Pore Level Modelling of Three Phase Flow in Porous Media

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ABSTRACT

We analyze the pore level displacement of three phases — water, oil and gas. The presence of a third phase dramatically alters the flow, because of the formation of a layer of oil between water and gas in the pore space. We derive simple conditions for the stability of the oil layer, which is governed by the spreading coefficient (which must be either zero or negative in thermodynamic equilibrium) and the ratio of oil/water and gas/oil capillary pressures. We also predict several new types of double displacement process, where one phase displaces another which displaces the third. We then describe a pore level numerical network model that incorporates all these processes. We demonstrate that the flow of oil at low saturation — which is important in enhanced oil recovery and pollutant transport — cannot be adequately described by the conventional multiphase Darcy law.

1. INTRODUCTION

Three phase flow is an important process in enhanced oil recovery, gravity drainage, solution gas drives and in pollutant transport and clean-up. Multiphase flow in porous media is characterized by capillary pressure and relative permeability functions. For three phase flow, they are extremely difficult to determine for the full range of saturation values. For a recent study see [Kalaydjian *et al.*, 1993]. Simulation studies rely on empirical correlations to compute relative permeability. These are either fits to the experimental data or correlations that extrapolate the two phase (gas/water, oil/water and gas/oil) functions into the three phase region

[Baker, 1988; Fayers, 1989; Stone, 1973]. These functions cannot properly represent the intricacies of the flow phenomena.

To understand three phase flow in porous media, we need to study the physics at the pore level. When three phases are in contact with other, their behavior is determined by the spreading coefficient C_s , which is defined as:

$$C_s = \gamma_{gw} - (\gamma_{ow} + \gamma_{go}) \quad (1)$$

where initially γ_{gw} , γ_{ow} and γ_{go} are the gas/water, oil/water and gas/oil interfacial tensions respectively, measured on pure fluids before they are brought into contact with each other. There are three different things that can happen [Hirasaki, 1993]. (i) If $C_s < 0$, the three phase contact line shown in Figure 1 is stable. Examples include medium and long chain alkanes, such as dodecane in contact with air and water. (ii) If $C_s > 0$, the contact line between the three phases is unstable and the oil spreads. Many solvents, hydrocarbons and crude oils (see p. 104, Table 5 of [Muskat, 1949]) have a positive spreading coefficient. We can

define an equilibrium spreading coefficient C_s^e from Equation (1), where the interfacial tensions are measured in thermodynamic equilibrium. If $C_s > 0$, the water surface is coated by a thin oil film, which lowers the effective gas/water interfacial tension and $C_s^e < 0$. Excess oil remains in a droplet in equilibrium with the film. Many hydrocarbons, such as benzene, and solvents, such as carbon

tetrachloride, have a positive initial spreading coefficient, but a negative equilibrium spreading coefficient. The film generally is approximately of molecular thickness, between 0.5 and 5 nm across. (iii) The third possibility is that the oil film can swell without limit. Once the oil film is thicker than the range of intermolecular forces, $C_s^e = 0$ [Adamson, 1990; Gibbs, 1928; Rowlinson and Widom, 1989]. An example of this behavior is Soltrol 170, a commercial mixture of hydrocarbons [Oren *et al.*, 1992; Vizika, 1993]. In the rest of this paper, we will assume that the system has reached thermodynamic equilibrium and hence the distribution of fluid is controlled by the equilibrium spreading coefficient, which is either zero or negative.

Figure 1. Three fluids in contact near a solid surface.

If gas is introduced into a system containing water and residual oil, spreading allows the oil to form a continuous layer between gas and water, enabling the oil to flow. This phenomenon has been suspected as an important mechanism for oil recovery by inert gas injection since the work of Dumoré and Schols [1974] and was confirmed by careful experimental measurements on sandstone cores and unconsolidated media [Blunt *et al.*, 1994; Chatzis *et al.*, 1988; Kantzas *et al.*, 1988a; Vizika, 1993]. The drainage of oil layers has been directly observed using two dimensional etched glass micromodels by Kantzas *et al.* [1988b], Oren *et al.* [1992] and Kalaydjian [1992]. Kalaydjian and Oren *et al.* demonstrated that a system with a positive value of C_s gives better oil recovery than one where $C_s < 0$. Recently, three phase gravity drainage has been studied theoretically and experimentally. It has been shown that flow in stable oil layers in crevices of the pore space enable very low residual oil saturations to be achieved [Blunt *et al.*, 1995].

Three phase flow allows a series of double displacement mechanisms, where one fluid displaces another that displaces the third. This was observed and described by Oren *et al.* [1992] with reference to double drainage, where gas displaces oil that displaces water.

In this paper we will describe a three phase pore level numerical model that incorporates the effects of oil layers and double displacement mechanisms. A percolation network model of three phase flow

was first proposed by [Heiba *et al.*, 1984], and more sophisticated models including the effects of flow in oil films [Soll and Celia, 1993] and both oil films and double drainage [Oren *et al.*, 1994] have been shown to reproduce the results of two-dimensional micromodel experiments. This model will extend the previous work to three dimensions and to include the full range of possible drainage and imbibition mechanisms. Since the configuration and displacement of the fluids at the pore scale is not well known, we will first describe the two novel features of three phase flow: the stability of an oil layer between water and gas, and the six possible double displacement processes. We then briefly describe the network model and demonstrate how our description of the pore level physics inevitably leads to a macroscopic description of three phase flow that is very different from the conventional Darcy law formulation.

2. A PORE LEVEL NETWORK MODEL

We represent the pore space as a cubic array of wide pores connected together by narrower throats. Arbitrary distributions of pore and throat radii may be specified, except that a pore is always larger than any of the six throats connected to it. In this model both the pores and throats have a square cross-section, although this restriction can be changed easily. The flow of three phases is simulated by allowing a sequence of individual pore events. These events are described below.

3. AN OIL LAYER IN THE PORE SPACE

Figure 2 shows three phases in a wedge. We will assume that the water is wetting and that the oil/water contact angle is smaller than the gas/oil contact angle. This arrangement may be stable even if the spreading coefficient is negative. The oil layer here will be of order a few microns thick — much thicker than the nanometer sized molecular oil films seen on flat surfaces. The radius of curvature of the gas/oil interface is r_{go} and the curvature of the oil/water interface is r_{ow} . We assume that there is no curvature in the direction perpendicular to the plane of Figure 2. Then from the Young-Laplace equation $P_{cgo} = \gamma_{go}/r_{go}$, where P_{cgo} is the local gas/oil capillary pressure, with a similar expression for P_{cow} , the oil/water capillary pressure. We define:

$$R = \frac{r_{go}}{r_{ow}} = \frac{\gamma_{go}P_{cow}}{\gamma_{ow}P_{cgo}} \quad (2)$$

For large values of R , the oil layer is thick. At a critical value, R_c , the arrangement of fluid shown in Figure 2(a) is no longer possible and it unlikely that the oil layer remains stable. This happens when the point of contact of the oil/water interface with the surface and the gas/oil contact coincide, as shown in Figure 2(b). The distance AB marked on Figure 2(b) is:

$$AB = r \frac{\cos(\theta + \beta)}{\cos \beta} \quad (3)$$

for an interface of radius r , contact angle θ and wedge of half angle β . Hence the critical ratio R_c is:

$$R_c = \frac{\cos(\theta_{ow} + \beta)}{\cos(\theta_{go} + \beta)} \quad (4)$$

If we consider the case where the water is completely wetting and covers the solid surface with a thin film of molecular thickness, then the microscopic arrangement of water, gas and oil at the solid surface is similar to that illustrated in Figure 1, except that the water surface is flat. The vertical force balance is maintained by intermolecular forces in the water film, but the horizontal balance of forces implies that:

$$\gamma_{gw} = \gamma_{go} \cos \theta_{go} + \gamma_{ow} \quad (5)$$

or:

$$\cos \theta_{go} = 1 + \frac{C_s^e}{\gamma_{go}} \quad (6)$$

as derived by [Kalaydjian, 1992; Kalaydjian et al., 1993]. Notice here we have used the equilibrium value of the spreading coefficient — the water film may itself be coated by a thin film of oil.

Figure 2(a). Three phases in a wedge of half angle β .
(b) At this point, the oil layer first becomes unstable.

If we use Equation (6) for the gas/oil contact angle and assume that $\theta_{ow}=0$, then, after some algebra, Equation (4) becomes:

$$\frac{1}{R_c} = 1 + \frac{C_s^e}{\gamma_{go}} - \left(-\frac{C_s^e}{\gamma_{go}} \right)^{1/2} \left(2 + \frac{C_s^e}{\gamma_{go}} \right)^{1/2} \tan \beta \quad (7)$$

As an example, consider benzene in contact with water and air, for which $C_s^e = -1.6 \text{ mNm}^{-1}$ and $\gamma_{go} = 28.8 \text{ mNm}^{-1}$. Then for a square wedge with $\beta = \pi/4$, $R_c = 1.6$. An oil layer is stable for larger values of R and is unstable for R below this critical value. If the equilibrium spreading coefficient is zero, $R_c = 1$.

This is a very simple geometric argument for the stability of an oil layer in a wedge that ignores the complex geometry of a real pore space. However, the analysis does give an indication of the expected behavior: oil layers are stable even for negative spreading coefficient, but that the range of capillary pressures over which a layer is stable decreases with decreasing spreading coefficient.

When oil layers are stable, the oil is connected and cannot be trapped in the presence of gas. This allows very low oil saturations to be achieved during gas injection. For $R < R_c$ there are no oil layers and oil can be trapped by both gas and water. If the initial spreading coefficient is positive, the water will still be coated by an oil film of molecular thickness, but this film is far too thin to allow any significant oil flow. The flow of oil through molecular films will be ignored in the calculations that follow.

4. DISPLACEMENT MECHANISMS

Three phase flow allows all possible combinations of two phase displacements. Drainage, or the invasion of a non-wetting fluid, occurs when gas displaces oil, gas displaces water and oil displaces water. To enter a pore or throat of radius r requires a capillary pressure $2\gamma \cos \theta / r$, where θ is the contact angle. Imbibition, or the invasion of wetting fluid, allows two distinct types of process. The first is snap-off [Roof, 1970], where a wetting film or layer of fluid swells until it invades the center of a narrow throat. For a throat of square cross-section with inscribed radius r the critical capillary pressure is $\gamma(\cos \theta - \sin \theta) / r$ [Lenormand and Zarcone, 1984]. This type of advance can only occur when the wetting fluid is present as a continuous layer in crevices of the pore space. By construction, we always allow water to be continuous, but oil layers are only stable when the condition discussed in section 3 is met. Thus examples of snap-off are water invasion into gas, when there is no oil layer, water into oil in a throat that contains no gas, and oil into gas, when an oil layer is stable. The second imbibition process is piston-like advance. In throats the threshold

capillary pressure is the same as drainage, but in pores the capillary pressure depends on the number of adjoining throats that are filled with wetting fluid. The more adjacent throats filled with wetting fluid, the higher the capillary pressure for invasion of the pore. These processes have been extensively described by [Lenormand and Zarcone, 1984; Lenormand et al., 1983] and are called I_n when n surrounding throats are filled with non-wetting fluid. Examples are water invasion of gas, water displacing oil and oil displacing gas.

In three phase flow it is also possible for one fluid (A) to displace another (B) which then displaces the third phase (C). For this to happen,

phases A and C must be continuous, but B may be discontinuous. If gas displaces disconnected oil that displaces water, we have a double drainage process by which waterflood residual oil can be mobilized in the presence of gas and water. The other, analogous process, is double imbibition, when water displaces oil that displaces gas. In all there are six such double displacement mechanisms for all possible combinations of phases A, B and C, and they are summarized in Table 1.

As an illustration, consider Figure 3, which describes a possible double imbibition process. The invasion of oil by water by snap-off in a throat of

Table 1. Double displacement mechanisms in three phase flow.

Mechanism	Favored when	Name
Drainage		
Gas→oil→water	Wider oil/water throat than any gas/water throats, or oil is trapped. Disfavored for strongly negative C_S .	Double drainage, DD
Gas→water→oil	$R < 1$ and negative C_S .	Drainage-imbibition, DDI
oil→gas→water	Negative C_S . Mechanism for the mobilization of trapped gas.	Imbibition-drainage, DID
Imbibition		
oil→water→gas	Not favored.	Drainage-imbibition, IDI
Water→gas→oil	Not favored.	Imbibition-drainage, IID
Water→oil→gas	$C_S < 0$ and oil occupies narrower throats than gas, or oil is trapped.	Double imbibition, II

Figure 3. Double imbibition. Water displaces oil in two throats as shown and then oil displaces gas from a pore.

radius r_{to} is followed by piston-like advance of oil displacing gas in a pore of radius r_{pg} and requires a gas/water capillary pressure, P_{cgw} greater than or equal to approximately $2\gamma_{go} \cos \theta_{go} / r_{pg} + \gamma_{ow} / r_{to}$. In contrast, direct displacement of gas by water by piston-like advance requires a gas/water capillary pressure greater than or equal to $2\gamma_{gw} / r_{pg}$. Double imbibition will occur if it has the larger capillary pressure, which is more likely to be the case for systems with a strongly negative spreading coefficient. In contrast, it has been shown that double drainage is more likely to occur in preference to the direct displacement of water by gas when the spreading coefficient is as large as possible [Oren *et al.*, 1992].

5. HOW THE NETWORK MODEL SIMULATES FLUID INVASION

Displacement proceeds by one pore or throat filling at a time. The capillary pressures for all the possible displacement processes mentioned in the previous section are stored in a sorted list. At the beginning, the model is completely saturated with water. Fluid is injected through one face of the model and produced through the opposite face. There are periodic boundary conditions in the other two directions. Oil is injected into the network. Subsequently, water, gas or oil may all be injected and displaced in any order. When all three phases are present in the model, two capillary pressures must be specified. If we specify P_{cgo} and P_{cow} , the gas/water capillary pressure is defined as $P_{cgw} = P_{cgo} + P_{cow}$. We hold one of the capillary pressures constant, say the gas/oil pressure. We then make a small change in the oil/water capillary pressure. Let us assume that we are considering drainage, which means that the oil/water capillary pressure is increasing. We then find, of all possible two phase and three phase displacements, the one that has the lowest oil/water capillary pressure assuming that P_{cgo} is some known, fixed value. This could be an event where oil displaces water, oil displaces gas, or gas displaces water, or one of the double displacement mechanisms. For imbibition, we would find the event with the highest oil/water capillary pressure. In the next step we may either keep P_{cgo} constant and proceed as before, or hold P_{cow} fixed at its previous value. In the latter case we perform the displacement with the lowest value of P_{cgo} (for a drainage step) or the highest value (for imbibition).

If a phase, for instance oil, does not span the network, we can still define local oil/water and gas/oil capillary pressures. These are found from the radii of curvature of the last pore or throat that oil either invaded or was displaced from.

The network model simulates any sequence of three phase flow by incremental changes in capillary pressure. The saturations of each phase at each step

are recorded.

As an example, Figure 4 is a picture of a two-dimensional three phase simulation on an 80 by 80 network. The picture shows gas breakthrough during gas injection into water and oil.

6. WHY A CONVENTIONAL DARCY LAW DESCRIPTION CANNOT BE VALID

Figure 5 shows the saturation path and corresponding capillary pressures for three phase displacements with a zero spreading coefficient simulated on a 20 by 15 by 15 network. Initially the network model is completely saturated with water. The oil/water capillary pressure is then increased to 11,000 Pa, where the water saturation is 15%. Waterflooding was then simulated and the residual oil saturation in water was just over 30%. We model the injection of gas for two cases. The first, indicated by the solid line, is when the oil/water capillary pressure is increased to and then maintained at 11,000 Pa. This represents the injection of gas into connate water and oil. All the oil is recovered. Before the gas is injected, all the oil is connected. The oil/water capillary pressure is determined by the smallest throat that the oil has entered. When the gas is first injected, oil layers are stable and so the oil remains connected. For zero spreading coefficient, the point at which oil layers disappear, when $R=R_c=1$ in Figure 5, also corresponds exactly to the gas/oil capillary pressure necessary for gas to enter the smallest oil filled throat. Thus the gas is able to displace all the oil while oil layers are present, resulting in 100% recovery. This is the ideal case.

Figure 4. Gas injection into oil and water at gas breakthrough simulated on an 80 by 80 square network. The fluids have a spreading coefficient of zero. Gas is gray, oil is black and water is white. Both the water and oil phases are connected through layers in the corners of the pore spaces.

The dotted line in Figure 5 indicates gas injection into waterflood residual oil and water. In this simulation the oil phase never spans the network. Oil layers are no longer stable at a lower value of P_{cgo} than in the first example. Not all the oil has been contacted by gas when the layers disappear. The remaining oil recovery for $R < R_c$ is the result of double drainage alone. The final oil saturation, when $P_{cgo}=42,000$ Pa (off the scale in Figure 5) is 20%, approximately 10% lower than the waterflood residual.

Figure 6 illustrates the same two displacements

for fluids with an equilibrium spreading coefficient of -4 mNm^{-1} , similar to a decane/water/air system [Hirasaki, 1993]. In this example, oil layers are stable for a more restricted range of capillary pressure, as indicated on the Figure. For both cases, drainage through stable oil layers makes very little contribution to recovery, and displacement of oil is predominantly by double drainage. Notice that for gas injection into waterflood residual oil, the final oil saturation is virtually the same as for the zero spreading coefficient case. In contrast, injection into a higher oil saturation now recovers much less oil and the remaining oil saturation (40%) is higher than the waterflood residual (35%).

Figure 5. Different pathways in capillary pressure and saturation space, representing gas injection into waterflood residual oil for fluids with a spreading coefficient of zero.

Figure 6. Different pathways in capillary pressure and saturation space, representing gas injection into waterflood residual oil for fluids with a spreading coefficient of -4 mNm^{-1} .

The conventional multiphase Darcy law relates the oil flow to a pressure gradient in the oil phase. If the oil is not connected, but there is recovery by double drainage, we have oil flow with no macroscopic pressure gradient in the oil. This process can only be modeled by cross-terms, where the flow of oil is related to pressure gradients in the continuous gas and water phases. This demonstrates one inadequacy of conventional three phase relative permeability models.

Hysteresis, where we get different final oil saturations after gas injection, depending on the saturation (or capillary pressure) history, is also seen in two phase flow, but in three phase flow, particularly at low oil saturation, we have shown that it is very significant.

How could we use the network model to predict the oil recovery from gas injection? We have demonstrated that the residual oil saturation is sensitive to capillary pressure history, but we have no way of knowing *a priori* what route in capillary pressure space a given displacement would take. Imagine that we attempt to predict a one-dimensional displacement where gas is injected into waterflood residual oil. Conventionally we would use predetermined relative permeability and capillary pressure functions in the conservation equations for the fluid phases. We could solve the equations and find the route in capillary pressure space that the displacement takes at some fixed spatial location. However, we have just shown that the final oil saturation and consequently the relative permeability and capillary pressure is a strong function of this path. For instance, if an oil bank of large oil saturation develops we would predict very good recovery for zero spreading coefficient, whereas if no oil bank is formed this corresponds to gas injection with a low value of P_{cow} and the recovery is much poorer. Using a network model we can compute capillary pressure and relative permeabilities for a given pathway in capillary pressure space. A discussion of this will be the topic of later work. We must find relative permeabilities and capillary pressures which when placed in a conservation equation give the same sequence of saturation changes that were used to compute them in the first place. This self-consistency requirement is particularly important for a correct understanding of the mobilization of residual oil by gas and water. This can be achieved using network modeling, but clearly cannot be incorporated in conventional numerical models, nor readily measured experimentally for the full range of possible types of displacement.

7. CONCLUSIONS

In thermodynamic equilibrium, the spreading coefficient of oil between water and gas is either zero, or negative. However, it is still possible for three bulk phases to coexist in a pore throat and we found the conditions in which a oil layer would be

stable in a wedge.

Three phase flow allows six different double displacement mechanisms, where one phase displaces another which displaces the third. If three phases cannot coexist in a pore throat, double drainage and double imbibition are the only mechanisms for the mobilization of residual oil.

We have described a three-dimensional, three phase network model that incorporates three phase drainage and imbibition displacement mechanisms. We have demonstrated that conventional models of capillary pressure and relative permeability are likely to give an inadequate representation of oil flow at low saturation, because of the significant and subtle effects of hysteresis. We showed this by considering different possible sequences of saturation changes during gasflooding. Further work on a description of three phase flow in a variety of different circumstances is planned.

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NOMENCLATURE

C_s	spreading coefficient
P_c	capillary pressure
r	radius of curvature
R	ratio of curvatures
R_c	critical ratio for three phases to be stable in a throat
γ	interfacial tension
θ	contact angle

Subscripts

o	oil
w	water
g	gas

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