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Liquid infiltration through the boiling-point isotherm in a desiccating fractured rock matrix.

by O.M. Phillips

Department of Earth and Planetary Sciences The Johns Hopkins University Baltimore, MD 21218

<u>Abstract</u>

A simple two-dimensional model is constructed for the infiltration of liquid water down a fracture in a permeable rock matrix, beyond the boiling-point isotherm. The water may derive from episodic infiltration or from the condensation of steam above a desiccating region. Boiling of the water in the fracture is maintained by heat transfer from the surrounding superheated matrix blocks.

There are two intrinsic length scales in this situation, (1): $l_r = \rho_l q_o L/(k_m\beta)$, which is such that the total heat flow over this lateral distance balances that needed for evaporation of the liquid water infiltration, and (2): The thermal diffusion distance $l_o = (\kappa_m t)^{1/2}$ which increases with time after the onset of infiltration. The primary results are: (a) for two-dimensional infiltration down an isolated fracture or fault, the depth of penetration below the (undisturbed) boiling point isotherm is given by $\frac{1}{2}\pi^{1/2}(l_r l_o)^{1/2}$, and

so increases as $l^{1/4}$. Immediately following the onset of infiltration, penetration is rapid, but quickly slows. This behavior continues until l_{0} (and D) become comparable with l_{s} . (b) With continuing infiltration down an isolated fracture or cluster of fractures, when $l_{0} \gg l_{s}$ the temperature distribution becomes steady and the penetration distance stabilizes at a value proportional to l_s . (c) Effects such as three-dimensionality of the liquid flow paths and flow rates, matrix infiltration, etc., appear to reduce the penetration distance. In most cases, the model provides an upper limit to the penetration to be expected in the field, for a given volume flux q_s per unit width of fracture.

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<u>1. Introduction</u>

The emplacement of radioactive wastes in a proposed repository above the water table in Yucca mountain requires containment for several thousands of years. The rock medium, the Topopah Springs Welded Tuff, surrounding the proposed repository site is generally described as having very low matrix permeability $(\sim 10^{-18} m^2)$, low-to-medium matrix porosity $(\sim 10\%)$ and a high density of fractures (>10 per meter). Over a long time interval, the integrity of the containment may be compromised by corrosion accelerated by intermittent wetting which could occur by episodic infiltration of meteoric water from above through the fracture network. A series of important papers by Buscheck, Nitao and Chesnut has examined the infiltration of a liquid front into a fractured, unsaturated porous medium, with specific attention to the Yucca mountain site.

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Buscheck, Nitao and Chesnut¹ list a number of pertinent references. Detailed theoretical studies have been supplemented by numerical modeling and they indicate that vertical water movement in a fracture can be extremely rapid, particularly for relatively large fractures in a relatively impermeable matrix. A more permeable matrix retards infiltration down the cracks because of absorption into the matrix blocks by capillary suction, but in a matrix of very small permeability, absorption is slow.

However, if the heat released by radioactive decay increases the rock temperature in the vicinity of the repository to levels above the boiling point of water, it is possible that infiltration of liquid water down fractures to the repository may be inhibited by boiling and the present contribution is devoted to an analysis of this question. The gases - air and vapor - in a connected fracture network are close to atmospheric pressure, so that boiling of liquid water seeping downward in the fractures will occur at a temperature near 100°C. The origin of the liquid water infiltrating downwards in the fractures is immaterial insofar as its percolation characteristics beyond the boiling point isotherm are concerned - it could derive from condensation of water vapor expelled from a desiccating rock mass, or from a pulse of surface precipitation. The time histories of the water flows are probably quite different, however, condensate appearing as a more or less continuous infiltration over a considerable time, surface percolation as a episodic, possibly intense event of shorter duration.

It will be found below that an important quantity involved in the infiltration process is q_o , the volume flux of liquid downwards per unit lateral extent of the fracture, with units (velocity x length). In principle, this could be related to the fracture characteristics, particularly geometry, but the single most remarkable hydrological characteristic of fractures is their variability. They may be open or filled partially or completely with detritus. They certainly contain contact areas where the aperture (for hydrologic purposes) vanishes and narrow throats in connected pathways that restrict the flow between wideraperture regions. The task of relating q_o to geometrical fracture characteristics, except in an orderof-magnitude sense, is rather unrewarding. The flux q_o can, however, be determined by seepage observations without reference to the fracture details; it is of course also extremely variable along the lateral extent of a natural fracture²

The dominant physical processes involved are fluid flow or percolation down a fracture crack or fault and boiling with heat transfer to the boiling region from the surrounding matrix. The primary analysis given here assumes a steady ambient temperature field with vertical heat flux, and a vertical fissure with laterally uniform flow. Field situations must be expected to be considerably more complicated. Liquid water may be absorbed from the fracture into the matrix block, forming an internal boiling front with elevated internal pressure needed to drive the vapor from the block. Although the simplest situation is twodimensional, with a uniform vertical fracture and steady temperature field, the liquid infiltration almost certainly occurs in nature in the form of fingers or along channels within the fracture, so that the effects of three-dimensionality on the behaviour of the system must be assessed. The temperature field may not be steady, with the boiling isotherm moving through the medium. Finally, the crack may be inclined to the direction of the ambient heat flux. From the practical point of view, the important effects among these are the ones that tend to augment the infiltration relative to the two-dimensional case. Fortunately, however, it is found below that these tend to inhibit the

infiltration, so that the simple model given provides a useful upper limit.

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2. Infiltration with fracture boiling.

Consider the two-dimensional situation illustrated in figure 1 with a vertical fracture or fissure carrying a volume flux q_{o} of liquid water (volume per unit lateral distance per unit time) downwards across the horizontal boiling point isotherm T_{b} . In this vicinity, the undisturbed temperature gradient $\partial T/\partial z = \beta$ is assumed constant, the temperature increasing downwards. The liquid flow downwards is assumed to start at t=0 and thereafter remain constant; if instead it ceases at some subsequent time, the liquid infiltration halts at the point it had reached.

Above the boiling point isotherm, as the water percolates down the fracture without boiling, the temperature of fluid elements increases in response to the ambient temperature field, but it can be shown that it remains close to thermal equilibrium with the matrix. The advective distortion of the isotherms in the neighboring rock by the downwards flow can be estimated from the thermal energy balance in the descending fluid, integrated across the fissure:

$$q \frac{\partial T}{\partial 3} = -\frac{2k_e}{(\rho C)_e} \frac{\partial T}{\partial x}\Big|_e = -\frac{2k_m}{(\rho C)_e} \frac{\partial T}{\partial x}\Big|_m$$
$$= -2\kappa \frac{\partial T}{\partial x}\Big|_m$$

where the lateral temperature gradient is at the interface into the medium, and z is measured downwards. The slope of the isotherms at the block surface, $(\partial T/\partial x)_m/(\partial T/\partial z)$ is thus $q_o/2\kappa$, or (half) the Peclet number. In a uniform open fissure of width $10^{-4}m$ with water in 'free fall' under gravity, $q \sim 5 \times 10^{-8} m^2 s^{-1}$ while

for most rocks $\kappa \sim 10^{-6} m^2 s^{-1}$, and the distortion of isotherms above the boiling zone is very small.

The water thus arrives at the boiling-point isotherm, itself essentially at the boiling point. Under natural conditions with a partially liquid saturated network of interconnecting fractures, the gas pressure is everywhere close to atmospheric, pressure differences needed to drive gas (or steam) flow being too small to influence the boiling point. Consequently, as the water percolates past the isotherm T_b , it begins to boil, its temperature remaining at T_{b} as it does so. Enthalpy or latent heat for boiling is supplied by conduction from the surrounding matrix blocks. As the boiling water moves downwards through the distance D(t) of figure 1, it remains at the boiling temperature T_{b} until it is all boiled away. The isotherms in the matrix blocks are then deflected downwards as shown on the left of figure 1, forming a thermal boundary layer along the fracture surface. which gradually thickens outwards. The pattern of the temperature field and the time history of the distance D(t) of penetration of liquid are governed by the conservation of liquid mass, thermal energy in the water and the diffusion of heat from the matrix on either side. If q(z,t)represents the volume flux of liquid water downwards, then

$$\rho_{2} \frac{\partial 2}{\partial 3} = -2E$$
 (2.1)

where *E* represents the rate of evaporation (by boiling) on each side (or half the total), having units mass per unit area per unit time. In the heat balance for the water, the advection terms vanish:

$$C_{e} \nabla \cdot (P_{e} \overset{u}{\sim} T)$$

= $C_{e} T \nabla \cdot (P_{e} \overset{u}{\sim}) + C_{e} P_{e} \overset{u}{\sim} \nabla \cdot T$

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The first term vanishes by mass conservation and the second since $T - T_b$, constant, below the boiling isotherm. The heat balance for the water, integrated across the fissure reduces simply to

$$O = 2 k_e \frac{\partial T}{\partial x} \Big|_e - 2 E L \quad (2.2)$$

where L is the latent heat of the boiling water and k_i the thermal conductivity of the water. Since in the heat transfer across the fracture surface

$$\frac{\partial T}{\partial x}\Big|_{e} = \frac{\partial T}{\partial x}\Big|_{m}$$
$$= (\rho C)_{m} \frac{\partial T}{\partial x}\Big|_{m},$$

equation (2.2) can be written

$$\mathcal{K}_{m} \frac{\partial T}{\partial \mathbf{z}} \bigg|_{m} = \frac{EL}{\left(\rho C\right)_{m}}$$
(2.3)

where κ_m is the thermal diffusivity in the matrix and $(\rho C)_m$ the product of density and specific heat for the matrix. Finally, following the onset of flow, the temperature distribution in the matrix is specified by the thermal boundary layer equation

$$\frac{\partial T}{\partial t} = \kappa_m \frac{\partial^2 T}{\partial x^2} \qquad (2.4)$$

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The boundary conditions on the temperature field are that

$$T = T_b = 0, say$$

$$at = 0, 3 < D(t),$$

$$T \rightarrow \beta 3 \quad at \quad t = 0$$

$$and \quad x \rightarrow \infty \quad all \quad t,$$

$$(2.5)$$

where, for convenience, the boiling point temperature is taken as zero. The volume flux q(z,t) is subject to the condition that

 $q=q_o$ at z=0 t>0 and q=0 at the nose of the wetted region z=D(t), say.

The detailed analytical solution will be given elsewhere, but the salient properties will be listed below and interpreted physically:

(a) The thermal boundary layer spreads laterally with thickness $\delta = [\kappa_m(t-t_0)]^{1/2}$, where $t_o(z)$ is the time at which the wetting front of boiling water reached the depth z below the undisturbed boiling-point isotherm. The factor $(t-t_o)$ is the time of contact with the boiling water. The temperature difference across the thermal boundary layer at depth z is simply βz . These results are in accord with simple intuition.

(b) The penetration distance D of the wetting front at a time t after it crosses the boiling-point isotherm is given by

$$D(t) = \left(\frac{2}{\pi}\right)^{1/4} \left(\frac{P_{e} q_{o} L}{k_{m} \beta}\right)^{1/2} (\kappa_{m} t)^{1/4}$$
(2.6)

The form of this solution is perhaps not obvious a priori but it can be obtained by the following simple physical argument. Water crosses the boiling-point isotherm at the boiling temperature, and is converted to steam at the same temperature by the addition of latent heat derived from cooling the hot

rock on either side of the fissure. The total mass of liquid water entering over the time interval t is $\rho_i q_o t$ (per unit lateral extent) and the heat required to vaporize this is $\rho_i q_o L t$. After time t the cooled area has depth D(t) and width $(\kappa_m t)^{1/2}$ and so is proportional to $D(\kappa_m t)^{1/2}$. In cooling the rock back to the boilingpoint temperature, the temperature change varies from zero (at the boiling-point isotherm) to βD (at the wetting tip), an average of about $\frac{1}{2}\beta D$. The total latent heat lost from the rock, then, is approximately

$$(\rho e)_{m} \cdot \mathcal{D} (\kappa_{m} t)^{\frac{1}{2}} \cdot \frac{1}{2} \beta \mathcal{D}$$

$$\simeq (\rho e)_{m} \beta (\kappa_{m} t)^{\frac{1}{2}} \mathcal{D}^{2},$$

Equating this to the heat needed for vaporization gives

$$P_{e} q_{o} L t$$

~ $(PC)_{m} / 3 (x_{m} t)^{1/2} D^{2},$

or

$$D^{2} \sim \frac{P_{e} q_{o} L t}{(\rho C)_{m} \beta \kappa_{m}^{\nu_{1}} t^{\nu_{1}}}$$
$$= \left(\frac{P_{e} q_{o} L}{\kappa_{m} \beta}\right) (\kappa_{m} t)^{\nu_{2}},$$

where $k_{\tilde{m}}^2(\rho C)_m \kappa_m$. This is precisely the same as (2.6), except for the order-unity numerical factor, which is not provided by this physical argument.

(c) This result can also be interpreted in terms of the intrinsic length scales of this problem. The configuration has no pertinent geometrical length scale, and the thermal diffusion distance $l_o = (\kappa_m t)^{1/2}$ depends on the time elapsed since onset of the flow. There is, however, an intrinsic length scale defined by the physical processes themselves. As before, the thermal power required to evaporate the descending water (per unit lateral distance) is $\rho_l q_o L$; if this were to be supplied by the heat flux over a horizontal distance l_s then

and the scale distance

$$l_{s} = \frac{P_{e} q_{o} L}{k_{m} \beta} \qquad (2.7)$$

depends on the flow rate and the temperature gradient, but not explicitly on elapsed time. The solution (2.6) can then be expressed as

$$D(t) = \left(\frac{2}{\pi}\right)^{1/4} \left(\ell_{\theta} \ell_{s}\right)^{1/2} \quad (2.8)$$

The penetration distance is, in effect, the harmonic mean of l_0 and l_x , so that its magnitude is intermediate between the two. The factor l_x depends on the fissure flow characteristics, l_0 essentially on time. A notable aspect of (2.6) and (2.7) is that they do not involve the medium permeabilities, whose values are subject to large uncertainties. The variability of D(t) is associated largely with the variability of q_0 .

(d) Since $l_0 \propto t^{1/2}$, and if q_0 is constant after time t=0, then $D(t) \propto t^{1/4}$; the initial penetration past the boiling-point isotherm is therefore rapid, but slows quickly.

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The solution (2.6) and (2.7) hold as long as the boundary-layer approximation is valid; that is as long as the boundary layer thickness l_{θ} remains small compared with *D*. From (2.7), this requires that

$$l_{\theta}/l_{s} \ll 1$$
 (2.9)

As time goes by, if the infiltration continues, l_{θ} increases as the isotherm distribution spreads laterally, as shown in figure 2. The upward heat flux is directed towards the fissure and the configuration approaches a steady state in which the upwards heat flux over the distance l_s is deflected to boil the water infiltrating downwards. There is a simple exact solution for this, homologous to a classical problem in hydrodynamics. The steady state penetration distance is in fact $\frac{1}{2}l_s$, l_s being the only length scale now pertinent. The scale l_s thus assumes additional importance by specifying the maximum distance over which penetration of liquid can occur.

(e) The infiltration depth,

$$D(t) = \left(\frac{2}{\pi}\right)^{\prime\prime 4} (l_{o} l_{s}), \quad l_{o} \ll l_{s},$$
$$= \frac{1}{2} l_{s}, \qquad l_{o} \gtrsim l_{s}.$$

Recall that the thermal diffusion scale l_0 depends essentially on elapsed time and the length scale l_s on the liquid volume flux, the largest possible values of which are of most interest. To give a sense of magnitude, one drop of water per meter of fracture per second corresponds to $q_o \sim 5 \times 10^{-9} m^2 s^{-1}$. With $\beta = 1 C m^{-1}$ and the other values given in the notation list, l_s is about 12 m. The following short table gives other representative values:

t	l.	q.	l,
1 hr	0.05 m	$10^{-10}m^2s^{-1}$	0.24 m
l day	0.25 m	10-9	2.4 m
l year	4.6 m	10-8	24 m
100 years	46 m	10-6	2.4x10 ³ m

Note that strong, continuous flows $q_o > 10^{-8}m^2s^{-1}$ or so are capable of infiltrating substantial distances vertically, but only if they continue for a substantial time. Thus if $q_o = 10^{-6}m^2s^{-1}$, and remains steady, the penetration is about 25 m after 1 day, 105 m after a year and 330 m after 100 years. If flow ceases before then, the penetration also stops.

3. Modifying factors.

The model described above is very simple and we need to assess the influence upon it of real-world complexities that one might expect.

(a) Three-dimensionality

Whether as a result of varying fracture aperture, variations in detrital content or fingering instability, an infiltrating tongue of liquid water must be expected to be finite lateral extent rather than a uniform sheet. The ribbons of fluid with the greatest flow rates infiltrate faster and further than others, so that even if initially there were a cluster of them, the ones with greatest flow rates become isolated. In a uniform sheet, the cooled region from which has been extracted to boil the water, extends a distance $(\kappa t)^{1/2}$ on either side. With an infiltrating tongue, an additional circular area of radius $(\kappa t)^{1/2}$ is cooled by the boiling, so that heat transfer per unit lateral width, or the boiling rate is increased. This would then reduce the rate of penetration below that given by the two-dimensional model, i.e. (2.6), for the same value of q_{\bullet} .

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The length scale l_{3s} characterizing the maximum penetration distance in three-dimensional flow can be found in a similar manner to be

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$$\mathcal{L}_{35} = \left(\frac{P_e Q_o L}{k_m/\epsilon}\right)^{1/2}, \quad (3.1)$$

where $Q_o(m^3 s^{-1})$ is the total liquid downflow rate across the boiling isotherm. In a ribbon of width Y, $Q_o = q_o Y$ and equation (3.1) is equivalent to

$$l_{3S}^2 = l_S Y$$

and if $Y < l_s$, $l_{3s} < l_s$; three-dimensional infiltration down a tube-shaped conduit may be more penetrative.

(b) Fracture slope

Vertical fractures seem to provide for the greatest liquid infiltration. The penetration in depth along inclined fractures is reduced by the cosine of the slope to the vertical for simple geometrical reasons and by an additional such factor when the liquid infiltration is gravity driven. After long time intervals, the enhanced interception of vertical heat flux provides additional boiling, supplementing that provided by cooling of superheated rock. These effects all reduce the vertical penetration.

(c) Moving isotherms.

During the early history of the repository when the boiling-point isotherm is expanding, steam generated by desiccation infiltrates outwards, and, when encountering cooler rock, condenses. In general, the rate of expansion of the boiling-point isotherm, of order $(k/t)^{1/2}$ (or $10^{-7}m/s$ after 3 years, $10^{-8}m/s$ after 300 years) is small compared with the

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downward fluid velocities in fractures with active liquid infiltration $(10^{-5}m/s \text{ or so})$, so that one would expect that the slow increase in the temperature field would leave the flow pattern quasi-steady rather than accurately steady. However, in an increasing temperature field above the repository, the temperature gradient (below the boiling-point isotherm, in particular) increases with depth, so that the heat transfer to an infiltrating liquid tongue is somewhat greater than in the model (constant $\partial T/\partial z$), and the penetration distance somewhat reduced.

(d) Absorption into matrix blocks.

It is intuitively fairly evident that absorption of water into the matrix blocks before boiling reduces the vertical infiltration along fractures, just as it does in the nonboiling case. (Buscheck et al^1). The properties and behaviour of boiling fronts, inside matrix blocks, the interior of which is superheated, are little explored, but they are certainly different from the movement of wetting fronts in a cold block. In the latter case, pressure gradi-ents in the flow of air displaced by water are usually neglected, since the dynamic viscosity for air is $O(10^{-2})$ that for water. In a boiling front, the volume of steam generated is much larger than the volume of water boiled. In a stream tube from the wetted fracture surface, across the boiling front to the point of emergence of steam from the matrix block, the mass flux ρU is constant. The pressure gradient

 $\nabla p = -k_p^{-1}\mu \underline{u} = -(k_p^{-1}p\underline{u})v$, where k_p is the intrinsic permeability and v the <u>kinematic</u> viscosity, larger for steam than for water by a factor of about 30 at 100°. The capillary pressure difference across the boiling front is thus balanced mostly by driving out steam and only secondarily by drawing in water. In fingering liquid infiltration and matrix-block absorption, the steam from any internal boiling front will emerge preferentially along the path of least resistance, usually between the liquid fingers.

(e) Dissolved solutes

The infiltrating liquid may contain dissolved solutes in low concentration, leached from the rock above. Solid residues left after boiling will tend to seal the fractures and reduce further infiltration, but geochemical reactions may be possible that would have the opposite effect.

In summary, each of these effects appears to generally reduce the rate of liquid infiltration down fractures past the boiling-point isotherm below that given by the simple twodimensional model, i.e. (2.6). This is fortunate, since many of them are difficult to quantify in detail and unless there are other effects that would increase the rate, the expression (2.6) provides an upper limit to the infiltration rate, which is conservative from the engineering viewpoint.

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<u>4. Notation</u>

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- C: specific heat
- D = D(t): penetration depth
- k_m k_i: thermal conductivity of matrix, liquid (~1.0.6 W/mK)
- $l_o = (\kappa t)^{1/2}$: thermal diffusion length scale
- l, = (p₁q_oL/k_mβ): 2-D infiltration length scale
- $l_{3s} = (\rho_l Q_o L/k_m \beta)^{1/2}$: 3-D infiltration length scale
- L: Latent heat of water (2.4x10⁶ J/kg

- q_- volume flux of liquid water per unit width of a 2-D fracture, moving past boiling-point isotherm.
- Q_o corresponding total volume flux in a ribbon of flow in (3-D).
- t = time elapsed since the onset of
 flow
- x,z = co-ordinates, horizontal and vertically down
- Y = width of flow ribbon
- β vertical temperature gradient at the boiling-point isotherm
- $\kappa_m = k_m / (\rho C)_m, \ \kappa = k_m / (\rho C)_l \sim 0.7 \times 10^{-6} m^2 s^{-1}$
- ρ_{l} = liquid water density $10^{3} kgm^{-3}$

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