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## Introduction

Heavy oil and oil sands are important hydrocarbon resources that account for over 10 trillion barrels (Meyer et al., 2007), nearly three times the conventional oil in place in the world. There are huge, wellknown resources of heavy oil, extra-heavy oil, and bitumen in Canada, Venezuela, Russia, the USA and many other countries. The oil sands of Alberta alone contain over two trillion barrels of oil. In Canada, approximately 20% of oil production is from heavy oil and oil sand resources.

The process of In-Situ Upgrading (ISU) by subsurface pyrolysis has been applied in various pilot projects and laboratory experiments (Fowler and Vinegar, 2009; Kumar et al., 2011). This process is only effective if the formation is heated above 300°C. At this temperature, the long chain oil molecules that mostly compose kerogen and bitumen decompose through a series of chemical reactions of pyrolysis and cracking. This results in the production of small hydrocarbon molecules, and thus improves the quality of the recovered oil. There are various potential advantages of using an ISU process instead of the more common process of steam injection (Butler and Stephens, 1981). Firstly, at the recovery stage, there would be no requirement for a nearby water supply and water recycling facilities. Secondly, since upgrading of the oil takes place in-situ, the heavy components like coke will be left in the reservoir, and so the produced oil is lighter and of higher commercial value (Snow, 2011). As a result, using the ISU process will lead to a reduction in the amount of required infrastructure and expenses on site for refining and pre-upgrading before transport.

Modelling ISU is complex as various physical and chemical phenomena need to be represented. In addition to the transport of fluids through porous media and the change of properties with varying pressure and temperature, ISU involves transport of heat, evaporation, condensation and several chemical reactions. The temperature scale goes from initial reservoir temperature to several hundreds of degrees celsius. As a result, thermodynamic and petrophysical properties vary significantly within the reservoir. Moreover, describing the complex chemistry accurately requires a large number of hydrocarbon components and chemical reactions. In this context, a compositional description is mandatory.

Despite the advent of faster and more powerful computers, numerical simulation of the ISU process is challenging because of the large number of physical mechanisms that need to be modelled and the non-linearity of the equations describing these processes. Various methods for reducing the Central Processing Unit (CPU) time in simulations can be considered. One can identify several numerical operators in the simulation: heat transport and diffusion, mass transport, and chemical reaction. The time constant of the system is driven by the most penalizing operator. Decoupling techniques, or so-called Operator Splitting (OS) methods, provide a framework to deal separately with each operator and then propose a dedicated resolution (special numerical schemes, explicit/implicit) that leads to smaller systems and improve computational efficiency (Barry et al., 1997; Lanser and Verwer, 1999). However, a significant drawback of splitting technique is that decoupling the governing equations introduces an additional source of numerical error, known as the splitting error (Valocchi and Malmstead, 1992).

In this paper, we develop a mathematical model that can be used to represent the ISU of heavy oil or oil shale. We then describe several operator splitting methods to solve the non-linear systems, and evaluate them on two test cases by considering the evolution of the discretization error with the size of the time-step compared with the result of a fully implicit simulation.

## Mathematical Model

The ISU process generally uses tightly spaced electrical heaters to slowly and uniformly heat the formation by thermal conduction to the conversion temperature of about 350° C (Fowler and Vinegar, 2009). In this paper, we define a one dimensional domain that contains one heater and one producer well (figure 1). To define the boundary conditions, we assume constant temperature around the heater and constant bottom hole pressure (bhp) at the producer. Due to the symmetry of the problem, we assume no heat

transfer by conduction around the producer.

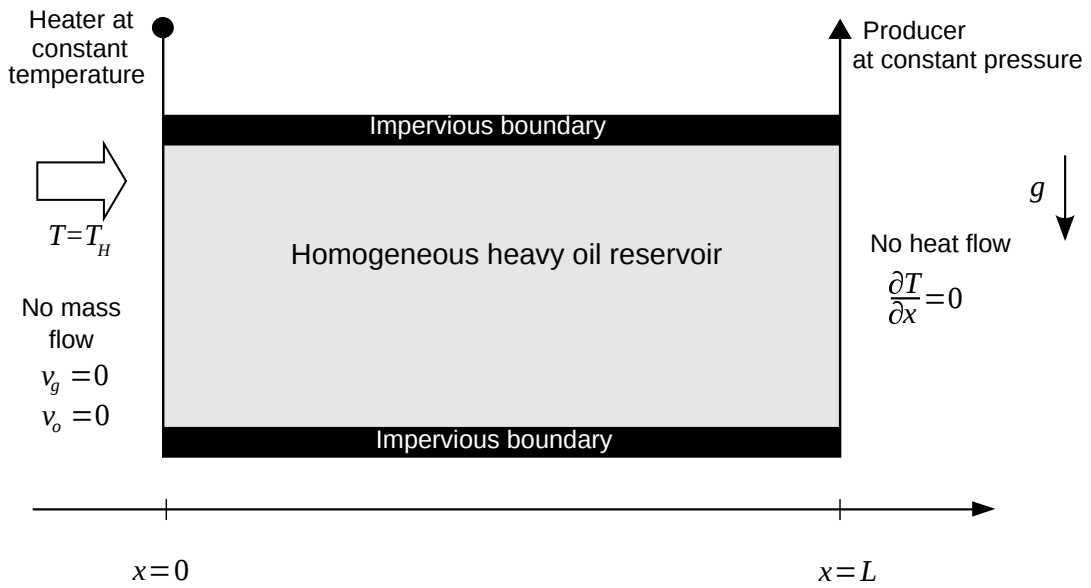


Figure 1 One dimensional model for ISU

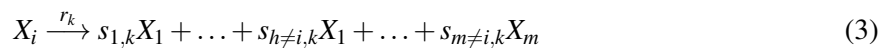
The model contains three phases: gas, liquid and solid. The solid phase is formed by kerogen and/or coke. Gravity is neglected so the model can be considered one dimensional. The mass-balance equation for compositional simulation for each fluid component  $j$  can be expressed as follows (Watts, 1986):

$$\frac{\partial}{\partial t} \left( \phi \sum_p \alpha_{j,p} \rho_p S_p \right) = - \frac{\partial}{\partial x} \left( \sum_p \alpha_{j,p} \rho_p v_p \right) + \sum_k s_{j,k} r_k \quad (1)$$

where  $\phi$  is the rock porosity,  $S_p$ ,  $\rho_p$  and  $v_p$  the saturation, molar density and velocity of phase  $p$ ,  $\alpha_{j,p}$  the mole fraction of component  $j$  in phase  $p$ ,  $s_{j,k}$  the stoichiometric coefficient for component  $j$  as a product ( $s_{j,k} > 0$ ) or a reactant ( $s_{j,k} < 0$ ) of reaction  $k$  and  $r_k$  the rate of reaction  $k$ . The velocity is given by Darcy's law:

$$v_p = -K \frac{k_{rp}}{\mu_p} k_s \frac{\partial P}{\partial x} \quad (2)$$

where  $P$  is the pressure,  $K$  is the rock permeability,  $k_{r,p}$  and  $\mu_p$  are the relative permeability and viscosity of phase  $p$  and  $k_s$  is the solid mobility multiplier, which is a function of the solid saturation. We assume that the thermally unstable chemical entities decompose with first-order kinetics. The reactivity of an entity  $X_i$  can be accounted for by one chemical reaction with one reactant:



The rate of reaction is modelled using an Arrhenius law of order 1:

$$r_k = A_k \exp \left( - \frac{E_k}{RT} \right) C_i \quad (4)$$

where  $A_k$  and  $E_k$  are the frequency factor and the activation energy of reaction  $k$ ,  $R$  is the universal gas constant and  $C_i$  is the mole concentration of the reactant  $X_i$  of reaction  $k$ . Phase equilibrium is modeled using Wilson  $K$ -values (Wilson, 1968). Heat transfer is accounted for in the overall energy balance equation (Mifflin et al., 1991):

$$\frac{\partial}{\partial t} \left( (1 - \phi) \rho_r u_r + \phi \sum_p \rho_p u_p S_p \right) = - \frac{\partial}{\partial x} \left( \sum_p \rho_p v_p h_p \right) + \frac{\partial}{\partial x} \kappa \frac{\partial T}{\partial x} + \sum_k \Delta h_{r,k} r_k \quad (5)$$

where  $\rho_r$  and  $u_r$  are the rock density and internal energy,  $u_p$  and  $h_p$  are the phase internal energy and enthalpy,  $\kappa$  is the thermal conductivity of the system and  $\Delta h_{r,k}$  is the reaction enthalpy of  $k$ . Finally, we obtain the following of equations for the boundary conditions:

$$\begin{aligned} \text{at } x = 0, \quad v_p &= 0, \quad \forall p \\ &T = T_H \\ \text{at } x = L, \quad P &= P_0 \\ &\frac{\partial T}{\partial x} = 0 \end{aligned} \tag{6}$$

Where  $L$  is the length of the domain,  $P_0$  the initial pressure and  $T_H$  the heater temperature. This mathematical model can be used to describe both thermal decomposition of oil shale and bitumen. In the next section, we explore the precision and convergence of OS methods to solve the governing equations.

### Operator Splitting Methods

Operator splitting methods have been previously applied to a wide range of applications, including groundwater transport simulations (Barry et al., 1997), air pollution modelling (Lanser and Verwer, 1999) and combustion-reaction problems (Pope and Ren, 2009). They provide a framework to deal separately with the transport and the chemical reaction steps. Thus, dedicated solvers can be applied to each operator. Accurate ODE (ordinary differential equation) solvers can be employed to cope with the sometimes stiff systems of equations describing the chemical reactions while Fully Implicit (FIM), Implicit Pressure Explicit Saturation (IMPES) or Adaptive Implicit (AIM) (Coats, 2003) method can be used to deal with the transport step. Different time-step strategies can be applied to the different operators, and in the case of ODE, local time-steps may be used. Moreover, in many cases, the chemical reaction operator depends on variables that do not affect the transport. Complex kinetic models sometimes require a large number of components, while the transport step can be described with a small number of pseudo-components (Kumar et al., 2011).

The convergence and precision of operator splitting methods have been extensively studied for linear or quasi-linear operators (Valocchi and Malmstead, 1992). Applying these methods to the modelling of ISU could potentially improve both precision and performance. There are a large number of operator splitting methods published in the literature (Carrayrou et al., 2004; Farago et al., 2008). In this paper, we describe the most common methods and evaluate their precision and convergence on two different test cases. Test case 1 is a one dimensional model representing ISU of oil shale adapted from Fan et al. (2010). In test case 2, pyrolysis is applied to a fluid representing Athabasca tar-sands adapted from Kumar et al. (2011). The best performing method is applied to test case 3, where a very large number of components is necessary to describe the kinetics of pyrolysis, but they are regrouped into a small number of pseudo-components for the transport steps. We describe our methods on a Cauchy problem of the form:

$$\begin{cases} \frac{\partial u}{\partial t} = A.u + K.u, & t \in (0, T]. \\ u(0) = u_0 \end{cases} \tag{7}$$

where  $A$  represents the advection and thermal conduction operator and  $K$  the chemical reaction operator.

#### *Sequential Non Iterative Approach*

Operator splitting methods offer two distinct approaches. In a Sequential Non-Iterative Approach (SNIA), each operator is applied once sequentially. The simplest and most common of these methods is the Sequential Split Operator (SSO) (Carrayrou et al., 2004), which is a sequence of one transport

step followed by one chemical step (SSO-AK):

$$\begin{cases} \frac{\partial u^*}{\partial t} = A.u^*, & t \in [t^n, t^{n+1}], u^*(t^n) = u(t^n) \\ \frac{\partial u^{n+1}}{\partial t} = K.u^{n+1}, & t \in [t^n, t^{n+1}], u^{n+1}(t^n) = u^*(t^{n+1}) \end{cases} \quad (8)$$

SSO can be done the opposite way with one chemical step followed by one transport step (SSO-KA):

$$\begin{cases} \frac{\partial u^*}{\partial t} = K.u^*, & t \in [t^n, t^{n+1}], u^*(t^n) = u(t^n) \\ \frac{\partial u^{n+1}}{\partial t} = A.u^{n+1}, & t \in [t^n, t^{n+1}], u^{n+1}(t^n) = u^*(t^{n+1}) \end{cases} \quad (9)$$

In SNIA the splitting error arises from the decoupling of the governing equations and has been extensively studied for linear operators (Valocchi and Malmstead, 1992). In this case, it can be linked to the asymmetry of the operator decoupling. The classical SSO can be modified by using two time-steps in an effort to cancel the splitting error, as is done in the Strang-Marchuk Split Operator (SMSO) sometime called the Alternate Split Operator (ASO) (Strang, 1968; Carrayrou et al., 2004):

$$\begin{cases} \frac{\partial u^*}{\partial t} = A.u^*, & t \in [t^{2n}, t^{2n+1}], u^*(t^{2n}) = u(t^{2n}) \\ \frac{\partial u^{2n+1}}{\partial t} = K.u^{2n+1}, & t \in [t^{2n}, t^{2n+1}], u^{2n+1}(t^{2n}) = u^*(t^{2n+1}) \end{cases} \quad (10)$$

and

$$\begin{cases} \frac{\partial u^{**}}{\partial t} = K.u^{**}, & t \in [t^{2n+1}, t^{2n+2}], u^{**}(t^{2n+1}) = u^{2n+1}(t^{2n+1}) \\ \frac{\partial u^{2n+2}}{\partial t} = A.u^{2n+2}, & t \in [t^{2n+1}, t^{2n+2}], u^{2n+2}(t^{2n+1}) = u^{**}(t^{2n+2}) \end{cases} \quad (11)$$

For constant linear operators, SMSO cancels the splitting error of order one (Valocchi and Malmstead, 1992), but these findings do not necessarily apply to ISU where the coupling between transport and chemical reactions is strongly non-linear. In this paper, we evaluate SSO-AK, SSO-KA and SMSO. First, we solve the full system of equations with no splitting using an implicit solution technique. We choose a small time-step (0.01 day) in order to obtain a reference solution  $\bar{P}$  for pressure,  $\bar{T}$  for temperature,  $\bar{S}_p$  for saturations and  $\bar{z}_j$  for overall compositions. We then study the evolution of the relative error between our reference solution and the three SNIA described above as a function of the time-step. Newton-Raphson's algorithm is applied to handle non-linearities. We use the following definitions for the normalized error for each variable:

$$\begin{aligned} e_P &= \max_n \left( \frac{1}{n_d} \sum_{x_j} \frac{|P(t^n, x_j) - \bar{P}(t^n, x_j)|}{P_0} \right), & e_T &= \max_n \left( \frac{1}{n_d} \sum_{x_j} \frac{|T(t^n, x_j) - \bar{T}(t^n, x_j)|}{\Delta T} \right) \\ e_S &= \max_p \max_n \left( \frac{1}{n_d} \sum_{x_j} |S_p(t^n, x_j) - \bar{S}_p(t^n, x_j)| \right), & e_z &= \max_j \max_p \left( \frac{1}{n_d} \sum_{x_j} |z_j(t^n, x_j) - \bar{z}_j(t^n, x_j)| \right) \end{aligned} \quad (12)$$

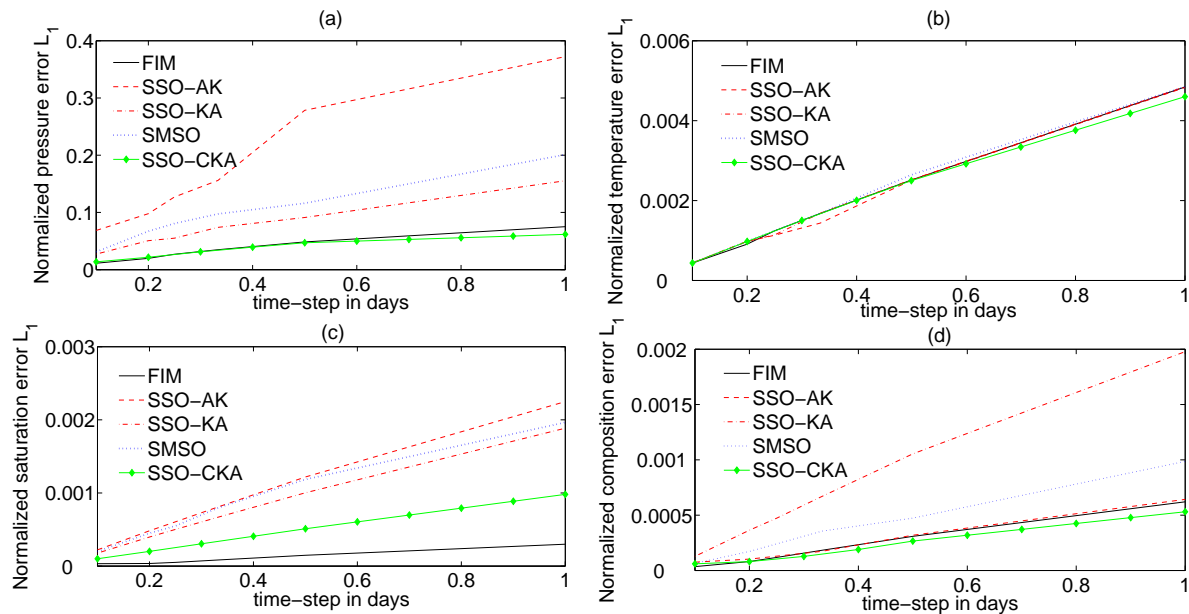
Figures 2 and 3 show the evolution of the normalized errors with the time-step for test case 1 and test case 2. For test case 1, we observe that the SSO-AK gives a large pressure error. The pressure rose during the chemical reaction step and could reach non-physical values if not relaxed by a transport step afterwards. However, we obtain a small composition error. On the other hand, SSO-KA has a limited pressure error but the saturation and composition errors are large. SMSO gives a compromise between the two methods but the pressure and saturation errors are still too large. For test case 2, the pressure error was less important. As a result, SSO-AK gives very good results but SSO-KA and SMSO still generate large saturation and composition errors.

A New Splitting Method : SSO-CKA

When the operator  $K$  is performed before  $A$ , as in SSO-KA and a half step of SMSO, the chemical reactions are computed with a temperature that has not been transported yet. The thermal conduction is the dominant process controlling the temperature for ISU, so we try to solve this problem by using a splitting scheme where the thermal conduction is performed first (operator  $C$ ), followed by a chemical reaction step (operator  $K$ ) and finally the advection part with no thermal conduction (operator  $A'$ ). This method is defined as SSO-CKA:

$$\begin{cases} \frac{\partial u^*}{\partial t} = C.u^*, & t \in [t^n, t^{n+1}], u^*(t^n) = u(t^n) \\ \frac{\partial u^{**}}{\partial t} = K.u^{**}, & t \in [t^n, t^{n+1}], u^{**}(t^n) = u^*(t^{n+1}) \\ \frac{\partial u^{n+1}}{\partial t} = A'.u^{n+1}, & t \in [t^n, t^{n+1}], u^{n+1}(t^n) = u^{**}(t^{n+1}) \end{cases} \quad (13)$$

The evolution of the normalized errors with the dimensionless time-step for SSO-CKA are also plotted on figures 2 and 3. We observe that it gives the best compromise in term of discretization error.

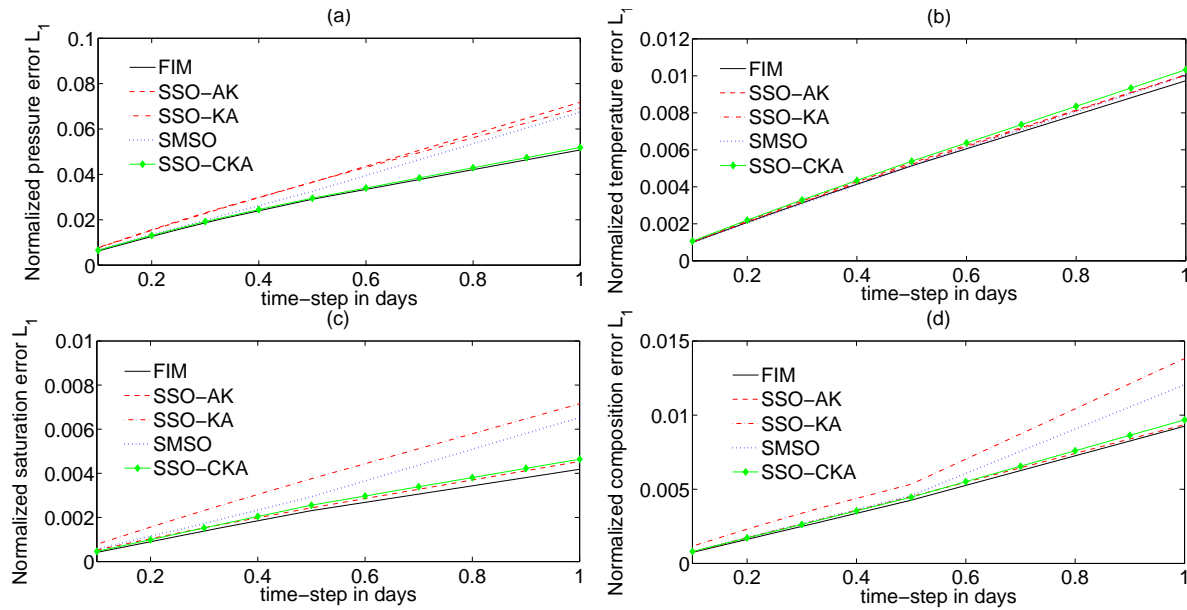


**Figure 2** Normalized error in (a) pressure, (b) temperature, (c) saturation and (d) composition with respect to the time-step size for test case 1. We observe that SSO-CKA gives the best compromise in term of discretization error.

Sequential Iterative Approach

The second category of operator splitting methods is the Sequential Iterative Approach (SIA), which attempts to eliminate or control the splitting error through an iterative process. Unlike SNIA, each sub-step of an iterative scheme solves an approximation to the fully coupled PDE system. The simplest of these methods is the Iterative Split Operator (ISO) (Fargo et al., 2008):

$$\begin{aligned} \frac{\partial u_{2i+1}^*}{\partial t} &= A.u_{2i+1}^* + K.u_{2i}^* & t \in [t^n, t^{n+1}]. \\ u_{2i+1}^*(t^n) &= u_n(t^n) \\ \frac{\partial u_{2i+2}^*}{\partial t} &= A.u_{2i+1}^* + K.u_{2i+2}^* & t \in [t^n, t^{n+1}]. \\ u_{2i+2}^*(t^n) &= u_n(t^n) \end{aligned} \quad (14)$$



**Figure 3** Normalized error in (a) pressure, (b) temperature, (c) saturation and (d) composition with respect to the time-step size for test case 2. We observe that SSO-AK and SSO-CKA give very good results in term of discretization error.

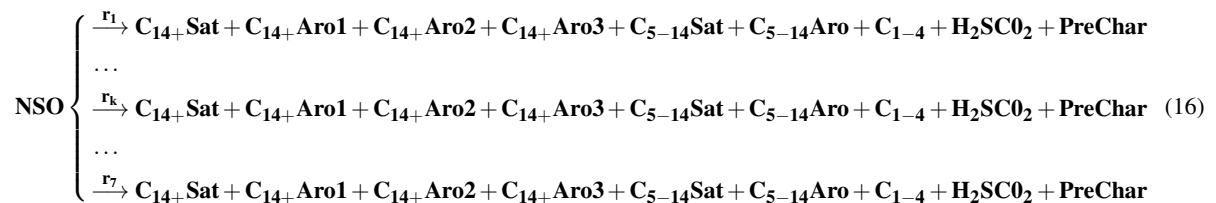
for  $i = 0, 1, \dots, m$  or until convergence. The function  $u_0^*$  is an arbitrarily chosen initial guess on the interval  $[t^n, t^{n+1}]$  and

$$u_{n+1}(t) = u_{2m+1}^*(t) \quad t \in [t^n, t^{n+1}]. \quad (15)$$

ISO converges for constant linear operators (Farago et al., 2008) but not necessarily for a complex model such as ISU. Indeed, we have tested ISO on test cases 1 and 2 and for both cases, ISO does not converge for time-steps larger than 0.1 day. The mass balance error decreases after one or two cycles, but then instabilities appear due to the explicit/implicit treatment of operators  $A$  and  $K$  leading to large unphysical errors.

### Application to large chemical model

In this section, we consider the ISU of Athabasca oil sand bitumen (test case 3). The decomposition of the unstable  $NSO$  compounds can be described by a set of seven parallel reactions (Kumar et al., 2011):



Each of the parallel reactions has its own stoichiometry and reaction constant parameters. To approximate the total decomposition, one can apply a constant weight for each reaction rate  $r_k$ , but this approximation generates a large error in the hydrocarbon production rate (about 15%). To describe correctly the decomposition rate, one needs to split the  $NSO$  component into seven chemical entities, which have the same thermophysical properties and only differ in the stoichiometry of the chemical reactions. The decomposition of the product components  $C_{14+}$ ,  $C_{5-14}$  and  $PreChar$  can also be accounted for by sets of parallel reactions, and so they need to be split into separate chemical entities as well. In total, the model contains 27 reactions between 11 components that are split into 30 chemical entities. The simulation of such a model using FIM is very slow for three reasons:

- The number of variables by cell (pressure, temperature and compositions of chemical entity) to be

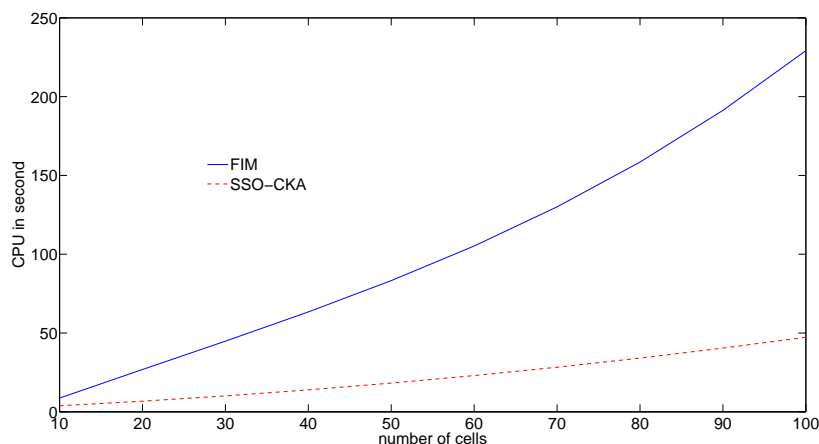


solved for each step of the Newton method is large (about 50% of the CPU time for test case 3)

- For each Newton iteration and for each cell, the thermal equilibrium between the 30 components must be calculated (about 20% of the CPU time for test case 3)
- For each Newton iteration and for each cell, the chemical reaction rate of each reaction (27) needs to be computed (about 30% of the CPU time for test case 3)

One can obtain a large speed-up when splitting the advection-conduction and the chemical reactions. The advection and conduction operators can be solved using only the 11 components because the thermal properties of the chemical entity inside one component are identical so the relative compositions inside one lumped component are constant during those steps. The linear system to be solved during a Newton step is significantly smaller (number of variables 13 instead of 32). The thermal equilibrium is calculated with the 11 components. Finally the chemical reaction rates are computed only when solving the operator  $K$ , which is fully local, so the chemical rates do not need to be computed for each cells at each Newton step but only for those which have not converged yet. In test case 3, the chemical reactions are significant only in the cells near the temperature front, so most of the cells (about 90%) have converged after 1 or 2 Newton iterations. Then for iteration 3 and above, we need to compute the chemical reaction rates only for the cells that have not converged yet.

Test case 3 has been simulated for 150 days with a time-step of 0.5 day, using a finite-volume code written in C++. We compared the results between one simulation using FIM and one using SSO-CKA. Figure 4 shows the CPU time for both methods. We obtained speed-ups between 3 and 5. Parallelisation



**Figure 4** Comparison of CPU time using FIM and SSO-CKA for test case 3. The simulations have been run for 150 days for different number of cells. We obtain a speed-up between 3 and 5.

could even further improve the speed-up since  $K$  is fully local. The bottleneck of the simulation is inside the advection which is solved with three time fewer variables than for FIM and with no chemical reactions. The precision of the chemical reaction operator could be improved by using smaller and local time-steps or higher order non-linear methods such as Runge-Kutta (Valocchi and Malmstead, 1992).

## Conclusions

This work has focused on the application of operator splitting methods (OS) to simulate the process of heavy oil ISU, where heavy components such as kerogen or  $NSO$  compounds decompose into lighter liquid and gas components. We showed that the simple Sequential Split Operator (SSO, in both direction AK or KA) applied to an oil shale test case adapted from Fan et al. (2010) (test case 1) and a bitumen test case adapted from Kumar et al. (2011) (test case 2) led to unacceptable time discretization errors.



Moreover, unlike for constant linear operators A and K, the Strang-Marchuk Split Operator (SMSO) did not significantly reduce the splitting error. We solved this issue with a splitting scheme where the thermal conduction was performed first, followed by a chemical reaction step and finally advection with no thermal conduction (SSO-CKA).

OS methods have the potential to improve the precision of the chemical reaction operator and decrease the computation time. To illustrate the later, we compared the CPU time of a simulation using FIM and one using SSO-CKA for a test case with 11 components that needs to be split into 30 components to represent accurately the chemical reactions (test case 3). The speed-ups obtained are between 3 and 5.

The method proposed led to small time discretization errors in the three cases presented here but the splitting error could be large for other applications. In order to ensure the applicability of SSO-CKA for the simulation of the ISU process, one could study the sensitivity of the splitting error with several physical parameters (reaction enthalpy, activation energy of chemical reactions...). We also observed that the Iterative Split Operator (ISO) was not converging for both test case 1 and 2. In practice, this method could not be applied on its own but may be used in future work to accelerate the fully implicit method in the non-linear or linear step.

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