IMPROVED PREDICTABILITY OF IN-SITU COMBUSTION ENHANCED OIL RECOVERY

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ABSTRACT. In-situ combustion (ISC) possesses advantages over surface-generated steam injection for deep reservoirs in terms of wellbore heat losses and generation of heat above the critical point of water. Additionally, ISC has drastically lower requirements for water and natural gas, and potentially a smaller surface footprint in comparison to steam. In spite of its apparent advantages, prediction of the likelihood of successful ISC is unclear. Conventionally, combustion tube tests of a crude-oil and rock are used to infer that ISC works at reservoir scale and estimate the oxygen requirements. Combustion tube test results may lead to field-scale simulation on a coarse grid with upscaled Arrhenius reaction kinetics. As an alternative, we suggest a comprehensive workflow to predict successful combustion at the reservoir scale. The method is based on experimental laboratory data and simulation models at all scales. In our workflow, a sample of crushed reservoir rock or an equivalent synthetic sample is mixed with water/brine and the crude-oil sample. The mixture is placed in a kinetics cell reactor and oxidized at different heating rates. An isoconversional method is used to estimate kinetic parameters versus temperature and combustion characteristics of the sample. Results from the isoconversional interpretation provide a first screen of the likelihood that a combustion front is propagated successfully. Then, a full-physics simulation of the kinetics cell experiment is used to predict the flue gas composition. The model combines a detailed PVT analysis of the multiphase system and a multistep reaction model. A mixture identical to that tested in the kinetics cell is also burned in a combustion tube experiment. Temperature profiles along the tube and also the flue gas compositions are measured during the experiment. A high-resolution simulation model of the combustion tube test is developed and validated. Finally, the high-resolution model is used as a basis for upscaling the reaction model to field dimensions. Field-scale simulations do not employ Arrhenius kinetics. As a result, significant stiffness is removed from the finite difference simulation of the governing equations. Preliminary field-scale simulation shows little sensitivity to grid-block size and the computational work per time step is much reduced.

INTRODUCTION

During in-situ combustion (ISC) air is injected into the reservoir with the intent of oxidizing a small fraction of the hydrocarbon in place. The significant heat generated by combustion reactions mainly contributes to enhanced oil recovery by reducing crude-oil viscosity and increasing drive energy through pressurization that results in a vigorous gas drive (Prats, 1982). Large temperature difference signifies heat transfer and results in phase change. Thus, ISC is a strongly coupled reactive transport process whose modelling is challenging. Compounding difficulties, crude-oil components, reactive intermediate products, and the reactions cannot be characterized exhaustively.

Conventionally, combustion tube tests are used to infer the likelihood of combustion at field scale and design the ISC process (Moore. et al., 1997). A combustion tube test gives an understanding of parameters affecting ISC such as air requirement, fuel deposition, and front propagation speed (Sarathi, 1999). The study of reaction kinetics in the combustion tube, however, is not appropriate. Likewise, there is interplay of transport, phase behavior, and reaction (Lin. et al., 1984) in a combustion tube that needs to be deconvoluted. Combustion tube tests are typically designed to operate in the so-called high-temperature oxidation (HTO) mode and feature the products of
bond-breaking reactions including CO$_2$, CO, and H$_2$O. Low temperature oxidation (LTO) and fuel formation reactions, while occurring in the combustion tube, are not easy to discern from combustion tube results. The products of LTO are partially oxygenated hydrocarbons and H$_2$O whereas fuel formation produces coke-like species. An ISC coke is a carbon-rich, hydrogen poor, high-molecular weight reaction product. Clearly, effective fuel formation is vital for successful combustion in the HTO mode.

Based on the air requirement obtained from combustion tube experiments and a selection of well patterns, the required air compression is estimatable and a project can be designed. Moore. et al. (1997) have suggested to use a line-drive pattern and restricted well-spacing to provide sufficient air to the field. Semi-empirical and analytical models, such as the Gates and Ramey (1980) method and Brigham et al. (1980), were developed to aid design without requiring extensive computation.

Prediction of field performance using reservoir simulation remains difficult, however. See, for example, Zhu. et al. (2011). Commercial and research thermal simulators have been developed to model and predict the in-situ combustion process (Coats, 1980; Eclipse, 2009; STARS, 2009). In all commercial thermal simulators, mass and energy conservation equations are solved coupled with chemical reaction terms calculated using Arrhenius kinetics. It is well known that for increasing the length scale to full field from laboratory, severe grid-size effects are encountered during in-situ combustion simulations (Coats, 1983; Gutierrez et al., 2009; Kristensen et al., 2007). That is, we are not able to achieve consistent predictions at field scale using typical large grid blocks.

To mitigate the grid-size effects in ISC simulations, various empirical techniques have been developed. In many cases, the reaction kinetics parameters were changed or tuned to force the oil to burn in field-scale simulations. This can be achieved, for example, by adjusting the activation energy to small or even zero values, thereby lowering the threshold crude oil burning energy requirement. In some cases, the temperature values in Arrhenius kinetics are also adjusted to make the oil easier to burn (Coats, 1983). A comprehensive summary of all these techniques is presented in Marjerrison and Fassihi (1992). Specialized numerical methods such as adaptive mesh refinement (Christensen et al., 2004) and operator splitting (Kristensen, 2008) have also been applied, leading to some improvement in simulator performance. Despite such improvements, there is a lack of applicability for field-scale simulation.

Motivated by the potential of ISC and the need for predictive capability, we propose a workflow and describe through example application the steps at each phase of the workflow. The scope of the workflow extends from laboratory measurement to upscaling of equivalent reaction effects within large volume grid blocks. Our goal is to develop laboratory procedures to measure indicators of combustion performance and to demonstrate a methodology for simulation of the effect of in-situ combustion reactions on the field scale accurately and without severe grid-size effects.

Our research efforts, to date, have aimed at developing the experimental and reservoir simulation components of the workflow. The intent of this paper is to present the workflow employing these components and illustrate it through example. This paper proceeds with a description of the workflow. Then each element of the workflow is illustrated and discussed. We pay special attention to the linkage of experimental data with numerical models to create a predictive mechanistic model of in-situ combustion. Succeeding sections discuss experimental tests to assess crude-oil oxidation kinetics, the calibration of a numerical model for kinetics, implementation of the kinetic model into a simulator to describe front propagation in a combustion tube, and the use of fine-scale mechanistic models to generate upscaled simulation input. Discussion and conclusions complete the paper.
Workflow

As an alternative to current ISC engineering and design (Moore. et al., 1997; Sarathi, 1999), we suggest a workflow (Fig.1) that integrates ramped temperature oxidation (RTO) experiments of crude-oil (referred to here as kinetics cell experiments), combustion tube experiment, compositional analysis of crude-oil, high resolution mechanistic models and combustion-specific upscaling to predict ISC at reservoir scale. In our approach, the kinetics cell experiment is used to probe the kinetics of combustion rather than a combustion tube (Cinar. et al., 2009, 2011; Lapene. et al., 2011-a). This workflow transitions naturally across length and time scales integrating experiment and numerical modeling. In this sense, the workflow for ISC is multiscale and multiphysics. Although ISC is applicable to heavy and light oils, this workflow was constructed from a heavy-oil perspective. We have yet to consider the extension to light oils.

We first prepare a sample of crushed reservoir rock or an equivalent synthetic sample mixed with brine/water and crude-oil. The mixture is put in the kinetic cell and oxidized at a given heating rate. The test is then repeated at different heating rates. We take advantage of the isoconversional method (Cinar. et al., 2011; Cinar et al., 2011-b) to distinguish different regions of reaction during combustion. The isoconversional interpretation provides a first screen of the likelihood that a combustion front can be propagated successfully. If the crude-oil sample shows a positive sign of being a good candidate for ISC, then the detailed compositional description and PVT properties of the crude-oil sample is obtained.

The isoconversional method also provides us with a plot of effective activation energy versus temperature. A reaction model (or models) is developed and tested to reproduce effluent gas production from the kinetics cell at various heating rates and the isoconversional fingerprint obtained experimentally. An optimization method is used to find the reaction parameters in a way that it matches the kinetics cell result. This provides a high-resolution reaction model to be used in the combustion tube simulation.

The next steps in the combustion study are combustion tube experiments that are performed on a mixture identical to that in the kinetic cell experiment. By understanding the multi-scale nature of ISC, we present a methodology for reaction upscaling. The reaction model is validated by comparing prediction and experimental result. The reaction model and/or the results from combustion tube experiments are then useful to provide quantities such as the amount of fuel formed during combustion. The high-resolution reaction model also, naturally, provides reference solutions for upscaling in the final stages of the workflow.

The remainder of this paper lays out the workflow. Throughout this paper, the heavy crude oil analyzed and characterized is from Venezuela. This sample is a so-called well-burning sample as shall be illustrated.

Kinetics Cell Experiment

Kinetics cell experiments probe the mechanisms of the kinetics of crude-oil oxidation. Ramped temperature oxidation (RTO) experiments with analysis of the effluent gas are conducted. The schematic of the apparatus used for experiments is given in Figure 2. Further details of the system are given elsewhere (Cinar. et al., 2009). The system pressure is kept fixed with a back pressure regulator and the air rate is controlled with a mass flow controller. The outlet gas is dehydrated and filtered before being sent to a gas analyzer. The sample is a mixture of sand (or crushed reservoir rock), clay, water, and an appropriate amount of oil. The mass of oil used is determined by a trial and error procedure. The amount of oil is small enough to minimize temperature deviations from the pre-programmed temperature history and large enough to produce sufficient effluent gas for
Figure 1. Proposed workflow.

Figure 2. Experimental apparatus for ramped temperature oxidation experiments.
different heating rates (Vyazovkin, 1997, 2001). All the other parameters, such as pressure, flow rate, initial temperature and so on are held fixed for all tests. Therefore, each experiment is conducted with great care to achieve satisfactory and consistent results with the proposed analysis technique. At least five consistent experiments are necessary for the isoconversional analysis to produce reliable results (Cinar. et al., 2009). Once the set is complete, the isoconversional analysis is applied.

**Isoconversional Method.** ISC reaction rates are commonly described as a function of fuel concentration and oxygen partial pressure (Bousaid. et al., 1968). Assuming Arrhenius behavior for the rate constant, this model is

\[ -\frac{dC_f}{dt} = Ae^{-\frac{E}{RT}} P_{O_2}^a C_f^b \]  

where \(a\) and \(b\) represent exponents for oxygen partial pressure and fuel concentration, respectively, \(E\) is the activation energy (J/mol), \(T\) is absolute temperature (K), \(R\) is the gas constant (J/mol-K) and \(A\) is a pre-exponential factor sometimes referred to as the Arrhenius constant. Similar forms are applied by various authors (Bousaid. et al. (1968), Burger and Sahuquet (1972), Fassihi. et al. (1984)).

Beyond its wide application, Eq. (1) is the simplest form of a combustion rate equation. In reality, oxidation of hydrocarbons involves a set of series and parallel reactions leading to a complicated reaction scheme with an overall reaction expression that may not be entirely represented by Eq. (1). The isoconversional method provides a way to bypass such complex, unknown reaction models. Numerous experiments at different heating rates are performed to probe and parameterize the reaction. Here, we lay out the general methodology for applying the isoconversional method to crude oils. Substantial details are available in the literature (Cinar. et al., 2009, 2011).

In a more general expression, the reaction rate is written as a product of rate constant and reaction model. The former is a function of temperature and the latter is a function of concentration or conversion. Representing the reaction model with \(f(X)\), we have

\[ -\frac{dX}{dt} = K(T)f(X) \]  

where \(K(T)\) is the rate constant (units depends on reaction model). The rate constant is expressed as a function of temperature. Assuming Arrhenius behavior we have,

\[ -\frac{dX}{dt} = Ae^{-\frac{E}{RT}} f(X) \]  

The isoconversional principle states that at constant extent of conversion, the reaction rate is only a function of the temperature. Eq. (3) is the basis of all isoconversional methods discussed in this work. Taking the logarithm of Eq. (3) gives,

\[ \ln(\frac{dX}{dt}) = \ln(A) + \ln[f(X)] - \frac{E}{RT} \]  

At constant values of conversion, \(f(X)\) is assumed to be constant. This is analogous to assuming that the chemistry of the process is independent of temperature and dependent only on the level of conversion (Friedman, 1964). As a consequence, for different temperatures at the same conversion levels or isoconversional values, \(f(X)\) is identical. Then,

\[ \ln(\frac{dX_x}{dt_x}) = m - \frac{E_x}{RT_x} \]
where

\[ m = \ln(A) + \ln[f(X)] \]  

(6)

here \( t_x \) and \( T_x \) are time and temperature, respectively, for any particular experiment at conversion, \( X \). The symbol \( E_x \) is activation energy at conversion \( X \). For different constant temperatures, we plot the left hand side (LHS) of Eq. (6) with respect to \(-1/T_x\). The slope of the graph gives \( E/R \) and the intercept is \( m \). This method was first introduced by Friedman (1964) and is referred to the differential isoconversional method. This method needs reaction rate values to be obtained and the rate values are usually calculated by numerical differentiation. It is well known that numerical differentiation amplifies error in experimental data. Therefore results are sensitive to experimental noise (Vyazovkin, 1997). In order to avoid numerical differentiation, integral isoconversional methods were developed (Kissinger (1957), Akahira and Sunose (1971), Ozawa (1965), Flynn and Wall (1966), Vyazovkin (1997) and Vyazovkin (2001)). These different methods are described and compared in their applicability to ISC kinetics by Cinar. et al. (2009). Based on synthetic examples and experimental analysis they concluded that Vyazovkin (2001) and Friedman (1964) methods work well for the kinetics analysis of ISC.

Isoconversional analysis yields effective activation energy versus conversion (or temperature). The plots show how effective activation energy changes with the extent of conversion and provides initial estimates for reaction parameters. Figure 3 shows the isoconversional fingerprint of a crude-oil sample (Cinar. et al., 2009). It is a typical example of a well-burning oil and encompasses the features of an isoconversional fingerprint. The LTO and HTO reaction regimes identified are shown in Fig.3. Also the valley in the figure is associated with the negative temperature gradient region (NTGR) (Cinar. et al., 2009). Isoconversional methods are useful as a diagnostic tool to recognize the underlying mechanisms of complex multi-step reactions.

Different parts of the graph are related to different reactions. The low temperature oxidation (LTO) at roughly 560 K is dominated by the NTGR that is centered about 600 K. In this region the effective activation energy decreases, achieves a minimum, and then increases up to the HTO region. A clear high temperature oxidation (HTO) plateau is observed. The smooth transition from NTGR to HTO is a typical of a good combustion candidate (Cinar. et al., 2011). Figure 4 shows the isoconversional fingerprint of a poor combustion candidate. Poor candidates exhibit
significant energy barriers in the low temperature region as shown by their fingerprints whereas good combustion candidates exhibit a smoother transition and, in general, smaller activation energies in the low temperature region (Cinar. et al., 2011). Thus, isoconversional method provides a first screening of combustion candidates.

![Graph showing Effective activation energy versus conversion and temperature](image)

**Figure 4.** Sample two, isoconversional fingerprint of a poor combustion candidate. Effective activation energy versus conversion (left) and temperature (right) (Cinar. et al., 2011).

**Phase Behavior.** If the interpretation of the result of the isoconversional method suggests that a crude-oil sample is potentially a good candidate for ISC, then a compositional description and PVT analysis of the crude-oil sample is obtained. For the purposes of compositional simulation of ISC and of kinetics cell results, a good characterization of the heavy components is desirable (Lapene. et al., 2011-a).

**Simulation of Kinetics Cell Experiment.** The governing equation system that models the kinetic cell experiment is composed of classical mass conservation equations. We have followed two parallel routes to simulate kinetics cell experiments to discern reaction schemes and pathways. In the first effort, the crude oil is treated in a fully compositional manner, reaction schemes are postulated, and a multiobjective match to kinetics cell effluent gas history is obtained using a genetic algorithm. The details of this first effort are reported by Lapene. et al. (2011-a) and Lapene. et al. (2011-b). The second effort employed extensive investigation of reaction intermediates and reaction products to infer a lumped reaction model consistent with observation (Cinar et al., 2011-b). While we have had excellent results from these complementary efforts, for reasons of space, this section focuses upon the second approach.

Based on experimental observations, the following simplified reaction scheme is proposed to mimic the experimental observations for oxidation of heavy oil including the isoconversional fingerprint. Cinar et al. (2011-b) explains how such a simplified reaction model was obtained. At least two different coke formation reactions are necessary because coke precipitated under nitrogen (inert gas) and under air flow have been demonstrated to be different. Thus, there should be two different coke species for LTO and HTO reactions. In combustion tube experiments, ignition is initiated under nitrogen flow so oxidation of Coke\(_1\) is necessary. The transformation of Coke\(_1\) to Coke\(_2\) was found to be a necessary reaction to obtain the correct response in the NTGR. Coke transformation is unique to such a simplified reaction scheme.
Oil + 4O$_2$ $\rightarrow$ 10Coke$_1$ + 22.3888H$_2$O \hspace{1cm} (7)

Coke$_1$ + 1.5O$_2$ $\rightarrow$ CO + CO$_2$ \hspace{1cm} (8)

Coke$_1$ $\rightarrow$ 2Coke$_2$ \hspace{1cm} (9)

Coke$_2$ + 1.4375O$_2$ $\rightarrow$ 0.5CO + CO$_2$ \hspace{1cm} (10)

where Oil is an oil species, Coke$_1$ is a coke species, and Coke$_2$ is a coke species. Coke species are hydrogen deficient and produce only carbon oxides during oxidation. For all of the reactions, the Arrhenius form of the rate constant is assumed.

There are two significant features of this reaction scheme. First, the scheme does not include any oil directly burning as experimental data strongly suggest that heavy oil does not burn directly. Second, it includes a reaction that represents the transformation of coke formed in the LTO region into the fuel (coke) that burns in HTO region.

Based on the reactions given above, kinetic cell simulations are carried out with a commercial simulator. A radial model with one grid block in the z direction and 4 blocks in the r direction is built. The details for the grid blocks used in the r direction are given in Cinar et al. (2011-b). The first grid block in the r direction represents the sample, the second the stainless steel tube, the third the spacing between the furnace wall and reactor and, the fourth the furnace. These grid blocks were necessary to mimic the exact programmed heating schedule in the experiments. The injected fluid temperature is increased at each time step according to the heating schedule. This is similar to the experiments where tubing is tightly coiled and placed within the furnace to allow heating of the inlet gas. Thus, the injected gas reaches the furnace temperature before it reacts. The challenge in modeling the kinetic experiments was to impose a linear heating rate. There is not an option in the version of the simulator that we used. This problem is solved by changing the target temperature for the heaters at each time step. Therefore, we impose a linear heating with different rates with pre calculated target temperature based on the rate. Note that this is done only for the pre-programmed temperature history not for the deviations resulting from reactions or water changing phase. These are a direct result of reaction enthalpy and enthalpy of vaporization. All parameters used in the simulations are given by Cinar et al. (2011-b). The molecular weights of the lumped components are shown in Table 1. The reaction parameters for the synthetic model 1 are given in Table 2.

Figure 5 shows the simulation results for the runs with heating rates spanning from 1.74 to 2.74 K/min. The first peak in O$_2$ consumption and temperature is representative of LTO while the second peak is representative of HTO. This figure indicates that the general trends observed in the experimental data are conserved in numerical simulations. Based on these simulated data, the isoconversional fingerprint is estimated and given in Figure 6. Compare this result to that in Fig. 3 for a well-burning experimental sample.

<table>
<thead>
<tr>
<th>Component</th>
<th>Molecular Weight (g/mole)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oil</td>
<td>515</td>
</tr>
<tr>
<td>Coke$_1$</td>
<td>24</td>
</tr>
<tr>
<td>Coke$_2$</td>
<td>12</td>
</tr>
</tbody>
</table>

Table 1. Molecular weights of lumped components
Table 2. Arrhenius parameters and heat of reaction for kinetics cell simulation.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Pre-exponential factor A</th>
<th>Units</th>
<th>Activation Energy, E (J/mol)</th>
<th>Heat of Reaction, ΔH (J/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>2.00 × 10^{12}</td>
<td>mol/cm³·min</td>
<td>9.30 × 10^{4}</td>
<td>-1.00 × 10^{5}</td>
</tr>
<tr>
<td>8</td>
<td>2.50 × 10^{8}</td>
<td>mol/cm³·min</td>
<td>5.20 × 10^{4}</td>
<td>3.00 × 10^{5}</td>
</tr>
<tr>
<td>9</td>
<td>4.00 × 10^{7}</td>
<td>l/min</td>
<td>9.50 × 10^{4}</td>
<td>0.00 × 10^{5}</td>
</tr>
<tr>
<td>10</td>
<td>1.00 × 10^{12}</td>
<td>mol/cm³·min</td>
<td>1.10 × 10^{5}</td>
<td>5.00 × 10^{5}</td>
</tr>
</tbody>
</table>

Figure 5. Kinetic cell simulation results with the given reaction model at 5 different heating rates: (left) oxygen consumed and (right) temperature within the kinetics cell.

Combustion Tube Experiment

The combustion tube experiment is designed to study in-situ combustion front propagation in one dimension. In this experiment, crude oil, water, sand (or field rock), and sometimes clay are mixed and then put in the combustion tube. The tube is held vertically and the gas is injected from the top. The upper part of the tube is heated using an electrical heater while nitrogen is injected. At roughly 400 °C, heaters are turned off and then air is injected. Temperature is measured along the tube using thermocouples placed at the center. It is observed that the temperature increases along the tube (with depth) and reaches a peak that indicates the combustion front and then sharply decreases. Oil and water production are recorded during the experiment. A gas analyzer that is placed at the end is used to capture the composition of the produced gases. The peak temperature, front propagation speed, and fuel requirement are obtained from the combustion tube experiment.

Figure 7 depicts a sample temperature history in the tube versus time (Glatz et al, 2011). Thermocouples are at fixed locations as indicated in the legend. Note that the sustained peak combustion temperature is about 620 °C. Figure 8 is an example of flue gas composition recorded (Glatz et al, 2011). The gas analyzer is able to record effluent oxygen, carbon dioxide, carbon monoxide, and methane. The combustion behavior may also be monitored using a CT-scanner.
Figure 6. Isoconversional fingerprint computed from synthetic model: (left) effective activation energy versus conversion and (right) effective activation energy versus temperature.

Figure 7. Typical temperature history from a combustion tube experiment that had successful front propagation.
allowing visualization of the movement of the burning front and the liquids, respectively (Hascakir. et al., 2010).

**Figure 8.** Typical gas production history from a combustion tube experiment that had successful front propagation.

**Combustion Tube Simulation**

Next, combustion tube simulations are run with the reaction model at the system backpressure, 100 psi in the example to follow. The 1 meter long combustion tube is modeled with a fine grid and grid refinement studies ensure a converged solution. In the example, 912 grid blocks in the \( z \) direction and 4 in the \( r \) direction. The first block in the \( r \) direction represents the porous medium, the second block is the tube wall, the third is the insulation, and the fourth block is the relatively large grid block (at room temperature) that is used to account for the heat losses. The results are given in Fig. 9. The temperature history at 5.5 cm intervals along the combustion tube is plotted as is the effluent gas rate. As it is shown by the temperature profiles, a combustion front propagates in the tube.

One noticeable behavior regarding Fig. 9 is the oscillations in gas rates after 2 hours. Interestingly, similar oscillations are in fact also present in our combustion tube experiments as well as those of different researchers (Baena et al., 1990; Fassihi, 1981; Mamora, 1993). Most of the time, these oscillations are attributed to the local differences in oil (consequently coke) concentration due to packing (Baena et al., 1990).

Careful investigation of combustion tube experiments reveals that the magnitude of these oscillations correlate well with the amount of oxygen that passes through the combustion front suggesting that oxygen addition reactions are responsible for the oscillatory behavior. The amount of oxygen consumed at the combustion front is directly proportional to the amount and the reactivity of the coke deposited. The reactivity of coke deposited is determined by the conditions during coke formation. These depend mainly on the availability of oxygen. As indicated in this study, the presence of oxygen during coke formation increases the concentration of the oxygen functional groups (active sites) on the coke surface. Also, it is well known that low temperature reactions increase the amount of coke deposited (Alexander et al., 1962). Oxygen is only available for coke formation reactions if the oxygen penetrates the combustion front. That is, more oxygen is supplied than required for
the combustion reaction. Note that these experiments are conducted at a constant air flow rate. In most of these experiments, the oxygen is present ahead of the combustion front where coke formation reactions take place increasing the amount and the reactivity of the coke deposited. When the combustion front reaches the region where the coke formed in the presence of oxygen, more oxygen is consumed due to the increase in the amount deposited and increased reactivity due to oxygen functional groups. More oxygen consumption decreases the amount of oxygen penetrating the combustion front. Consequently, coke deposited is less in amount and also less reactive. When this coke is burned, more oxygen penetrates and coke deposited is again more reactive completing and starting another cycle. This behavior could be the reason for the oscillations in the effluent gas concentrations.

In the simulations two different kinds of coke are assumed to play a role in the combustion with different reactivity. The relative amount of these components change with the amount of oxygen available for coking reactions. The formation of Coke\(_1\) in Eq. 7 competes with the transformation of Coke\(_1\) to Coke\(_2\) in Eq 9 leading to an oscillatory lay down of coke and subsequent oxidation.

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**Figure 9.** Front propagation in the combustion tube simulation.

**Reaction Upscaling for Field Scale Simulation**

We use Arrhenius kinetics to model the reactions and history-match laboratory experiments. We use a large number of small grid blocks with enough resolution to ensure convergence and accuracy at lab scale. The high resolution kinetics model obtained is used to perform ISC reaction upscaling. The full description of the method is found elsewhere (Zhu. et al., 2011; Zhu, 2011). A first step in the upscaling is to extract the most important parameter: the fuel amount \(S_{o,fuel}\). The fuel amount is the equivalent oil saturation that is converted to the fuel for in-situ combustion. Through
fine-scale calibration tests or experiment, we generate a table for fuel amount, $S_{o,fuel}$, with respect to different operating conditions such as pressure, initial condition, type of porous media, and so on. This information is then fed into field-scale reservoir simulation.

For field-scale simulation, non-Arrhenius kinetics are used. In a sense, $S_{o,fuel}$ is assumed to burn instantaneously. This simplifying assumption appears to be warranted in large grid blocks where the rates of reaction are quite large relative to the rate of fluid movement. The method treats the in-situ combustion reaction front as a sub-grid phenomenon. We focus on the equivalent reaction effects on a large field-scale simulation grid. That is, the amount of heat released, oil burned, and reaction products generated on a field-scale simulation grid block. In this way, we achieve consistency when scaling up from lab to field.

Although this approach requires calibration of the above mentioned input parameters, it is attractive because it significantly reduces grid-size dependencies. In this way, the reaction terms are insensitive to grid size. This approximate approach also removes the severe stiffness encountered in the traditional ISC simulation, and can be effectively used for large field-scale simulation and optimization studies.

An example in one dimension is given in Fig. 10. The domain is 2.1 m long and so is of the same order as a laboratory combustion tube test. Simulations with full Arrhenius kinetics are compared to the upscaling procedure. To resolve fully the temperature profile, 600 equally sized grid blocks are used during simulations with Arrhenius kinetics. Coarse simulations employing only 10 grid blocks are compared to the fine-grid result. The first coarse grid solution is computed using Arrhenius kinetic parameters. The second coarse grid solution is computed using the upscaling procedure with an $S_{o,fuel}$ of 8% as obtained from combustion tube experimental results. In both cases, only 10 grid blocks are used. Comparing the fine and coarse grid solutions teaches that the upscaling procedure has produced results for which the peak temperature and its location well approximate the fine-grid solution. The leading edge of the oxygen bank is also well approximated as is the concentration within the oxygen bank.

The coarse grid simulation implementing Arrhenius kinetics disagrees substantially with the fine-grid result. Note that the combustion front is significantly retarded on the coarse grid and the peak temperature is over 1000 °C. Essentially, the large grid blocks and fast reaction kinetics have created a situation where too much coke is generated, relative to the fine-grid result. Because there is too much coke, excessive oxygen is consumed, excess heat is generated, and the front lags behind where it is predicted in a fully converged simulation.

The second upscaling exercise shown here is a grid coarsening study in a three-dimensional volume. In this case, fully converged Arrhenius-based kinetic simulations are too costly to compute. Only results from the upscaling methodology are given. The reservoir volume is homogeneous and is 150m by 63m by 15m. A vertical air injector is on the left and a producer on the right. The $S_{o,fuel}$ is set to 8%. Three different grid resolutions are used: 50 by 21 by 10 blocks, 25 by 11 by 10 blocks, and 10 by 11 by 5 blocks.

Comparison of the $O_2$ concentration and temperature profiles in the top view shows that all grid resolutions track front movement horizontally. For the grid resolutions of 50 by 21 by 10 and 25 by 11 by 10, gravity override of air is clearly captured. When using the 10 by 11 by 5 grid, the simulation has some problem in representing the gravity override because of the coarse grid in the vertical direction, as expected.

Importantly, the simulation results are consistent across the three different grid sizes for identical input. In this fashion, our upscaling methodology is fundamentally different from parameter adjustment within an Arrhenius kinetics based model. A different set of parameters would be needed for each grid resolution and these parameters are determined in a trial and error manner. This
Figure 10. One-dimensional upscaling of ISC. Kinetic and upscaled model use different grid resolutions. The coarse upscaled model matches the fine-scale kinetics based reference solution while the coarse scale kinetic model fails.

Discussion

A single experiment or characterization procedure is insufficient to probe fully the complex (and numerous) series and parallel reactions as well as the highly exothermic reactive transport that is characteristic of in-situ combustion. The workflow presented here integrates a suite of experiments along with high-resolution mechanistic simulation consistently in space and time. A particular reaction model is calibrated by matching multiple experiments conducted at different heating rates. Experimental design is driven in part to yield data that is useful for model development. For example, the isoconversional, apparent activation energy fingerprint of an oil is useful for both screening and to be assured that the ensemble of reactions mimics the measured RTO kinetic behavior.

With respect to screening based on the isoconversional fingerprint, Fig. 4 is an example fingerprint of a crude-oil/rock system that does not burn well in a combustion tube experiment. We did not dwell on examples that fail to propagate a combustion front. Elsewhere (Cinar et al., 2011), we have demonstrated the considerable predictability obtained by screening based on isoconversional fingerprint. That study examined the RTO kinetics and combustion tube performance of 10 crude-oil/rock samples. Isoconversional fingerprints, such as those in Figs. 3 and 4 indicated that 6 samples should and 4 samples should not propagate a combustion front at test conditions. Combustion tube tests subsequently confirmed the predictions from isoconversional analysis.

Reaction schemes developed to reproduce the effluent gas history from RTO kinetics experiments accurately portrayed successful combustion front propagation, as shown here. Similar reaction schemes developed for poor combustion candidates failed to show ignition and propagation during simulation of combustion tube tests (Cinar et al., 2011-b). Our workflow, potentially, reduces the
number of more difficult and time intensive combustion tube tests through our novel screening process.

Due to space considerations, we only described one method to obtain a calibrated reaction model. Elsewhere (Lapene. et al., 2011-a,–b), we describe the parallel approach whereby a reaction model with initial estimation of reaction parameters is introduced to a fully compositional simulation model of the kinetics cell experiment. A multiobjective genetic algorithm optimization is used to obtain the reaction parameters such that the simulation result matches the kinetics cell experiment. An inherent advantage in this alternate approach is that the optimization produces multiple reaction models that match the data equally well. As these different reaction models are easily propagated forward in the workflow, a natural approach to uncertainty evaluation is available.
The literature documents the clear limitations and numerical errors associated with simulation of ISC at reservoir scale employing large grid blocks and Arrhenius kinetics (Gutierrez et al., 2009). The literature also makes clear that it is difficult to extract parameter values from laboratory tests to use in field and laboratory-scale simulations. The upscaling methodology eliminates ad hoc treatment of reaction kinetics and in-situ combustion at reservoir scale. The multireaction mechanistic model of one-dimensional combustion provides a means to explore combustion success at conditions not investigated experimentally. Such mechanistic models also provide the means to predict the fuel amount under a variety of oxygen partial pressure and temperature histories. The fuel amount is the main parameter needed in the upscaled, non-Arrhenius model of combustion.

**Summary**

A workflow combining experimental measurements, full-physics mechanistic simulation, and upscaling is proposed to predict the likelihood of successful and unsuccessful ISC at field scale. The development of useful simulation parameters is a natural feature of the workflow. Measurements of crude-oil combustion characteristics at lab scale are important to the overall effort and, importantly, the combination of RTO kinetics and combustion tube measurements suggests a high resolution pseudo-reaction model that is predictive of combustion at lab scale. Successively, this high-resolution model is used to provide the oil saturation that is converted to fuel and subsequently burned as a function of oxygen partial pressure, oxygen flux, rock type and heterogeneities and so on. Field-scale simulations do not employ Arrhenius kinetics. As a result, significant stiffness is removed from the finite difference simulation of the governing equations. Accordingly, field-scale simulations run quickly in comparison to cases employing Arrhenius kinetics. Results employing the new upscaling methodology show very little sensitivity to grid block size.

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