



## Full Length Article

# Temperature prediction via reaction heat calculation of burned pseudo-components during in-situ combustion



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## ABSTRACT

This work proposes a novel method of temperature prediction during heavy oil in-situ combustion according to the fuel availability (FA) of true boiling point fractions, which is also called pseudo-components. Six kinds of *n*-alkanes with different carbon number and three crude oil samples from Karamay oil field were used and each oil sample was chosen to get seven true boiling point (TBP) fractions respectively. Kinetic cell experiment with ramped temperature oxidation (RTO) was conducted on each *n*-alkane and pseudo-component to get the total mole amount of CO and CO<sub>2</sub>. Combustion tube (CT) experiment was performed to obtain the deviation between the calculated value and measured result, which can be used to validate the accuracy of the new method. The results revealed that the FA of *n*-alkanes presented linear relationship to the carbon number and the average carbon number for different pseudo-components as well as heavy crude oil could be figured out based on this standard curve. Then the reaction heat for pseudo-components and the whole oil could be calculated and used to predict the temperature of fire front in CT experiment. There is a deviation below 50 °C between the calculation and the thermocouples measurement during the CT experiment, which can be acceptable in reservoir temperature prediction.

## 1. Introduction

In-situ combustion (ISC) is considered as a great potential EOR technique for heavy oil recovery. During ISC, a huge temperature drop appears between the fire front to all parts of the reservoir not yet reached by the heat front, with the maximum temperature gradient found between the fire front and the cracking region [1]. Most of the heat sustaining fire front propagation derives from the combustion process of coke. The fire front is the highest temperature zone. The heat and mass transfer of upgrading oil or air causes the temperature of other regions rising [2]. This reveals that the key to temperature prediction in ISC is to obtain relatively accurate combustion parameters of each pseudo-component and reaction heat of the whole crude oil.

There were numerous studies concerning temperature calculation and measurement of the combustion process of hydrocarbons in areas of internal combustion engine, porous burner and factors prediction based on element composition and molecular structure [3–18]. Innerly-fixed thermocouples and infrared camera were common tools for temperature measurement of internal combustion engine and porous burner [3–6]. However, due to the inability to monitor inner

temperature of porous media, the infrared apparatus is inutile in ISC experiment. Jared Dunnmon et al. [7] employed X-ray Computed Tomography (XCT) to determine internal flame structure in porous media and capture temperature profiles of the three-stage porous burner clearly. In their study, combustion process occurred in a transparent quartz tube under atmosphere pressure and the attenuation of X-ray in the linear distance was converted into temperature at a single loci, and this was quite different from the conditions of ISC experiment. Whether XCT method could be introduced into ISC experiment was still undecided. Quantitative structure-property relationship (QSPR) was another way to predict combustion temperature, and plenty of models based on molecular structure and atom properties for predicting combustion heat of organic compounds were established in various studies [8–11]. QSPR prediction would be a potentially effective method when the formation mechanism and molecular structure of coke are certain. In a word, a generally applicable and accurate temperature prediction method for ISC is still in the course of exploration, with the existing techniques used for ISC experiments mostly being fixed thermocouples and simple visualization models [12,13].

Available commercial softwares and theoretic models are starting to

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**Nomenclature**

K	quantity of coke for HTO
n	mole amount of substance
N	carbon number
M	relative molecular weight
$Q_j$	reaction heat of each pseudo-component
C	instantaneous gas concentration
$\rho_{bj}$	TBP proportion of each pseudo-component in crude oil
$\rho_{cj}$	fuel availability of each pseudo-component
$\Delta t$	time interval

H	standard combustion heat
m	mass of substance
$\Delta T$	temperature difference
c	specific heat
q	gas flow
	point in time
Q	reaction heat of the whole oil
$N_c$	carbon number of coke
$M_c$	molecular weight of coke

offer a number of numerical results for temperature field profile during thermal recoveries. Greaves M et al. [14] developed a new model to accurately predict dynamic ISC flooding conditions. Fatemi S.M. [15] simulated characteristics of ISC in fractured carbonate systems. Although these studies provide relatively reasonable results, they still need to be validated by field application and laboratory experiments.

The existing numerical simulations and experimental investigations help better understand the trends of variation of temperature distribution in ISC, but it remains challenging to predict the dynamic temperature field. The crux of predicting temperature change in the combustion zone during ISC is to obtain thermal factors of oil components. Belgare JDM [16] divided heavy crude components into saturate, aromatic, resin and asphaltene (known as SARA) according to the polarity, but SARA component of different oil sample was not uniform, and the distinction of SARA caused by the variation of oil production sites made this method less reliable to general research. Alternatively, in the previous work of R.B. Zhao [17,18], TBP fractions was used to represent heavy oil components in ISC, thus simplified experimental operations and broadened the application range. Further research is reported in this paper.

In the present work, the mole amount of CO and CO<sub>2</sub> produced by combustion of *n*-alkane and pseudo-component were compared. When the amount was equivalent, it was reasonable to correlate combustion processes of the two materials.

## 2. Apparatus and methodology

### 2.1. Materials and sample preparation

The materials used in this study contained *n*-alkanes ( $n = 12, 16, 22, 28, 34, 40$ ), three heavy oil samples and the TBP fractions of each oil. The heavy oil samples from Karamay oil field (Xinjiang, China) were collected directly from the production wellheads. The *n*-alkanes including dodecane ( $n = 12$ ), hexadecane ( $n = 16$ ), docosane ( $n = 22$ ), octacosane ( $n = 28$ ), tetratriacontane ( $n = 34$ ) and tetracontane ( $n = 40$ ) were regarded as standard materials in this work. Characteristics of each oil were given in Table 1, and HAAKE RS6000 Rotor Rheometer (Thermo Scientific, Germany) was used to obtain viscosity of each oil sample at a constant temperature of 40 °C. Information of *n*-alkanes was given in Table 2.

Electric dehydration instrument (Petroleum Analytical Instrument Company, China) was used to dehydrate the oil samples. True boiling point distillation setup (Petroleum Analytical Instrument Company, China) was used to prepare pseudo-components out of the dehydrated oil by standard procedures (ASTM Standard D5236, 2013 [19]). Mass proportion of pseudo-components (listed in Table 3) was used to represent the distribution of components of different oil samples, and components with boiling point range over 500 °C derived from each oil are much richer than any other component.

### 2.2. Apparatus and experimental operation

In this study, combustion process took place in kinetic cell and combustion tube. Detailed information of the apparatus and experimental operations was presented in the work of Cinar et al. [20–22]. The reaction parameters of CT experiments and kinetic cell experiments in this study were listed in Tables 4 and 5.

The flow chart of the temperature prediction of fire front and the evaluation of fuel availability of pseudo-components is shown in Fig. 1. An extra mass of nonvolatile oil reacted in kinetic cell, which was vertically placed through the whole process. The total amount of CO and CO<sub>2</sub> generated in the experiment was larger than that generated in the field, because the nonvolatile part of crude oil would have been flooded through the porous media in the field. This causes the temperature calculated by gas concentration curve of RTO slightly higher than that measured by thermocouples in CT experiment. Similarly the calculated quantity of coke and reaction heat by our model tends to be higher than actual experiment values.

#### 2.2.1. Kinetic cell experiment

The size of quartz sand used the in ISC experiment was 40–60 mesh. The sand was mixed adequately with a certain *n*-alkane or pseudo-component at a mass ratio of 10 to 0.5 to prepare oil sand for kinetic cell experiment. Fig. 2 showed the packing situation of the cell.

Nitrogen was used to flush with the injection rate of 2 L/min, and then followed with air the same rate. When oxygen content became stable, the heating furnace was started. The heating rate of furnace was maintained at 3.84 °C/min for 2.5 h. The composition of vent gas was monitored in real time by a gas analyzer (Wuhan Cubic Optoelectronics Co. Ltd, China).

#### 2.2.2. Combustion tube experiment

Combustion tube experiment was used to simulate ISC in real formation to get variation of combustion temperature during fire front propagation. The deviation of temperature values measured by thermocouples and calculated from kinetic cell experiment validated the new temperature prediction method. As shown in Fig. 3, the tube is 60.0 cm in length and made of titanium alloy with the inner diameter 3.8 cm and the outside diameter 6.0 cm. An igniter, which is 10.0 cm in length and denoted by T<sub>1</sub>, was mounted on the inlet flange. Five thermocouples (T<sub>2</sub>–T<sub>6</sub>) are located at 12.0 cm intervals along the tube's length to monitor centerline temperature of oil sand. A rotatable disc that is mounted on the bracket was used to fix the combustion tube to realize the tilt angle adjustment.

**Table 1**  
Density and apparent viscosity of oil samples.

Oil sample	Density, 10 <sup>-3</sup> kg/m <sup>3</sup>	Apparent viscosity, mPa·s
Sample 1	0.959	14,582
Sample 2	0.958	14,275
Sample 3	0.951	12,874

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