Development of a Thermo-Hydro-Geochemical Model for Low Temperature Geoexchange Applications

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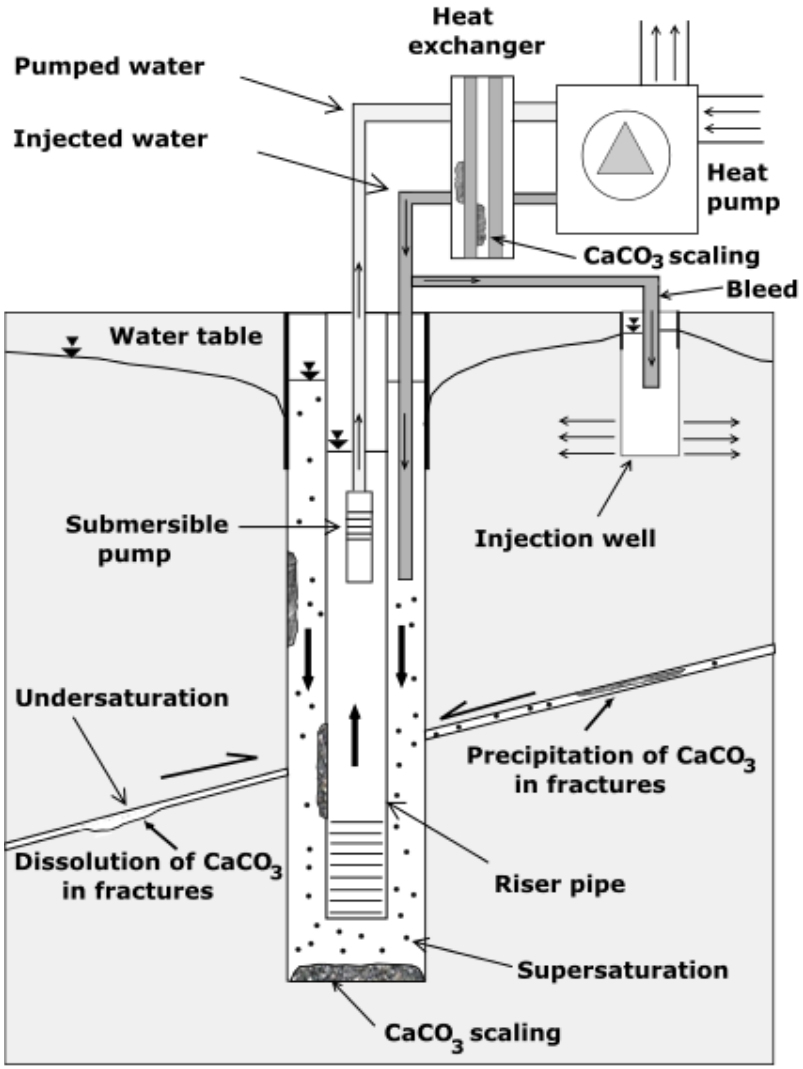
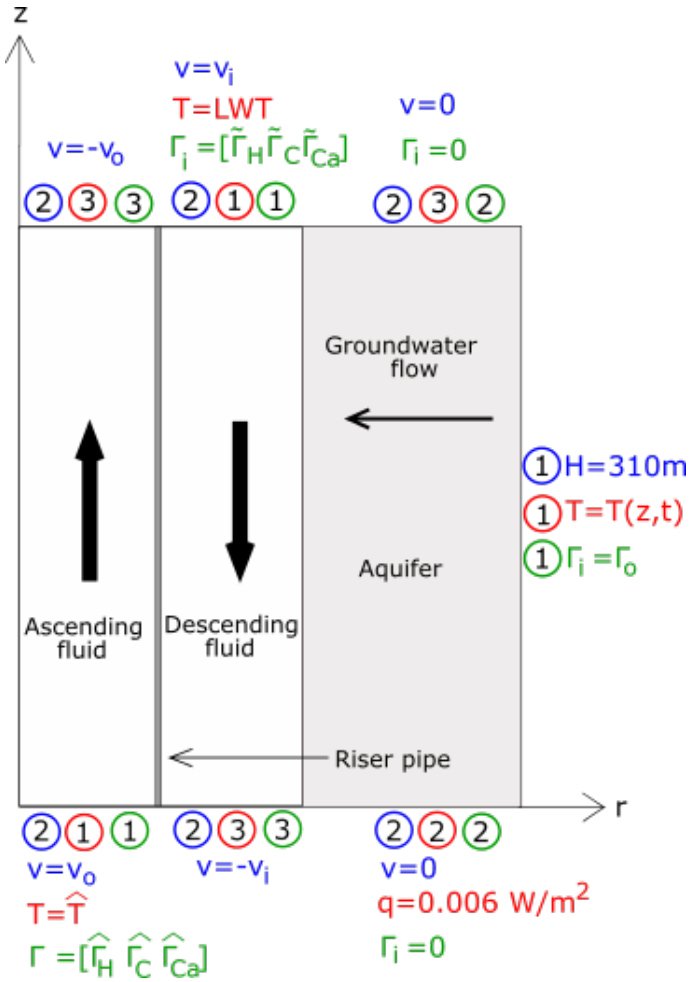
INTRODUCTION



- SCWs are a type of ground heat exchanger which uses groundwater as heat carrier fluid;
- Mineral scaling may occur in the heat exchanger, the well and the geological formation;
- Temperature influences the rate of chemical reactions.

METHODOLOGY - GEOMETRY

Thermo-Hydro-Geochemical (THG) processes are coupled in a 2D axisymmetric model inspired by the work of Nguyen and al. (2012, 2015).



Parameters	Value (m)
Domain length	300
Domain radius	40
Inner pipe radius	0.070
Outer pipe radius	0.076
Borehole radius	0.102

Legend:

Groundwater flow model

Heat transfer model

Geochemical model

1: Dirichlet

2: Neumann

3: Open Boundary

METHODOLOGY – MULTIPHYSICS COUPLED MODEL

The model uses three different physics from the Subsurface flow module and an ODEs and DAEs module. The governing equations are:

Groundwater flow model:

(Darcy's law)

$$\rho S \frac{\partial p}{\partial t} + \nabla \cdot (\rho v) = 0 \qquad v = -\frac{K}{\rho g}(\nabla p + \rho g \nabla D_v)$$

Heat transfer model:

(Heat transfer in porous media)

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p v \cdot \nabla T = \nabla \cdot (\lambda \nabla T)$$

Geochemical model:

(Solute transport and ODEs and DEAs domain)

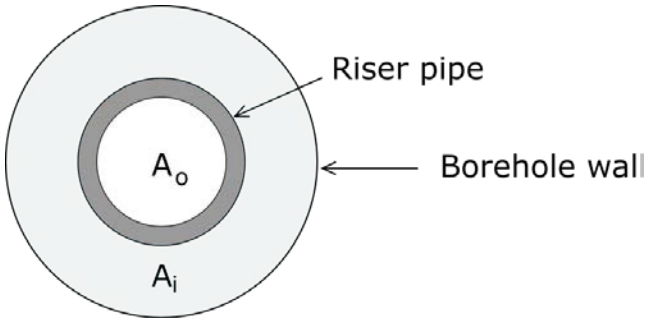
$$\varphi \frac{\partial \boldsymbol{\Gamma}}{\partial t} = \nabla \cdot (D \nabla \boldsymbol{\Gamma}) - \nabla \cdot (\vec{v} \boldsymbol{\Gamma}) + \boldsymbol{U S_k' r_k}$$

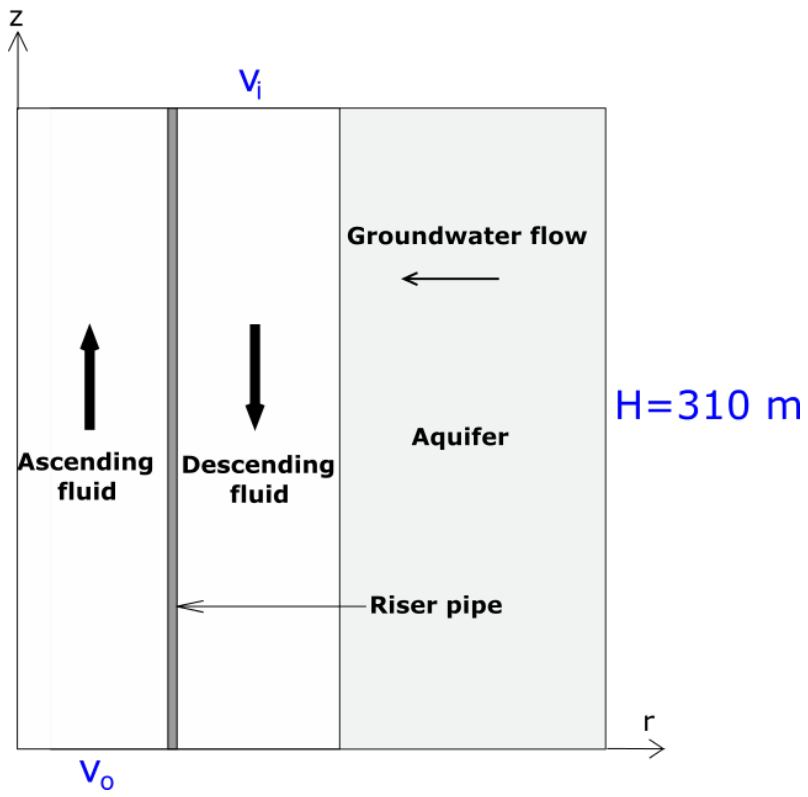
$\boldsymbol{\Gamma}$	: vector of total activities	[-]
$\mathbf{S_k}$	: stoichiometric matrix for kinetic reactions	[-]
$\mathbf{r_k}$	: vector of reaction rates for kinetic reactions	[-]
$\mathbf{U}$	: transformation matrix	[-]

METHODOLOGY – GROUNDWATER FLOW MODEL

The normal velocity of the ascending (v_o) and descending (v_i) fluid is defined by the two following equations:

$$v_0 = \frac{\dot{V}}{A_o} \qquad v_i = \frac{\dot{V} \cdot (1 - B)}{A_i}$$





when

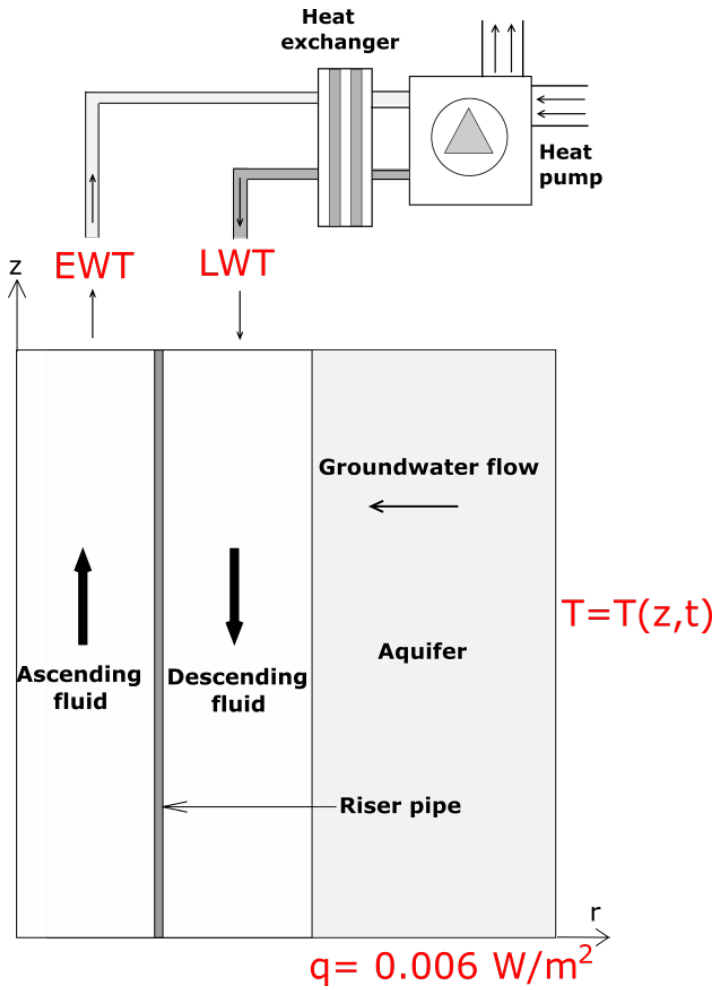
- B=0 : all the pumped water is re-injected in the well
- B=1 : all the pumped water is discharged outside the well

METHODOLOGY – HEAT TRANSFER MODEL

The heat pump and heat exchanger are not simulated directly but integrated through:

$$LWT = EWT + \frac{\dot{Q}_g}{\dot{V} \cdot \rho \cdot C_p}$$

Temperature variation induced by the heat pump operation



Transport processes

The nine species involved in the system are grouped in three total activities (Γ) according to the Tableaux method (Morel and Hering, 1993), allowing solving only three transport equations instead of nine:

$$\Gamma_H = [H^+] - [OH^-] + [H_2CO_3] - [CO_3^{2-}] - \left[CaCO_{3(aq)}\right] - [CaOH^+]$$

$$\Gamma_C = [HCO_3^-] + [H_2CO_3] + [CO_3^{2-}] + [CaHCO_3^+] + \left[CaCO_{3(aq)}\right]$$

$$\Gamma_{Ca} = [Ca^{2+}] + [CaHCO_3^+] + \left[CaCO_{3(aq)}\right] + [CaOH^+]$$

METHODOLOGY –TRANSPORT PROCESSES

The matrix U corresponds to:

$$\boldsymbol{U} = \begin{array}{c} \begin{matrix} \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 & \alpha_6 & \alpha_7 & \alpha_8 & \alpha_9 \end{matrix} \\ \begin{bmatrix} 1 & 0 & 0 & -1 & 1 & -1 & 0 & -1 & -1 \\ 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix} \end{array} \begin{matrix} \Gamma_H \\ \Gamma_{HCO3} \\ \Gamma_{Ca} \end{matrix}$$

At the equilibrium (Saaltink and al., 1998; Holzbecher, 2012):

$$\boldsymbol{U} \cdot \boldsymbol{\alpha} - \boldsymbol{\Gamma} = 0$$

with

$$\boldsymbol{\alpha} = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_9 \end{pmatrix} \qquad \boldsymbol{\Gamma} = \begin{pmatrix} \Gamma_H \\ \Gamma_{HCO3} \\ \Gamma_{Ca} \end{pmatrix}$$

A first set of 3 (N_s-N_r) nonlinear differential equations is locally solved in an ODEs and DAEs module over the domain to simulate the transport processes and to link the transport with equilibrium and kinetic reactions.

Reaction kinetics

$$CaCO_{3(s)} + H^+ \underset{k_{-1}}{\overset{k_1}{\leftrightarrow}} Ca^{2+} + HCO_3^-$$

$$CaCO_{3(s)} + H_2CO_3 \overset{k_2}{\underset{k_{-2}}{\leftrightarrow}} Ca^{2+} + 2HCO_3^-$$

$$CaCO_{3(s)} + H_2O \underset{k_{-3}}{\overset{k_3}{\leftrightarrow}} Ca^{2+} + HCO_3^- + OH^-$$

The direct reaction rate constants are calculated as follow (Plummer et al., 1978):

$$\log k_1 = 0.198 - (444/T) \qquad \log k_3 = -5.86 - (317/T) \quad T \leq 25°C$$

$$\log k_2 = 2.84 - (2177/T) \qquad \log k_3 = -1.10 - (1737/T) \quad T > 25°C$$

The reverse reaction rate constant can be defined as follow:

$$k_{-j} = \frac{k_j}{K_{eq,j}}$$

METHODOLOGY – REACTION KINETICS

The reaction rates of the three kinetic reactions can be defined as follow:

$$\hat{R}_1 = k_1 \cdot \alpha_{H^+} - k_{-1} \cdot \alpha_{Ca^{2+}} \cdot \alpha_{HCO_3^-}$$

$$\hat{R}_2 = k_2 \cdot \alpha_{H_2CO_3} - k_{-2} \cdot \alpha_{Ca^{2+}} \cdot \alpha^2_{HCO_3^-}$$

$$\hat{R}_3 = k_3 \cdot \alpha_{H_2O} - k_{-3} \cdot \alpha_{Ca^{2+}} \cdot \alpha_{HCO_3^-} \cdot \alpha_{OH^-}$$

The kinetic reactions are integrated in the model through a reaction term in the Solute Transport module as follow:

$$\boldsymbol{U} \cdot \boldsymbol{S'_k} \cdot \boldsymbol{r_k} = \begin{bmatrix} -\hat{R}_1 - \hat{R}_2 - \hat{R}_3 \\ \hat{R}_1 + \hat{R}_2 + \hat{R}_3 \\ \hat{R}_1 + \hat{R}_2 + \hat{R}_3 \end{bmatrix}$$

where

$$\boldsymbol{S_k} = \begin{array}{c} \begin{matrix} \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 & \alpha_6 & \alpha_7 & \alpha_8 & \alpha_9 \end{matrix} \\ \begin{bmatrix} 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2 & -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \begin{matrix} r_1 \\ r_2 \\ r_3 \end{matrix}$$

$$\boldsymbol{r_k} = \begin{array}{c} R_j \\ \begin{bmatrix} \hat{R}_1 \\ \hat{R}_2 \\ \hat{R}_3 \end{bmatrix} \end{array}$$

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METHODOLOGY – EQUILIBRIUM REACTIONS

Equilibrium reactions

$$H^+ + OH^- \leftrightarrow H_2O \qquad Ca^{2+} + HCO_3^- \leftrightarrow CaHCO_3^+ \qquad Ca^{2+} + CO_3^{2-} \leftrightarrow CaCO_{3(aq)}$$

$$H^+ + CO_3^{2-} \leftrightarrow HCO_3^- \qquad H^+ + HCO_3^- \leftrightarrow H_2CO_3 \qquad H^+ + CaOH^+ \leftrightarrow Ca^{2+} + H_2O$$

At the equilibrium (Saaltink and al., 1998, Holzbecher, 2012):

$$\boldsymbol{S_e} \cdot \log \boldsymbol{\alpha} - \log \boldsymbol{K} = 0$$

with

$$\boldsymbol{S_e} = \begin{array}{c} \begin{matrix} \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 & \alpha_6 & \alpha_7 & \alpha_8 & \alpha_9 \end{matrix} \\ \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & -1 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{matrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \\ r_6 \end{matrix} \end{array}$$

$$\boldsymbol{K} = \begin{pmatrix} K_1 \\ \vdots \\ K_6 \end{pmatrix}$$

A second set of 6 (N_r) nonlinear differential equations is locally solved in an ODEs and DAEs module over the domain to simulate the equilibrium reactions.

SUMMARY

- The system of 9 equations (one for each reaction) and 9 unknown (one for each species) is solved at each point of the domain through an ODEs and DAEs module.

- The first set of 3 (N_s-N_r) nonlinear differential equations is solved to simulate the transport processes and to link the transport with equilibrium and kinetic reactions:

$$\boldsymbol{U} \cdot \boldsymbol{\alpha} - \boldsymbol{\Gamma} = 0$$

- The kinetic reactions are integrated in the model through a reaction term in the Solute Transport module:

$$\boldsymbol{U} \cdot \boldsymbol{S_k'} \cdot \boldsymbol{r_k} = \begin{bmatrix} -\hat{R}_1 - \hat{R}_2 - \hat{R}_3 \\ \hat{R}_1 + \hat{R}_2 + \hat{R}_3 \\ \hat{R}_1 + \hat{R}_2 + \hat{R}_3 \end{bmatrix}$$

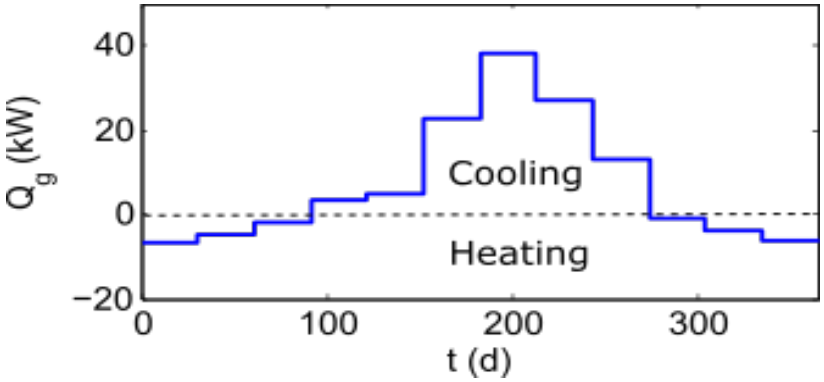
- The second set of 6 (N_r) nonlinear differential equations is solved to simulate the equilibrium reactions:

$$\boldsymbol{S_e} \cdot \log \boldsymbol{\alpha} - \log \boldsymbol{K} = 0$$

RESULTS

Simulation of a 1-year typical operation ($\dot{V}$ =3e-3m^3/s, initial pH=7 and initial PCO_2=4.1e-2 atm):

a)



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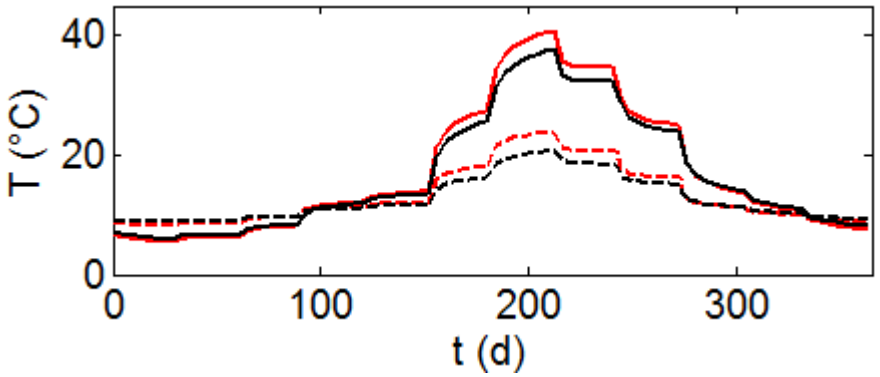
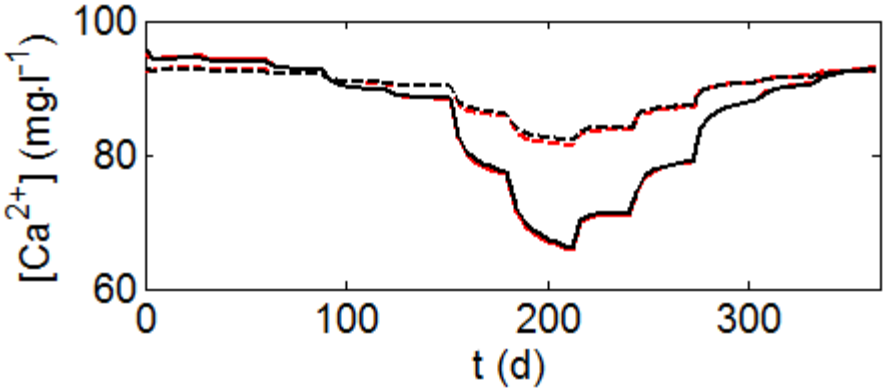
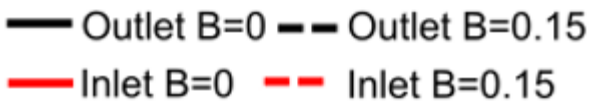


c)

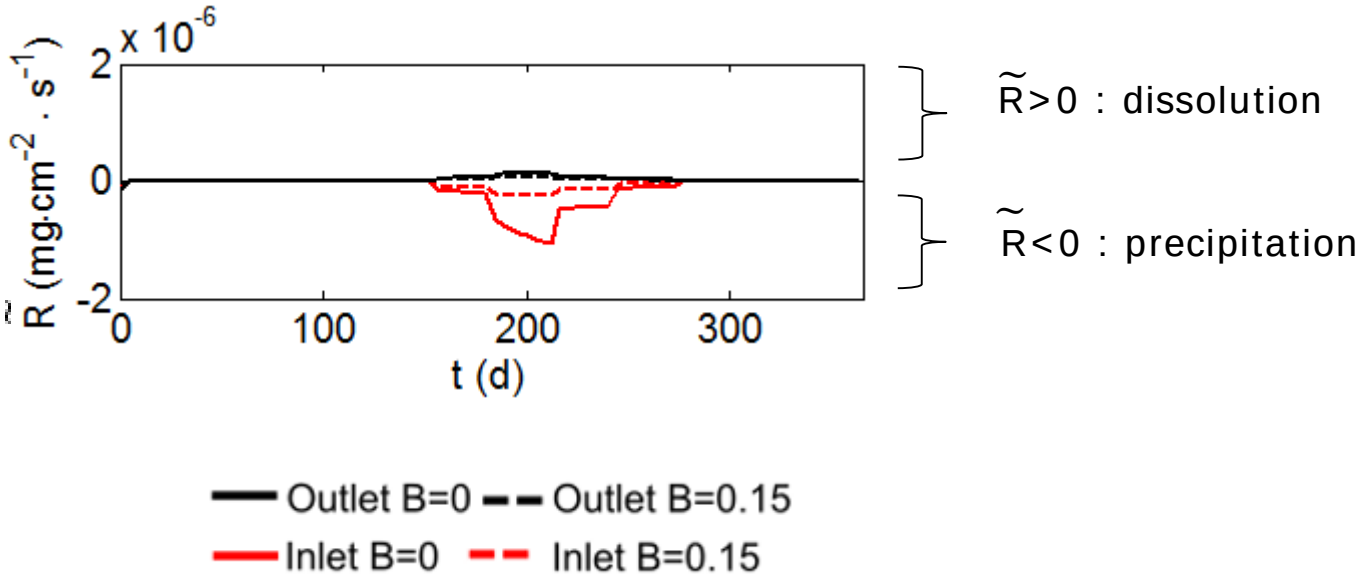




RESULTS

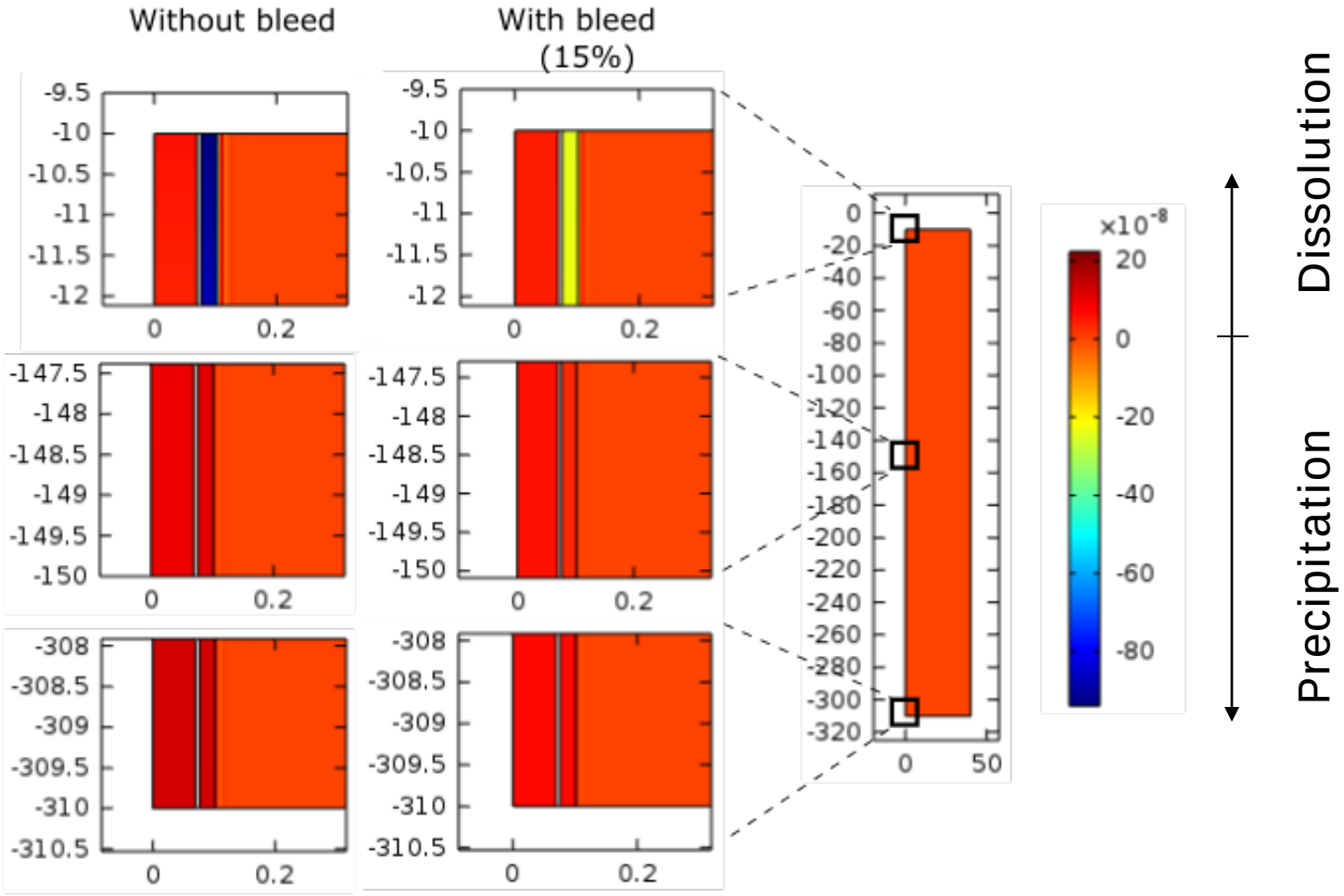
The overall rate of precipitation and dissolution of calcite is given by (Plummer and al., 1978):

$$\tilde{R} = k_1 \alpha_{H^+} + k_2 \alpha_{H_2CO_3} + k_3 \alpha_{H_2O} - k_{-1} \alpha_{Ca^{2+}} \alpha_{HCO_3^-} - k_{-2} \alpha_{Ca^{2+}} \alpha_{HCO_3^-}^2 - k_{-3} \alpha_{Ca^{2+}} \alpha_{HCO_3^-} \alpha_{OH^-}$$



RESULTS

Rate of reaction of calcite (mg/(cm^2·s)) after 200 days of simulation without bleed and with 15% of the pumped water discharged outside the well:



CONCLUSIONS

1. The developed model allows simulating the thermo-hydro-geochemical processes in a SCW and the geological formation.

2. The results show that:
    1. Mineral scaling in SCWs should be considered;
    2. In the well, the concentration of Ca^{2+} is inversely proportional to the temperature and thus calcite precipitation is likely to occur in summer;
    3. The bleed tends to stabilize the parameters and thus, limit the risk of precipitation of calcite.

CONCLUSION - REFERENCES

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4) Nguyen, A., Pasquier, P., Marcotte, D., 2012. Multiphysics modelling of standing column well and implementation of heat pumps off-loading sequence. In : Comsol Conference, Boston, USA.

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6) Nguyen, A., Pasquier, P., 2015. An Adaptive Segmentation Haar Wavelet Method for Solving Thermal Resistance and Capacity Models of Ground Heat Exchangers, Applied Thermal Engineering 89, 70-79.

7) Nguyen, A., Pasquier, P., Marcotte, D., 2015. Influence of Groundwater Flow in Fractured Aquifers on Standing Column Wells Performance, Geothermics, In Press.

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9) Plummer, L., Wigley, T., Parkhurst, D., 1978. The kinetics of calcite dissolution in co2 -water systems at 5 to 60°C and 0 to 1 atm co2. Am Jour Sci 278, 179–216.

10) Saaltink, M.W., Ayora, C., Carrera, J., 1998. A mathematical formulation for reactive transport that eliminates mineral concentrations. Water Resources Research 34, 1649–56.

QUESTIONS

http://69.18.148.120/~/media/Files/resources/oilfield_review/ors99/aut99/fighting.pdf

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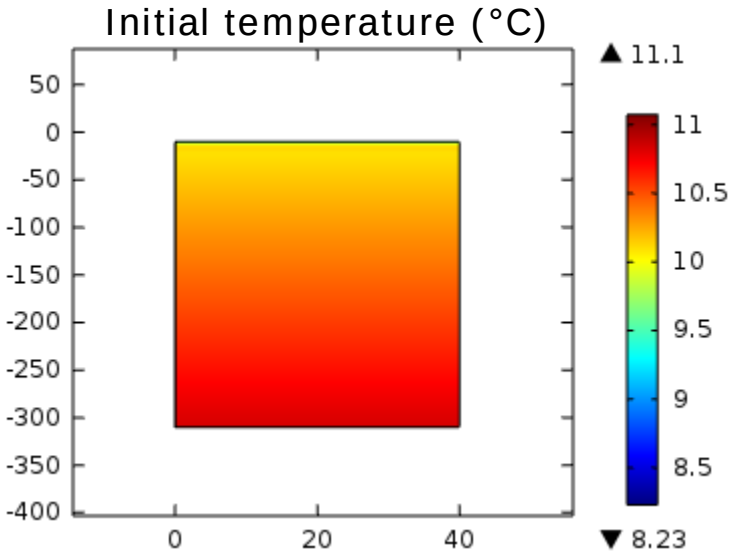
ANNEX 1– LUNARDINI (1981) MODEL

Lunardini (1981) model

$$T(z,t) = T_m + \frac{q_g \cdot z}{k_{eq}} - T_0 \cdot e^{-z\cdot\sqrt{\frac{2\pi}{2\alpha P}}} \cdot \cos\left(\omega \cdot (t - t_d) - z \cdot \sqrt{\frac{2\pi}{2\alpha P}}\right)$$



T_m	: mean annual air temperature	[°C]	10
z	: depth below the ground surface	[m]	
T_o	: amplitude of the seasonal variation relative to T_m	[°C]	15.08
P	: period of the cycle	[s]	$3.1536 \cdot 10^7$
ω	: angular frequency	[1/s]	2π·P
α	: thermal diffusivity	[m^2/s]	$9.77 \cdot 10^{-7}$
t_d	: time lag corresponding to the lowest annual temperature after January 1st	[s]	20.7·24·3600
q_g	: heat flux	[W/m^2]	0.006
K_{eq}	: equivalent thermal conductivity	[W/m/K]	2.31

ANNEX 2 – TABLEAUX METHOD

Tableaux method (Morel and Hering, 1993) with H^+, HCO_3^- and Ca^{2+}:

Species	Combination	Components		
		H	HCO3	Ca
H^+	$(H^+)_1$	1	0	0
HCO_3^-	$(HCO_3^-)_1$	0	1	0
Ca^{2+}	$(Ca^{2+})_1$	0	0	1
OH^-	$(H_2O)_1(H^+)_{-1}$	-1	0	0
H_2CO_3	$(HCO_3^-)_1(H^+)_1$	1	1	0
CO_3^{2-}	$(HCO_3^-)_1(H^+)_{-1}$	-1	1	0
$CaHCO_3^+$	$(Ca^{2+})_1(HCO_3^-)_1$	0	1	1
$CaCO_{3(aq)}$	$(H^+)_{-1}(HCO_3^+)_1(Ca^{2+})_1$	-1	1	1
$CaOH^+$	$(H_2O)_1\ (H^+)_{-1}(Ca^{2+})_1$	-1	0	1

$$\Gamma_H = [H^+] - [OH^-] - [CO_3^{2-}] + [H_2CO_3] - [CaCO_{3(aq)}] - [CaOH^+]$$

$$\Gamma_C = [CaHCO_3^+] + [CO_3^{2-}] + [H_2CO_3] + [HCO_3^-] + [CaCO_{3(aq)}]$$

$$\Gamma_{Ca} = [Ca^{2+}] + [CaHCO_3^+] + [CaCO_{3(aq)}]$$

ANNEX 4 – RESULTS

THG model - parameters

Groundwater flow and heat transfer model			
Parameters	**Fluid**	**Soil**	**Pipe**
Density (kg/m3)	1000	2700	1300
Normal velocity of the fluid inner (m/s)	$7.24 \cdot 10^{-7}$	-	-
Normal velocity of the fluid outer (m/s)	$7.24 \cdot 10^{-7}$	-	-
Porosity	-	0.1	-
Pumping rate (l/min)	151	-	-
Hydraulic conductivity (m/s)	-	$2 \cdot 10^{-6}$	$1 \cdot 10^{-9}$
Thermal conductivity (W/K/m)	0.6	2.5	0.0974
Volumetric heat capacity (J/K/kg)	4200	800	1200
Borehole length (m)	300		
Borehole radius (m)	0.102		
Inner pipe radius (m)	0.07		
Outer pipe radius (m)	0.076		
Soil radius (m)	40		

Chemical model	
Parameters	**Initial values**
pH (-)	7
PCO_2 (atm)	$4.1 \cdot 10^{-2}$
$[H^+]$	10^{-pH}
$[HCO_3^-]$	$\frac{K_1 \cdot [H_2CO_3]}{[H^+]}$
$[Ca^{2+}]$	$\frac{K_{sp}}{[CO_3^{2-}]}$
$[OH^-]$	$\frac{K_w}{[H^+]}$
$[H_2CO_3]$	$K_H \cdot PCO_2$
$[CO_3^{2-}]$	$\frac{K_2 \cdot [HCO_3^-]}{[H^+]}$
$[CaHCO_3^+]$	$\frac{[Ca^{2+}] \cdot [HCO_3^-]}{K_{CaHCO3}}$
$[CaCO_{3(aq)}]$	$\frac{[Ca^{2+}] \cdot [CO_3^{2-}]}{K_{CaCO3(aq)}}$
$[CaOH^+]$	$\frac{K_{CaOH} \cdot [Ca^{2+}]}{[H^+]}$