Case study

EQUILGAS: Program to estimate temperatures and in situ two-phase conditions in geothermal reservoirs using three combined FT-HSH gas equilibria models ☆

Rosa María Barragán [a,*], José Núñez [b], Víctor Manuel Arellano [a], David Nieva [a]

[a] Instituto de Investigaciones Eléctricas, Gerencia de Geotermia, Reforma 113, Col Palmira, 62490 Cuernavaca, Morelos, México
[b] Universidad de La Ciénega del Estado de Michoacán de Ocampo. Avenida Universidad 3000, Fraccionamiento Lomas de la Universidad, 59103 Sahuayo, Michoacán, México

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ABSTRACT

Exploration and exploitation of geothermal resources require the estimation of important physical characteristics of reservoirs including temperatures, pressures and in situ two-phase conditions, in order to evaluate possible uses and/or investigate changes due to exploitation. As at relatively high temperatures (> 150 °C) reservoir fluids usually attain chemical equilibrium in contact with hot rocks, different models based on the chemistry of fluids have been developed that allow deep conditions to be estimated. Currently either in water-dominated or steam-dominated reservoirs the chemistry of steam has been useful for working out reservoir conditions. In this context, three methods based on the Fischer–Tropsch (FT) and combined H_2S–H_2 (HSH) mineral-gas reactions have been developed for estimating temperatures and the quality of the in situ two-phase mixture prevailing in the reservoir. For these methods the mineral buffers considered to be controlling H_2S–H_2 composition of fluids are as follows. The pyrite-magnetite buffer (FT-HSH1); the pyrite-hematite buffer (FT-HSH2) and the pyrite-pyrrhotite buffer (FT-HSH3). Currently from such models the estimations of both, temperature and steam fraction in the two-phase fluid are obtained graphically by using a blank diagram with a background theoretical solution as reference. Thus large errors are involved since the isotherms are highly nonlinear functions while reservoir steam fractions are taken from a logarithmic scale. In order to facilitate the use of the three FT-HSH methods and minimize visual interpolation errors, the EQUILGAS program that numerically solves the equations of the FT-HSH methods was developed. In this work the FT-HSH methods and the EQUILGAS program are described. Illustrative examples for Mexican fields are also given in order to help the users in deciding which method could be more suitable for every specific data set.

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1. Introduction

Geothermal reservoirs can be considered closed systems in which fluid-rock interaction processes take place at relatively high temperatures ($\geq$ 150 °C) and hence the assumption of chemical equilibrium is justified (Truesdell et al., 1987). For this reason the chemistry of fluids discharged by geothermal wells reflects important characteristics of the deep conditions, which are useful for evaluating the resource and deciding on its optimal utilization. In order to estimate the capacity of liquid and steam-dominated reservoirs to produce power the volumetric liquid saturation, which is defined in terms of temperature and in situ amount of steam in

the two-phase original fluid, should be investigated (D'Amore and Pruess, 1986; D'Amore, 1992; D´Amore and Truesdell, 1995). When the liquid saturation is close to zero in a reservoir, in most cases the flow will decrease rapidly and will not support electric power generation. In two-phase reservoirs when water is produced this is taken as a good indication of relatively high liquid saturations in the reservoir. Besides, the chemical composition of water helps in estimating reservoir conditions like deep temperatures through liquid geothermometers. By contrast, in steam-dominated reservoirs the liquid remains in the rock as an immobile phase and no water is produced to give an indication of actual liquid saturation conditions at the reservoir which are needed to evaluate the resource potential. For both wet two-phase and dry geothermal wells the chemistry of steam through the modeling of mineral-gas reactions allows estimation of deep conditions in terms of reservoir temperatures and in situ two-phase conditions. Among a number of existing steam models (D'Amore and Panichi,

1980; Giggenbach, 1980; Nieva et al., 1987) those based on the Fischer–Tropsch reaction together with H_2S-H_2 gas-mineral reactions have been documented and are readily available (D'Amore and Truesdell, 1985; D'Amore, 1992; 1998; Siega et al., 1999). Such methods named FT-HSH1, FT-HSH2 and FT-HSH3 consider combined pyrite-magnetite, pyrite-hematite and pyrite-pyrrhotite mineral buffers respectively, to be controlling the H_2S concentration in fluids (D'Amore and Truesdell, 1985; D'Amore, 1998; Siega et al., 1999, Arellano et al., 2003; Salonga et al., 2004). According to such methods, both the reservoir temperatures and the quality of the mixture in two-phase reservoirs can be estimated by calculating two parameters from gas equilibria: FT and HSH. These parameters are then represented graphically on suitable background grids as reference, which contain theoretical curves calculated for both parameters for specific temperatures and steam contents. However, although results can be inferred from the graphical method, large errors may occur since the steam fractions are taken from a logarithmic scale while isotherms from which temperatures are obtained are highly non-linear functions. Then, in order to allow better estimations of reservoir temperatures and steam fractions from FT-HSH1, FT-HSH2 and FT-HSH3 methods, the EQUILGAS program, that numerically solves the non-linear equations on which the methods are based, was developed. In this work the three FT-HSH methods and the EQUILGAS program are described. Some examples for Mexican fields are also included.

## 2. Description of the FT-HSH gas equilibrium methods (Siega et al. 1999)

For the three equilibrium models FT-HSH1, FT-HSH2 and FT-HSH3, the Fisher–Tropsch reaction (FT) which is given in Eq. (1) is considered.

$$(FT): CO_2 + 4H_2 = CH_4 + 2H_2O \tag{1}$$

For the FT-HSH1 method, the pyrite-magnetite (HSH1) mineral buffer is considered to be controlling the concentration of H_2S in fluids. This reaction is given in Eq. (2):

$$(HSH1)\ H_2 + 2H_2O + 3/2FeS_2 = 3H_2S + \tfrac{1}{2}Fe_3O_4 \tag{2}$$
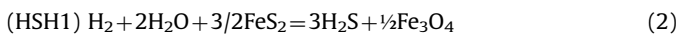
While for the FT-HSH2 method, the concentration of H_2S in fluids is considered to be controlled by a mineral buffer resulting from the combined pyrite-magnetite and pyrite-hematite equilibria, according to Eq. (3):

$$(HSH2)\ 5/4H_2 + \tfrac{3}{4}Fe_2O_3 + 3/2FeS_2 + 7/4H_2O = 3H_2S + Fe_3O_4 \tag{3}$$
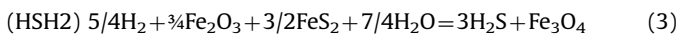
And for the FT-HSH3 method, the concentration of H_2S in fluids is considered to be controlled by a mineral buffer resulting from the combined pyrite-magnetite and pyrite-pyrrhotite equilibria, according to Eq. (4):

$$(HSH3)\ H_2 + FeS_2 = H_2S + FeS \tag{4}$$

Thermodynamic equilibrium constants for the reactions given in Eqs. (1)–(4) expressed in molar proportion with respect to H_2O are given as follows:

$$Log\ KFT = 4\log P_{H2} + \log P_{CO2} - \log P_{CH4} - 2\log P_{H_2O} \tag{5}$$

$$Log\ KHSH1 = 3\log P_{H2S} - \log P_{H2} - 2\log P_{H_2O} \tag{6}$$

$$Log\ KHSH2 = 3\log P_{H2S} - 5/4\log P_{H2} - 7/4\log P_{H_2O} \tag{7}$$

$$Log\ KHSH3 = \log P_{H2S} - \log P_{H2} \tag{8}$$

and writing the constants in terms of the water partial

pressure, according to (D'Amore, 1992):

$$\log P_i = \log (n_i/n_{H_2O}) - \log A_i + \log P_{H_2O} \tag{9}$$

where (n_i/n_{H_2O}) is the molar ratio of "i" component regarding the total water. The coefficient A for every species "i" is defined as a function of temperature and the steam fraction "y". In following equations $y > 0$ refers to vapor gain while $y < 0$ refers to vapor loss:

$$\text{If } y \geq 0: A_i = y + (1-y)/B_i \tag{10}$$

$$\text{If } y < 0: A_i = 1/\big(B_i(1 + y - yB_i)\big) \tag{11}$$

B_i is the distribution coefficient for every gas which is a function of temperature (Giggenbach, 1980; D'Amore, 1992). For temperatures between 100 and 340 °C, (t in °C):

$$\log B_{CO_2} = 4.7593 - 0.01092t \tag{12}$$

$$\log B_{H_2S} = 4.0547 - 0.00981\,t \tag{13}$$

$$\log B_{CH_4} = 6.0783 - 0.01383\,t \tag{14}$$

$$\log B_{H_2} = 6.2283 - 0.01403\,t \tag{15}$$

Thus, equilibrium equations for every reaction are as follows.

$$FT = \log_{KFT} + 4\log A_{H_2} + \log A_{CO_2} - Log\,A_{CH_4} - 2\,Log\,P_{H_2O} \tag{16}$$

$$HSH1 = \log K_{HSH1} + 3\log A_{H_2S} - \log A_{H_2} \tag{17}$$

$$HSH2 = \log K_{HSH2} + 3\log A_{H_2S} - 5/4\log A_{H_2} \tag{18}$$

$$HSH3 = \log K_{HSH3} + \log A_{H_2S} - \log A_{H_2} \tag{19}$$

Equilibrium constants of the general form, where T is in K:

$$\log K = a + b/(T) + c\log(T) \tag{20}$$

Table 1 gives the constants a, b and c for every reaction.
The equilibrium equations can be expressed as a molar proportion of every species with respect to H_2O. The logarithm used is base 10.

$$FT = 4\log(H_2/H_2O) + \log (CO_2/H_2O) - \log (CH_4/H_2O) \tag{21}$$

$$HSH1 = 3\log (H_2S/H_2O) - \log (H_2/H_2O) \tag{22}$$

$$HSH2 = 3\log (H_2S/H_2O) - 5/4\log (H_2/H_2O) \tag{23}$$

$$HSH3 = \log (H_2S/H_2O) - \log (H_2/H_2O) \tag{24}$$

The graphical solutions of (Eqs. (16) and 17); (16) and (18) and (16) and (19) provide the theoretical grids in the coordinates (HSH1, FT), (HSH2, FT) and (HSH3, FT), given in Figs. 1–3 respectively, to be used as frame references. The parameters FT, HSH1, HSH2 and HSH3 are obtained from the gas compositions according to Eqs. (21–24) where concentrations of gas species are taken in

Table 1
Coefficients a, b and c for the reactions (Siega et al., 1999).

Equilibrium constant K	a	b	c
K_{FT}	−4.330	−8048	4.635
K_{HSH1}	6.449	−6150	−0.412
K_{HSH2}	7.609	−6087	−0.412
K_{HSH3}	4.940	−2874	–
P_{H2O}	5.510	−2048	–