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CALCULATION OF STEAM FRACTIONS IN VAPOUR-DOMINATED GEOTHERMAL SYSTEMS USING AN EMPIRICAL METHOD

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ABSTRACT

Steam fractions can be calculated via an empirical method using the steam fraction model conditions developed by earlier researchers (eg Giggenbach, 1980; D'Amore et al, 1982). The only exception is that prior knowledge of the reactions controlling the gas composition of the reservoir fluid is not required. Two techniques, one graphical and the other numerical, of calculating steam fractions by this new method are presented and their respective performances are assessed. The advantages and limitations of the new method compared with previous steam fraction calculation methods are discussed.

INTRODUCTION

In recent years numerous investigations have been directed towards the use of gas geochemistry as a reservoir evaluation tool for vapour-dominated geothermal fields. Most interest has centred upon the calculation of steam fractions (y) from wellhead steam gas compositions due to their possible use in the estimation of reservoir fluid reserves. The steam fraction is defined as the proportion of produced steam which is original reservoir vapour as opposed to vaporised reservoir liquid. Since the initial studies of Giggenbach (1980), 12 types of steam fraction calculation have been proposed in the literature for use on vapour-dominated systems (D'Amore et al, 1982; D'Amore and Celati, 1983; D'Amore et al, 1983; D'Amore and Truesdell, 1985; D'Amore et al, 1987), all of which are based on the same mixing/boiling model.

One of the principal uncertainties with current steam fraction calculation methods lies in the need for prior knowledge of the reactions controlling the gas composition of the reservoir fluid, and the thermodynamic equilibrium constants of these reactions. If either are incorrect, the calculated steam fractions will be erroneous. Previous researchers have relied on gas equilibrium calculations from liquid-dominated systems, or mineralogical evidence, to determine the most likely reactions at equilibrium in vapour-dominated systems (see Table 1). It is difficult, however, to determine which, if any, of these reactions are valid for any given selection of produced steam samples. For example, Arnorsson (1985) has found that the Fischer-Tropsch reaction (Reaction 7, Table 1) is not in equilibrium in all geothermal waters over 200°C and yet this reaction has been widely incorporated in previous steam fraction calculations (Table 1). Likewise, where multiple generations of secondary minerals are present, it is not always evident which are controlling the fluid gas composition.

D'Amore and Pruess (1986) have recently found that the current calculation methods do not produce correct steam fractions unless all fluids derived from production sites feeding a well have the same chemical composition (ie they are derived from the same fluid type; McCartney and Haizlip, this volume). In this paper we introduce an empirical steam fraction calculation technique which has an advantage over previous methods in that it does not require knowledge of the reactions controlling the gas composition of fluids in vapour-dominated reservoirs. Instead, it utilises the new condition imposed by D'Amore and Pruess (op cited). The new method also differs from those used previously in that it is applied to sets of steam analyses as opposed to individual samples. We discuss the potential use and limitations of the new technique.

STEAM FRACTION MODEL CONDITIONS AND MOLE RATIO DATA

All current steam fraction calculation methods are based on a vapour-liquid boiling model which incorporates the following conditions:

1 Liquid and vapour are in phase and chemical equilibrium in the reservoir.

2 The reactions and thermodynamic equilibrium constants controlling the gas composition of both phases in the reservoir are known.

3 The temperature of the reservoir fluid is known.

TABLE 1 EQUILIBRIUM REACTIONS USED IN PREVIOUS STEAM FRACTION CALCULATIONS

YNN	$NH_3 = \frac{1}{2}N_2 + \frac{3}{2}H_2$	Ref 1
YCN1	$3C + 4NH_3 = 3CH_4 + 2N_2$	Ref 1
YCN2	$C + NH_3 + \frac{1}{2}H_2 = \frac{1}{2}N_2 + CH_4$	Ref 1
YCN3	$C + \frac{1}{2}N_2 + \frac{7}{2}H_2 = NH_3 + CH_4$	Ref 1
YH	(a) $H_2O = H_2 + \frac{1}{2}O_2$	Ref 1
	(b) $CH_4 + 2H_2O = CO_2 + 4H_2$	
YS	(a) $H_2S = H_2 + \frac{1}{2}S_2$	Ref 1
	(b) $CH_4 + 2H_2O = CO_2 + 4H_2$	
YHC (≡ YFT)	$CH_4 + 2H_2O = CO_2 + 4H_2$	Ref 3
YSC	$10H_2O + CH_4 + 6FeS_2 = 2Fe_3O_4 + 12H_2S + CO_2$	Ref 3
YFT	$CH_4 + 2H_2O = CO_2 + 4H_2$	Ref 4
Y_C	$CO_2 + H_2 = CO + H_2O$	Refs 5,6
Y_{C2}	$CH_4 + 3CO_2 = 4CO + 2H_2O$	Ref 5
YHSH (YSHC in Ref 6)	$Fe_3O_4 + 6H_2S = 2H_2 + 3FcS_2 + 4H_2O$	Refs 6,7
YHSC	$Fe_3O_4 + 6H_2S + CO_2 + 2H_2 = 3FeS_2 + 6H_2O + CH_4$	Ref 7

Ref 1	D'Amore et al (1983)
Ref 2	D'Amore and Gianelli (1984)
Ref 3	D'Amore et al (1982)
Ref 4	D'Amore and Celati (1983)
Ref 5	Bertrami et al (1985)
Ref 6	D'Amore et al (1987)
Ref 7	D'Amore and Truesdell (1985)

4 Whilst the liquid may boil and be transferred as steam along with the original vapour, there is no mass gain or loss during transport from the reservoir to the wellhead.

5 The gases do not re-equilibrate either chemically or between phases at any stage between the production site and the wellhead.

6 All fluids derived from production sites feeding a well have the same chemical composition.

A further condition of current methods is that the simple mixing model of Equation 1 is obeyed.

$$C_s = C_v.y + C_l.(1-y) \qquad (1)$$

Our new model conditions only differ from those above in that condition 2 is ignored.

The distribution of gases between the reservoir liquid and vapour phases can be described by the partition coefficient:

$$B = C_v/C_l \qquad (2)$$

Partition coefficients are temperature dependent and can generally be described by equations such as (see D'Amore and Truesdell, 1986 for a review):

$$\text{Log } B = a + bT \qquad (3)$$

For gases normally analysed in steam from vapour-dominated geothermal systems, the order of affinity for the vapour phase (ie the order of decreasing distribution coefficient) is:

$N_2 > H_2 > CH_4 > CO_2 > H_2S > NH_3$

The partition coefficients of each of these gases are in excess of unity below the critical temperature, but decline as temperature increases. From Equations 1 and 2 it is evident that these gases favour the vapour phase and that as the steam fraction increases, so will the gas concentrations in produced steam samples given our model conditions.

Produced steam gas data sets which satisfy our model conditions display a distinctive distribution on graphs depicting mole ratio (A/B) against A, B or C concentration (see Figure 1, where A, B and C are gaseous species). Curves such as those in Figure 1 are generated through the use of Equations 1 and 2 for all gases, and by knowing the reservoiar temperature and vapour (or liquid) composition. The shape of the data curves is determined by the partition coefficients of the gases (and therefore the reservoir temperature) involved on the graph. The species which are more soluble in the liquid phase and have a lower partition coefficient are enriched in produced steam which has a lower steam fraction and, therefore, a lower gas concentration. Mole ratios tend to be more constant at higher steam fractions because most of the gas resides in the vapour phase; high dilution with vaporised liquid is usually required before the mole ratios in the

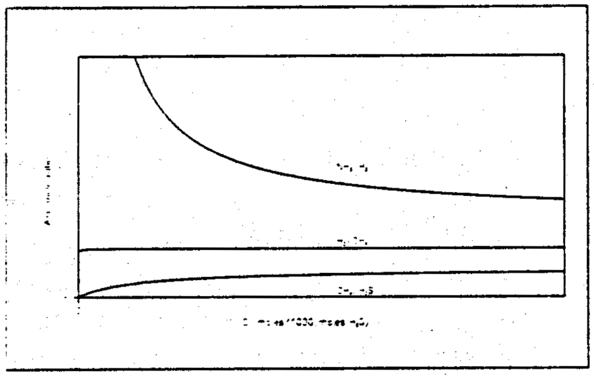

FIGURE 1 EXAMPLE MODEL DATA TRENDS. CURVES WERE GENERATED USING EQUATIONS 1 AND 2, GIVEN C_v AND B_i WITH y AS A VARIABLE

steam change significantly. Thus, the position of data along the curves is determined by the steam fraction of the produced steam sample. Data satisfying the model are also sensitive to the vapour (and liquid) phase gas concentrations and mole ratios which determine the position of the curves relative to the x and y axes, respectively.

CALCULATION OF STEAM FRACTIONS USING A MANUAL FITTING TECHNIQUE

Steam gas mole ratio data, which are evidently sensitive to the steam fraction of a produced steam sample and the vapour (or liquid) phase composition of the reservoir fluid, can be useful in two ways when displayed on graphs such as that in Figure 1. Firstly, they may be used to identify data which potentially satisfy the model conditions described above. For example, examination of data on such graphs will indicate which samples, and which gas analyses of those samples, follow the trends predicted by the model conditions.

Secondly, if the data appears to satisfy the model conditions, and an estimate of reservoir temperature is available, the observed data on the graphs can be 'fitted' by a mixing line such as those shown in Figure 1 after initial selection of the appropriate vapour (or liquid) phase composition. This allows estimation of the steam fraction of each of the samples used in the 'fit'. For example, fitting can be achieved by initially estimating the vapour mole ratios from the mole ratios in the highest gas samples (which will have the highest steam fraction). The vapour gas concentrations can then be selected and using Equations 1 and 2 for all gases involved, mixing lines can be generated and compared with the field data. Better visual fits of the mixing lines to the data can be achieved by judicious variation of the vapour composition. Equations 1 and 2 can then be used with the best-fit vapour composition to calculate one steam fraction for each gas analysed in each sample. These steam fractions can be used to determine the average steam fraction for the sample and errors on each. Evidently, the method also provides an estimate of the reservoir vapour (and liquid) composition.

This method is tedious and prone to bias so we have developed an automated minimisation technique for the calculation of steam fractions based on similar principles to those of the manual fitting method.

CALCULATION OF STEAM FRACTIONS USING A MINIMISATION TECHNIQUE

The minimisation technique also produces estimates of the steam fraction for each sample and the reservoir vapour composition, but does so through the solution of a set of simultaneous equations (one for each gas of every sample):

$$C_{sij} = C_{vi} \cdot y_j + C_{vi} (1-y_j)/B_i(T_j) + E_{ij} \tag{4}$$

All the samples need to be analysed for the same gases and the minimum necessary for the calculation is two gases.

It is also assumed that the temperatures of all samples (T_j) are the same and this constant temperature must be provided as an input to the algorithm.

If B values are large or y is close to 1, the equations reduce to:

$$C_{sij} = C_{vi} \cdot y_j + E_{ij} \tag{5}$$

In such cases it will be impossible to estimate the values of C_{vi} or y_j since any solution (y_j, C_{vi}) will be indistinguishable from the solution (y_j/R, $C_{vi}.R$) where R is any constant. This scaling effect is the major source of error in fitting Equation 4. Our model pays special attention to this scaling error.

Let

$$s = \sum_{j=1}^{Ns} \sum_{i=1}^{Ng} \frac{(C_{sij} - C_{vi} \cdot y_j - C_{vi}(1-y_j)/B_i)^2}{\sigma_{ij}^2} \tag{6}$$

σ_{ij} are estimates of sampling/analytical error and would typically be found from the analysis of duplicate samples. Partial differentiation with respect to C_{vi} and y_j leads to:

$$\frac{ds}{dy_j} = -2 \sum_{i=1}^{Ng} \frac{(C_{sij} - C_{vi} \cdot y_j - C_{vi}(1-y_j)/B_i)}{\sigma_{ij}^2} (C_{vi} - C_{vi}/B_i) \tag{7}$$

and

$$\frac{dS}{dC_{vi}} = -2 \sum_{j=1}^{Ns} \frac{(C_{sij} - C_{vi} \cdot y_j - C_{vi}(1-y_j)/B_i)}{\sigma_{ij}^2} \left(y_j + \frac{1-y_j}{B_i}\right) \qquad (8)$$

For any set of y_j,C_{vi} that minimise S, we must have $dS/dy_j = 0$ for all j and $dS/dC_{vi} = 0$ for all i. Given estimates of the steam fractions y_j^{K-1}, we can use Equation 7 to derive new estimates of the vapour concentrations C_{vi}^K. Similarly we can use the C_{vi}^K in Equation 8 to derive new steam fraction estimates y_j^K. We have expanded Equations 7 and 8 into explicit equations for y_j and C_{vi}, these are Equations 9 and 10.

$$Y_j^K = \frac{\sum_i (C_{sij} - C_{vi}^K/B_i)/\sigma_{ij}^2}{\sum_i (C_{vi}^K - C_{vi}^K/B_i)^2/\sigma_{ij}^2} \qquad (9)$$

$$C_{vi}^K = \frac{\sum_j C_{sij} \left(y_j^{K-1} + \frac{1-y_j^{K-1}}{B_i}\right)/\sigma_{ij}^2}{\sum_j \left(y_j^{K-1} + \frac{1-y_j^{K-1}}{B_i}\right)^2/\sigma_{ij}^2} \qquad (10)$$

The calculation follows the following procedure:

a Set all initial estimates y_j0 to 0.5 for all j. Set the iteration count k to 0.

b Increment k.

c Calculate C_{vi}^K from Equation 9.

d Calculate y_j^K from Equation 10.

e If the relative change in any parameter C_{vi} or y_j is greater than a given tolerance (eg 1%) go back to step b.

At this point we have derived estimates y_j^K and C_{vi}^K, however because of the ill conditioned nature of the equations (4), we now rescale the y_j^K by a common factor R such that $S(y_j/R, C_{vi}^K*R)$ is a minimum. If the computed factor R is not close to 1 (ie within 0.005), we now go back to step b. Otherwise the algorithm has converged, typically this rescaling occurs between two and five times before convergence.

A number of numerical test cases were examined to evaluate the performance of the method (Table 2). Dummy sample analyses were generated using Equation 11. The sampling/analytical errors were set to 10% RSD for each gas. The y_j were randomly selected from a uniform distribution. The vapour concentration was as shown in Table 3. Different sets of samples were generated for each test case.

$$C_{sij} = \left(C_{vi} + e_{ij}\right)\left(y_j + \frac{(1-y_j)}{B_i}\right) \qquad (11)$$

TABLE 2 TEST CASES USED IN MODELLING

	No of Samples	Y range	Temperature (°C)	Gases Used	Mean Error	SD	Mean % Error	SD of % Error
1	50	0-1	240	All	0.02	0.07	5	14
2	50	0-1	240	NH_3,H_2	-0.02	0.07	-5	17
3	50	0-1	240	H_2,CH_4	-0.06	0.33	-12	57
4	50	0-1	220	All	-0.10	0.08	-20	10
5	50	0-1	260	All	+0.12	0.11	26	15
6	10	0-1	240	All	0.02	0.16	10	34
7	10	0-1	240	NH_3,H_2	0.06	0.17	18	43
8	10	0-1	240	H_2,CH_4	No convergence			
9	25	0-0.2	240	All	0.01	0.02	14	23
10	25	0-0.2	240	NH_3,H_2	0.03	0.04	44	53
11	25	0-0.2	240	H_2,CH_4	No convergence			
12	25	0.8-1.0	240	All	0.65	0.41	-11	55
13	25	0.8-1.0	240	NH_3,H_2	No convergence			
14	25	0.8-1.0	240	H_2,CH_4	No convergence			
15	10	0-0.2	240	All	0.00	0.02	7	24
16	10	0-0.2	240	NH_3,H_2	0.05	0.20		
17	10	0-0.2	240	H_2,CH_4	No convergence			

TABLE 3 RESERVOIR VAPOUR COMPOSITION*

Moles/1000 moles H_2O	
CO_2	3.6469
H_2S	0.3234
NH_3	0.1756
N_2	0.1019
CH_4	0.9303
H_2	1.0363

* Calculated from Truesdell et al (1987) (Central and West Geysers medium sample, Table 1) assuming y=0.5

Six gases were used in the calculations (CO_2, H_2S, NH_3, CH_4, H_2) and partition coefficients were determined from the equations of D'Amore and Truesdell (1986). The temperature was generally set to 240°C except in cases 4 and 5. For each test case the percentage error between the original and estimated steam fractions have been calculated (Table 2)*.

RESULTS

The test cases produced the following results.

1 The principal errors are related to the scaling of the y values.

2 As indicated earlier, the method fails where either steam fractions or partition coefficients are high (Figure 3).

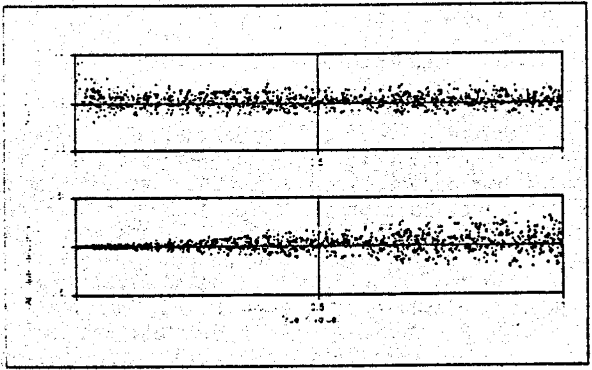

FIGURE 2 TEST CASE 1 : COMPARISON OF THE PERCENTAGE AND ABSOLUTE ERRORS BETWEEN THE TRUE AND CALCULATED STEAM FRACTIONS

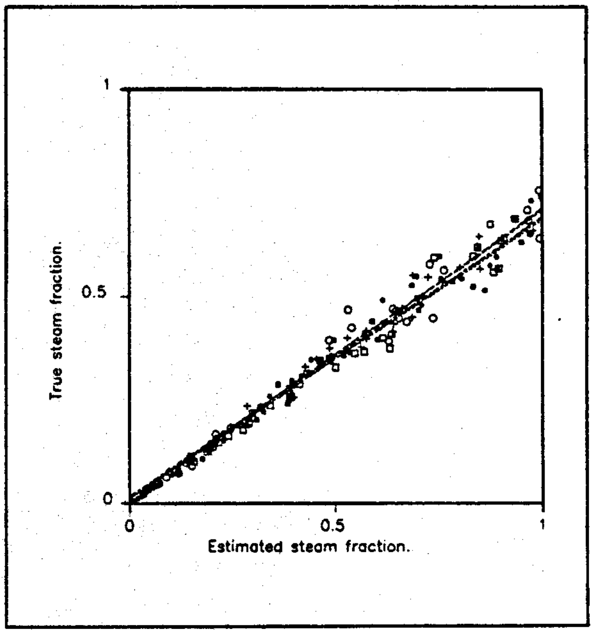

FIGURE 3 TEST CASE 3 : RELATION BETWEEN THE TRUE AND CALCULATED STEAM FRACTIONS. DIFFERENT SYMBOLS REPRESENT DIFFERENT DATA SETS. DASHED LINES ARE 'BEST-FIT' LINES

3 Reasonable results are achieved when a) at least one gas used in the calculation has a low partition coefficient (eg NH_3); b) the spread in sample gas concentrations (and steam fractions) is large and c) low steam fraction samples are present (eg Figure 4). In test case 1 85% of the calculated steam fractions are within 20% of the input values (eg Figure 2).

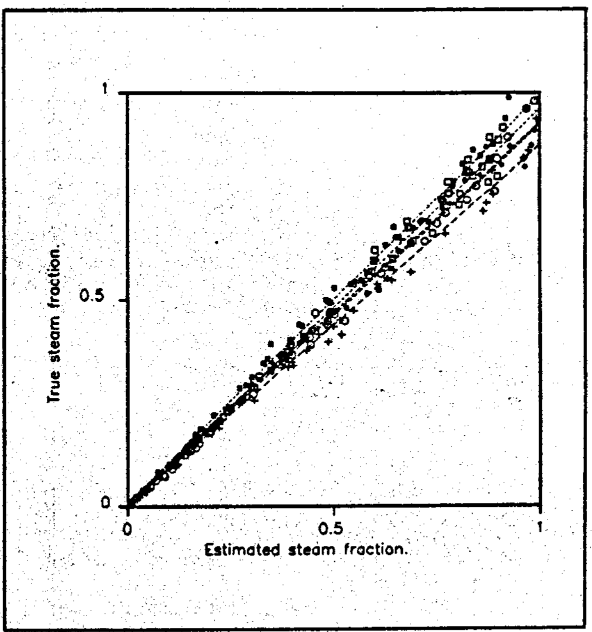

FIGURE 4 TEST CASE 1 : RELATION BETWEEN THE TRUE AND CALCULATED STEAM FRACTIONS. DIFFERENT SYMBOLS REPRESENT DIFFERENT DATA SETS. DASHED LINES ARE 'BEST-FIT' LINES

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* We have only quoted percentage errors for samples with steam fractions greater than 0.01, and absolute errors for all samples. This is because the percentage errors of lower steam fraction samples distort what are relatively constant values in higher steam fraction samples (Figure 2).

4 The accuracy and precision of the method increases with the number of samples.

5 Where the input temperature is over-estimated so are the steam fractions. Steam fractions are correspondingly under-estimated when the input temperature is lower than that of the reservoir.

We examined the test case mole ratio data and the corresponding vapour liquid mixing lines generated via the calculated vapour composition and Equations 1 and 2. In each case the fit of the mixing line to the mole ratio data was as good as that expected from hand-fitting (Figure 5). Indeed the limitations of the minimisation method and the ideal conditions for its use are those anticipated when using the manual fitting method. Mole ratio data evidently provides an independent check on the reliability of the steam fractions calculated by the minimisation technique.

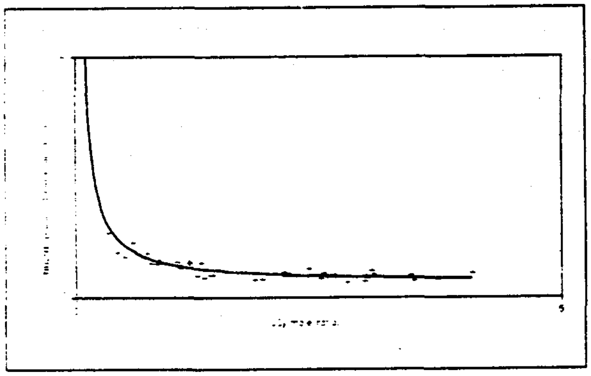

FIGURE 5 EXAMPLE OF THE RELATION BETWEEN THE MINIMISATION DERIVED VAPOUR-LIQUID MIXING LINE AND A TEST DATA SET

DISCUSSION

The principal advantages of the above empirical methods compared with existing steam fraction calculation techniques are a) no information concerning the reservoir reactions are required, and b) the data upon which the new methods are most likely to be successful can be readily identified. It should be noted however, that a good correlation between the mixing line and sample data only indicates that the data could be produced under the conditions defined by the model. We are currently investigating the processes and conditions which may mimic the mole ratio trends produced by the steam fraction model, but actually produce erroneous steam fraction values.

At this stage, the disadvantages of the technique might be perceived as being the relatively stringent data requirements, the accuracy and precision of the calculated steam fractions and the need to know the reservoir temperature. Although few localities produce the type of data required by the calculation method, it may be appplied to the Unit 15 area at The Geysers (McCartney and Haizlip, this volume; McCartney and Haizlip, 1989).

The precisions quoted earlier include the sampling/analytical error associated with the data, and as such may be acceptable for certain applications. On the other hand, the calculated empirical steam fractions could be compared with those calculated by existing methods to help determine which reactions are indeed controlling gas compositions in the reservoir fluid. More precise steam fractions could then be calculated using existing methods incorporating these reactions. It is hoped that the accuracy and precision may also be improved by refinement of our current numerical technique.

More accurate steam fractions depend on knowing the reservoir temperature at which the reservoir vapour and liquid equilibrated. Whilst endeavours should be made to use other information to correctly estimate the reservoir temperature, it is evident that even errors in the calculated steam fractions of +/- 20°C do not significantly affect the estimates of the steam fractions when the overall accuracy and precision of the method are considered.

CONCLUSIONS

We have presented two empirical methods for calculating steam fractions of steam samples from vapour dominated systems. The methods rely on the assumption that the steam is being produced from a single fluid type, however assumptions concerning reaction equilibria are not required. Steam gas mole ratio data may be used to identify samples to which the methods may be applied, and to check the accuracy of the calculated steam fractions.

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NOMENCLATURE

a,b	Constants in Equation 3
B	Gas partition coefficient
C_l	Concentration of gas in reservoir liquid (moles/1000 moles H_2O)
C_s	Concentration of gas in produced steam (moles/1000 moles H_2O)

C_v	Concentration of gas in reservoir vapour (moles/1000 moles H_2O)
E_{ij}	Sampling/analytical error in sample j for gas i
i	Gas identifier
j	Sample identifier
K	Iteration count in numerical scheme
N_g	Number of gases analysed
N_s	Number of samples
T	Reservoir temperature estimate (°C)
y	Steam fraction
σ_{ij}	Estimate of sampling/analytical error
e_{ij}	Gaussian random variable

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