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NonArrhenius kinetics for reactive transport simulations of in situ combustion

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ABSTRACT

In situ combustion (ISC) is a substantially exothermic reactive transport process. Due to the multicomponent nature of crude oil, ISC reactions are time consuming to characterize and represent accurately in a compact mathematical form. We have developed a methodology for simulation of thermal reactive flow with fidelity to reaction kinetics without construction of a model for reaction. The progress of ISC reactions is represented in a three-dimensional space bounded by conversion (extent of reaction), temperature, and heating rate that may be obtained experimentally. The representation may be either in continuous or tabular form (preferred). The reaction model free approach as applied to ISC is outlined and demonstrated for the first time. Comparison to the predictions of ISC from a conventional simulator is favorable. The results of the reaction-model free method match the common reaction model approach for one and two dimensional combustion processes. The reaction model free approach simplifies the numerical representation of reactive transport. The approach covers the whole range of heating rates that exist in combustion processes and it is as accurate as current methods.

1. Introduction

In situ combustion (ISC) is an enhanced oil recovery method that is applicable to various types of oil reservoirs. Despite successful field projects around the world (Moritis, 1998; Marjerrison and Fassihi, 1994; Gadelle et al., 1981; Counihan, 1977), prediction of the likelihood of a successful in situ combustion field project from first principles is unclear. Historically, combustion tube tests of a crude-oil and rock are used to design an in situ combustion process and to infer whether one expects the process to work at reservoir scale (Hascakir et al., 2013; Greaves et al., 1990; Prats, 1982; Gates and Ramey, 1980; Penberthy and Ramey, 1966). Ideally, such tests are completed in combination with simulation for prediction and design of combustion recovery processes (Chavez et al., 2015; Belgrave et al., 1997; Coates et al., 1995; Gottfried, 1965). To simulate combustion recovery processes, fairly sophisticated reaction models for formation of crude-oil intermediates and their oxidation have been proposed based on kinetics studies (Lapene et al., 2011; Cinar, 2011; Sequera et al., 2010; Dechelette et al., 2006).

Conventionally, kinetics cell experiments are used to find the reaction parameters for the suggested models (Sarathi, 1999; Burger and Sahuquet, 1972). In a ramped temperature oxidation (RTO) test, a small sample of crude oil mixed with sand, clay, and water is oxidized while increasing the temperature at a prescribed rate (Marjerrison and Fassihi, 1994). The results of the RTO experiment including effluent gas compositions and temperature history (i.e., deviation of the history from the prescribed heating rate due to the heat of reaction), are used to find the reaction parameters for a proposed kinetics scheme (e.g., Bazargan et al. (2011)). Clearly, the number of crude-oil components and their potential reaction intermediates is very large, and potentially intractable. A typical approach for description of ISC is to replace detailed chemical component and reaction details with pseudocomponents and simplified equivalent reaction schemes, respectively.

Additionally, even when simplified reaction models with a small number of pseudocomponents are implemented in the numerical simulator, a severe grid-block size effect is observed due to numerical stiffness (Zhu et al., 2011; Gutierrez et al., 2009). Rigorous grid-block upscaling (Yang et al., 2015) of the combustion process is an open area of study. Several numerical approaches that resolve a combustion front with fine spatial grid-blocks have been suggested (Younis and Gerritsen, 2006; Kristensen et al., 2006; Gerritsen and Lambers, 2008; Nilsson et al., 2005). Other researchers have tried to simulate ISC on the field-scale without resolving the combustion front and by tuning the reaction parameters (Marjerrison and Fassihi, 1992; Le Thiez et al., 1990; Onyekonwu et al., 1986). Apart from the finite-volume methods, there are numerous simulation studies to predict the position of the combustion front (Akkutlu and Yortsos, 2003; Davies, 1989; Hwang et al., 1982).

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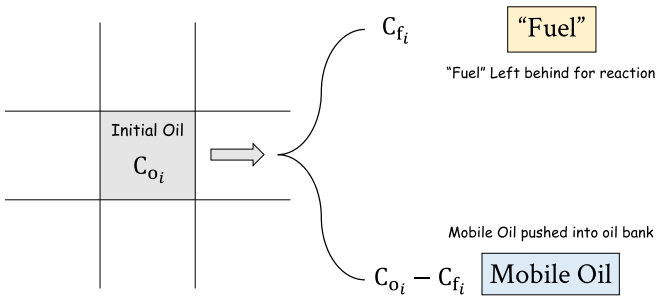

Fig. 1. Schematic of the different parts of the crude-oil in RMFK.

A rigorous procedure (Arce et al., 2005) to lump ISC reactions to a small set of equivalent reactions is also an open area of study and complements grid-block upscaling. A novel reaction model-free kinetics (RMFK) procedure was proposed by Bazargan and Kovscek (2015). The technique uses only kinetics cell measurements thereby bypassing the construction of a multi-step reaction model. In their method, results of the RTO experiments are used directly to predict the oxidation profile for any arbitrary temperature history. Additionally, Bazargan et al. (2013) presented the design, verification, and validation of a new reactor for use in measuring crude-oil oxidation kinetics. The reactor is capable of covering a range of heating rate from 1 to 30 $^{\circ}C$/min and is, thus, capable of reaching the heating rate of the combustion front that is typically 10 to 30 $^{\circ}C$/min. RMFK is able to predict crude-oil oxidation for any arbitrary temperature profile provided that the RTO lab results bound the physically realistic heating rates.

This paper extends the RMFK technique from zero dimensional batch reactors to one and two dimensional ISC. This is the first instance of the application of the RMFK technique to reactive transport. RMFK replaces detailed multi-step reactions schemes that are used for high-resolution combustion simulations. To permit a meaningful comparison, flow simulation results using the RMFK procedure are compared directly to a commercial simulator that implements a full Arrhenius reaction kinetics model. After explanation of the RMFK methodology, this paper proceeds by describing combustion in a one-dimensional combustion tube, laying out the necessary mass and energy balances, presenting the RMFK technique as applied to reactive transport, and comparing results obtained with the RMFK technique and conventional numerical reservoir simulation.

2. RMFK methodology

This section outlines how RMFK solves reactions at the scale of a grid block. Assume that grid block i (Fig. 1), representing a block for a finite-volume discretization of a reservoir that undergoes ISC, has an initial oil saturation of S_{o_i} (corresponds to the initial oil concentration of C_{o_i}). Before the combustion front reaches the grid block i, S_{o_i} changes because of flow and/or phase change. Temperature increases as the combustion front approaches the grid block i until it reaches T_{ignition}, at which oxidation starts if oxygen is present. The concentration of the "organic material" remaining in grid block i at T_{ignition}, is C_{f_i}. In RMFK, this immobile amount of organic matter is referred to as "Fuel" (Fig. 1), because C_{f_i} is the reactive, immobile part of the oil.

For a given amount of oil, for any specified or arbitrary temperature history, Bazargan and Kovscek (2015) suggested a novel reaction model-free method to obtain the oxygen consumption and carbon oxides oxidation profiles based on the results of a given set of RTO experiments. In the conventional approach, a reaction model employing Arrhenius-type reaction constants is typically used. The reaction model is usually calibrated to match experimental behavior. In the RMFK technique, the results of a set of RTO experiments obtained at heating rates that bound ISC conditions are used directly instead of a reaction model.

Importantly, conversion of the fuel is defined in RMFK based on oxygen consumption (X_{O_2}) and carbon oxides (X_{CO_2} and X_{CO}) production profiles (Bazargan and Kovscek, 2015). In other words, we focus on the evolution of the oxygen consumed and carbon oxides produced by the fuel instead of measuring the change of the mass of the fuel when applying RMFK. For an RTO experiment, the conversion of the fuel in terms of oxygen consumption (X_{O_2}) is (Cinar et al., 2009):

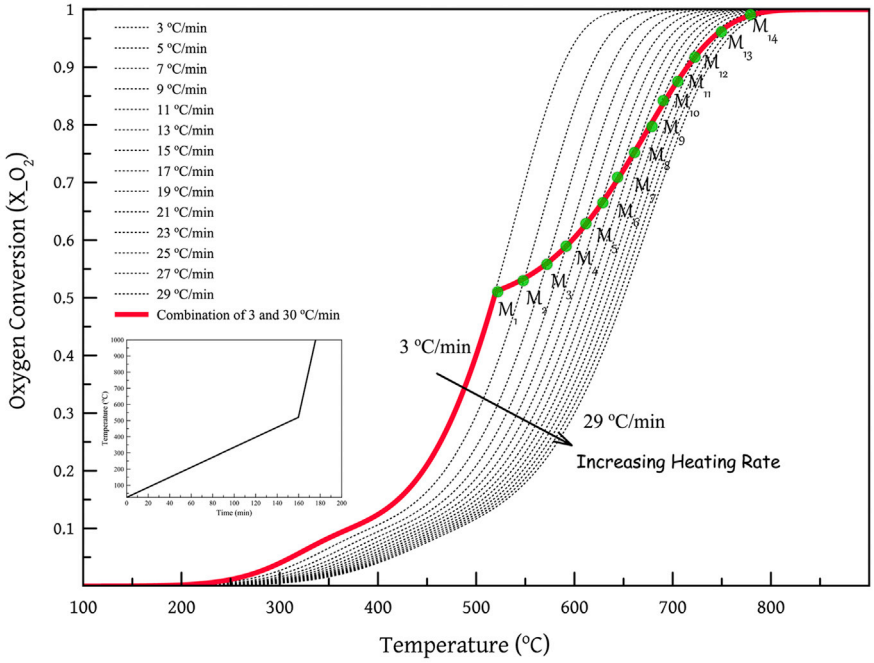

Fig. 2. Example application of the RMFK method. Dotted lines represent results from synthetic kinetics cell measurements at constant heating rate. The solid red line is the path followed by a series combination of 3 and 30 $^{\circ}C$/min heating rates. For ISC simulation, the temperature history is obtained by solving the energy balance. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)