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MASS BALANCE AND DAMKtJHLER NUMBERS IN FLOW SYSTEMS - FLUID THROUGHPUT AT OHAAKI-BROADLANDS

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ABSTRACT - Theoretical approaches to 1-dimensional infiltration of a homogeneous aquifer lead to precise distance profiles of 6^{*8}0 and similar parameters in aquifer rock as a function of the dimensionless Damkohler number of chemical engineers. Reasonably complete 6^{18}0 data in real systems can determine the infiltration distance and therefore actual fluid throughput; for flow systems this information is more relevant than fluid/rock ratios. At Ohaaki-Broadlands a theoretical infiltration distance of 78 km, now well past the discharge interface, is postulated.

INTRODUCTION

Fluids consisting largely of H2O and CO2 dominate geochemical activities in the lithosphere. Chemical and isotopic reactions between minerals are accelerated by even small quantities of H2O which act catalytically. Reactions in which H2O or CO2 (or their constituent isotopes) are being consumed or produced are equally common and their progress is obviously determined by how much fluid arrives at (or is released from) a local area of reaction. It has been shown in previous papers, how cumulative water/rock ratios determined from oxygen isotope shifts of reservoir rock and throughput water in a box model can be used to better understand geothermal hydrologies (Blattner 1985). Here we extend this approach to a flow model; the water/rock ratio becomes ambivalent and the role it plays in a box model is taken over by infiltration distance, porosity, and (for kinetics) DamkOhler number.

FLUID/ROCK RATIOS : 0-DIMENSIONAL

Geochemical processes are logically and historically appraised by reference to representative elementary volumes (EV, REV) in which the phases present are thoroughly and intimately mixed (e.g., Lichtner 1985). Traditional O-dimensional box models of geochemistry (Taylor 1977; Blattner 1985) simply employ an enlarged EV in their model of reality, and, in view of this limitation, they are remarkably successful. In such models the cumulative fluid/rock ratio V (oxygen in fluid/oxygen in solid) depends directly on how many times the pore volume of the reservoir rock has been filled (or partially filled) in the course of the interaction. By strict adherence to this EV-based concept, and with the assumption of instantaneous isotope exchange (LEA - local equilibrium approximation) one can use the measured isotope shifts of the EV rock (the reservoir rock) and the recharge fluid to calculate y'. Even within LEA both over- and under-estimates can result, depending on how well the chosen batch size for the fluid simulates the real flow and circulation process in a system. If isotope exchange is kinetically limited,purely LEA-based estimates would of course tend to be minimum estimates for the actual hydrological fluid/rock ratio. Whatever the details, the fluid/rock ratio in a 0-dimensional box is always conceptually simple, in that it consists of the sum of batches of fluid that have passed through. A geometric illustration involves no distance and the geochemical evolution consists of a monotonic change (usually drop) of 6^{18}0 of the reservoir rock.

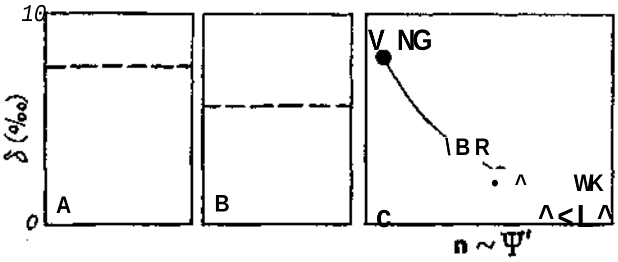

Fig. 1. Fluid/rock ratios in box model, oxygen porosity 25% and instantaneous exchange (LEA). A,one filling drops the 6_{roc}|< by one quarter of the total possible shift P to equilibrium with input fluid. B, two fillings' shift is V+(V^3<); C, for n fillings and n-*» the shift approaches -P. Approximate positions for Ngawha, Broadlands and Wairakei as increasingly hydrologically mature systems, y'iscumulative water/rock ratio.

ONE-DIMENSIONAL ADVECTION AND KINETICS

Kinetically limited isotope exchange between fluid and rock in purely advective flow has been modelled numerically by McKibbin et al. (1986). Blattner(1986), Blattneretal(1987)and Blattnerand Absar(1988) have drawn attention to the fast reaction limit (i.e., **LEAJ** of this approach, which leads to the concept of geochemical fronts. Lassey and Blattner (1988) present an analytic solution to the transport and kinetic equations, employing Goldstein's (1953) J-function. Their solution can handle any magnitude of reaction rate constant, as well as different steady state temperature profiles over the achieved length of advection or infiltration.

Additional definitions

$6 = 6^{18}0 = [(R/R_reference) -1] 10^3$
(in permille)
where R = I80/I60
$Ai\_2 \doteq A^{18}0i\_2 = 6 1 - 6 2$ (Function of temperature T)
z = distance
L = distance infiltrated by advective process
q = z/t, interstitial (longitudinal) velocity of fluid
v = tq/L, non-dimensional time
Z = z/L, (non-dimensional distance)
Reaction rate constant K:

$$\frac{\partial\delta_1}{9T} = - \kappa (6_r - 6_w - 4_{rw})$$

y, the 'oxygen porosity' is more strictly the ^{18}0-porosity (cf. Lassey and Blattner 1988)
Units in this paper: m, s.

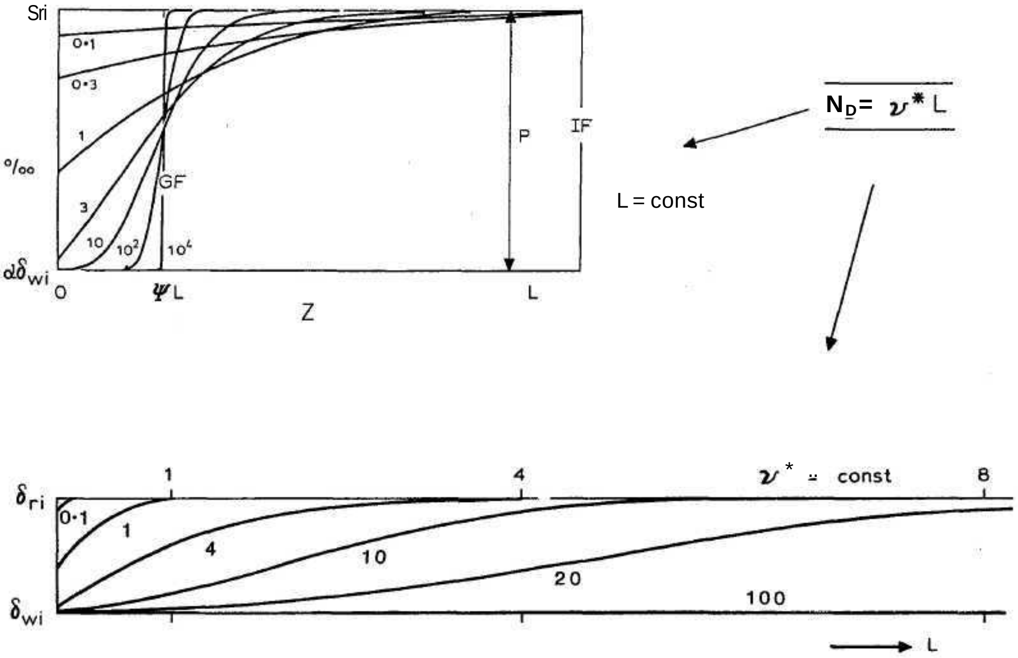

Fig. 2 . (Above) Non-dimensional or constant length Damköhler plot for pure advection and constant $A_{roc}k\_fi_ujH$, with only 6_r shown. IF = infiltration front, GF = exchange (geochemical) front, a = fractionation factor (= exp 10~3A), U* = K/q = exchange intensity. - (Below) Fronts defined by the marked Damköhler numbers, in real space. Since u* has to be constant, *HQ* is proportional to the infiltration length L. Our distance measure here implies that u* = 1. Slopes of <S^{18}0 in real space *are* tabulated in Lassey and Blattner (1988). P is total potential isotope shift of rock.

Solving the differential equations for isotope transport and first order reaction kinetics, leads to unequivocal distance profiles of isotope compositions in an aquifer. The shape, over the whole infiltration distance, of these profiles is expressed by a single dimensionless parameter

$$NQ = \frac{JLL}{q} \quad \text{(Damköhler number)} \qquad (1)$$

where K is the isotope exchange rate constant q the interstitial velocity of the infiltrating fluid, and L the total achieved infiltration distance. Where there is a surface discharge, this distance will be theoretical only. If, for that reason, an arbitrary reference distance L_{re}f is chosen instead of L, the dimensionless time T becomes L/L_{re}f and indicates how often the pore space up to L_{re}f has Deen filled so far. (A characteristic reference length for a given system - e.g. Fig. 4 - is of course that to the actual discharge cross section. This we call L_s, for •-solid-) Fig. 2 shows the basic pattern of profiles for a simple infiltrated aquifer of length L, constant temperature (i.e., constant Arock.fiuid) constant oxygen porosity ¥, with initial 6_r = $10^o/_{oo}$ initial (input) 6_W= $0°/_{oo}$ and fixed reaction rate constant κ and fluid velocity q.

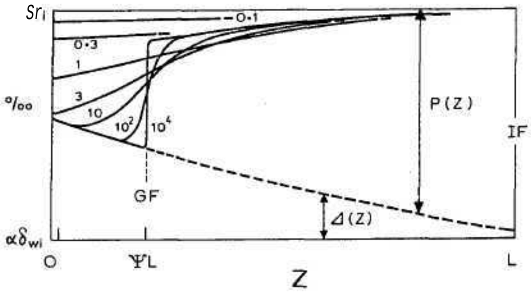

Fig. 3. As Fig. 2a but with a A(T) value dependent on distance: A(Z) = 5.45 exp (-1.8θ) *1 °/oo,* i.e., a linear temperature gradient from 300°C to 600°C at z = L (Z = 1). Note how the relationships between the different curves is similar as in the case of constant A (Fig. 2a).

The non-dimensional "Damköhler scheme" of Fig. 2a has the remarkable property to capture all possible profile shapes for advective models as defined above. It has to be kept in mind only that in real space (Fig. 2b) the total profile expands with L and this flattens the geochemical exchange front more than the increased NQ (eq. 1) sharpens it. For *HQ* values >>1 the slope 6_r/z is proportional $L^{"1}$^.

APPLICATION TO OXYGEN ISOTOPE DATA FROM 0HAAKI-BROADLANDS

Values of 6^{18}0 for altered rock and fluid at Ohaaki-Broadlands are given by Absar (1988). To make full use of the 1-dimensional concept, we consider here meteoric recharge on the margins of the field, and assume the water to enter a zone hot enough for significant isotope exchange to take place, about 6.5 km

Theoretical IF
at Z = 1 , T = 1

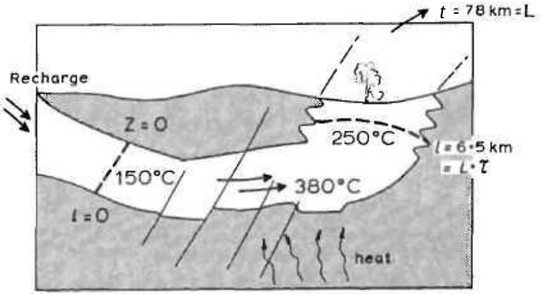

Fig. 4. Conceptual picture of a geothermal system with meteoric surface recharge. A first approximation to a 1-dimensional isotope exchange model for Ohaaki-Broadlands. Note that in actual fact the recharge could be from a]J_ sides (circular on a map) and still satisfy the 1-D approach. Exchange is assumed to take place only above 150°C. This in part counteracts the adoption of a fixed exchange rate constant < (since in actual fact K will increase with temperature). Exchange is assumed to end at 250°C to also roughly counteract a perceived faster fluid velocity toward the discharge area.

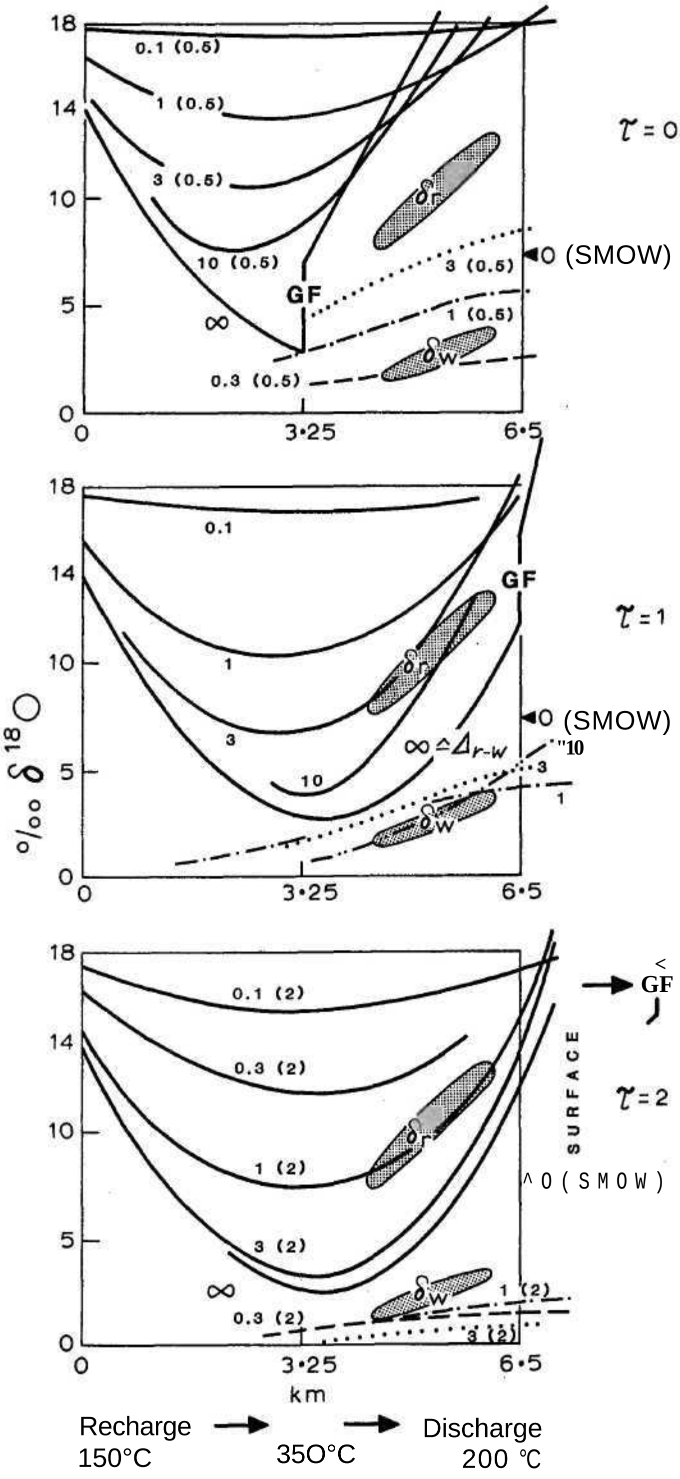

Fig. 5. Ohaaki-Broadlands simulation, using model of Lassey and Blattner (1988). We plot the distance of L_s = 6.5 km from the 150°C isotherm to the 250°C cross section, which is effectively the discharge surface, as shown in Fig. 4, and oxygen isotope compositions for each distance. The 6-scale on the left is arbitrary, its zero point being the local meteoric water.

The data to be matched are the preferred values 6_r for reservoir rock and $<5_w$ for the infiltrating fluid, of Absar (1988) from wells BR 15, 24, 34 and 43 (grey fields). The oxygen porosity is approximately <? = 0.1. To be close to T = 1, we have chosen a reference length $L_{re}f$ = 65 km. For T = 0.5 (top) the geochemical or isotope exchange front GF is at VLT = 0.1 x 65 x 10^ x 0.5 = 3250 m. For T = 1 (middle) the GF is just at the present day discharge surface, and for T = 2 well past it. In comparison to Fig. 2 the 6_r profiles appear distorted and this is simply due to the more complicated profiles A = f(T), where T = f(Z). Expected kinetic constraints are expressed in the reference Damkohler numbers N_r^f = v* $L_{re}f$, marked at each corresponding 6_r profile (with T in brackets). For ND = ^{ro} sharp fronts are apparent, but these are smoothed out for $N_{re}f$ = 10 already. The dotted and dashed curves show values for the fluids (6_w) for selected $N_{re}f$ values.

Since for any given infiltration process within our model, v* and therefore $N_{re}f$ are fixed by the rock properties, any possible evolutionary path in Fig. 5 has to move among curves with equal $N_{re}f$ and increasing x, e.g., from 0.1 (0.5) to 0.1 to 0.1 (2), so that the shape-determining Np = $N_{re}f$ T evolves, for example, from 0.05 to 0.1 to 0.2. The same is true for the fluid profiles 6_w.

While it is difficult to obtain accurate $<5_w$ values, the availability of both $<5_r$ and 6_w data can critically constrain desired estimates for data as those presented for Ohaaki-Broadlands in Fig. 5, since the same $N_{re}f$ and T must always hold for both rock and fluid. The plots now tell us - (1) that T should be much greater than 0.5, (2) that with T greater 2, the 6_w drops off way below the data field, so that 0.5 < T < 2; and finally (3) that a good match obtains for T = 1 and $N_{re}f$ = 5. More detailed analysis actually points to T = 1.2 and NQ = 4. This means that the total theoretical infiltration distance must be 1.2 x 65 = 78 km, with a theoretical GF for v = 0.1 at 78 km, just past the present discharge cross section.

upstream from the Ohaaki-Broadlands surface activity (Fig. 4). The temperature then slowly rises and begins to drop again toward the surface discharge, after having reached a peak of c. 380°C.

An analysis of the data in terms of 1-D advection follows in Fig. 5. Because of the temperature profile from cool to hot to cool, the DamkBhler plot becomes more complex than in Figs 2 and 3, but it remains exactly analogous. An arbitrary reference distance of 65 km has been chosen and it is clear from the cases shown for x = 0.5, x = 1, and x = 2, that the actual value must have been greater x = 0.5. Therefore, due to f ≈ 0.1, the infiltration distance L must be greater than 32.5 km. It is seen, too, that because of the kinetically caused lack of complete equilibration, the profiles of 6_r and 6_w evolve differently over a given distance. While the slope of the 6_r and 6_w fields may not be all that important, the fact that estimates for both are available can therefore be critical (Fig. 5).

As explained in the analysis of Fig. 5, we obtain a match of the Ohaaki-Broadlands data with a total infiltration length of about 78 km, with a theoretical GF or isotope exchange front (for ¥ ≈ 0.1) at 7.8 km, a little past the present discharge area. Because the Damköhler number is only = 4, however, this front appears relatively flat (distended). Having allowed for the actual temperature profile in Fig. 5 in order to gain the real NQ value, we can now simplify the situation again by looking, in Fig. 6, at an 'NQ = 4[1] profile for constant temperature. From eq. (1) it is also seen that v* = </q; therefore if q^ lO"^{9}m/s (McKibbin et al. 1986) it would follow that K≃IO~13 s~l. The cumulative water/rock ratio for the system length L_s = 6.5 km would be yL/L_s = 0.1 x 78/65 =1.2, but cannot be geochemically compared to similarly obtained ratios for other fields where L_s is different.

LIMITATIONS AND OUTLOOK

Compared with actual aquifers, the present model is still relatively simple. Its greatest virtue may be its analytical character which provides transparency and an understanding of the behaviour of stable isotope profiles.

All relevant geochemical and hydrological information on an advective flow system is contained in the porosity, infiltration distance and Damköhler number (Fig. 6). In addition, so-called water/rock ratios contain an arbitrary distance element and represent information of a lower order of generality.

As usual in geology many additional complicating issues can be raised. A major one is that of dispersion in the fluid. Following an updated model by Lassey (in prep.) the Ohaaki-Broadlands data can also be matched by a combination of a Damköhler number NQ = 10 with a Péclet number, Np = 10; this would correspond to an overall dispersion coefficient D ≈ 10~6. In general the model that combines advection and dispersion provides plots similar to Fig. 3 but for fixed pairs of *HQ* and Np values.

Finally, more detailed isotope data on separate minerals could allow a more sophisticated analysis of what is now an overall average Damköhler number.

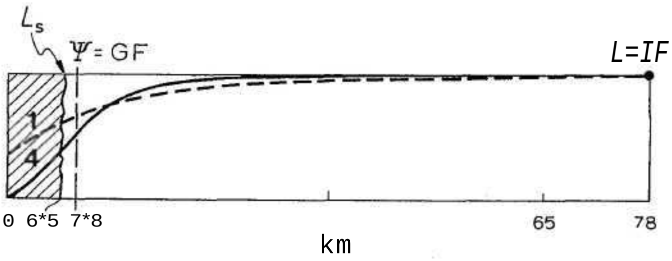

Fig. 6. Present situation at Ohaaki-Broadlands, after correction for the complex temperature effects. The actual system of length L_s, is shaded, the idealised (theoretical) exchange front, at *v,* is slightly past the discharge cross-section. The deduced *HQ* value is c.4. If part of the 'front flattening' was due to dispersion, a reasonable NQ could be 10 (with a PSclet number also of c.10).

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