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# The oxidation of heavy oil to enhance oil recovery: The numerical model and the criteria to describe the low and high temperature oxidation

Yue Chu [a], Cheng Fan [a], Qiang Zhang [a,*], Cheng Zan [b], Desheng Ma [b], Hang Jiang [b], Yao Wang [a], Fei Wei [a]

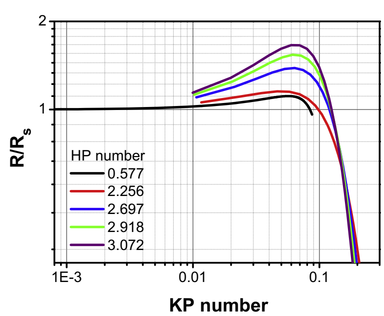
[a] Beijing Key Laboratory of Green Chemical Reaction Engineering and Technology, Department of Chemical Engineering, Tsinghua University, Beijing 100084, China
[b] State Key Laboratory of Enhanced Oil Recovery, Research Institute of Petroleum Exploration & Development, China National Petroleum Corporation, Beijing 100007, China

## HIGHLIGHTS

- A model to describe the temperature distribution of heavy oil oxidation.
- The high- and low-temperature oxidation processes.
- KP and HP factors are proposed to describe the oxidation reaction strength.

## GRAPHICAL ABSTRACT

A mathematical model to describe the temperature distribution during the oxidation of heavy oil. Both KP and HP factors are proposed as the criteria to determine the strength of the oxidation reactions.

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## ABSTRACT

The *in situ* oxidation of heavy oil brings exothermic reaction between the hydrocarbon and the oxygen, which renders advantages in high efficiency in heat utilization and displacement for oil recovery. The simulation of oxidation is very convenient to investigate the influence of operation parameters and reflect the dynamic response. In this contribution, a mathematical model to simulate the temperature distribution during the oxidation of heavy oil with the injection wells and the production wells arranged in the hexagonal pattern was developed. The effects of convection, diffusion, oxidation reaction, and coking were considered. The temperature distributions in the high- and low-temperature oxidation processes were simulated. The results exhibited that the modeling domain can be heated by both processes. The significant change in the kinetic parameters of oxidation and coking with temperature induced the different oxidation behaviors between the high- and low-temperature oxidation processes. Two dimensionless parameters, KP and HP factor, were proposed based on the simulation results as the criteria to determine the strength of the oxidation reactions in the enhanced oil recovery process.



## 1. Introduction

Heavy oil which possesses high content of asphaltene and high viscosity is an important feedstock the resources of which are nearly three times those of the conventional oil [1,2]. Nowadays, more and more attention has been paid on the recovery of heavy oil as the conventional reserves decline significantly. The cost-effective production and processing of heavy oil remains to be a much sought after prize [3].

The recovery of the heavy oil is a complex process because of the high viscosity, high density, and low fluidity properties [4–6].

* Corresponding author. Tel.: +86 10 6278 9041; fax: +86 10 6277 2051.
*E-mail address:* zhang-qiang@mails.tsinghua.edu.cn (Q. Zhang).

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**Nomenclature**

| | |
|---|---|
| $A$ | pre-exponential factor in the oxidation reaction, $s^{-1}$ |
| $A_c$ | pre exponential factor in the coking reaction, $h^{-1}$ |
| $c$ | oxygen concentration, mol $m^{-3}$ |
| $c_g$ | heat capacity of gas, J $kg^{-1}$ $K^{-1}$ |
| $c_s$ | heat capacity of solid, J $kg^{-1}$ $K^{-1}$ |
| $c_{coke}$ | weight percentage of produced coke, 1 |
| $c_{oil}$ | weight percentage of heavy oil, 1 |
| $c_s$ | oxygen concentration in the injection well, mol $m^{-3}$ |
| $D$ | effective diffusion coefficient, $m^2$ $s^{-1}$ |
| $d_e$ | diameter of rock particles, m |
| $E$ | activation energy in the oxidation reaction, J $mol^{-1}$ |
| $E_c$ | activation energy in the coking reaction, J $mol^{-1}$ |
| $F$ | mass generated by the oxidation reaction, kg $m^{-3}$ $s^{-1}$ |
| $k$ | oxidation reaction rate constant, $s^{-1}$ |
| $L$ | distance from the injection well, m |
| $M_c$ | molar weight of carbon, kg $mol^{-1}$ |
| $m$ | mass of the heavy oil in the TG, kg |
| $N$ | molar flux of oxygen in the TG, mol $s^{-1}$ |
| $P_0$ | initial pressure in the reservoir, Pa |
| $P_{IW}$ | pressure of the injection well, Pa |
| $P_{EW}$ | pressure of the production well, Pa |
| $P_{TG}$ | pressure in the TG reactor, Pa |
| $Q$ | heat generated by the oxidation reaction, J $m^{-3}$ $s^{-1}$ |
| $R$ | rate of oxidation reaction, mol $m^{-3}$ $s^{-1}$ |
| $T_0$ | initial temperature in the reservoir, K |
| $T_{TG}$ | temperature in the TG reactor, K |
| $T_s$ | ignition temperature, K |
| $u$ | gas velocity, m $s^{-1}$ |

*Greek letters*

| | |
|---|---|
| $\beta$ | HP dimensionless number, dimensionless |
| $\varepsilon$ | porosity of the reservoir, dimensionless |
| $\eta$ | viscosity of the gas phase, Pa s |
| $\kappa$ | gas permeability, $m^2$ |
| $\lambda$ | thermal conductivity, W $m^{-1}$ $K^{-1}$ |
| $\rho_s$ | density of the rocks, kg $m^{-3}$ |
| $\rho_g$ | density of the gas, kg $m^{-3}$ |
| $\varphi$ | KP dimensionless number, dimensionless |
| $\Delta P$ | pressure drop between the injection and producing wells, Pa |
| $\Delta H$ | molar reaction heat, J $mol^{-1}$ |

The thermal enhanced oil recovery is proposed based on the characterization of the heavy oil that the oil viscosity can be reduced by several orders of magnitude through the increase of temperature [7]. Based on the mechanism of energy generated, the thermal enhanced oil recovery (EOR) falls into two types: for the former, like steam huff and puff process, the thermal energy at ground is transported into the reservoir to improve its fluidity; in the latter process, oxidative gas is injected into the reservoir and the heat is *in situ* generated by the exothermic reactions between the hydrocarbon and the oxygen (such as the *in situ* combustion) [8–11]. The latter process brings many advantages such as a high efficiency in heat utilization, highly efficient displacement drive mechanism, and less total environmental impact [7].

The oxidation reactions of hydrocarbon were classified as high temperature oxidation (HTO) that occurs at temperatures above 350 °C and low temperature oxidation (LTO) that corresponds to temperatures lower than 350 °C [12]. In the HTO process, the heavy oil is fired, in which the carbon–hydrogen bonds are broken and water and carbon dioxide were produced [13], therefore, continuous combustion is guaranteed, the huge amount of heat release during the underground combustion facilitates the temperature of the reservoir higher than 600 °C. While in the LTO process, it is believed that LTO reactions produce oxygenated hydrocarbons such as carboxylic acids and sulfones with negligible amounts of carbon oxides [14–16]. Although the reaction mechanism is very complex [17], the released reaction heat is beneficial to increase the temperature of reservoir, therefore, the temperature of the whole reservoir is controlled to be lower than the ignition point of heavy oil to thermally reduce the viscosity of the heavy oil to a required level and simultaneously avoid coke generation at high temperature. The LTO process renders advantages on the high efficiency of energy utilization [1,18]. Both the HTO and LTO are very important since their products play a significant role with respect to the sustainability of the combustion process. The use of heterogeneous catalysts is a promising way to mediate the reaction pathway and related characters [13,19]. In most cases, the temperature is a very important index to describe the HTO and LTO with different reaction mechanisms. However, the synergy between the reaction and transport phenomena is not well illustrated yet. If the important parameters in the EOR process are integrated to dimensionless number, the correlation between the strength of the oxidation reaction and the dimensionless number is anticipated to serve as the guidance for choosing rational operation region.

Attributed from the numerous operation parameters and the complex conditions in the heavy oil reservoir, the physical and mathematical simulation becomes necessary before experiments in the field [16,20–24]. The mathematical simulation is widely investigated because of its convenience in studying the influence of operation parameters and reflecting the dynamic response [15,19,22,25–29]. In this work, a mathematical model to describe the EOR process is developed. The conservation of momentum, mass, and energy is considered. The kinetic sub-model is set up based on the characterization of the heavy oil using thermal gravimetric analysis (TGA) with differential scanning calorimeter (DSC). The temperature distribution in the modeling domain is investigated both in HTO and LTO processes. The similarities and differences in the temperature distribution in the two processes are explored. The KP and HP Number are proposed as the dimensionless numbers to describe the oxidation behavior.

## 2. Mathematical model and numerical simulations

Air was employed as the oxidizing gas to improve oil recovery in the thermal enhanced oil recovery. The injection wells and the production wells are usually located in a meshwork [18,30,31]. Herein wells with hexagonal shaped arrangement are modeled based on the laboratory scale experiment. The six injection wells are located on the points with one producing well in the center as shown in Fig. 1a. The modeling domain is reduced to a 2D geometry (Fig. 1b) only considering the horizontal temperature, concentration, and velocity distribution. The wells are separated from the surrounded rocks by an outside boundary $\Gamma_D$. Circle boundary is used to guarantee that the same distances between the injections wells and the outside boundary. The distance between the injection wells ($\Gamma_{IW}$) and the production wells ($\Gamma_{EW}$) is 1.0 m. The outside boundary ($\Gamma_D$) is 0.5 m away from the injection wells.