



An optimization algorithm for evaluation of kinetic parameters for crude oil combustion



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ABSTRACT

The design of enhanced oil recovery processes that employ in-situ combustion requires high-fidelity simulation models that accurately describe the physics and chemistry of reactive, exothermic multiphase fluid flow. Therefore, a detailed description of oil combustion kinetics is required. The goal of this work is to present and apply a workflow to define and match pseudo-kinetic reaction models based on Arrhenius kinetics. These models are meant to be used at the laboratory scale with high-resolution, fully-resolved simulation models as a tool to generate high density data required by upscaled models at reservoir scale.

The workflow starts by performing ramped temperature oxidation (RTO) experiments for a wide range of heating rates. New experimental equipment has allowed us to obtain data for large heating rates ($>15 \frac{^{\circ}\text{C}}{\text{min}}$) that were not achievable in the past. A subset of the experiments are selected to match the oxygen consumption curves by tuning kinetic parameters of several global reaction models using pattern search optimization. Those models that obtain a match are validated by predicting a second subset of the data that was not considered during the optimization. The workflow is tested using a heavy oil and two satisfactory matches with two different global reaction models are obtained.

1. Introduction

Reactive flow arises in many processes observed in oil reservoirs, especially during secondary and tertiary recovery processes (e.g., low salinity water injection, foam injection, In-Situ Combustion (ISC)).

Given the complex nature of reactions, modeling reactive flow usually involves finding a global set of reactions that captures the main mechanisms. The proposed reaction model is validated by matching the pseudo-reaction parameters to representative laboratory experiments. This process is iterative, computationally expensive and highly uncertain because it relies strongly on optimization algorithms that may or may not find a global minimum given the large parameters space and the strongly non-linear nature of the problem. In other words, it may be hard to unequivocally dismiss a set of pseudo reactions even if a match is not achieved, as it may be an issue with the optimization procedure (e.g., bad initial guess, not enough iterations, and so on) or inherent to the optimization itself (e.g., stuck in a local minima). Furthermore, comparing the different pseudo-reaction schemes is complicated and arguments on why one is better than the other are highly subjective.

Modeling reactive flow in the context of ISC further complicates matters for two reasons: the small size of the reaction zone, or combustion front, and the exponential dependence of reaction rates on

temperature. The first requires one to resolve the simulation grid to at least the size of the combustion front, that is estimated to be on the order of inches. Such small grids are impractical for reservoir-scale simulations.

The second means that any averaging of properties due to grid size and property upscaling results in large errors due to diffused and incorrect temperature estimations. These errors accumulate through time and result in inaccurate predictions.

Other issues include numerical stability problems due to the multiscale character in reaction vs. flow timescales and the inability to match simultaneously all scaling parameters between lab vs reservoir scales. A comprehensive review of the challenges involved in modeling ISC from laboratory experiments are summarized by Gutierrez et al. (Gutierrez et al., 2009, 2012).

Given modeling limitations, research efforts have shifted towards representing reaction kinetics with an explicit model such as Reaction Model Free Kinetics (RMFK) both at lab-scale (Bazargan, 2014; Bazargan and Kovscek, 2015) and at field-scale (Zhu et al., 2011a; b; Nissen et al., 2015). These models are combined into general ISC workflows that feed accurate lab-scale data for calibrated full-field predictions. Experimental data is needed to validate these upscaled reaction-free kinetic models.

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Yet, the large quantity of data required to build accurate models, including dense tables of fuel conversion and accurate fuel lay-down, make lab-scale Arrhenius models a valuable tool as they can be used to generate data for large numbers of scenarios that are impractical to run experimentally and to compute sensitivities to parameters that cannot be changed easily, and controlled, in the experimental lab settings.

Matching lab-scale Arrhenius models is not trivial and the problem has been traditionally approached as a history matching problem, where a single global reaction model is selected and parameters are manually tuned until a single match is obtained (Fassihi et al., 1984; Belgrave et al., 1993; Freitag et al., 2003; Jia et al., 2006; Cinar et al., 2011; Cinar, 2011; Chen, 2012; Chen et al., 2014; Dechelette et al., 2006). Even though there is agreement on the principal reaction regimes involved in ISC, proposed reaction models differ greatly from investigator to investigator. Belgrave et al. (1993) and Jia et al. (2006) propose global reaction models based on maltenes, asphaltenes, coke and gas a pseudo components whereas Freitag et al. (2003) does so using Saturates, Aromatics, Resins and Asphaltenes (SARA) fractions. Most recently, global reaction models consider intermediate coke pseudo-components whose properties can be used as a matching parameter (Dechelette et al., 2006; Cinar et al., 2011; Cinar, 2011; Chen, 2012; Chen et al., 2014). All global reaction schemes are backed by some consistent physical understanding of the process and more importantly have achieved satisfactory matches within calibration ranges. Nevertheless, all these models are simplifications of reality where thousands of components are grouped into a small number of pseudo-components making it hard to justify why a particular model is better than the other based solely on physical arguments. The only true valid measure of their performance is their ability to predict new experiments.

This manuscript focuses on the modeling of reaction kinetics for ISC. It seems necessary to evaluate many pseudo reaction schemes that can match the same data and then test their predictability. Hence, we model a laboratory reactor and compare experimental and best-match numerical results. We proceed by describing the experimental effort, various reaction models, a reaction matching algorithm and results.

2. Workflow description

The methods presented in this work are consistent with the high-level workflow presented by Kovscek et al. (2013) for improved predictability of ISC. This work focuses mainly on the generation of high resolution reaction models using experimental data. Specifically, it attempts to formalize the reaction matching scheme proposed and used by Cinar et al. and Chen et al. (Cinar et al., 2011; Cinar, 2011; Chen, 2012; Chen et al., 2014).

Fig. 1 employed the steps to obtain matched high resolution models. The workflow begins by performing ramped temperature oxidation (RTO) experiments for a range of heating rates expected in a field application. Experiments must be designed to reflect reservoir conditions as closely as possible, especially those that affect reaction kinetics such as clay content. Using the experimental data, the isoconversional fingerprint is obtained to identify important reaction zones and their corresponding apparent activation energies (Cinar et al., 2011; Cinar, 2011; Chen, 2012; Chen et al., 2014; Padilla et al., 2016, 2017). Based on this information, several global reaction models are proposed under different but equally possible assumptions, including number of fuel components and fuel laydown conditions.

For each global reaction scheme, numerical optimizers and a simulation model of the experimental set-up are used to match the experimental data. A match may, or may not, be achieved at this point depending on the optimizer, its parameters, and the global reaction model itself. Given the large parameter space of the problem, it is probable that more than one solution is achieved.

The solutions are then validated by predicting additional RTO experiments that were not considered during the regression process.

Finally, the validated models are used in an uncertainty analysis and tested in more complicated models such as two or three dimensions.

2.1. Experiments at large heating rates

Until recently, kinetic cell experiments had been performed for small heating rates in the range of $0.5\text{--}3\frac{^{\circ}\text{C}}{\text{min}}$ mainly due to the limitations of typical experimental set-ups using furnaces. Bazargan et al. (2013) constructed a new kinetic cell reactor based on induction heating that allows experiments to be performed with accuracy for heating rates up to 30°C . Bazargan (2014) calculated the instantaneous heating rate at various points of a combustion tube experiment and found values as large as $40\frac{^{\circ}\text{C}}{\text{min}}$. This experimental achievement provides new calibration data for matching models.

2.1.1. Induction cell reactor

Samples are prepared by mixing dead oil with silica sand that has been fired at 750°C to remove active/organic minerals and to passivate clays. The samples consist of 1% dead oil by weight and are meant to be below or equal to residual oil saturation. This mixture is then introduced into the reactor and packed with clean sand on both sides. The reactor is then heated by an induction coil that is controlled to the desired heating rate by a temperature controller. The thermocouples are introduced into the sample by means of a thermowell. The effluent gas composition is continuously analyzed using a gas analyzer and the temperature for the reactor is also recorded. This is all the data required to obtain an isoconversional fingerprint.

2.1.2. Behavior at high heating rates

Historical RTO experimental data has shown a consistent trend in oxygen consumption curves at low heating rates. These curves are characterized by having two oxygen consumption "humps" corresponding to two dominating reaction zones commonly referred to as low temperature oxidation (LTO) and high temperature oxidation (HTO). New experiments with the induction cell reactor show that LTO and HTO zones tend to merge with increasing heating rates. Fig. 2 shows the oxygen consumption of experiments at different heating rates as a function of time. Converging peaks are clearly observed. The oxygen consumptions peaks also increase while total oxygen consumption seems to stay constant. This observation supports the idea that the primary reaction mechanisms are not changing with heating rate.

2.2. Evaluation of global reaction models

One way to evaluate different global reaction models is to test them in numerical experiments. Results help us discard any models that do not reproduce expected physical behaviors. Given the new intuition provided by experiments at large heating rates, existing global reaction models may be tested to see if they behave, as expected, under these conditions. Specifically, the models proposed and matched by Cinar (2011) and Chen (2012) are tested. These models were matched using experimental data for heating rates in the range of $0.5\text{--}3\frac{^{\circ}\text{C}}{\text{min}}$.

When RTO numerical experiments are performed in the range of $2\text{--}30\frac{^{\circ}\text{C}}{\text{min}}$, both reaction models show collapsing oxygen consumption peaks with increasing heating rates. The relative heights of the LTO and HTO peaks are reversed, however. This could be due to the specifically matched parameters or to an underlying constraint related to the reaction model itself. In the following subsections, a more detailed analysis is performed.

2.2.1. Cinar et al. (2011); Cinar (2011) 6-reaction model

Cinar proposed a 6-reaction model to match RTO experiments performed using Hamaca crude, among others (Cinar et al., 2011; Cinar, 2011).

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