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

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Abstract

Air sometimes is pumped in injection wells in order to preserve the pressure and to expel oil to producing wells. A low temperature oxidation usually occurs in such a situation. The aims are increasing the oil production and guaranteeing that all the oxygen is consumed before reaching the production wells, where it would be a safety hazard. In this work we consider a simplified model for the flow and we find some oxidation fronts, described by heteroclinic connections in a non-hyperbolic system of three ordinary differential equations associated to the model.

1 Introduction

In this work we study oxidation fronts for a system of gas and oil moving linearly in porous media. We assume that the injected gas is pure oxygen, and that it forms carbon dioxide in a 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, it will be assumed 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. The effect of carbon dioxide concentration on the oil phase viscosity will be ignored. 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

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oil have the same density. We assume that the heat capacity of oil and gas is negligible compared to rock capacity, so that all generated heat is used to warm the rock. 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. In [8] and [9] it was shown that if this heat loss is not neglected, the combustion 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 oleic phases, at reservoir temperature. At the left of the front, there is only an oleic phase, with a certain dissolved carbon dioxide, at a higher temperature resulting from oxidation. We remark that if air is injected, we have to keep track of the portion of the gaseous phase which has been oxidized, so an extra variable and an extra equation are needed.

The Arrhenius type reaction rate law we use states that the total amount of oxygen mass consumed per unit time is proportional to the oxygen available and to a temperature dependent factor, see [2].

$$q = A_r e^{-\frac{E_a}{R(\theta-\theta_0)}}, \quad \text{if} \quad \theta > \theta_0 \qquad \text{and} \qquad q = 0 \quad \text{if} \quad 0 \leq \theta \leq \theta_0\,, \tag{1}$$

where A_r is the Arrhenius´s rate coefficient, E_a is the activation energy, and θ_0 is the temperature where the reaction starts.

Our aim in this paper is to discuss the oxidation fronts as traveling waves. We show that under certain conditions such waves exist and are well determined.

The equations for the model are obtained as in [4], and they are described in Section 2. In Section 3, we describe the chemical reaction fronts as traveling waves. In Section 4, the orbits of the ordinary differential equations for the traveling waves are found. Section 5 is devoted to discussion of our results.

2 The model

Throughout this section, the subscripts g and o refer to the gaseous and oleic phases, respectively, and r to the porous rock phase. We will follow Reference [1]. The flow is described by state quantities depending on (x,t), the space and time coordinates. They are denoted as follow: $s_j = s_j(x,t)$, $j = g$, o, is the saturation of phase j in the fluid, i.e., the fraction of the porous volume occupied by phase j; and $\theta = \theta(x,t)$, is the temperature, which is assumed to be the same for gas, oil, and rock at each (x,t). The density of phase j, $j = g$, o, r, is denoted by ρ_j. The other relevant quantities related to phase j, $j = g$, o, are denoted by: v_j is the seepage velocity; and λ_j is the relative mobility, which is a function of saturation s_j and temperature θ, defined by

$$\lambda_j(s_j, \theta) = \frac{k_j(s_j)}{\mu_j(\theta)} \,. \tag{2}$$

Here, μ_j is the viscosity, i.e, its intrinsic resistance to motion; and k_j is the relative permeability, it is a dimensionless function of saturation s_j, measured in the laboratory, also, it is a phase dependent quantity such that Kk_j is the porous medium capability of allowing the flow of phase j, where K is the absolute permeability of the rock, which measures the porous medium capability of allowing fluid flow. Gas viscosity and the absolute permeability are assumed to be constant. However, oil viscosity depends strongly on temperature. Finally, the porosity of the rock is denoted by ϕ, which is the total fraction of the rock volume available to the fluids, where we take it to be constant by assuming that the rock is homogeneous.

The conservation of mass of the gaseous phase is

$$\frac{\partial}{\partial t}(\phi \rho_g s_g) = -\frac{\partial}{\partial x}(\rho_g v_g) - (\phi \rho_g s_g)(\phi \rho_o s_o) q \,. \tag{3}$$

The conservation of mass of the oleic phase is

$$\frac{\partial}{\partial t}(\phi \rho_o s_o) = -\frac{\partial}{\partial x}(\rho_o v_o) + (\phi \rho_g s_g)(\phi \rho_o) s_o q \,. \tag{4}$$

The total flow of the fluid is given by

$$v = v_g + v_o \,, \tag{5}$$

while the total mobility of the fluid, is

$$\lambda = \lambda_g + \lambda_o \,, \tag{6}$$

and hence

$$v = -K\lambda_g \frac{\partial p_g}{\partial x} - K\lambda_o \frac{\partial p_o}{\partial x} \,. \tag{7}$$

Considering the capillary pressure $p_c(s_o) = p_g - p_o$, with $\frac{\partial p_c}{\partial s_o} < 0$, and Eq. (7), we have

$$\frac{\partial p_g}{\partial x} = f_o \frac{\partial p_c}{\partial x} - \frac{v}{K\lambda} \text{ and } \frac{\partial p_o}{\partial x} = -f_g \frac{\partial p_c}{\partial x} - \frac{v}{K\lambda} \,, \tag{8}$$

where f_j is called the "fractional flow function" of phase $j = g, o$. These functions depend on s_j and θ; they are defined by

$$f_j(s_j, \theta) = \lambda_j(s_j, \theta)/\lambda. \tag{9}$$

Substituting (5)-(9) in (3) and (4), after some manipulations we obtain

$$\frac{\partial}{\partial t}(\phi \rho_g s_g) + \frac{\partial}{\partial x}(\rho_g f_g v) = \frac{\partial}{\partial x}(K \rho_g \lambda_o f_g \frac{\partial p_c}{\partial x}) - (\phi \rho_g s_g)(\phi \rho_o s_o) q \ , \tag{10}$$

$$\frac{\partial}{\partial t}(\phi \rho_o s_o) + \frac{\partial}{\partial x}(\rho_o f_o v) = -\frac{\partial}{\partial x}(K \rho_o \lambda_o f_g \frac{\partial p_c}{\partial x}) + (\phi \rho_g s_g)(\phi \rho_o s_o) q \ . \tag{11}$$

To avoid effects due to volumetric changes, we make the unphysical assumption that the fluid densities are constant and identical ($\rho_g = \rho_o = \rho$). This assumption becomes our analysis easier because the two last equations may be substituted by only one equation, as the following: Eqs. (10) and (11), after to be divided by ρ, are equivalent to the following equations,

$$\frac{\partial}{\partial t}(\phi s_o) + \frac{\partial}{\partial x}(v f_o) = -K \frac{\partial}{\partial x}(\lambda_o f_g \frac{\partial p_c}{\partial x}) + \phi^2 \rho s_g s_o q \ , \tag{12}$$

$$\frac{\partial v}{\partial x} = 0 \ . \tag{13}$$

This last equation shows that $v = v(t)$, which may be given by the boundary condition, and will be assumed to be constant.

Since we are assuming that all generated heat is used to warm the rock, the conservation of energy may be written as

$$\frac{\partial}{\partial t}(\rho_r C_r \theta) = \frac{\partial}{\partial x}\left(\rho_r \kappa_r \frac{\partial \theta}{\partial x}\right) + \phi^2 \rho^2 \Lambda s_g s_o q \ . \tag{14}$$

where C_r, κ_r and Λ, are the heat capacity of the rock at constant pressure, the heat conductivity of the rock, and the energy released by oxidation, respectively. Here, all these quantities are assumed to be constant.

From now on we will substitute s_g by $1 - s_o$. Let us also introduce the positive constants

$$\eta = \frac{\phi^3 \rho^2 \Lambda}{\rho_r C_r}, \quad \gamma = \frac{\phi \kappa_r}{v^2 C_r}, \quad \text{and} \quad \chi = \phi^2 \rho \, , \tag{15}$$

and the nonnegative function

$$h(s,\theta) = -\frac{K}{v^2}\lambda_g f_o \frac{dp_c}{ds}\,, \tag{16}$$

where we use that $\lambda_o f_g = \lambda_g f_o$. In principle, $h(s,\theta)$ vanishes for $s = 0$ and $s = 1$, but to simplify our analysis we consider it as a positive function in $0 \leq s \leq 1,\ \theta \geq 0$.

We will omit the index o in s_o and in f_o. So, the oil saturation will be denoted by s, and the fractional flow function of oil, which depend on s and T, will be denoted by f. To scale out ϕ and v, we can set

$$t = \phi\tilde{t} \quad \text{and} \quad x = v\tilde{x}\,. \tag{17}$$

For simplicity of notation, we drop the tildes, obtaining from (12) and (14), the following system

$$\frac{\partial s}{\partial t} + \frac{\partial f}{\partial x} = \frac{\partial}{\partial x}(h\frac{\partial s}{\partial x}) + \chi(1-s)sq\ , \tag{18}$$

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}(\gamma\frac{\partial \theta}{\partial x}) + \eta(1-s)sq\ . \tag{19}$$

Following standard modeling of two-phase flow in porous media, see [1], we will assume that $f(s,\theta)$ is a nonnegative C^2-function, S-shaped in s for each θ, with $f(0,\theta) \equiv 0$ and $f(1,\theta) \equiv 1$. Also, we assume that $\frac{\partial f}{\partial s}$ vanishes for $s = 0$ and $s = 1$ for each θ, and that $\frac{\partial f}{\partial \theta} > 0$ for $0 < s < 1$.

3 Oxidation traveling waves

Since the effects of capillary pressure and thermal conductivity have been take in account the system (18)-(19) has parabolic terms, characterized by the second derivatives. Thus, it is natural to look for solutions as *traveling waves*, see [11].

Next, the following definition will be needed.

Definition 1 *A state (s,θ) is called non-oxidized if $s < 1$ and $\theta \leq \theta_0$, and it is called oxidized if $s = 1$ and $\theta > \theta_0$, where θ_0 is the temperature where the reaction starts.*

In this model traveling waves must represent oxidation fronts propagating with certain speed, leaving an oxidized state behind, denoted by (s^-,θ^-), which advances into a non-oxidized state ahead, denoted by (s^+,θ^+). In the non-oxidized region the reaction rate q, from Definition 1 vanishes because $\theta \leq \theta_0$. In this case the system (18)-(19) is decoupled. We can first find the temperature by solving the linear heat equation obtained from (19) and then find the saturation by solving the scalar Buckley-Leverett's equation obtained form (18).

In the oxidized region, since $s \equiv 1$ we have that $f \equiv 1$. Thus the source terms in (18)-(19) vanish. In this case the Eq. (18) is trivially satisfied, and (19) becomes a forced linear diffusion equation.

In order to do the analysis of the oxidation fronts it is helpful to write the source terms in (18) and (19) as derivatives. So, we will introduce an auxiliary variable Q defined by

$$Q = Q(x,t) \;=\; \int_x^{\infty} (1-s)\, s\, q\, dx' \,. \tag{20}$$

With this new variable the system (18)-(19) has to be augmented by one equation and may be rewritten as

$$\frac{\partial s}{\partial t} + \frac{\partial f}{\partial x} = \frac{\partial}{\partial x}(h\frac{\partial s}{\partial x}) - \chi\frac{\partial Q}{\partial x}\,, \tag{21}$$

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}(\gamma\frac{\partial \theta}{\partial x}) - \eta\frac{\partial Q}{\partial x}\,, \tag{22}$$

$$\frac{\partial Q}{\partial x} = -\,(1-s)\, s\, q(\theta)\,. \tag{23}$$

From (20), the auxiliary variable value related to a non-oxidized state is given by

$$\lim_{x\to\infty} Q = Q^+ = 0\,, \tag{24}$$

and it related to an oxidized state by

$$\lim_{x\to-\infty} Q = Q^-\,, \tag{25}$$

where we assume that $0 < Q^- < \infty$. In the (s,θ,Q)-space, a non-oxidized state will be denoted by (s^+,θ^+,Q^+), and an oxidized state by (s^-,θ^-,Q^-). We recall that from Definition 1 we have that $s^- = 1$, $s^+ < 1$, $\theta^+ \le \theta_0$ and $\theta^- > \theta_0$, and from (24) $Q^+ = 0$. We will assume that $\theta^+ = \theta_0$.

Definition 2 *Given two arbitrary states $U^+ = (s^+,\theta^+,Q^+)$ and $U^- = (s^-,\theta^-,$ $Q^-)$, a traveling wave solution of system (21) - (23) with propagation speed σ, connecting U^- on the left to U^+ on the right, is a smooth solution $\big(s(\tau),\theta(\tau),$*

$Q(\tau)\big)$ of this system, depending on the single variable $\tau = x - \sigma t$ with $-\infty < \tau < \infty$, such that

$$\lim_{\tau\to-\infty}(s(\tau),\theta(\tau),Q(\tau)) = U^-, \quad \lim_{\tau\to+\infty}(s(\tau),\theta(\tau),Q(\tau)) = U^+, \tag{26}$$

and

$$\lim_{\tau\to-\infty}(\dot{s}(\tau),\dot{\theta}(\tau),\dot{Q}(\tau)) = (0,0,0)\,, \quad \lim_{\tau\to+\infty}(\dot{s}(\tau),\dot{\theta}(\tau),\dot{Q}(\tau)) = (0,0,0)\,. \tag{27}$$

Substituting $s(\tau)$, $\theta(\tau)$ and $Q(\tau)$ in (21)-(23), we can easily prove the following proposition relating traveling waves to solutions of an ordinary differential equations system. We use the notation $f^+ = f(s^+,\theta^+)$ and $f^- = f(s^-,\theta^-)$.

Proposition 1 *Given a non-oxidized state $U^+ = (s^+,\theta^+ = \theta_0, Q^+ = 0)$ and an arbitrary state $U^- = (s^-,\theta^-,Q^-)$, a traveling wave solution of system (21) - (23) with propagation speed σ, connecting U^- on the left to U^+ on the right, is an orbit of the following ordinary differential equations system, satisfying (26) and (27),*

$$\dot{s} = X(s,\,\theta,\,Q) = \sigma(s^+ - s) - (f^+ - f) + \chi Q\,, \tag{28}$$

$$\dot{\theta} = Y(s,\,\theta,\,Q) = \frac{h}{\gamma}\{\sigma(\theta^+ - \theta) + \eta Q\}\,, \tag{29}$$

$$\dot{Q} = Z(s,\,\theta,\,Q) = -h(1-s)sq\,, \tag{30}$$

where γ is the parameter defined in (15) and h is the positive function of s and θ defined in (16).

Also, the speed σ and the states U^+ and U^- are related by the following Rankine-Hugoniot conditions,

$$\sigma(s^+ - s^-) - (f^+ - f^-) + \chi Q^- = 0\,, \tag{31}$$

$$\sigma(\theta^+ - \theta^-) + \eta Q^- = 0\,, \tag{32}$$

$$-(1-s^-)s^- q(\theta^-) = 0\,. \tag{33}$$

Eqs. (31)-(33) are obtained by taking the limit as $\tau \to -\infty$ in (28)-(30), respectively.

Remark 1 *Eqs. (28)-(33) show that the states U^+ and U^- are singular points of the system (28)-(30).*

Remark 2 *If we consider the state $U^- = (s^-,\theta^-,Q^-)$ such that $s^- > 0$ and $\theta^- > \theta_0$, we have $q(\theta^-) > 0$, and from Eq. (33) we have $s^- \equiv 1$. Consequently, in this case, U^- is forced to be an oxidized state.*

4 Heteroclinic orbits

In order to formulate our results, the system (28)-(30) will be considered as depending only on the speed parameter σ. The other parameters γ and χ will be fixed. We rewrite this system as the following one-parameter family of vector fields

$$\Phi_\sigma = X(s,\,\theta,\,Q;\,\sigma)\,\frac{\partial}{\partial s} \;+\; Y(s,\,\theta,\,Q;\,\sigma)\frac{\partial}{\partial \theta} \;+\; Z(s,\,\theta,\,Q;\,\sigma)\frac{\partial}{\partial Q}\,. \tag{34}$$

In this section we consider the non-oxidized state $U^+ = (s^+, \theta^+ = \theta_0, Q^+ = 0)$ as a fixed state with $0 < s^+ < 1$. The problem that we will consider is the following: given a value for the speed σ, we first find all states $U^-(\sigma) = (s^-(\sigma), \theta^-(\sigma), Q^-(\sigma))$ satisfying the Rankine-Hugoniot conditions (31)-(33). Then, we ask if there exist an orbit φ of the system (28)-(30) such that $\omega(\varphi) = U^+$ and $\alpha(\varphi) = U^-(\sigma)$ i. e., if there exist a heteroclinic orbit φ connecting $U^-(\sigma)$ to U^+. Notice from Remark 1 that U^+ and $U^-(\sigma)$ are singular points of this system. Also, from (33) we have $s^-(\sigma) = 1$ or $s^-(\sigma) = 0$ or $\theta^-(\sigma) \le \theta_0$. Since we are looking for oxidation fronts, the case of interest is when $U^-(\sigma)$ is an oxidized state. Therefore, we will consider $s^-(\sigma) = 1$ and $\theta^-(\sigma) > \theta_0$, as in Definition 1.

We will prove the following result.

Theorem 1 *Consider the family of systems of differential equations (28)-(30), or equivalently, the one parameter family of vector fields Φ_σ given by (34). Let σ be such that $\sigma > f_s^+ = \frac{\partial f}{\partial s}(s^+, \theta^+) > 0$. If σ is large enough, then there exists a unique heteroclinic orbit connecting the two singular points $U^- = U^-(\sigma) = (1, \theta^-(\sigma), Q^-(\sigma))$ and $U^+ = (s^+, \theta^+ = \theta_0, 0)$. Here $\theta^-(\sigma) > \theta^+ = \theta_0$ and $Q^- > 0$.*

In what follows we will describe the structure of the singular points of Φ_σ.

Lemma 1 *Assume that $0 < s^+ < 1$. Then the curves $\sigma \to C_0(\sigma) \equiv (0, \theta^-, Q^-)$ and $\sigma \to C_1(\sigma) \equiv (1, \theta^-, Q^-)$, defined by $\Phi_\sigma(C_0(\sigma)) = (0,0,0)$ and $\Phi_\sigma(C_1(\sigma)) = (0,0,0)$, are hyperbolas parametrized by σ as in Fig. 1.*

Proof. From the equation $Z = 0$ it follows that $s = 0$, $s = 1$ or $q(\theta) = 0$. Let us first consider the case, $s = 1$ and $X = Y = 0$. It yields

$$Q = \frac{f^+ - 1}{\chi} + \frac{(1 - s^+)}{\chi}\sigma = Q_1 + v_1\,\sigma\;, \tag{35}$$

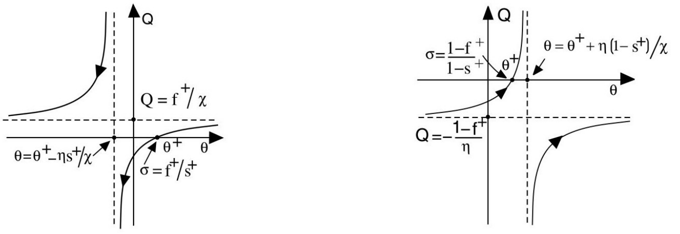

Figure 1: Hyperbolas for $s^- = 0$ and $s^- = 1$.

$$\theta = \theta^+ + \frac{\eta(1-s^+)}{\chi} + \left(\frac{\eta(f^+-1)}{\chi}\right)\frac{1}{\sigma} = \theta_2 + v_2\,\frac{1}{\sigma}\,. \tag{36}$$

Eliminating σ in (35)-(36) we obtain

$$(Q-Q_1)(\theta-\theta_2) = v_2 v_1 = -\,\frac{\eta(1-s^+)(1-f^+)}{\chi^2} < 0,$$

which is clearly a hyperbola with asymptotes $\theta = \theta_2$ and $Q = Q_1$.

In the same way the equations $s = 0$ and $X = Y = 0$ implies that

$$Q = \frac{f^+}{\chi} - \frac{s^+}{\chi}\sigma = Q_3 + v_3\,\sigma\,, \tag{37}$$

$$\theta = \theta^+ - \frac{\eta s^+}{\chi} + \left(\frac{\eta f^+}{\chi}\right)\frac{1}{\sigma} = \theta_4 + v_4\,\frac{1}{\sigma}\,. \tag{38}$$

Therefore,

$$(Q-Q_3)(\theta-\theta_4) = v_3 v_4 = -\frac{\eta s^+ f^+}{\chi^2} < 0\,.$$

The parametric form of the two branches of the hyperbola, in each case, follows from (35)-(36) and (37)-(38), respectively. □

Remark 3 *Lemma 1 shows that for each $\sigma \in \mathbb{R}$, $\sigma \neq 0$, the vector field Φ_σ has only one equilibrium point on the plane $s = 0$ and only one equilibrium on the plane $s = 1$.*

Remark 4 *When $\sigma \to \infty$ we easily have the following limits along curve C_1, $Q^-(\sigma) \to \infty$ and $\theta^-(\sigma) \to \theta^+ + \eta(1-s^+)/\chi$; along curve C_0 we have $\theta^-(\sigma) \to \theta^+ - \eta s^+/\chi$.*

In order to understand the structure of the singular point $U^+ = (s^+, \theta^+, 0)$, which is an equilibrium of Φ_σ for all $\sigma \in \mathbb{R}$, we consider the function

$$F(s, \theta, Q) = (f - f^+ + \chi Q)(\theta^+ - \theta) - \eta Q(s^+ - s)$$

obtained from the elimination of σ in the equations $X = 0$ and $Y = 0$ in (28)-(29).

Lemma 2 *The set $S = \{(s, \theta, Q) \mid F(s, \theta, Q) = 0\}$ is a regular surface away from the point U^+. It contains the curves C_0 and C_1 as described in Lemma 1. The topological structure of S near U^+ is of an index-2 Morse singular point (cone).*

Proof. A direct calculation at the point $(s^+, \theta^+, 0)$ gives $F = \dfrac{\partial F}{\partial s} = \dfrac{\partial F}{\partial \theta} = \dfrac{\partial F}{\partial Q} = 0$. Also,

$$Hessian(F, (s^+, \theta^+, 0)) = \begin{pmatrix} 0 & -f_s^+ & \eta \\ -f_s^+ & -2f_\theta^+ & -\chi \\ \eta & -\chi & 0 \end{pmatrix}, \tag{39}$$

where $f_s^+ = \frac{\partial f}{\partial s}(s^+, \theta^+) > 0$ and $f_\theta^+ = \frac{\partial f}{\partial \theta}(s^+, \theta^+) > 0$, as stated in the last paragraph of Section 2.

The three real eigenvalues λ_1, λ_2 and λ_3 of Hessian$(F, (s^+, \theta^+, 0))$ satisfy the following relationships:

$$\lambda_1 \lambda_2 \lambda_3 = 2f_s^+ \eta \chi + 2 f_\theta \eta^2 > 0$$
$$\lambda_1 + \lambda_2 + \lambda_3 = -2f_\theta^+ < 0\,.$$

Therefore, two eigenvalues are negative and one is positive. By Morse Lemma it follows that, locally, $F^{-1}(0)$ has the topological structure of a cone. By Lemma 1, $C_0\,, C_1 \subset F^{-1}(0)$. □

Lemma 3 *Assume that $\sigma > f_s^+$. Then the singular point $U^+ = (s^+, \theta^+ = \theta_0, Q^+ = 0)$, with $0 < s^+ < 1$, is not an isolated singular point of Φ_σ. More precisely, $U^+ \in S_\sigma = \{(s, \theta, Q) \mid \sigma = \frac{f^+ - f - \chi Q}{s^+ - s} = \frac{\eta Q}{\theta - \theta^+},\ \theta \leq \theta^+\ \}$ where S_σ is a regular curve ending at U^+; the tangent space at U^+ is given by the vector*

$$v_\sigma = (f_\theta^+ \eta + \chi \sigma,\ \eta(\sigma - f_s^+),\ \sigma(\sigma - f_s^+))^T\,. \tag{40}$$

Proof. The singular points of Φ_σ are defined by the equation $X = Y = Z = 0$. As $0 < s^+ < 1$ it follows that $Z = 0$ if and only if $q(\theta) = 0$. So $\theta \leq \theta^+ = \theta_0$. Therefore, $S_\sigma = \{(s, \theta, Q) \mid X = Y = 0 \text{ and } \theta \leq \theta^+ = \theta_0\}$. Direct calculations give $v_\sigma = \nabla X \wedge \nabla Y$. □

Proposition 2 *Suppose $\sigma > f_s^+$, with $0 < s^+ < 1$. Then the line of singularities S_σ is normally hyperbolic(attracting). The stable manifold of $U^+, W^S(U^+, \Phi_\sigma)$ is a regular surface tangent to the $s\theta$-plane at U^+. The center manifold of $U^+, W^c(U^+, \Phi_\sigma)$ is one-dimensional and tangent to v_σ at U^+. The phase portrait of Φ_σ near U^+ is sketched in Fig. 2.*

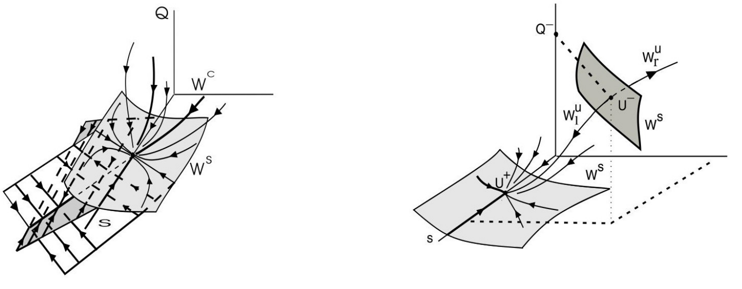

Figure 2: Singular line ending at U^+. Stable manifold at U^+ and unstable manifold at U^-.

Proof. At the point $U^+ = (s^+, \theta^+, 0)$,

$$D\Phi_\sigma(U^+) = \begin{pmatrix} -\sigma + f_s^+ & f_\theta^+ & \chi \\ 0 & -\frac{\sigma h^+}{\gamma} & \frac{\eta h^+}{\gamma} \\ 0 & 0 & 0 \end{pmatrix}, \tag{41}$$

where $f_s^+ = f_s(s^+, \theta^+)$, $f_\theta^+ = f_\theta(s^+, \theta^+)$ and $h^+ = h(s^+, \theta^+)$.

The eigenvalues of $D\Phi_\sigma(U^+)$ are given by

$$\lambda_1 = -\sigma + f_s^+ < 0, \qquad \lambda_2 = -\frac{\sigma h^+}{\gamma} < 0 \qquad \text{and} \qquad \lambda_3 = 0.$$

The corresponding eigenvectors are $v_1 = (1, 0, 0)^T$, $v_2 = (f_\theta^+, \sigma - f_s^+ - \frac{\sigma h^+}{\gamma}, 0)^T$ and v_σ given in (40).

Therefore, by Invariant Manifold Theory, see [5] and [7], it follows that there exists an invariant surface (stable manifold $W^s(U^+, \Phi_\sigma)$) tangent to the eigenspace spanned by $\{v_1, v_2\}$ and a center manifold, $W^c(U^+, \Phi_\sigma)$, tangent to v_σ at U^+. Also, by continuity and Invariant Manifold Theory, it follows that S_σ is a normally (attracting) hyperbolic set with splitting defined by the eigenvectors of $D\Phi_\sigma(S_\sigma)$. As $\dot{Q} < 0$ it follows that the local region above $W^s(U^+, \Phi_\sigma)$ lies in the attracting basin of U^+. □

Proposition 3 *Suppose* $0 < s^+ < 1$ *and* $\sigma > 0$. *Then the singular point* $U^- = (1,\, \theta^-(\sigma),\, Q^-(\sigma))$ *is a hyperbolic singular point of* Φ_σ *with dim*$(W^s(U^-, \Phi_\sigma)) = 2$ *and dim*$(W^u(U^-, \Phi_\sigma)) = 1$. *The tangent space to the unstable manifold* $W^u(U^-, \Phi_\sigma)$ *is generated by a vector* v, *where* v *is a negative vector, i.e., the three components of* v *are negative. See Fig. 2.*

Proof. Recall that at U^-, we have $\theta^- > \theta^+ = \theta_0$ and so $q(\theta^-) > 0$. Also,

$$D\Phi_\sigma(U^-) = \begin{pmatrix} -\sigma & 0 & \chi \\ 0 & -\frac{\sigma h^-}{\gamma} & \frac{h^-\eta}{\gamma} \\ h^-q^- & 0 & 0 \end{pmatrix},$$

where $h^- = h(s^-, \theta^-)$ and $q^- = q(\theta^-)$.

The eigenvalues of $D\Phi_\sigma(U^-)$ are given by the equation

$$(-\frac{\sigma h^-}{\gamma} - \lambda)(\lambda^2 + \sigma\lambda - \chi h^- q^-) = 0.$$

Therefore, the eigenvalues of $D\Phi_\sigma(U^-)$ are

$$\begin{aligned} \lambda_1 &= -\frac{\sigma h^-}{\gamma} < 0, \\ \lambda_2 &= \frac{-\sigma - \sqrt{\sigma^2 + 4\chi h^- q^-}}{2} < 0, \\ \lambda_3 &= \frac{-\sigma + \sqrt{\sigma^2 + 4\chi h^- q^-}}{2} > 0. \end{aligned}$$

The corresponding eigenvectors are

$$\begin{aligned} v_1 &= (0, 1, 0)^T, \\ v_2 &= (\chi\gamma(\lambda_1 - \lambda_2),\, -\eta h^-(\sigma + \lambda_2),\, \gamma(\sigma + \lambda_2)(\lambda_1 - \lambda_2))^T, \\ v_3 &= (\chi\gamma(\lambda_1 - \lambda_3),\, -\eta h^-(\sigma + \lambda_3),\, \gamma(\sigma + \lambda_3)(\lambda_1 - \lambda_3))^T. \end{aligned}$$

Direct calculations show that all components of v_3 are negative. □

Proposition 4 *Suppose* $0 < s^+ < 1$ *and* $\sigma > f_s^+$ *is large enough. Then a branch of* $W^u(\Phi_\sigma, U^-)$*, where* $U^- = (1, \theta^-, Q^-)$*, is contained in the region defined by* $R = \{(s, \theta, Q) \mid X(s, \theta, Q) < 0,\ Y(s, \theta, Q) < 0\}$*. Moreover, if* σ *is large enough then a branch of* $W^u(\Phi_\sigma, U^-)$ *is above* $W^s(\Phi_\sigma, U^+)$*.*

Proof. By Proposition 3, $W^u(\Phi_\sigma, U^-)$ is spanned by the negative vector $v_3 = (\chi\gamma(\lambda_1 - \lambda_3), -\eta h^-(\sigma + \lambda_3), \gamma(\sigma + \lambda_3)(\lambda_1 - \lambda_3))^T$. Consider the surfaces $S_2 = \{(s, \theta, Q) : X(s, \theta, Q) = 0\}$ and $\Sigma = \{(s, \theta, Q) :\ Y(s, \theta, Q) = -\sigma\theta + \eta Q = 0\}$, see Fig. 3. The vector field $\Phi_\sigma = (X, Y, Z)$ is transversal to both surfaces and $Z|_{S_2} < 0$ and $Z|_\Sigma < 0$, except in the singularities of this vector field. So, the region $R_\sigma = \{(s, \theta, Q) : X(s, \theta, Q, \sigma) < 0, Y(s, \theta, Q, \sigma) < 0\}$ is an invariant region for the flow of Φ_σ.

We have that $\nabla X = (f_s - \sigma,\ f_\theta,\ \chi)$ and $\nabla Y = \frac{h}{\gamma}(0, -\sigma, \eta)$. At $U^- \in S_2 \cap \Sigma$ it follows that $< \nabla X,\ v_3 >= \chi\gamma(\lambda_1 - \lambda_3)(\lambda_3) < 0$ and $< \nabla Y,\ v_3 >= -\eta(\sigma + \lambda_3)\lambda_3 h^- < 0$. Therefore, as $T_{U^-} W^u(\Phi_\sigma, U^-) = v_3$, a branch of $W^u(\Phi_\sigma, U^-)$ is contained in the invariant region R_σ. The portion of this region inside of the parallelepiped $0 \le s \le 1$, $\theta^+ \le \theta \le \theta^-$, $0 \le Q \le Q^-$ is shown in Fig. 3.

Now, consider the vector field $\Psi_{\frac{1}{\sigma}} = \frac{1}{\sigma}\Phi_\sigma$. For all $\sigma \neq 0$, $\Psi_{\frac{1}{\sigma}}$ and Φ_σ have the same orbits with the same orientation when $\sigma > 0$. Letting $\sigma \to \infty$, we have that $\Psi_0 = \lim_{\sigma\to\infty} \Psi_{\frac{1}{\sigma}}$ is given by $\Psi_0 = (s^+ - s)\frac{\partial}{\partial s} + \frac{h}{\gamma}(\theta^+ - \theta)\frac{\partial}{\partial \theta} + 0\frac{\partial}{\partial Q}$.

For the vector field Ψ_0 the $s\theta$-plane is invariant and $W^s(U^+, \Psi_0) = \mathbb{R}^2$. In fact, $U^+ = (s^+, \theta^+, 0)$ is the unique singular point of $\Psi_{0|_{Q=0}}$ and $V(s, \theta) = (s - s^+)^2 + (\theta - \theta^+)^2$ is a Liapunov function for the vector field $\Psi_{0|_{Q=0}}$, [10].

By the continuity of the stable manifold it follows, for σ large enough, that $W^s(\Phi_\sigma, U^+) = W^s(\Psi_{\frac{1}{\sigma}}, U^+)$ is close to $W^s(\Psi_0, U^+)$ in any compact region of the $s\theta$-plane.

In fact, for any $\rho > 0$, the invariant surface $W^s(\Phi_\sigma, U^+)$ is a graph over the ball $B_\rho(U^+) = \{(s, \theta, 0) : s^2 + \theta^2 \le \rho^2\} \subset \mathbb{R}^2 \times \{0\}$ and

$$W^s(\Phi_\sigma, U^+) \cap \{(s, \theta, Q) : s^2 + \theta^2 \le \rho^2\}$$

is C^1- close to $B_\rho(U^+)$ for $\sigma > 0$ large enough and any $\rho > 0$.

Now, as $W^s(\Phi_\sigma, U^+)$ is an invariant set it follows that

$$\{(s, \theta, Q) : d((s, \theta, Q), W^s(\Phi_\sigma, U^+)) > 0\} \cap R_\sigma$$

is an invariant region for Φ_σ for all σ large enough. Here $d(.,.)$ means a distance with signal, positive if (s, θ, Q) is above $W^s(\Phi_\sigma, U^+)$ and negative otherwise.

Therefore, for $\sigma > 0$ large enough and taking $\rho > 2\theta^-(\sigma) = 2[\theta_2 + v_2 \frac{1}{\sigma}]$, see Eq.(36) and Remark 4, it follows that $W_l^u(U^-, \Phi_\sigma)$ lies in

$$\{(s, \theta, Q) : d((s, \theta, Q), W^s(\Phi_\sigma, U^+)) > 0\} \cap R_\sigma.$$

As $(1, \theta^-, 0) \in B_\rho(U^+)$ and $U^- = (1, \theta^-, Q^-)$ is above $W^s(\Phi_\sigma, U^+)$ it follows that $W_l^u(U^-, \Phi_\sigma) \subset R_\sigma$ is above $W^s(\Phi_\sigma, U^+)$. This ends the proof. $\square$

Proof of Theorem 1. Consider $\sigma > 0$ large enough. According to Proposition 4, the left branch of $W^u(\Phi_\sigma, U^-)$ (see Fig. 2), denoted by $W_l^u(\Phi_\sigma, U^-)$, is contained in the invariant region R_σ, exhibited in Fig. 3, and the curve $W_l^u(\Phi_\sigma, U^-)$ lies above the surface $W^s(\Phi_\sigma, U^+)$. Thus, it follows that the ω-limit set of the orbit $W_l^u(\Phi_\sigma, U^-)$ is the singular point U^+. This ends the proof of Theorem 1. $\square$

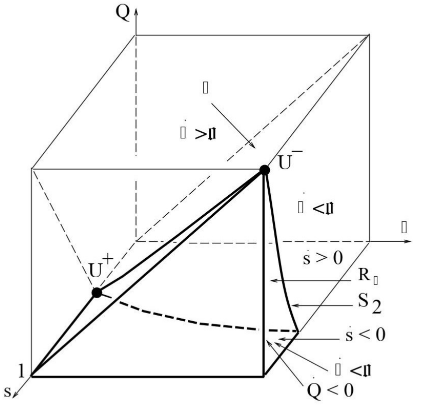

Figure 3: Surface S_2 where $\dot{s} = 0$ and Σ where $\dot{\theta} = 0$. Portion of the region R_σ inside of the parallelepiped $0 \le s \le 1$, $\theta^+ \le \theta \le \theta^-$, $0 \le Q \le Q^-$.

5 Discussion

In this work we used methods of qualitative theory of ordinary differential equation applied to a mathematical model of partial differential equation describing an oxidation process in petroleum reservoirs, and we find oxidation fronts as heteroclinic connections in the ordinary differential equation. For other mathematical models and applications, see [3], [6], [8], [9] and [11].

A problem left is to show that if

$$\sigma > f_s^+ = \frac{\partial f}{\partial s}(s^+, \theta^+) > 0,$$

then there exists a heteroclinic connection as stated in the Theorem 1. This problem is suggested by numerical evidence.

The model considered is oversimplified because we consider that all heat generated by combustion is used to warm the rock, and that the carbon dioxide generated dissolves immediately into the oil phase. We also consider that densities of oil and gas are equal. If we do not make these simplifications, the system (18)-(19) has to be augmented by one or two equations, and it becomes more difficult to apply the qualitative theory. This work is a first step in finding oxidation fronts in a more realistic model.

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