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Multicomponent effects in liquid–gas filtration combustion

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ABSTRACT

This paper develops the theory of liquid–gas filtration combustion, when an oxidizer (air) is injected into porous rock containing two-component liquid fuel. We found a qualitatively new combustion mechanism controlled by the successive vaporization and condensation of the liquid phase sustained by the reaction. Motivated by the problem of recovery of light oil by air injection, as an enhanced oil recovery method, we consider a liquid composed of light and medium pseudo-components. The light part is allowed to oxidize and vaporize, while the medium part is non-volatile and only oxidizes. The liquid mobility depends strongly on its composition, with a small viscosity (high mobility) of the purely light component and a high viscosity for the purely medium (immobile) component. We show that the combined vaporization and condensation in the combustion wave leads to accumulation of the light component in the upstream part of the wave, considerably increasing mobility and, therefore, playing a crucial role in the mechanism of the combustion process. We describe physical implications of this effect, as well as its importance for applications. The results are confirmed by numerical simulations.

1. Introduction

Filtration combustion, when an oxidizer is injected into a porous medium containing fuel, has numerous applications in technology and nature (enhanced oil recovery by in situ combustion, coal gasification, self-propagating high-temperature synthesis, smolder waves etc.). A large number of theoretical studies in this area consider solid (immobile) fuels [1,2]. Then the combustion process can be described using a single-phase flow model for an oxidizer. Examples of such studies are forced forward smoldering [3], downward buoyant filtration combustion [4] and the advance of in-situ combustion fronts in porous media [5]. These models can be extended to study the effects of gas–solid non-equilibrium in filtration combustion [6] and the transition from smoldering to flaming regimes [7], for example. When the fuel is a liquid with a relatively low viscosity and boiling temperature, the two-phase flow model becomes essential. In this case, combustion process couples both to the multi-phase flow and to the phase transition mechanism, increasing the complexity of the problem. Recent theoretical [8,9], numerical [10] and experimental [11] advances in this problem showed the fundamental difference of the combustion process with liquid fuels, compared to the classical filtration combustion for solid fuels. In this paper, our goal is to deepen the understanding of this process by considering multicomponent liquid fuels. We show that the presence of multiple components in a liquid fuel with different physical properties has a dramatic effect on the internal structure of the combustion wave, manifesting itself in a highly counterintuitive way.

The model considered in this work is motivated by the petroleum engineering applications, where in situ combustion is considered as a technique for enhancing the recovery rate due to a lowering of the oil viscosity thus increasing its mobility [12–14]. This technique is usually applied for heavy oils. However, due to thermal expansion and gas drive promoted by the oxidation reaction and vaporization, it can improve the recovery of light oils [15–17]. When air is injected into the reservoir at medium pressures (10–90 bar), the oxidation mechanism is fundamentally different for light and heavy oils. The heavy oil undergoes cracking, due to the increase in temperature, which generates coke deposited on the rock surface. This coke reacts with the injected oxygen, leading to the formation of a high-temperature oxidation (HTO) wave that propagates in the reservoir [5,18]. On the other hand, the oxidation of light oil leads to the scission of liquid molecules, generating a gaseous product. In this case, the temperature is bounded by the boiling point of the oleic phase, such that it does not get large. This is termed the medium-temperature oxidation (MTO) mechanism and recent experiments support the

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Nomenclature

A_{rl}, A_{rm}	frequency factors for light (l) and medium (m) component reactions (1/s)
c_g	heat capacity of gas (J/mol K)
C_m, C_o	heat capacities of rock and oil (J/m^3 K)
f_o, f_g	oil and gas fractional flow functions
k_o, k_g	oil and gas relative permeabilities (m^2)
n	reaction order
P	prevailing gas pressure (Pa)
P_{atm}	atmospheric pressure (Pa)
Q_{rl}, Q_{rm}	enthalpies of light and medium component reactions per mole of oxygen (J/mol)
Q_v	light component vaporization heat (J/mol)
R	ideal gas constant (J/mol K)
s_o, s_g	oil and gas saturations
t	time (s)
T	temperature (K)
T_b	light component boiling temperature (K)
T_{bn}	boiling temperature at P_{atm} (K)
T_{ini}	initial temperature (K)
T_l^{ac}, T_m^{ac}	activation temperatures for reactions of light and medium components (K)
u_o, u_g, u	oil, gas and total Darcy velocities (m/s)
u_{gl}, u_{gk}, u_{gr}	Darcy velocities of light (l), oxygen (k) and remaining (r) gas components (m/s)
u_{ol}, u_{om}	Darcy velocities of light and medium component (m/s)
u_{inj}	air injection Darcy velocity (m/s)
W_v	vaporization rate (mol/m^3 s)
W_{rl}, W_{rm}	reaction rates of light and medium components (mol/m^3 s)
X_l, X_m	volumetric fractions in oleic phase
X_m^{ini}	medium component fraction in initial oil
x	spatial coordinate (m)
Y_l, Y_k, Y_r	molar fractions in gas phase (mol/mol)
Y_k^{inj}	oxygen fraction in injected gas
λ	thermal conductivity of porous rock (W/m K)
μ_o, μ_g	viscosities of oil and gas (Pa s)
μ_l, μ_m	viscosities of purely light and purely medium oleic phases (Pa s)
ν_{ol}, ν_{gl}, ν_{om}, ν_{gm}	stoichiometric coefficients for light and medium component reactions
ρ_o, ρ_g	molar densities of oil and gas (mol/m^3)
ρ_l, ρ_m	molar densities of purely light and purely medium oleic phases (mol/m^3)
φ	rock porosity

existence of reaction occurring at low temperatures [11]. Pascual et al. [19] performed a high pressure tube test using light crude oil to simulate the LTO process, with a stable reaction front at a temperature of 250 °C. They showed that reservoir oil had excellent burning characteristics, which made the process technically feasible. When thermal losses through the rock are high, or if the heat released by the reaction is not sufficient to increase the temperature significantly, the oxidation reaction occurs not far from the initial reservoir temperature [20]. In this case, oxidation is slow and can be incomplete, and oxygen consumption occurs in a larger reservoir zone [21].

The MTO process for light oil requires the two-phase (liquid–gas) flow model. The combustion (MTO) wave was analyzed theoretically [8,9] for a simplified two-phase model with one pseudo-component oil (single component liquid fuel) and the solution to this problem was obtained as a series of traveling waves. Inside the combustion wave the reaction region separates the vaporization zone upstream and the condensation zone downstream. Note that the position of the vaporization zone in the upstream part of the combustion wave is opposite to the HTO process, where it travels on the downstream side [18]. The speed of the wave was shown to be equal to the Buckley–Leverett characteristic speed evaluated at a point separating the vaporization and condensation regions (called a resonance condition), and this condition allowed determining all macroscopic parameters of the combustion wave. The MTO process within a two-component oil model was studied in [22] by numerical simulations, where an oleic mixture composed of light (low viscosity) and medium (high viscosity) fractions was considered. The light component was allowed to vaporize and oxidize, while the medium non-volatile component only oxidized. Numerical simulations showed that the light component has a tendency to accumulate in the upstream part of the combustion wave despite of vaporization and the much higher mobility, indicating the importance of multicomponent considerations. However, for mixtures composed predominately of a medium non-volatile fraction, the transient behavior featuring the HTO process was reported.

In the present work we provide the analytical theory for liquid–gas filtration combustion with a two-component oil as a liquid fuel. In our formulation, following the model of [22], we consider a two-component oil mixture, consisting of light and medium pseudo-components, where the medium component is non-volatile and immobile. The latter property is represented by the liquid mobility depending on the composition, which is high for a purely light oil and vanishes for purely medium oil. Such model is the simplest possible that considers multicomponent effects and it mimics a wide variety of oil types from very light to very heavy ones. The result of this paper is the detailed study of the combustion wave profile providing analytic formulas describing its macroscopic properties: limiting states and speed. We show that, due to the phase transition mechanism, the medium component is almost completely expelled from the reaction region to the downstream side of the wave and, thus, it does not react. This important property, which is valid for any initial oil composition cannot be captured with one pseudo-component models, e.g., [8,9]. Furthermore, the described effect is very counterintuitive: the medium component decreases the oil mobility and, thus, would be expected to accumulate on the opposite upstream side. The consequences are dramatic: the combustion wave speed turns out to be independent on the initial oil composition even if the medium component dominates in the initial oil. For such heavy initial mixtures, the coupled reaction/flow/phase-transition mechanism in the combustion wave yields a strong increase of gas drive and provides high downstream oil saturations, both favorable for oil recovery applications. Finally, we perform numerical simulations supporting our theoretical conclusions.

2. Two pseudo-component oil model

We study a combustion front in two-phase flow in which a gaseous oxidizer (air) is injected into a porous rock filled with oil composed of a light and a medium fraction. The light oil (volatile component) can both vaporize and oxidize, whereas the medium oil (non-volatile component) can only oxidize. In our applications we disregard gaseous phase reactions, as annihilation of free radicals at pore walls reduces drastically the corresponding reaction rates [23]. We summarize the reaction process of liquid components in the following reaction equations:

$$\nu_{ol}(\text{light component}) + O_2 \rightarrow \nu_{gl}(\text{gaseous products}),$$
$$\nu_{om}(\text{medium component}) + O_2 \rightarrow \nu_{gm}(\text{gaseous products}), \quad (2.1)$$