A SIMPLIFIED OXIDATION MODEL FOR TWO-PHASE FLOW IN POROUS MEDIA

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ABSTRACT
This paper describes a simplified mathematical model for thermal recovery by oxidation for flow of oxygen and oil in porous media. Some neglected important physical effects include gravity, compressibility and heat loss to the rock formation, but heat longitudinal conduction and capillary pressure difference between the phases are considered. The mathematical model is obtained from the mass balance equations for air and oil, energy balance and Darcy’s law applied to each phase. Based on this model some typical features in low temperature oxidation concerning the wave structure are captured. Numerical simulations showing saturations and temperature profiles are reported.

Key words: porous media, mathematical model, numerical simulations.

INTRODUCTION
A procedure that is sometimes used to increase oil production in petroleum reservoirs consists of pumping air into injection wells in order to maintain pressure and to expel oil to producing wells. This procedure usually leads to low temperature oxidation and it is necessary to guarantee that all oxygen is consumed before reaching the production wells, because of safety concerns.

General models and numerical simulations for multiphase multicomponent thermal oil recovery are given in Crookston and Gottfried, for instance. In this work we present a simplified model in which we consider a two-phase flow consisting of gas and oil moving linearly in porous media with saturations $s_g$ and $s_o$, respectively. We assume that the injected gas is pure oxygen, and that it forms carbon dioxide in an exothermic chemical reaction. We also assume that this carbon dioxide becomes totally dissolved in the oil phase as soon as it is generated. For simplicity, in the current work we assume that the density of the oil phase is independent of the concentration of the dissolved carbon dioxide. The viscosity of the oil phase depends on the temperature. We ignore the effect of carbon dioxide concentration on the oil phase viscosity. Densities of gas and oil will be assumed to be independent of temperature. To avoid effects due to volumetric changes, we make the unphysical assumption that gas and oil have the same constant density. We use an Arrhenius type law for the reaction rate. We neglect heat loss to the rock formation, so that this oxidation gives rise to a temperature front with small amplitude. Marchesin and Schecter in their work proved that if this heat loss is not neglected, the oxidation may give rise to pulses rather than fronts, and oxidation will be incomplete.

We assume that at the right of the front there is a non-oxidized mixture of gaseous (oxygen) and oil phases, at a
reservoir temperature \( \theta \). At the left of the front, there is only an oleic phase, with a certain concentration of dissolved carbon dioxide, at a higher temperature resulting from oxidation. We remark that if air is injected, we have to keep track of the gaseous phase that has been oxidized, so an extra variable and an extra equation are needed.

The Arrhenius type reaction rate law we use states that

\[
q = (\phi \rho_{j} \phi_{k} K_{p} \rho_{k} \phi_{h})(\Delta \phi) \rho_{j} \phi_{h} \theta_{h} \exp(-\frac{E_{j}}{RT}) \quad \text{if} \quad \theta_{h} > \theta_{0}, \quad \text{and} \quad q = 0 \quad \text{if} \quad \theta_{h} < \theta_{0} \leq 0
\]

(1.1)

In formula (1.1) we have the following constants: \( \phi \) is the porosity, \( \rho_{j} \) and \( \rho_{k} \) are the gas and oil densities respectively, \( K_{p} \) is the Arrhenius constant, \( E_{j} \) is the activation energy and \( \theta_{0} \) is the temperature for which oxidation starts.

The mathematical model for the flow is described in Section 2. In Section 3 some illustrative numerical simulations are reported. Section 4 is devoted to conclusions and discussion of our results.

**THE MODEL**

The conservation of mass of the gas phase may be written as:

\[
\frac{\partial}{\partial t}(\phi \rho_{j} \phi_{k} s_{j}) = -\frac{\partial}{\partial x}(\rho_{j} \phi_{k} v_{j}) - q,
\]

(2.1)

The conservation of mass of the oleic phase may be written as:

\[
\frac{\partial}{\partial t}(\phi \rho_{j} \phi_{k} s_{j}) = -\frac{\partial}{\partial x}(\rho_{j} \phi_{k} v_{j}) + q.
\]

(2.2)

The conservation of energy may be written as:

\[
\frac{\partial}{\partial t}(\phi \rho_{j} \phi_{k} E_{j} + \phi \rho_{j} \phi_{k} E_{j} + \rho_{j} E_{j}) = \frac{\partial}{\partial x}(\rho_{j} \phi_{k} v_{j} E_{j} + \rho_{j} \phi_{k} E_{j}) + \frac{\partial}{\partial x}\left( \phi \left( \rho_{j} \phi_{k} K_{p} \rho_{k} \phi_{h} \theta_{h} \frac{\partial}{\partial x} \phi \left( \rho_{j} \phi_{k} s_{j} + \rho_{j} \phi_{k} \theta_{h} + \frac{\partial}{\partial x} \phi \right) \right) + \Delta q \right)
\]

(2.3)

where \( \Delta \) is the heat generated per unit mass of consumed oxygen. We will consider \( \Delta \) being constant.

The seepage velocity \( v_{j} \) is given by Darcy’s law (without gravitational effects):

\[
v_{j} = -K_{j} \frac{\partial p_{j}}{\partial x} \quad \text{if} \quad j = g, o
\]

(2.4)

In formula (2.4), \( K \) is the absolute permeability of rock; \( \lambda_{j} \) and \( \rho_{j} \) are the relative mobility and pressure of phase \( j = g, o \), respectively. Each relative mobility \( \lambda_{j} \) is a function of saturation \( s_{j} \) and temperature \( \phi \) defined by

\[
\lambda_{j}(s_{j}, \phi) = \frac{k_{j}(s_{j})}{\mu_{j}(\phi)}
\]

(2.5)

where \( \mu_{j} \) is the viscosity of phase \( j \), i.e., its intrinsic resistance to motion and \( k_{j} \) is the relative permeability of phase \( j \). Gas viscosity will be assumed constant. Oil viscosity, however, depends strongly on temperature.

The total seepage velocity of the fluid is defined by

\[
v = v_{g} + v_{o}
\]

(2.6)

while the total mobility of the fluid, which depends on saturation and temperature, is

\[
\lambda = \lambda_{g} + \lambda_{o}
\]

(2.7)

Therefore

\[
v = -K \lambda \frac{\partial p_{g}}{\partial x} - K \lambda \frac{\partial p_{o}}{\partial x}
\]

(2.8)

Considering the capillary pressure equation \( p_{s}(s_{j}) = p_{i} - p_{w} \), with \( \frac{\partial p_{s}}{\partial s_{j}} \), and Eq. (2.8), we get that

\[
\frac{\partial p_{g}}{\partial x} = f_{g} \frac{\partial p_{o}}{\partial x} - \frac{v}{K} \quad \text{and} \quad \frac{\partial p_{o}}{\partial x} = -f_{g} \frac{\partial p_{g}}{\partial x} - \frac{v}{K}
\]

(2.9)

where \( f_{g} \) is called the “fractional flow function” of phase \( j = g, o \). Each of these functions depends on \( s_{j} \) and \( \theta_{h} \); they are defined by

\[
f_{g}(s_{j}, \theta) = \frac{\lambda_{g}(s_{j}, \theta)}{\lambda}
\]

(2.10)

Considering the relations (2.4)-(2.10) above, the equations (2.1), (2.2) and (2.3) become, respectively,

\[
\frac{\partial}{\partial t}(\phi \rho_{j} \phi_{k} s_{j}) + \frac{\partial}{\partial x}(\rho_{j} \phi_{k} v_{j}) = \frac{\partial}{\partial x}\left( K \rho_{j} \lambda_{j} f_{j} \frac{\partial p_{j}}{\partial x} \right) - q,
\]

(2.11)

\[
\frac{\partial}{\partial t}(\phi \rho_{j} \phi_{k} s_{j}) + \frac{\partial}{\partial x}(\rho_{j} \phi_{k} v_{j}) = \frac{\partial}{\partial x}\left( K \rho_{j} \lambda_{j} f_{j} \frac{\partial p_{j}}{\partial x} \right) + q,
\]

(2.12)

\[
\frac{\partial}{\partial t}(\phi \rho_{j} \phi_{k} E_{j} + \phi \rho_{j} \phi_{k} E_{j} + \rho_{j} E_{j}) = \frac{\partial}{\partial x}(\rho_{j} \phi_{k} v_{j} E_{j} + \rho_{j} \phi_{k} E_{j}) + \frac{\partial}{\partial x}\left( K \rho_{j} \lambda_{j} f_{j} \frac{\partial p_{j}}{\partial x} \right) + \Delta q
\]

(2.13)

where \( \Delta \phi = \phi \rho_{j} \phi_{k} K_{p} \rho_{k} \phi_{h} \theta_{h} \frac{\partial}{\partial x} \phi \left( \rho_{j} \phi_{k} s_{j} + \rho_{j} \phi_{k} \theta_{h} + \frac{\partial}{\partial x} \phi \right) \) is the effective longitudinal thermal conductivity.

Under the assumption that \( \rho_{j} = \rho_{0} \) and that they are constant, we can divide equation (2.11) by \( \rho_{0} \) and equation (2.12) by \( \rho_{0} \) and add the results to replace equation (2.11) by

\[
\frac{\partial}{\partial x} v = 0,
\]

(2.14)

From Eq. (2.14), we see that \( v = v(t) \) can be related to the inflow boundary condition; for simplicity, we assume it to be constant. Thus we will eliminate equation (2.14).

Recall that \( E_{t} = CR \), where \( j = g, o, r \) and \( C_{i}, C_{j}, C_{o} \) are the thermal capacities of the gaseous phase (at constant pressure), oil and rock per unit mass. In this work, we will make the simplifying assumptions that \( C_{i} = g, o, r \) are constant.

Considering that \( s_{r} = 1 - s_{g} - s_{o} = 1 - f_{g} \) and \( \lambda_{f} = \lambda_{j} \), equation (2.13) becomes:
\[
\frac{\partial}{\partial t} \left( \rho_s (C_p \rho_x - C_p \rho_z) \frac{\partial}{\partial x} \right) + \frac{\partial}{\partial x} \left( \rho_f (C_p \rho_x - C_p \rho_z) \frac{\partial}{\partial x} \right) = \frac{\partial}{\partial x} \left( \frac{\partial P}{\partial x} \right) + \frac{\partial}{\partial x} \left( \frac{\partial P}{\partial x} \right) + \Delta q
\]

(2.15)

Let us introduce the positive constants

\[
a = C_p \rho_x, \quad \beta = C_p \rho_z, \quad \gamma = C_p, \quad \delta = C_p \rho_x, \quad \eta = \frac{\partial P}{\partial x} \quad \text{and} \quad \chi = \frac{1}{\rho_x}
\]

We will omit the index \( s \) and \( f \). So, from now on, oil saturation is denoted by \( \phi \) and the fractional flow function of oil is denoted by \( f \). To scale out \( \phi \) and \( v \), we can set

\[
t = \phi t \quad \text{and} \quad \tau = \frac{v t}{\phi}
\]

(2.16)

For simplicity of notation, we drop the tildes.

To shorten notation we also introduce the nonnegative function

\[
h(x) = \frac{K}{\nu^2} \int_x^\infty \frac{dp}{ds}
\]

After dividing equation (2.12) by \( \rho_x \), equation (2.15) by \( (C_p \rho_x - C_p \rho_z) \) and using the constants and the function above defined, we obtain, respectively,

\[
\frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \right) + \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \right) + \Delta q
\]

(2.17)

\[
\frac{\partial}{\partial x} \left( \alpha + \beta \phi \right) + \frac{\partial}{\partial x} \left( \alpha f + \delta \phi \right) = \frac{\partial}{\partial x} \left( \alpha \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial x} \left( \eta \frac{\partial h}{\partial x} \right) + \Delta q
\]

(2.18)

The system consisting of Eqs. (2.17), (2.18) is appropriate for time simulation of the Cauchy problem.

**NUMERICAL EXPERIMENTS**

In this section we show some numerical results in order to illustrate the solution to the simplified model developed in the previous section. We obtain these results by implementing a linearized finite difference Crank-Nicolson scheme.

To perform the simulations we considered Corey-type functions for permeabilities:

\[
k_w(s_x) = s_x^2, \quad k_m(s_x) = s_x^3
\]

Consequently, the oil fractional flow function was given by

\[
f(s) = \frac{s^2}{\mu_s(T)} \left( \frac{1-s}{\mu_e(T)} \right)
\]

The gas viscosity \( \mu_e \) is constant while the oil viscosity \( \mu_s(T) \) is a linear decreasing function of the temperature. The gas-oil capillary pressure we considered is a linear decreasing function depending only on the oil saturation.

In Figures 1-5 oil saturation (with dissolved carbon dioxide or not, indistinctly) and temperature profiles are displayed at several time steps to illustrate the propagation of the fundamental waves present in the figure. When it is convenient to follow the wave propagation, the oil saturation and the temperature profiles are displayed in the same, top and bottom, respectively. In these figures there are labels indicating the time steps. They are \( t = 0 < t_1 < t_2 \). Since the main purpose of simulations was to show the qualitative behavior of the solutions, we did not use appropriate scales for temperature and other physical quantities. We paid attention only to whether chemical oxidation reaction is present or not. The scaled length of the reservoir was considered to be one.

The simulations were performed considering initial conditions on saturations and temperature as constant-by-part functions. To be more precise, denoting \( (s, \theta) \) by \( U \) and \( x_1 \) a position in the interval \((0,1)\), the initial condition considered had the following form:

\[
U(x,0) = \begin{cases} 
(s_1, \theta_1), & \text{if } 0 \leq x \leq x_1, \\
(s_2, \theta_2), & \text{if } x_1 \leq x \leq 1.
\end{cases}
\]

In the first three numerical experiments we present simulations considering no oxidation reactions separating the left and the right states. In the simulation illustrated in 1 we consider that the reservoir was premixed with oxygen and oil under a constant temperature \( \theta_1 \neq \theta_2 \) below the ignition temperature \( \theta_2 \) and only one finite jump in saturations with \( s_1 = 0.2 \) and \( s_2 = 0.8 \). From the reaction term equation given in (1.1) and from equations (2.17), (2.18) it is easy to see that \( \theta(x,t) = \theta_2 \) is a solution of system (2.17)+(2.18), since \( \theta_1 = \theta_2 = \theta_0 \) and provided that \( s(x,T) \) satisfies Buckley-Leverett's two-phase flow equation (2.17).

Yet in the non-oxidized situation, if we consider possible temperature variations in a range below \( \theta_2 \) after dividing equation (2.17) by \( \alpha \) we get a system similar to the "hot-water" system studied by Barkve and da Mota. An advection-diffusion temperature wave may be included in the solution besides the Buckley-Leverett wave. This solution is illustrated in Figure 2 considering also \( s_1 = 0.2, s_2 = 0.8 \) and \( \theta_1 < \theta_2 < \theta_0 \).

In the opposite situation, we considered that both left and right initial states were in the oxidized region. Since we assumed that all oxygen is consumed and the produced carbon dioxide is totally dissolved in the oil phase, we have that \( s(x, t) \equiv 1 \) (and consequently \( f(x, \theta, t) \equiv 1 \) and \( q(s, \theta, t) \equiv 0 \)) is a solution of system (2.17)+(2.18), provided that the linear advection-diffusion equation (2.18) for the temperature is satisfied. Thus the solution consists only of a temperature diffusive wave as illustrated in Fig. 3, with \( \theta_1 > \theta_2 > \theta_0 \).

In the fourth experiment, illustrated in Figure 4, we considered that at the left boundary there was an initial oxidized
state ($x_i = 1$) at a temperature $\theta_i$, higher than $\theta_0$, and at the right there was a non oxidized initial state corresponding to a mixture of oxygen and oil with $x_i = 0.98$ and $x_0 = 0.98$. We remark that in Figure 4 the oil saturation axis is shown only in the range $[0.96, 1]$. As it is proved by da Mota et al., neglecting heat loss to the rock formation, under generic conditions, there is an oxidation reaction front propagating from left to right as a traveling wave. In this case, initially the temperature increases up to a maximum value. This maximum is proportional to the amount of oxygen available. Because of the boundary condition on the left temperature, a diffusive temperature wave is formed behind the oxidation front. This temperature wave also propagates to right (but slower than the oxidation front), causing temperature profile peak widening with time evolution.

Finally we considered, a situation with a “square pulse” in the initial data, as illustrated in Figure 5. This situation would represent “hot” oxygen injected into the reservoir during a finite time, after which injection ceases. Thus there is a finite region in the reservoir with a premixed mixture of oxygen and oil at a temperature higher than $\theta_0$. Away from this region the temperature is initially below $\theta_0$. This is illustrated in Figure 5 with $u(x,0) = 0.8$ if $0 < x < x_0 = 1$, and $u(x,0) = 1$ if $0 < x < 1$. We remark also that in Fig 5 only part of the oil saturation axis corresponding to the interval $[0.5, 1]$ is shown. As Figure 5 shows, the oxidation reaction is uniform in the finite region with temperature increase up to the maximum value when all available oxygen is consumed. After that, the pulse in the temperature starts to propagate to the right as two diffusive waves that tend asymptotically to cancel each other. Again the maximum temperature is proportional to the amount of available oxygen and it will reach the right edge of the reservoir depending on the temperature.
Fig. 3 - Diffusive temperature wave in the oxidized region.

Fig. 4 - Oxidation front separating an oxidized state from a non-oxidized one.

Fig. 5 - A pulse on the temperature when all available oxygen is consumed.
CONCLUSIONS AND DISCUSSION

We have presented a simple model capturing some features typical of low temperature oxidation, and which is amenable to mathematical analysis.

The most important step for making this model useful for practical simulations is replacing the injected gas by air, which consists of 21% oxygen and 79% nitrogen. It will be necessary to introduce a new variable besides gas saturation. This variable will measure the fraction of the gaseous phase that consists of oxygen components. We can still think that the carbon dioxide generated by oxidation dissolves immediately into the oleic phase.

The second most important improvement is the introduction of gravity terms, since the injection of gas is often done at the top part of a slanted reservoir.

Instead of two-phase flow, studying three-phase flow (water, oil and gas phases) allows using a more realistic chemical reaction of the type

\[ C_n F_{2m} + (n + \frac{m}{2}) O_2 \rightarrow nCO_2 + mH_2O. \]

We can then assume that the water generated in the chemical reaction goes to the water phase, and that the carbon dioxide generated partitions into the oleic and water phases according to the partial pressure law.

The next improvement in the model is to remove the simplification that the carbon dioxide generated by the chemical reaction dissolves instantly. There will be a solution rate, related to partial pressure of the carbon dioxide. Variation of the oleic phase viscosity with carbon dioxide content should also be taken into account.

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