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GEOCHEMICAL CALCULATION WORKFLOW TO ESTIMATE FLUID CHEMISTRY OF WATER DOMINATED GEOTHERMAL RESERVOIR

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ABSTRACT

Sampled aqueous chemistry at surface, is altered from reservoir chemistry due to boiling, degassing of non-condensable gases (mostly CO_2), and conductively or adiabatically cooling in wellbore at water dominated geothermal field. Geochemical modelling studies, from reservoir to surface or reinjection, begin by computing the initial equilibrium state of the system at temperature and pressure of geothermal reservoir. Practically, however, physical and chemical properties of fluid in reservoir cannot be measured. Therefore, in such cases, fluid chemistry is calculated from chemical analysis of surface samples. Consequently, some geochemical calculation steps should be combined to estimate reservoir chemistry.

Aqueous chemical analysis reveals just bulk composition of the solution. In order to distribute bulk composition among concentrations of ionic and molecular species, speciation step should be conducted. This process is the first step of the geochemical calculation workflow. Following steps are; mixing, increasing temperature, dissolution and equilibration. In this paper, governing equations that used in geochemical calculations and computation sequence of geochemical models are introduced to estimate reservoir fluid chemistry.

1. INTRODUCTION

Geochemical monitoring studies are conducted in exploitation stage of water dominated geothermal field to observe changes in thermal fluid properties and get insight about the ongoing processes. Practically, thermal waters (brine) and gas phases are sampled by using separators at surface instead of the reservoir. However, physical and chemical properties of thermal fluids which at or close to equilibrium with host rocks in a reservoir, change as ascending throughout the well and some minerals may precipitate in wellbore. Mineral scaling is mainly related to both evaporation of brine which increases dissolved species concentrations and simultaneously degassing of CO_2 which trigger some consecutive reactions that increase saturation index of carbonate dependent minerals as a result of pH rising (Akin et al 2015).

On the other hand, initial fluid chemistry (reservoir) is essential for observation of variations in water-rock interactions and partial pressure of CO_2 in reservoir during production time of the field. In addition, reservoir chemistry is also input parameter for evaluation of flash point depth in well by geochemical modelling.

Therefore, fluid chemistry at reservoir level should be calculated from chemical analysis of surface samples to get relevant data along with conducting geochemical modelling. To do this, speciation of brine and steam bulk compositions, mixing of aqueous and gas phase according to steam fraction, increasing reaction temperature to reservoir state, reacting and equilibrating solution with measured NCG along with observed mineral phase should be conducted in a sequence of given workflow.

2. GOVERNING EQUATIONS

Derivation of governing equations is necessary for describing equilibrium state of the geochemical system. All independent reactions among species, minerals and gases should be rewritten in terms of mass action equations. Mass balance equations should also be derived for all components in the system. Final governing equations which can be solved directly to find equilibrium state of the system should be derived by rewriting mass balance equations in terms of the mass action equations.

A geochemical system can be expressed by reaction much more than independent reaction number however, remaining reactions (dependent reactions) are linear combination of the independent reactions. Thus it is not necessary to take dependent reactions in to account. Independent reactions must be written between secondary and basis species (figure 1).

The independent reactions are those between the secondary species and the basis. In general form, the reactions are,

$$A_j \Leftrightarrow v_{wj}A_w + \sum_i v_{ij}A_i + \sum_i v_{kj}A_k + \sum_i v_{mj}A_m \qquad [2.1]$$

Here, v represents the reaction coefficients, v_{wj} is the number of moles of water in the reaction to form A_j, v_{ij} is the number of moles of the basis species A_i, k and m subscripts for the minerals and gases in same manner. Because of no reaction can be written between basis species, primary (basis) species must be selected based on the rule.

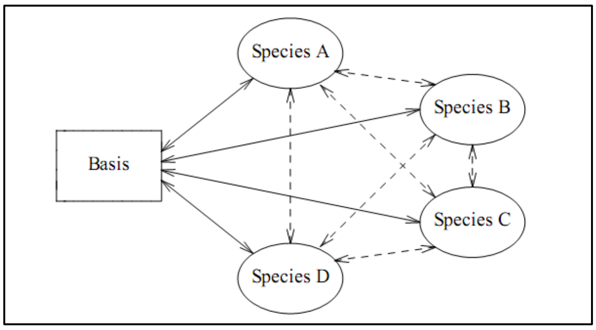


Figure 1: Independent (solidlines) and dependent (dashedlines) reactions in a chemical system composed of a basis and four secondary species A through D. Only the independent reactions need to be considered (Bethke 2008).

Each independent reaction in the equation 2.1 has an associated equilibrium constant K at the temperature of interest and, hence, a mass action equation of the form;

$$K_j = \frac{a_w^{v_{wj}}.\prod^i (\gamma_i m_i)^{v_{ij}}.\prod^k a_k{}^{v_{kj}}.\prod^m f_m{}^{v_{mj}}}{\gamma_j m_j} \qquad [2.2]$$

Here, a represents activity, f is the fugacity of gas, γ is the activity coefficient, m is the molality of the species. As Bethke (2008) has stated that aim in deriving the governing equations is to reduce the number of independent variables by eliminating the molalities m_j of the secondary species. For this purpose, equation 2.2 can be rearranged to get final mass action equation of m_j as;

$$m_j = \frac{1}{K_j\gamma_j}\left[a_w^{v_{wj}}.\prod^i(\gamma_i m_i)^{v_{ij}}.\prod^k a_k{}^{v_{kj}}.\prod^m f_m{}^{v_{mj}}\right] \qquad [2.3]$$

Mass balance equations state that component mass must be conserved during the speciation or any kind of geochemical calculation step. This means that analyzed bulk compositions are distributed among species, minerals and gases that form the system. According to equation 2.1, each mole of species A_j is composed of v_{wj} moles of the water component. The mole number M_w of water component is given by

$$M_w = n_w\left(55.5 + \sum_j v_{wj}m_j\right) \qquad [2.4]$$

Where 55.5 is the number of moles of H_2O in a kilogram of water. Multiplying molality units by the mass n_w of solvent water gives result in moles, as desired. Similar logic gives the mass balance equations for the species and mineral components (eq. 2.5-2.6).

$$M_i = n_w\left(m_i + \sum_j v_{ij}m_j\right) \qquad [2.5]$$

$$M_k = n_k + n_w\sum_j v_{kj}m_j \qquad [2.6]$$

Where M_i is primary species component, M_k is mineral components and n_k is the mole number of the mineral corresponding to the component.

3. CALCULATION WORKFLOW

Fluid sampling at surface is conducted in two phase (water + gas) flow conditions at water dominated geothermal fields. Liquid and gas phase should be sampled by using separator to avoid any contamination due to mixing of phases. Gas phase should also be sampled separately as steam condensate and non-condensable gas (NCG). Therefore, geochemical calculation workflow includes speciation, mixing, increasing temperature, dissolution and equilibration steps to estimate reservoir chemistry (figure 2).

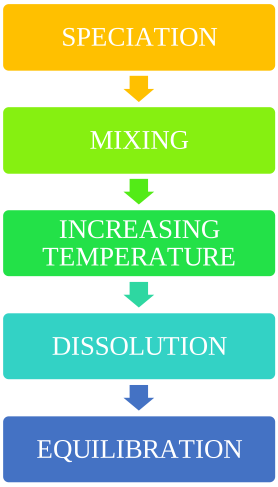


Figure 2: Workflow of geochemical calculations

Aqueous chemical analysis just reveals bulk composition of the solution. In order to determine saturation states with respect to various minerals in the system and hence, the direction of reactions that might occur toward achieving equilibrium, one should calculate distribution of bulk composition among concentrations of ionic and molecular species according to their activities. This process is called speciation in geochemical modelling and constitutes the first step of computations. Speciation must obey the mass balance of components and mass action law of considered reactions.

3.1 Speciation

Some bulk composition analysis such as total inorganic carbon (TIC), six valence sulphur (SO_4^{-2}), K, Na, Ca, Si are considered in order to explain details of the speciation and other steps of the workflow. In this case 16 reactions can be written among dissolved species (table 1). The reaction number may differs based on obtained database.

Table 1: Considered reactions

ID	Reaction	Log K (25 °C)
R1	$H_2O = OH^- + H^+$	-14
R2	$CO_3^{-2} + H^+ = HCO_3^-$	10.329
R3	$CO_3^{-2} + 2H^+ = CO_2 + H_2O$	16.681
R4	$SO_4^{-2} + H^+ = HSO_4^-$	1.988
R5	$Ca^{+2} + H_2O = CaOH^+ + H^+$	-12.78
R6	$Ca^{+2} + CO_3^{-2} = CaCO_3$	3.224
R7	$Ca^{+2} + CO_3^{-2} + H^+ = CaHCO_3^+$	11.435
R8	$Ca^{+2} + SO_4^{-2} = CaSO_4$	2.25
R9	$Ca^{+2} + HSO_4^- = CaHSO_4^+$	1.08
R10	$K^+ + SO_4^{-2} = KSO_4^-$	0.85
R11	$Na^+ + OH^- = NaOH$	-10
R12	$Na^+ + CO_3^{-2} = NaCO_3^-$	1.27
R13	$Na^+ + HCO_3^- = NaHCO_3$	-0.25
R14	$Na^+ + SO_4^{-2} = NaSO_4{}^-$	0.7
R15	$H_4SiO_4 = H_3SiO_4{}^- + H^+$	-9.83
R16	$H_4SiO_4 = H_2SiO_4{}^{-2} + 2H^+$	-23

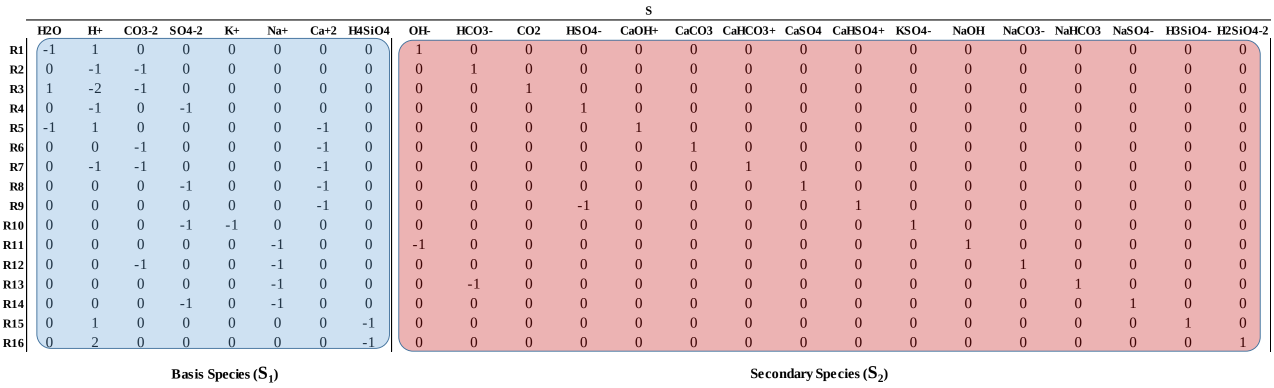
Reactions in the table 1 can be demonstrated in stoichiometry matrix (figure 3). Reaction coefficients at left hand side of the equations (reactants) is negative whereas it is positive at right hand side (products) according to conventional rule. There is 24 species in 16 reactions. 8 basis species (component) is needed according to phase rule. Selecting components to make up the basis should subject to three rules; each species and phase considered in the geochemical model can be formed from some combination of the components in the basis, the number of components in the basis is the minimum necessary to satisfy the previous rule and any balanced reaction could not be written to form one component in terms of the others. Therefore, H_2O, H^+, CO_3^{-2}, SO_4^{-2}, K^+, Na^+, Ca^{+2}, H_4SiO_4 species can be selected for basis species. Any other combination of basis species from other species, which obeys the mentioned rules, can also be chosen.

Linear algebra rules can be used due to reactions are demonstrated in matrix form. Hence, transforming dependent reactions to independent ones and calculating mass action along with mass balance equations can be easily done by forming of component matrix (figure 4). Component matrix can be designed by using equation 3.1. If there is any dependent reaction exist in the equation system like R9 and R13 in the table 1, equilibrium constant of the reaction should also be recalculated for transformed independent reaction by using equation 3.2. If values of basis species is known, concentration of secondary species can be calculated by using equation 2.1.

$$U = (I|-S_1^T(S_2^T)^{-1}) = (I|(S_1^*)^T) \qquad [3.1]$$

$$Log\ K^* = (S_2)^{-1} Log\ K \qquad [3.2]$$

In addition, pH is measured directly by using probes, which means that it is not bulk composition of the hydrogen combined species, it is just free H^+ ions in the solution. Therefore bulk composition of the hydrogen combined species (H component) should be calculated by constraining pH value in the mass balance equation of the M_H.

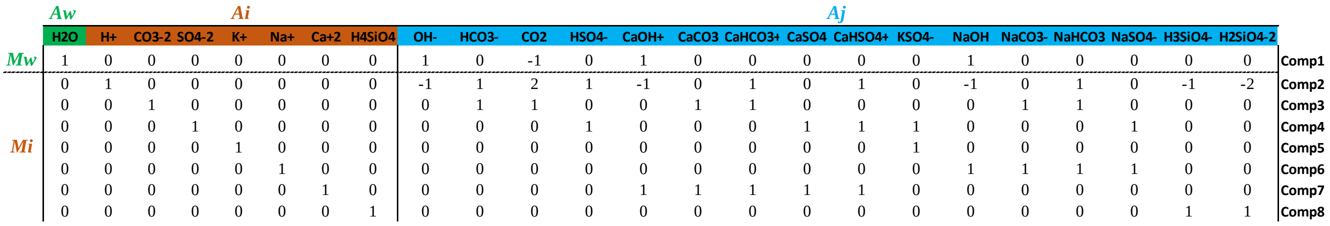


S	H2O	H+	CO3-2	SO4-2	K+	Na+	Ca+2	H4SiO4	OH-	HCO3-	CO2	HSO4-	CaOH+	CaCO3	CaHCO3+	CaSO4	CaHSO4+	KSO4-	NaOH	NaCO3-	NaHCO3	NaSO4-	H3SiO4-	H2SiO4-2
R1	-1	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
R2	0	-1	-1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
R3	1	-2	-1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
R4	0	-1	0	-1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
R5	-1	1	0	0	0	0	-1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
R6	0	0	-1	0	0	0	-1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
R7	0	-1	-1	0	0	0	-1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
R8	0	0	0	-1	0	0	-1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
R9	0	0	0	0	0	0	-1	0	0	0	0	-1	0	0	0	0	1	0	0	0	0	0	0	0
R10	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
R11	0	0	0	0	0	-1	0	0	-1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
R12	0	0	-1	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
R13	0	0	0	0	0	-1	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	1	0	0	0
R14	0	0	0	-1	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
R15	0	1	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
R16	0	2	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

Basis Species (S_1)

Secondary Species (S_2)

Figure 3: Demonstration of equilibrium reactions in stoichiometry matrix form.



	Aw	Ai							Aj																
	H2O	H+	CO3-2	SO4-2	K+	Na+	Ca+2	H4SiO4	OH-	HCO3-	CO2	HSO4-	CaOH+	CaCO3	CaHCO3+	CaSO4	CaHSO4+	KSO4-	NaOH	NaCO3-	NaHCO3	NaSO4-	H3SiO4-	H2SiO4-2	
Mw	1	0	0	0	0	0	0	0	1	0	-1	0	1	0	0	0	0	0	1	0	0	0	0	0	Comp1
	0	1	0	0	0	0	0	0	-1	1	2	1	-1	0	1	0	1	0	-1	0	1	0	-1	-2	Comp2
	0	0	1	0	0	0	0	0	0	1	1	0	0	1	1	0	0	0	0	1	1	0	0	0	Comp3
	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	1	1	1	0	0	0	1	0	0	Comp4
Mi	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	Comp5
	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	0	0	Comp6
	0	0	0	0	0	0	1	0	0	0	0	0	1	1	1	1	1	0	0	0	0	0	0	0	Comp7
	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	Comp8

Figure 4: Component matrix. Columns of Aj represents eq. 2.1. Mass balance equations (2.4, 2.5, 2.6) can be calculated by rows of the matrix.

In the same manner, water mass can also be constrained in the mass balance equation of water (M_w). Because, chemical analysis are performed in laboratory condition and water mass is almost equal to 1 kg. Next steps of the workflow need all bulk mass of the systems so, speciation should be the first step.

3.2 Mixing

Water and hydrogen components are known after speciation calculation of brine and steam condensate. The next step is to multiply all bulk mass of the brine and condensate with steam fraction of the sampled well. Steam fraction of geothermal well is calculated based on equation 3.3.

$$H_{res} = (1 - x)H_l + xH_v \qquad [3.3]$$

Here H_{res} is reservoir enthalpy of water dominated system, H_l is liquid whereas H_v is vapour phase enthalpy at sampling temperature and x is steam fraction. After updating bulk masses of mixture, new speciation can be conducted. In this case, however, water mass and pH are not constrained, which means that their values can be changed during distribution of bulk masses among dissolved species in speciation step.

3.3 Increasing Temperature

Equilibrium constants of reactions are important in calculation of secondary species (eq. 2.3) so, they should be recalculated to represent reservoir conditions. While variations in pressure have negligible effect on the equilibrium constant, the temperature variations are significant. The value of equilibrium constant at various temperature is usually calculated with the Van't Hoff equation:

$$\frac{dlnK}{dT} = \frac{\Delta H_r}{RT^2} \qquad [3.4]$$

Where ΔH_r is the reaction enthalpy, K is the equilibrium constant, R is the ideal gas constant and T is the temperature in Kelvin. However, if the database includes essential coefficients, equilibrium constant can be calculated from an analytical expression of the type:

$$\log k = A_1 + A_2.T + A_3/T + A_4.logT + A_5/T^2 \qquad [3.5]$$

Where T is temperature in Kelvin and the numbers are fit parameters. Increasing temperature step just updating log K of the reactions based on reservoir conditions.

3.4 Dissolution

Generally, carbon dioxide is the main non condensable gas in water dominated geothermal fields. In two phase flow condition, carbon dioxide and water vapour generates first gas bubble to compensate for the pressure difference at the depth where total partial pressure of both dissolved CO_2 and H_2O exceed dynamic pressure. The gas exsolution shifts equation 3.8 to left by combining bicarbonate with hydrogen. As a result, pH increases and some consecutive reactions that involve carbonate species occur. Decreases of hydrogen and bicarbonate concentration lead to rearrangement of ion activities based on equation 3.7 and 3.9.

$$CaCO_{3(s)} \leftrightarrow Ca^{+2}_{(aq)} + CO^{-2}_{3(aq)} \qquad [3.6]$$

$$CaCO_{3(s)} + H^{+}_{(aq)} \leftrightarrow Ca^{+2}_{(aq)} + HCO^{-}_{3(aq)} \qquad [3.7]$$

$$CO_{2(g)} + H_2O_{(l)} \leftrightarrow H^{+}_{(aq)} + HCO^{-}_{3(aq)} \qquad [3.8]$$

$$HCO^{-}_{3(aq)} \leftrightarrow CO^{-2}_{3(aq)} + H^{+}_{(aq)} \qquad [3.9]$$

These kind of consecutive reactions differ sampled brine chemistry while fluid ascending throughout the well. If gas phase includes NCG and the main constituents of NCG is CO_2 in the field, CO_2/H_2O ratio of gas phase should be measured during sampling with gas flow meter or any other relevant method (figure 5). Thus, mole of dissolved CO_2 per kg of thermal water at reservoir state can be calculated by using gas/steam ratio and steam fraction (table 2).

Figure 5: In situ measurements of gas/steam ratio.

Table 2: Calculation of steam fraction and dissolved CO_2 at reservoir condition.

Well head pressure (Barg)	12.5
Separator pressure (Barg)	11.5
Separator temperature (^{0}C)	182
Casing inlet temperature (^{0}C)	215
Water enthalpy at separator (kJ/kg)	771.895
Steam enthalpy at separator (kJ/kg)	2778.93
Steam enthalpy at casing inlet	920.527
Steam Fraction (%)	7.41
nCO_2/nH_2O at separator	0.186
nCO_2/nH_2O at reservoir	0.0138
nCO_2/mH_2O at reservoir (mole/kg)	0.765

As Bethke (2008) stated, the basis serves two purposes; each chemical reaction considered in the model is written in terms of the members of the basis set, and the system's bulk composition is expressed in terms of the components in the basis. However, dissolved CO_2 was not be selected for basis species as shown in the figure 3. Therefore, basis should be adapted to match current system by swapping method. In our cases, CO_3^{-2} can be swapped with CO_2 based on rules of choosing component. New basis species is written in terms of old basis and this is called transformation matrix (eq. 3.10). Bulk mass of already exist CO_2 in the system can be calculated by multiplying invers of the transformation matrix with CO_3^{-2} bulk mass (eq. 3.11).

$$\begin{vmatrix} H_2O \\ \mathrm{H}^+ \\ CO_2 \\ SO_4^{-2} \\ \mathrm{K}^+ \\ \mathrm{Na}^+ \\ \mathrm{Ca}^{+2} \\ H_4SiO_4 \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{vmatrix} \begin{vmatrix} H_2O \\ \mathrm{H}^+ \\ CO_3^{-2} \\ SO_4^{-2} \\ \mathrm{K}^+ \\ \mathrm{Na}^+ \\ \mathrm{Ca}^{+2} \\ H_4SiO_4 \end{vmatrix} \qquad [3.10]$$

$$\begin{vmatrix} H_2O \\ \mathrm{H}^+ \\ CO_3^{-2} \\ SO_4^{-2} \\ \mathrm{K}^+ \\ \mathrm{Na}^+ \\ \mathrm{Ca}^{+2} \\ H_4SiO_4 \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{vmatrix} \begin{vmatrix} H_2O \\ \mathrm{H}^+ \\ CO_2 \\ SO_4^{-2} \\ \mathrm{K}^+ \\ \mathrm{Na}^+ \\ \mathrm{Ca}^{+2} \\ H_4SiO_4 \end{vmatrix} \qquad [3.11]$$

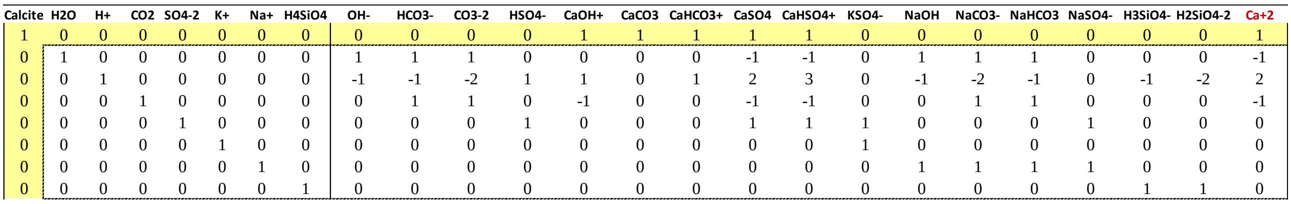
Hence, calculated amount of degassed CO_2 can be added into existed CO_2 bulk mass of the system (figure 6). After modifying bulk composition, new speciation step can be run to calculate species distribution, especially for pH.

3.5 Equilibration

Calcite scaling is widely encountered in geothermal wells and it has to be inhibited since it prevents production. As a result of a pressure drop, thermal fluids start to boil and degas of CO_2 while fluids rise in a wellbore. Thermal fluid becomes saturated to calcite as a result of both CO_2 exsolution and concentration increase of calcium and carbonates as a consequence of boiling. In order to prevent calcite scaling effectively, inhibitor must be injected into the wellbore at a depth below gas breakout point where thermal fluid is still in liquid phase. If inhibitor was not being used while sampling, the amount of calcium in the brine sample would be lower than initial quantity of reservoir. In such cases equilibration step should be conducted to estimate initial amount of dissolved species of calcite.

In order to equilibrate solution with calcite, dissolution reaction of the mineral phase should be added to stoichiometry matrix and swapped with any basis species based on rules of choosing component. In this case, calcium was selected for swapping (figure 6). By this way, bulk mass of calcite M_k is computed and speciation step can be performed to calculate final distribution of species.

Unlike CO_2, calcite is not be necessarily added to numerical solution part. Because equation 2.6 is linear and there is only one unknown n_k. In other words, M_k is constant and secondary species m_j are updated in iteration steps so, n_k is easily calculated by substitution. n_k is the dissolved or precipitated mass of calcite. If it is negative, this means dissolution. Otherwise, it means precipitation.



Calcite	H2O	H+	CO2	SO4-2	K+	Na+	H4SiO4	OH-	HCO3-	CO3-2	HSO4-	CaOH+	CaCO3	CaHCO3+	CaSO4	CaHSO4+	KSO4-	NaOH	NaCO3-	NaHCO3	NaSO4-	H3SiO4-	H2SiO4-2	Ca+2
1	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	0	0	0	0	0	0	0	1
0	1	0	0	0	0	0	0	1	1	1	0	0	0	0	-1	-1	0	1	1	1	0	0	0	-1
0	0	1	0	0	0	0	0	-1	-1	-2	1	1	0	1	2	3	0	-1	-2	-1	0	-1	-2	2
0	0	0	1	0	0	0	0	0	1	1	0	-1	0	0	-1	-1	0	0	1	1	0	0	0	-1
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0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	0	0	0
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0

Figure 6: Component matrix after swapping. In this case CO_2 and Calcite are basis species. Representing CO_3^{-2} and Ca^{+2} in terms of new basis species is calculated by transformation matrix.

3. CONCLUSIONS

Currently, there is special tools for fluid sampling from reservoir but these operations are not practical especially for inhibitor used production wells. In such cases, geochemical calculation workflow can be used to estimate reservoir fluid chemistry. Moreover, variations in water-rock interactions and partial pressure of CO_2 in reservoir can be monitored by the workflow during production time of the field.

Effective inhibition to mineral scaling can be achieved by injecting chemical inhibitors into liquid phase in casing. The depth of gas bubble formation in a geothermal well can be estimated more precisely using modelled or measured PT along with geochemical calculation (Akin et al, 2015). To do this, initial reservoir chemistry is essential and it can be estimated by workflow.

The sequence of workflow starts with speciation step to calculate bulk mass of constrained species like H_2O and pH. Because of the two phase flow condition, bulk composition of brine and steam should be multiplied with steam fraction related to sampled condition. Equilibrium constants of reactions are main parameters to effect calculation of secondary species (eq. 2.3) so, log K should be recalculated in increasing temperature steps to represent reservoir conditions. If gas phase includes NCG (mostly CO_2), mole of dissolved NCG per kg of thermal water at reservoir state should be calculated and added to bulk mass of mixture in dissolution step. If mineral scaling is exist before fluid sampling, dissolution of relevant mineral phase should be added to equation system and swapped with suitable basis in equilibration step.

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