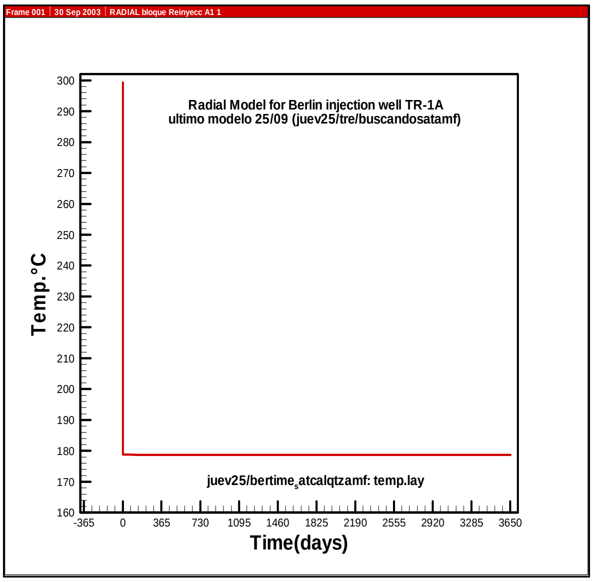

Fig. 13 Temperature change with time

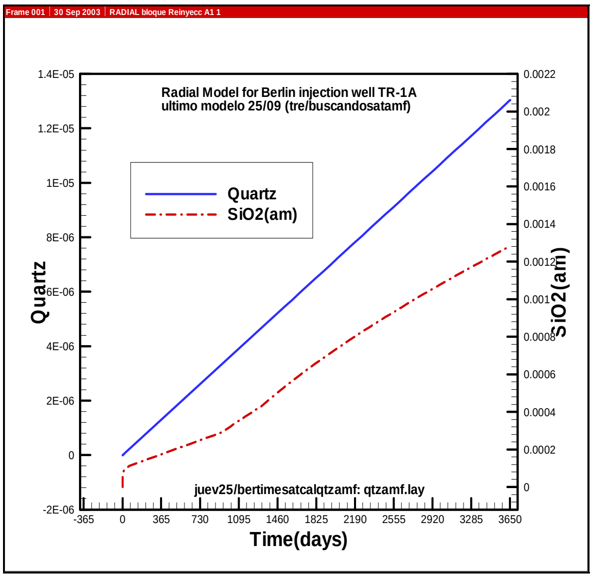

Fig. 14 Quartz and amorphous silica saturation with time

The temperature simulation in the reinjection well TR-1A in Fig. 13 shown instant decreasing in a short period of simulation time, that is the well bore is cooled reaching the water injection temperature.

In Fig. 14 the oversaturation of quartz and amorphous silica against the time of injection is shown. Fig. 15 shows that wairakite and prehnite are in equilibrium.

Fig. 16 shows clearly the drop in temperature and permeability due to the silica scaling in the well bore and probably occurring at some distance in the formation (mass transport). In Fig. 17 the change in amorphous silica is more likely deposited near the well, but quartz also should be present at some distance from the well . Other minerals like chlorite, illite, wairakite and prehnite shows equilibrium state, but the calcite seems to be also oversaturated.near the well (Fig. 18 and 19).

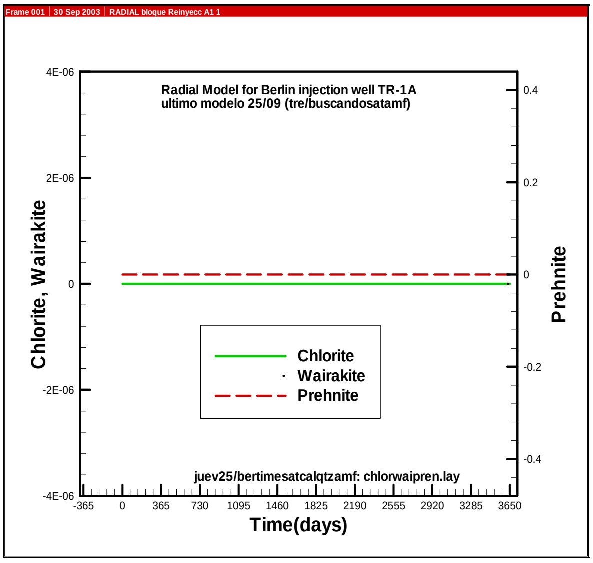

Fig. 15 Wairakite and prehnite are in equilibrium.

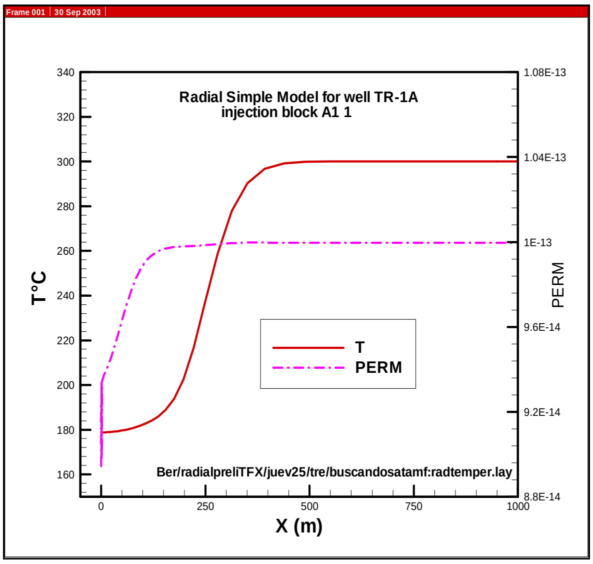

Fig. 16 Change in temperatureand permeability with distance

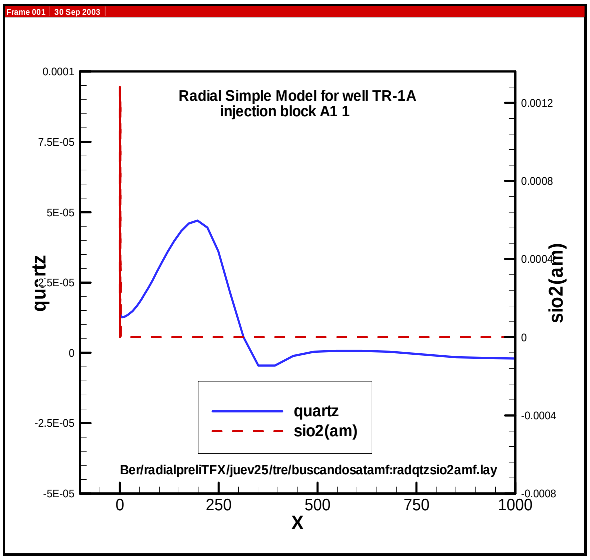

Fig. 17 Change in quartz and amorphous silica saturation with distance

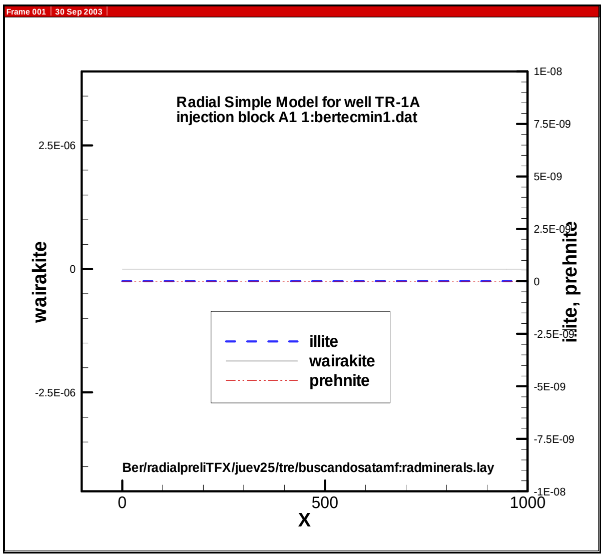

Fig. 18 Minerals in equilibrium with distance

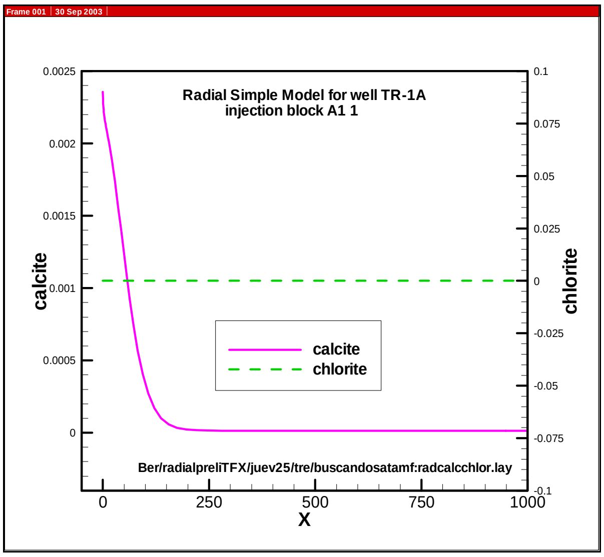

Fig. 17 Change in calcite saturation and chlorite equilibrium with distance

5. CONCLUSIONS

Generally the application of the TOUGHREACT gives a useful evaluation tool for the physical and chemical simulation processes occurring in a geothermal reservoir. The results of computer modeling agrees for comparative analysis rather than for examination of absolute saturation values. Also there is in agreement with the theoretical calculations by comparison with real data from wells where scaling has been observed.For the calcite case of Ahuachapan well AH-33B, the simulation shows an increasing calcite volume fraction suggesting increasing mineral saturation over the time, according to the presence of higher content of Ca^{+2} and HCO_3^- as a product of mineral disolution, producing a calcite scaling into the wellbore. Quartz and Pyrite shows increasing volume fraction that could be produce also mineral precipitation in the wellbore and possibly in the formation (at this time there is not evidence for that).Other mineral shows undersaturated conditions like amorphous silica, wairakite, illite, chlorite and prenite.

Respect to distance it is clear the rapid decrease in temperature but the permeability does not change (in this case is necessary improve new simulation in order to calibrate the decrease in permeability due to the scaling). The calcite saturation (or volume mineral fraction) decreases radially so it is more likely that the scaling is occurring near the well bore. For the case of silica scaling due to waste water injection for the Berlin field, the simulation reproduces in some way the decline in absorption capacity in the well TR-1A due to the increase in quartz volume fraction and mostly for amorphous silica volume fraction. In the radial model results shows declining temperature but in this case is clear the change in permeability due to the silica scaling. The same for the amorphous silica and quartz and probably calcite. Other minerals are still in undersaturation conditions.

6. RECOMMENDATIONS

For the Ahuachapan calcite case could be suggested improve new model using the CO_2 module (eosCO_2) and make a more detailed grid and simulation in order to get permeability decrease. For monitoring silica transport and to understand the scaling process and loss of injectivity in hot brine injectors, Ontoy et al. (2003) identified factors that cause the deposition of amorphous silica in the near-well formation and the extent of their effect using TOUGHREACT. These factors include the silica concentration in the hot brine injectate, the temperature of the injectate, the flowrate of the injectate, the pH of the injectate, and the temperature and pressure conditions of the reservoir in the vicinity of the injector. It is suggested to continuing with these data collection for simulation purposes, also define and study the mineral content in different parts of the reservoir (production or injection zones). Xu et al. (2003c) conducted a large number of numerical simulations to reproduce the loss of injectivity and its recovery by acid injection. This case study can be used for applying the code using specific data.

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REFERENCES

Tianfu Xu, Sonnenthal,E., Spycher, N.' and Pruess, K. TOUGHREACT User’s Guide: A Simulation Program for Non-isothermal Multiphase Reactive Geochemical Transport in Variably Saturated Geologic Media. Earth Sciences Division, Lawrence Berkeley National Laboratory University of California, Berkeley, CA 94720. April 2003

Finsterle, S. ITOUGH2 User’s Guide. Earth Sciences Division, Lawrence Berkeley National Laboratory University of California, Berkeley, CA 94720. January 1999

Pruess, K. TOUGH2 – A General-Purpose Numerical Simulator for Multiphase Fluid and Heat Flow Earth Sciences Division, Lawrence Berkeley National Laboratory University of California, Berkeley, CA 94720. May 1991.

Pruess, K. TOUGH USER’S GUIDE. Earth Sciences Division, Lawrence Berkeley National Laboratory University of California, Berkeley, CA 94720. June 1987

Sinclair Knigth Merz . Ahuachapan geothermal field. Review and assessment of calcite scaling.. June 2003.

LaGeo, internal reports.