Chapter 3

In-Situ Thermal Remediation of Contaminated Soil

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3.1 Background

Recently, a method for removing contaminants from soil (several meters under the ground) has been proposed by McMillan-McGee Corp. The process can be described as follows. Over a period of several weeks, electrical energy is introduced to the contaminated soil using a multitude of finite length cylindrical electrodes. Current is forced to flow through the soil by the voltage differentials at the electrodes. Water is also pumped into the soil via the injection well and out of the ground at the extraction well. The soil is heated up by the electrical current and the contaminated liquids and vapours are produced at the extraction well. The temperature of the contaminated soil, during the process, is believed to reach the maximum value (the boiling temperature of water). Normally, the electrodes are placed around the contaminated site and the extraction well is located in the centre of the contaminated region. The distance between the electrodes is usually seven to eight meters. The distance between the

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extraction well and an electrode is about four meters. The diameter of the electrodes is 0.2 meter and the extraction well is 0.1 meter in diameter.

The reason for using the electrical current is that "flushing" the soil using water alone is not effective for removing the contaminants. By heating up the soil and vaporizing the contaminated liquid, it is anticipated that rate of extraction will increase as long as the recondensation is not significant. A major concern, therefore, is whether recondensation will occur. Intuitively, one might speculate that liquid phase may dominate near the injection well. Moving away from the injection site towards the extraction well, due to the combined effects of lower pressure and higher temperature (from heating), phase change occurs and a mixture of vapour and liquid may co-exist. There may also be a vapour-only region, depending on the values of temperature, pressure, and other parameters. In the two-phase zone, since vapour bubbles tend to rise due to the buoyancy force, and the temperature decreases along the vertical path of the bubbles out of the heated region, it is possible that the bubbles will recondense before reaching the extraction well. As a consequence, the probability exists that part of the contaminants stay in the soil. Obviously, to predict transition between single-phase and two-phase regions and to understand the transport phenomenon in detail, a thermal capillary two-phase flow model is needed. However, to simplify the problem, here we only consider the case when two-phases co-exist in the entire region.

The main objective of this modelling exercise is to determine the necessary vacuum pressure (pressure drop from the electrodes to the extraction well) so that the chemical bubbles are removed at the extraction well before they rise too high and condense to the liquid state.

3.2 Flow and Temperature Fields

To make the problem tractable, we consider an idealised situation where the extraction well and an electrode are both placed at the centre of a circle and the current as well as the mixture of liquid and vapour are flowing towards the centre. The domain of interest becomes a cylindrical region with the extraction well and an electrode at the centre. To further simplify the problem, we assume radial symmetry and the electrical current is in the radial direction only. Even with these simplifications, the problem at hand is still a complicated one and in principle a multi-phase flow model will be an appropriate starting point. However, we take a simplistic approach in this report by decoupling the complicated process into several sub-processes.

First of all, since the main components in the system are water and water vapour, we will not distinguish various components in the system and treat it as a one-component system with two phases: liquid and vapour. Secondly, we assume that the two-phase flow under consideration falls into the slug flow regime since the flow rates are relatively low - typically in the range of 10^{-2} m^3/s. As a result, in the horizontal direction r, the vapour (generated by the heating) moves with the liquid phase. Therefore, we will not distinguish the two phases and a single-phase model will be used with a common radial mixture discharge velocity u. Furthermore, the mass exchange happens mainly in the r direction due to an applied pressure drop between the extraction well and the injection well. Therefore, conservation of mass will be applied to the horizontal velocity component only. In the vertical z direction the bulk of the liquid phase is at rest, except the part displaced by vapour due to buoyancy force. Following [4], the r-component of the velocity is determined by the Darcy's law

$$u = -\frac{k}{\mu}\frac{\partial P}{\partial r} \tag{3.1}$$

where k is the effective permeability, μ is the effective viscosity, and P is the effective pressure. The mass conservation (assuming that the vertical z component is small) can be written as

$$\frac{\partial \rho_f}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(ru\rho_f) = 0. \tag{3.2}$$

The mixture density ρ_f and r-velocity u are defined as

$$\rho_f = \alpha\rho_l + (1-\alpha)\rho_v, \quad \rho_f u = \alpha\rho_l u_l + (1-\alpha)\rho_v u_v$$

where α is the liquid volume fraction (saturation), u_l and u_v are the liquid and vapour velocity components in the r-direction, ρ_l and ρ_v are the liquid and vapour densities.

The temperature of the soil, liquid and vapour mixture is determined by the energy conservation law

$$\rho c\frac{\partial T}{\partial t} + \rho_f c_f u\frac{\partial T}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(\kappa r\frac{\partial T}{\partial r}\right) + \sigma|E|^2 - LM, \tag{3.3}$$

where $\sigma|E|^2$ is the Joule heating of the soil with an the electrical resistivity σ and electric field E. The term LM represents the heat lost in the formation of the bubbles with L is the latent heat of vapourization of the fluid and M the mass rate of vapourization. The soil fluid mixture is characterized by a heat capacity ρc and thermal conductivity κ. Note that we have assumed that there is no temperature variation in the vertical z direction.

Now, we use dimensional analysis to further simplify (3.1)-(3.3), by keeping the dominant terms. With this in mind we make the following assignments:

$$P = P_0 + \Delta P\hat{P}, \;\; r = x\hat{r}, \;\; t = \beta\hat{t}, \;\; u = \frac{x}{\beta}\hat{u}$$

where the quantities with hats are dimensionless and the collection $\{\Delta P, x, \beta\}$ are representative values. Under this assignment the expression for the pressure becomes

$$\frac{\partial \hat{\rho}_f}{\partial \hat{t}} - \frac{\beta k}{\mu}\frac{\Delta P}{x^2}\frac{1}{\hat{r}}\frac{\partial}{\partial \hat{r}}\left(\hat{r}\hat{\rho}_f\frac{\partial \hat{P}}{\partial \hat{r}}\right) = 0.$$

Representative values for the various quantities can be found in Table 3.1. Typical orders of magnitude in SI units [8] are $x \sim 10$, $\beta \sim 10^5$, $k \sim 10^{-9}$, $\mu \sim 10^{-3}$ and $\Delta P \sim 10^5$ yielding $\beta k\Delta P/(\mu x^2) \sim 10^2 \gg 1$. Consequently the temporal variations of $\hat{\rho}_f$ can be ignored to first approximation giving a pressure field expression[12]

$$\frac{1}{\hat{r}}\frac{\partial}{\partial \hat{r}}\left(\hat{r}\hat{\rho}_f\frac{\partial \hat{P}}{\partial \hat{r}}\right) = 0. \tag{3.4}$$

Turning to the expression for the thermal energy we make the further assignment that

$$T = T_0 + \Delta T\hat{T}.$$

[12]For the purposes of the dimensional analysis the relative permeability has been taken as a constant.

The expression for the temperature becomes

$$\rho c \frac{\partial \hat{T}}{\partial \hat{t}} + \rho_f c_f \hat{u} \frac{\partial \hat{T}}{\partial \hat{r}} - \frac{\beta \kappa}{x^2} \frac{1}{\hat{r}} \frac{\partial}{\partial \hat{r}} \left(\hat{r} \frac{\partial \hat{T}}{\partial \hat{r}} \right) - \frac{\sigma |E|^2}{\Delta T} \beta + \frac{LM}{\Delta T} \beta = 0.$$

The first two terms have coefficients of $\rho c \sim 10^6$ and $\rho_f c_f \sim 10^6$. Since the thermal conductivity $\kappa \sim 10$, the coefficient of the third term has a magnitude of $\beta\kappa/x^2 \sim 10^4 \ll 10^6$ indicating that diffusion of the temperature field can be ignored to first order. For the last two terms we use [8] $\Delta T \sim 10^2$, $\sigma|E|^2 \sim 10^3$, $L \sim 10^6$ and $M \sim 10^{-4}$ giving $\sigma|E|^2\beta/\Delta T \sim 10^6$ and $LM\beta/\Delta T \sim 10^5$ and to first order the temperature field satisfies

$$\rho c \frac{\partial \hat{T}}{\partial \hat{t}} + \rho_f c_f \hat{u} \frac{\partial \hat{T}}{\partial \hat{r}} - \frac{\sigma |E|^2}{\Delta T} \beta = 0. \tag{3.5}$$

We should mention that the phase-change term may become important when the mass rate M increases. In that case, the temperature and the flow fields will be coupled and numerical or asymptotic methods have to be used.

Dropping the hat notation and assuming ρ_f is spatially uniform allow one to express (3.4) and (3.5) as

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial P}{\partial r} \right) = 0, \tag{3.6}$$

$$\rho c \frac{\partial T}{\partial t} + \rho_f c_f u \frac{\partial T}{\partial r} = \frac{\sigma |E|^2}{\Delta T} \beta. \tag{3.7}$$

Finally, we use the motion of a long gas bubble inside a small channel to describe the relative vapour rising velocity in the vertical z direction due to buoyancy force. This problem was first investigated by Taylor [11] and studied subsequently by many researchers as a model to gain insights into slug multi-phase flows (in oil and gas recovery) [2, 7, 9, 10, 12].

For low viscosity and high surface tension systems such as the water-vapour two phase flows in a moderate-sized circular tube, Tung and Parlange [12] proposed that the terminal velocity v_b of the rising bubble is given by the phenomenological expression

$$v_b = \sqrt{0.272 g d} - 0.472 \frac{\gamma}{\Delta \rho d}, \quad d \geq d_{\text{min}} = 0.936 \left[\frac{\gamma^2}{g (\Delta \rho)^2} \right]^{1/3} \tag{3.8}$$

where d is the diameter of the tube, γ is the surface tension coefficient and $\Delta\rho = \rho_l - \rho_v$ is the density difference of the liquid and vapour. Note that for a sufficiently small tube, $d = d_{\text{min}}$, this formula predicts the vapour slug velocity becomes zero.

On the other hand, experimental investigations in micro non-circular channels have shown that the elongational bubbles always rise even for a channel with effective diameter as small as 0.866×10^{-3} meter [1]. More recently, numerical simulation of long gas bubbles rising through micro channels with triangular and rectangular cross section filled with stagnation liquid has been carried out [7]. The terminal velocity of the rising bubble as a function of the effective diameter is given in a non-dimensional form as

$$\text{Ca} = c_1 \text{Eo}^{d_1} + c_2 \text{Eo}^{d_2} \tag{3.9}$$

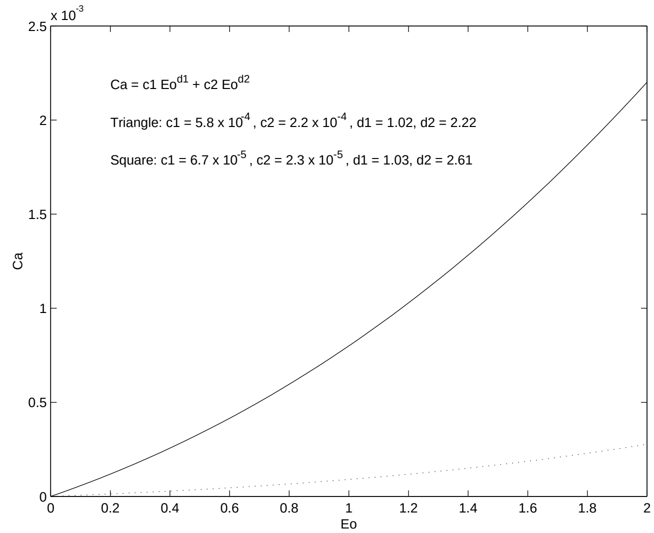

Figure 3.1: Illustrated is the capillary number as a function of the Eötvös number for channels with a triangular (solid) and square (dotted) cross section.

where the capillary number Ca and the Eötvös number Eo are defined as

$$\mathrm{Ca} = \frac{\mu v_b}{\gamma}, \quad \mathrm{Eo} = \frac{\Delta \rho g d^2}{\gamma}.$$

The parameters c_i and d_i are fit using numerical results. Figure 3.1 illustrates this relationship for channels with a triangular and rectangular cross section.

3.2.1 Pressure

Now let us consider the following equation for the pressure distribution in the system, assuming that the relative permeability is a constant one has equation (3.6)

$$\frac{\partial}{\partial r}\left(r \frac{\partial P}{\partial r} \right) = 0$$

with boundary conditions

$$P(r_w) = P_w, \quad P(r_e) = P_e,$$

where r_w is the radius of the domain (where the injection well is placed) and r_e is the radius of the extraction well, P_w is the pressure at the extraction well and P_e is the pressure at the electrode. The solution to this equation is

$$P(r) = (P_w - P_e)\frac{\ln r - \ln r_e}{\ln r_w - \ln r_e} + P_e. \tag{3.10}$$

3.2.2 Velocity

We have two equations for velocity distribution: lateral velocity and vertical velocity. Let us first consider equation for lateral velocity field:

$$u = -\frac{k}{\mu}\frac{dP}{dr}. \tag{3.11}$$

Using expression (3.10) we find

$$u = -\frac{k}{\mu}\frac{P_w - P_e}{\ln r_w - \ln r_e}\frac{1}{r}. \tag{3.12}$$

For the vertical component of the vapour velocity, we use the dimensional form of (3.9), which gives

$$v_b = \frac{\gamma}{\mu_l}\mathrm{Ca} = \frac{\gamma}{\mu_l}\left(c_1 \mathrm{Eo}^{d_1} + c_2 \mathrm{Eo}^{d_2}\right). \tag{3.13}$$

From which we can obtain the (average) discharge velocity in the vertical direction

$$v_v = \tau\phi(1-\alpha)v_b = \tau F V_\infty \tag{3.14}$$

where $V_\infty = \Delta\rho g d^2/(3\mu_l)$ is a representative terminal velocity of the rising vapour bubbles, and τ is the tortuosity factor of the bubble in the porous media relative to the terminal velocity of a vapour bubble in straight vertical channel with diameter d. The factor

$$F = \phi(1-\alpha)\frac{\gamma}{\mu_l V_\infty}\left(c_1 \mathrm{Eo}^{d_1} + c_2 \mathrm{Eo}^{d_2}\right) \tag{3.15}$$

where ϕ is the porosity of the medium

3.2.3 Temperature

Assuming constant electrical current inside the electrode I_t, the magnitude of the electrical field in the porous medium can be written as $E = I_t/(2\pi r\sigma H)$ where H is the height of the electrode. The energy equation (3.7) can be written in the form

$$\frac{\partial T}{\partial t} + \frac{b}{r}\frac{\partial T}{\partial r} = \frac{a}{r^2} \tag{3.16}$$

with initial and boundary conditions

$$\begin{cases} T(r,0) = T_0(r), \\ T(r_e,t) = T_e \end{cases} \tag{3.17}$$

with $T_0(r) = T_e$ for $0 < r \le r_e$ and where

$$a = \frac{10^3 I_t^2}{4\sigma\pi^2 H^2 \rho c}, \quad b = -\frac{q}{2\pi H}\frac{\rho_f c_f}{\rho c}.$$

Here we have replaced u by the volume flow rate q using the relationship $q = -2\pi r H u$. Unlike pressure, the temperature of the system is time dependent. In order to solve (3.16)-(3.17) we use method of characteristics which gives us:

$$T(r,t) = \begin{cases} \frac{a}{b}\ln\left(\frac{r}{\sqrt{r^2-2bt}}\right) + T_0(\sqrt{r^2-2bt}), & r \geq \sqrt{r_e^2+2bt} \\ \frac{a}{b}\ln\left(\frac{r}{r_e}\right) + T_e, & r < \sqrt{r_e^2+2bt}. \end{cases} \tag{3.18}$$

3.3 Transport of Contaminants

Let C_v and C_l be the mass concentration of the contaminant in the vapour and liquid phase. The total amount of contaminant is conserved and satisfies

$$\frac{\partial}{\partial t}(C_v + C_l) + \nabla \cdot (\vec{u}_v C_v + \vec{u}_l C_l) = 0$$

with $\vec{u}_i = \langle u_i, v_i \rangle$ being the radial and vertical components of the velocity vector of either the vapour $(i = v)$ or liquid $(i = l)$ phase.

Fast reaction assumption yields

$$C_l = K C_v$$

where

$$K = P \times 10^{-A+B/(T+C)}$$

with [8] $A = 7.098$, $B = 1238.71$ and $C = 217$. Here T and P are temperature and pressure, respectively. Eliminating C_l gives the expression

$$\frac{\partial}{\partial t}(1+K)\,C_v + C_v \nabla \cdot (\vec{u}_v + K\vec{u}_l) + (\vec{u}_v + K\vec{u}_l)\,\nabla C_v = 0. \tag{3.19}$$

Therefore, assuming that K is independent of time, we have

$$\frac{\partial}{\partial t}C_v + \frac{C_v}{1+K}\nabla \cdot (\vec{u}_v + K\vec{u}_l) + \left(\frac{\vec{u}_v + K\vec{u}_l}{1+K}\right)\nabla C_v = 0. \tag{3.20}$$

Solving by the method of characteristics, we have

$$\frac{dC_v}{dt} + \frac{C_v}{1+K}\nabla \cdot (\vec{u}_v + K\vec{u}_l) = 0 \tag{3.21}$$

where the characteristic base curves are determined by the two ODEs

$$\begin{aligned} \frac{dr}{dt} &= \frac{u_v + K u_l}{1+K}, \\ \frac{dz}{dt} &= \frac{v_v + K v_l}{1+K}. \end{aligned}$$

From these we have

$$\frac{dr}{dz} = \frac{u_v + Ku_l}{v_v + Kv_l}. \tag{3.22}$$

From the flow and temperature model we have

$$u_l = u_v = -\frac{q}{2\pi rH}, \quad v_l = 0, \quad v_v = \tau F V_\infty$$

where q is the volume flow rate at the extraction well, F is given by (3.15) and τ is a free parameter.

Assume that a parcel of contaminant at the base of the injection electrode ($z = 0$, $r = r_w$) moves towards the extraction electrode located at $r = r_e < r_w$. According to equation (3.22) the vertical displacement of this parcel is given by the monotonically increasing function

$$z = \frac{2\pi H v_v}{q} \int_r^{r_w} \frac{\xi}{1+K} d\xi.$$

If we let h be the height above the contaminant region which has been heated up by the electrodes then the parcel will be successfully extracted provided it reaches $r = r_e$ before $z = h$. Let $z_e = z(r_e)$ denote the height of this characteristic when it reaches the extraction well $r = r_e$. By assuming that the factor $1 + K$ does not vary significantly over the interval $r_e \le r \le r_w$ the condition that $z_e \le h$ can be converted into a lower bound on the volumetric flux of

$$q \ge \frac{\pi\tau FHV_\infty(r_w^2 - r_e^2)}{h(1+K)}.$$

With $H = 5$ m, $h = 1$ m, $r_w = 5$ m, $r_e = 0$ m, $\Delta\rho = 10^3$ kg/m^3, $\mu_l = 10^{-3}$ Pa s, and $\tau = 0.01$, for a mean throat size of $d = 10^{-3}$ m, we obtain $F = 1.7 \times 10^{-4}$ for a medium with square channels. Based on these values, we can compute the value of $q = 6.8 \times 10^{-4}$ m^3/s. The calculation was done based on the parameter values listed in Table 3.1. We note that there is no physical basis for choosing this value. However, viewing the possibility that bubbles may get trapped in a particular porous medium, it is not unreasonable to expect that it will take a much longer time for the bubbles to travel vertically.

3.4 Conclusions and Recommendations

In this report we have proposed a simple model for estimating the transport of contaminants using thermal remediation. Based on the model, the minimum extraction rate of fluid is calculated and its value is within the practical range. However, many questions remain unanswered. For example, we have not addressed the effect of temperature variation in the vertical direction and near the edge of the heated zone. We have not attempted to examine the effect of possible condensation near the cold/low pressure region. Finally, we have not considered the possibility that bubbles may be trapped in the isolated pore space and the effects of heating and the accumulation of vapour bubbles on the soil.

We should also mention that we have not tried to identify transitions between liquid-only, vapour-only and two-phase regions and the transportation of contaminants in the liquid and vapour only regions. However, this may not be as critical as other issues since it is relatively simpler to determine the velocity of the liquid or gas in the one-phase region.

Data	Symbol	Value
Operating Properties		
Maximum Temperature	$T_{\max}$	100^oC
Initial Temperature	$T_{\min}$	20^oC
Initial Pressure	P_0	101.325 kPa
Target Thickness	H	5 m
Electrode Length	L_e	5 m
Electrode Spacing	Z_e	10 m
Extraction Well Spacing	Z_x	10 m
Physical Properties		
Initial Permeability[13]	k	10.0 mD
Viscosity[14]	μ	1.0 cP
Surface Tension of Water[15]	γ	0.0717 N m^{-1}
Producing Pressure Drop	ΔP	500 kPa
Total Heat Capacity	ρc	2.8×10^6 J m^{-3}K^{-1}

Table 3.1: Input Data for the sample calculations.

Evidently further improvements are needed before the model can be used for prediction and to answer the other issues raised. In particular, a proper flow and temperature model must be derived and reference [5] should provide a good starting point where thermal two-phase flow in porous media is discussed. Secondly, the effects of the phase change (vapourization and condensation), capillary pressure and the existence of vapour only regions, which have been neglected, may be important in certain domains, especially near the boundary of the heated zone where the change of soil temperature is more significant. Models analyzing condensation and vapourization in porous media have been studied for other applications which may be helpful, see for example [3] and references therein. Finally, the effect of different types of porous media and the impact of heating and vapour bubbles may be important as well. Models of gas penetrating elastic media have been studied [6], which may be useful if fracturing of the media needs to be considered.

[13] 1 Darcy = 9.87×10^{-12} m^2.

[14] 1 centipoise = 1×10^{-3} kg m^{-1}s^{-1} $= 1 \times 10^{-3}$ Pa s.

[15] at 25^oC.

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