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Modelling in-situ upgrading of heavy oil using operator splitting method

Julien Maes¹ · Ann H. Muggeridge¹ · Matthew D. Jackson¹ · Michel Quintard^{2,3} · Alexandre Lapene⁴

Abstract The in-situ upgrading (ISU) of bitumen and oil shale is a very challenging process to model numerically because of the large number of components that need to be modelled using a system of equations that are both highly non-linear and strongly coupled. Operator splitting methods are one way of potentially improving computational performance. Each numerical operator in a process is modelled separately, allowing the best solution method to be used for the given numerical operator. A significant drawback to the approach is that decoupling the governing equations introduces an additional source of numerical error, known as the splitting error. The best splitting method for modelling a given process minimises the splitting error whilst improving computational performance compared to a fully implicit approach. Although operator splitting has been widely used for the modelling of reactive-transport problems, it has not yet been applied to the modelling of ISU. One reason is that it is not clear which operator splitting technique to use. Numerous such techniques are described in the literature and each leads to a different splitting error. While this error has been extensively analysed for linear operators for a wide

range of methods, the results cannot be extended to general non-linear systems. It is therefore not clear which of these techniques is most appropriate for the modelling of ISU. In this paper, we investigate the application of various operator splitting techniques to the modelling of the ISU of bitumen and oil shale. The techniques were tested on a simplified model of the physical system in which a solid or heavy liquid component is decomposed by pyrolysis into lighter liquid and gas components. The operator splitting techniques examined include the sequential split operator (SSO), the Strang-Marchuk split operator (SMSO) and the iterative split operator (ISO). They were evaluated on various test cases by considering the evolution of the discretization error as a function of the time-step size compared with the results obtained from a fully implicit simulation. We observed that the error was least for a splitting scheme where the thermal conduction was performed first, followed by the chemical reaction step and finally the heat and mass convection operator (SSO-CKA). This method was then applied to a more realistic model of the ISU of bitumen with multiple components, and we were able to obtain a speed-up of between 3 and 5.

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Keywords Heavy oil · Oil shale · Operator splitting method

1 Introduction

Heavy oil and oil sands are important hydrocarbon resources that account for over 10 trillion barrels [1], nearly three times the conventional oil in place in the world. There are huge, well-known 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 [2, 3]. This process is only effective if the formation is heated above 300 °C. At this temperature, the long chain hydrocarbon 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 [4]. 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 [5]. 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, change of phase and several chemical reactions. The temperature scale goes from initial reservoir temperature (between 10 and 40 °C) to several hundreds of degrees Celsius. As a result, thermodynamic and petro-physical properties vary significantly within the reservoir. Moreover, describing the complex chemistry accurately may require 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 [6, 7]. However, a significant drawback of splitting techniques is that decoupling the governing equations introduces an additional source of numerical error, known as the splitting error [8].

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 time-step size compared with the result of a fully implicit simulation. We observe that the error is least for a splitting scheme where the thermal conduction is performed first, followed by the chemical reaction step and finally the heat and mass convection operator (SSO-CKA). This method is then applied to a more realistic model of the ISU of bitumen with multiple components.

2 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 [2]. In this paper, we define a one-dimensional domain that contains one heater and one producer well (Fig.

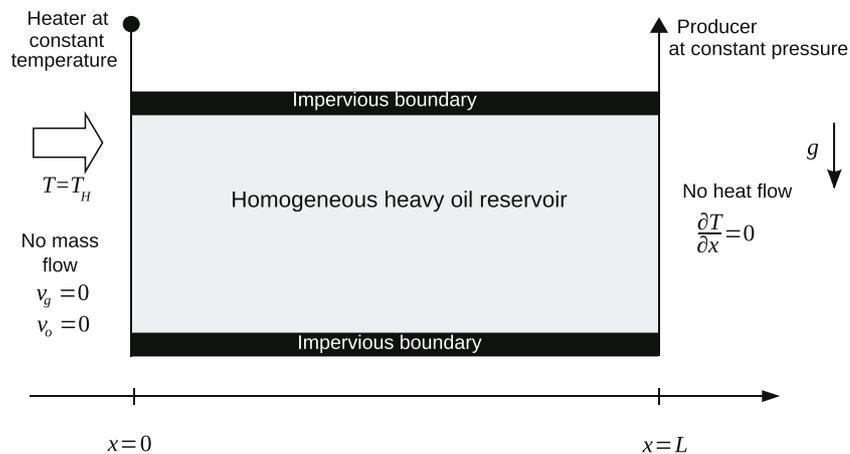


Fig. 1 One-dimensional model for ISU

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.

The model contains an inert rock phase r , with the pore-space occupied by three phases: gas (g), liquid (l), and solid phase (s). 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 [9]:

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

where ϕ is the rock porosity, S_p , ρ_p and v_p are 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 of phase p is given by Darcy's law:

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

where P is the pressure, K the rock permeability and $k_{r,p}$ and μ_p are the relative permeability and viscosity of phase p . The impact of the solid saturation on the permeability is given by a simple heuristic exponential relationship [10]:

$$K = K_0 \exp \left(a \frac{\phi_f - \phi_0}{1 - \phi_0} \right) \quad (3)$$

where ϕ_f is the current fluid porosity. K_0 and ϕ_0 are the initial permeability and fluid porosity, respectively. The fluid porosity is given by:

$$\phi_f = \phi (1 - S_s) \quad (4)$$

where S_s is the saturation of solid in the pores. The coefficient a determines how strongly the permeability varies with the change of solid saturation. Typically, a has a value between 5 and 50 [10]. We assume that the thermally unstable chemical entities decompose with first-order kinetics. The decomposition of an entity X_i can be accounted for by one chemical reaction with one reactant:



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

$$r_k = A_k \exp \left(- \frac{E_k}{RT} \right) C_i \quad (6)$$

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 modelled using Wilson K -values [11]. Heat transfer is accounted for in the overall energy balance equation [12]:

$$\frac{\partial}{\partial t} \left((1 - \phi) \rho_r u_r + \phi \sum_p \rho_p u_p S_p \right) = - \frac{\partial}{\partial x} \left(\sum_p \rho_p v_p h_p \right) + \frac{\partial}{\partial x} \left(\kappa \frac{\partial T}{\partial x} \right) + \sum_k \Delta h_{r,k} r_k \quad (7)$$

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

$$\begin{aligned} \text{at } x = 0, \quad v_p &= 0, \quad \forall p \\ &T = T_H \\ \text{at } x = L, \quad P &= P_0 \\ &\frac{\partial T}{\partial x} = 0 \end{aligned} \quad (8)$$

and the top and bottom surface are impervious boundaries. Here, L is the length of the domain, P_0 is the initial pressure and T_H is 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.

3 Operator splitting methods

A recurrent problem in reservoir simulation involving heat transfer and chemical reactions is to develop robust and accurate methods to solve these non-linear equations. Conventional reservoir simulations generally use one of three approaches: the fully implicit method (FIM), the sequential implicit method (SIM) and the implicit pressure explicit saturation (IMPES) method. FIM, in which all the unknown variables are treated implicitly, is the most common approach for thermal reservoir simulation [12]. This method is stable and can take very large time-steps, but is computationally expensive. For the same time-step, the IMPES formulation is computationally more efficient and also more accurate (introduces less numerical dispersion) than FIM [13]. However, treating some variables explicitly introduces limits on the size of the stable time-step that can be taken. To improve the efficiency of the method, the adaptive implicit method (AIM) [14, 15] combines the two approaches by treating some unknowns in the discrete model implicitly and other unknowns explicitly using a switching criterion. Alternatively, the SIM approach separates the solutions of the pressure and saturation equations

and solves each of these equations separately and implicitly [16]. SIM and AIM are more efficient in terms of computational time than FIM but less stable. For thermal reactive transport, high volumetric flow rates and large changes in gas volume create stability difficulties that are too severe to overcome and the transport is generally solved with a FIM approach. However, the choice of method to treat the chemical reactions remains open.

Operator splitting (OS) methods have been previously applied to a wide range of problems, including groundwater transport simulations [6], air pollution modelling [7] and combustion-reaction problems [17]. They provide a framework to deal separately with the transport and the chemical reaction steps and therefore simplify the resolution of the system. However, decoupling the equations introduce an additional source of error [8]. The convergence and precision of OS methods have been extensively studied for linear or quasi-linear operators [8, 19].

The control of this splitting error generates extra computational effort to obtain the same accuracy as a fully coupled approach, for example by decreasing the time-step size. Therefore, OS methods present an advantage in term of computational efficiency only if we can obtain large speeds-up for each steps.

Two methods can be considered to reduce the computational time. Dedicated solvers can be applied to each operator. Accurate ordinary differential equation (ODE) solvers can be employed to cope with the sometimes stiff systems of equations describing the chemical reactions while FIM, IMPES or AIM [14] methods can be used to deal with the transport step. Different time-step strategies can be applied to the different operators, and local time-steps may be used, especially in the case of ODEs, for which the operator is fully local.

Another method to reduce the CPU time is to use a lumped compositional model for one of the operator. In many cases, accurate kinetic modelling requires a large number of components, while the transport step can be described with a small number of lumped pseudo-components [3]. In this case, we can obtain a large speed-up by using the full model for the chemical reaction step and the lumped model for the transport step.

In this paper, we describe the most common methods and evaluate their precision and performance on three test cases. To simplify the notation, we describe the various splitting methods on a Cauchy problem of the form:

$$\begin{cases} \frac{\partial u}{\partial t} = A.u + K.u, & t \in (0, T]. \\ u(0) = u_0 \end{cases} \quad (9)$$

where A represents the advection and thermal conduction operator and K the chemical reaction operator. In the general case, A and K are non-linear operators.

3.1 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) [18], which is a sequence of one transport step followed by one chemical step:

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

which will be denoted SSO-AK to indicate the sequence of operator used. SSO can be done the opposite way with one chemical step followed by one transport step (SSO-KA):

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

For SSO-AK and SSO-KA, the splitting error arising from decoupling the governing equations is of order 1 [8]. For linear operators, this error can be related to the asymmetry of the decoupling. The classical SSO can be modified by using two time-steps and alternating the operators in an effort to cancel the splitting error of order 1, as is done in the Strang-Marchuk split operator (SMSO) (sometimes called the alternate split operator (ASO)) [18, 24]:

$$\begin{cases} \frac{\partial u^*}{\partial t} = A.u^*, & t \in [t^n, t^{n+1/2}], u^*(t^n) = u(t^n) \\ \frac{\partial u^{**}}{\partial t} = K.u^{**}, & t \in [t^n, t^{n+1}], u^{**}(t^n) = u^*(t^{n+1/2}) \\ \frac{\partial u^{n+1}}{\partial t} = A.u^{n+1}, & t \in [t^{n+1/2}, t^{n+1}], u^{n+1}(t^n) = u^{**}(t^{n+1}) \end{cases} \quad (12)$$

For linear operators, SMSO cancels the splitting error of order 1 [8] and so is of order 2. However, these findings do not necessarily apply to ISU where the coupling between transport and chemical reactions is strongly non-linear.

3.2 A new splitting method: SSO-CKA

When the operator K is performed before A , as in SSO-KA and in a half step of SMSO, the chemical reactions are computed with the temperature calculated at the previous time-step. 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:

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

SSO-CKA tries to take advantage of the fact that most of the effect of advection-diffusion on the chemical reaction comes from heat conduction if (1) reactants are transported slowly in the domain and (2) reaction enthalpies are small. Condition (1) implies that the mass advection A' has only a small effect on the operator K . It is true if only a small proportion of the reactant exists in the gas phase. Condition (2) implies that K has a small effect on C . Reaction enthalpies are generally neglected in the modelling of ISU [20, 21] and we follow this approximation in this work. However, we note that it could have a large impact on the process [22].

3.3 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) [19]:

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

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 is stable and converges for linear operators [19]. Note that each of the sub-steps is not necessarily stable. For example, if the chemical constants in K are larger than 1, the first step is obviously unstable. It is the iterations over the splitting scheme and the alternating between implicit and explicit treatment for each operators that stabilize the method in linear systems. However, we do not have such a result for non-linear operators.

4 Comparison of FIM and SNIA methods

We evaluate the precision of FIM, SSO-AK, SSO-KA, SMSO and SSO-CKA on two test cases. For each test case, we define a reference solution by solving the full system of equations with FIM with a time-step of 0.01 days and a $100 \times 1 \times 1$ mesh. The reference solution is denoted by \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 with the reference solution for the FIM and the three SNIA described above as a function of the time-step for a $50 \times 1 \times 1$ mesh. We use the following definitions for the normalized error L_1 for each variable:

$$\begin{aligned} e_P &= \max_n \left(\frac{1}{n_d} \sum_{x_j} \frac{|P(t^n, x_j) - \bar{P}(t^n, x_j)|}{P_0} \right), \\ e_T &= \max_n \left(\frac{1}{n_d} \sum_{x_j} \frac{|T(t^n, x_j) - \bar{T}(t^n, x_j)|}{\Delta T} \right), \\ e_S &= \max_p \max_n \left(\frac{1}{n_d} \sum_{x_j} |S_p(t^n, x_j) - \bar{S}_p(t^n, x_j)| \right), \\ e_z &= \max_j \max_p \left(\frac{1}{n_d} \sum_{x_j} |z_j(t^n, x_j) - \bar{z}_j(t^n, x_j)| \right) \end{aligned} \quad (16)$$

For SMSO, we use two time-steps to solve the chemical reactions. This way, the four methods perform the same number of transport steps and the same number of chemical reaction steps. For SSO-CKA, we perform one additional heat conduction step. However, since the heat conduction has been extracted from the operator A , the temperature can be treated explicitly in the transport step [15]. This way, the computational effort is roughly the same for the four SNIA methods.

All numerical simulations are performed using a C++ code developed for the modelling of ISU. We use finite volume method for the discretization and the Newton-Raphson algorithm for the treatment of non-linearities [23].

4.1 Test case 1

First, we consider the ISU of oil shale in a one-dimensional tube of length 5 m. The reactions included in the model are described in [20] and reported in Table 1. We note that values for the pre-exponential factors and activation energy are smaller than those reported by [25]. The rock properties are shown in Table 4 and the fluid properties in Table 5, adapted from [10, 20, 21]. The viscosity of the gas phase is given by:

$$\mu_g = 1.4360 \times 10^{-5} + 3.8 \times 10^{-8} T \quad (17)$$

Table 1 Chemical reactions for test case 1

Reaction	Pre-exponential factor (s^{-1})	Activation energy (kJ/mol)
$KER \rightarrow 0.0096 IC_{37} + 0.0178 IC_{13} + 0.045 IC_2 + 0.0054 CO_2 + 0.49 \text{ PreChar}$	4.33×10^7	161.6
$IC_{37} \rightarrow 0.206 IC_{13} + 2.36 IC_2 + 30.0 \text{ PreChar}$	7.23×10^{11}	206.0
$IC_{13} \rightarrow 0.573 IC_2 + 12.69 \text{ PreChar}$	1.14×10^{12}	219.3

These data are adapted from [20]

and the viscosity of the liquid phase is given by [26]:

$$\log_{10} \mu_o(T) = \frac{4.1228}{\left(1 + \frac{T-30}{303.15}\right)^{3.564}} - 3.002 \quad (18)$$

where μ_g and μ_o are in $Pa.s$, and T is in $^{\circ}C$.

Figure 2 shows the saturation and temperature profiles. At the initial temperature, the chemical reactions are very slow. As the heat conduction in the domain causes the temperature to increase, the reaction constants increase too. A reaction front forms where the temperature and the concentration of reactant are both large. Near this reaction front, the time scale of decomposition is between 1 and 5 days.

Figure 3 shows the evolution of the normalized errors with time-step. The time-steps represented in the x-axis is dt for SSO and $dt/2$ for SMSO, so that the four SNIA methods perform the same number of transport steps and the same number of chemical reaction steps. We observe that SSO-AK gives a large pressure error. The pressure rises 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. We observe that SSO-CKA gives the lowest discretization error of the spitting methods.

4.2 Test case 2

In test case 2, pyrolysis is applied to Athabasca tar-sands [3] in a one-dimensional tube of length 5 m. Table 2 lists the chemical reactions included in the model. They are adapted from [27]. The viscosity of the gas phase is given by Eq. 17 and the viscosity of the liquid phase is given by Andrade's equation [28]:

$$\log \mu_o(T) = A + \frac{B}{T - T_0} \quad (19)$$

Here, $A = -10.07$, $B = 1416.6$ and $T_0 = -63.15$ $^{\circ}C$.

Figure 4 shows the saturations and temperature profile. As in test case 1, the chemical reactions are very slow at initial temperature. Near the reaction front, the time scale of decomposition is between 0.1 and 1 day.

Figure 5 shows the evolution of the normalized errors with the time-step with dt for SSO and $dt/2$ for SMSO, so that the four SNIA methods perform the same number

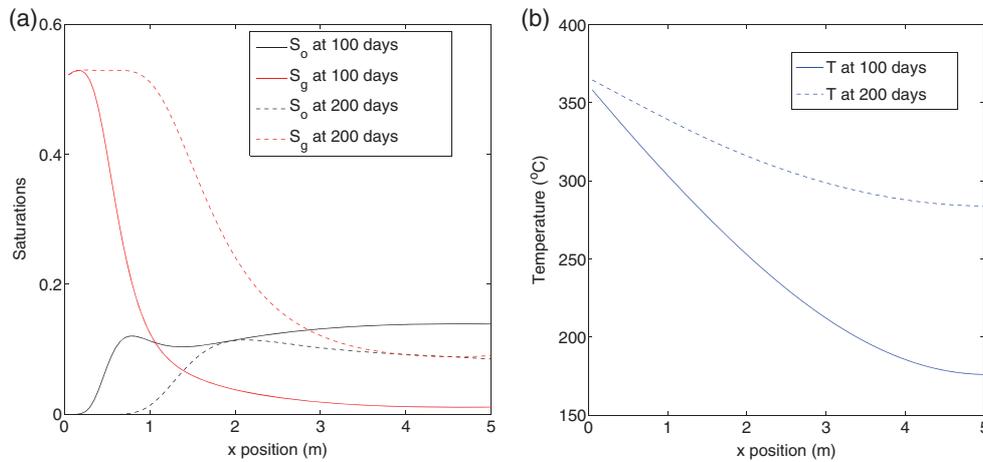
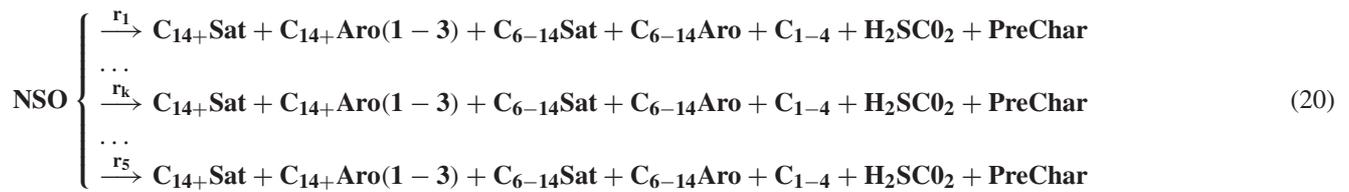


Fig. 2 a Saturation profile and b temperature profile for the ISU of oil shale (test case 1) after 100 and 200 days. The saturation front is progressing through the domain as the temperature increases. The time scale of the heat conduction in the domain is approximately 200 days

of transport steps and the same number of chemical reaction steps. The results are similar to those given by test case 1 (Fig. 3), except that the pressure errors are much lower and the saturation errors are higher. SSO-AK gives large pressure and saturation errors while SSO-KA gives a large composition error. SMSO does not reduce significantly the error. We observe that SSO-CKA again gives the lowest splitting error.

5 Convergence of ISO method

Since the ISU model is non-linear, we do not have any results concerning the stability and convergence of ISO. To assess its applicability, we compare the convergence behaviour with FIM for test cases 1 and 2. Figure 6 shows the number of non-linear iterations used to solve the transport step for each case, using FIM and ISO methods. For both test cases, ISO performs a lot more iterations because of convergence failures. Therefore, ISO cannot be applied to ISU. The stability error arising from the explicit treatment



For each reaction, a certain fraction of initial reactant decomposes with its own activation energy (column labeled

of one of the operator in each sub-step is too large and is not cancelled by alternating and iterating over the splitting scheme.

6 Comparison of computational efficiency of SSO-CKA and FIM for simulations with a full kinetic model

ISU compositional models generally need a large number of components in order to simulate accurately the chemical reactions. For example, Braun and Burnham's compositional model [25] includes 32 liquid and gas species and 19 solid species. Fan et al. [20] considered 15 components that are lumped into 5 pseudo-components. In Behar et al. [27], an overall kinetic model is used to describe the cracking of a crude oil from Safaniya, a reservoir in Saudi Arabia. This model uses 12 chemical classes such as NSO , C_{14+} saturates and C_{3-4} . Five of these classes decompose by pyrolysis. These decompositions can be described by a set of parallel reactions. For example, the decomposition of the unstable NSO compounds can be described by [3]:

E in Table 3). To describe correctly the decomposition rate, one needs to split the NSO class into five components,

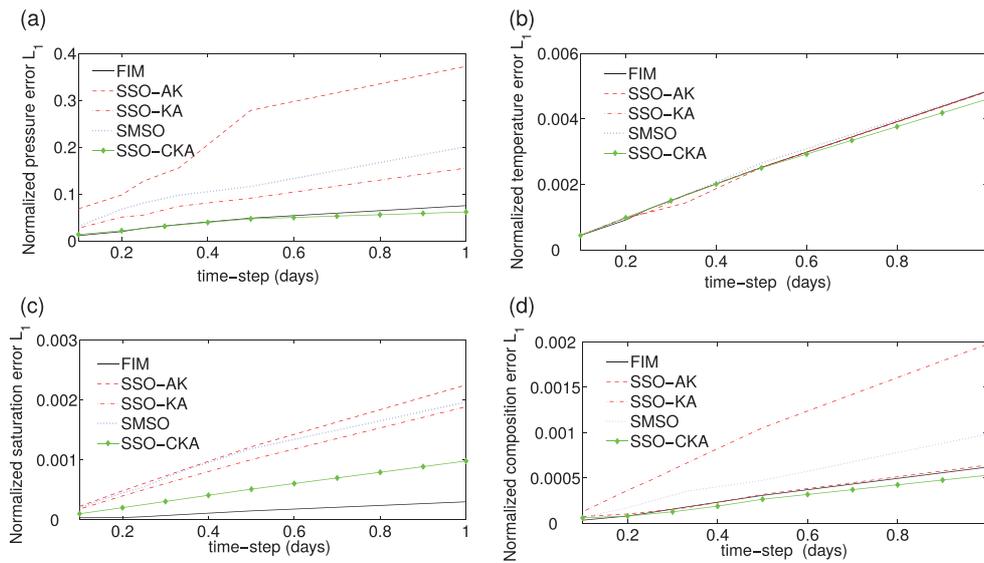


Fig. 3 Normalized error in **a** pressure, **b** temperature, **c** saturation and **d** composition with respect to the time-step size for test case 1. We observe that SSO-CKA gives the lowest discretization error

Table 2 Chemical reactions for test case 2

Reaction	Pre-exponential factor (s^{-1})	Activation energy (kJ/mol)
$NSO \rightarrow 0.616 IC_{37} + 0.360 IC_{13} + 0.755 IC_2 + 0.105 CO_2 + 11.63 \text{ PreChar}$	3.16×10^{12}	209.2
$IC_{37} \rightarrow 1.477 IC_{13} + 4.0 IC_2 + 7.85 \text{ PreChar}$	3.85×10^{16}	267.8
$IC_{13} \rightarrow 3.68 IC_2 + 4.96 \text{ PreChar}$	3.85×10^{16}	281.2

These data are adapted from [27]

which have the same thermophysical properties. Then, the full compositional model includes a large number of components (21 in this case). Numerical simulation with FIM using this large compositional model can be computationally expensive.

To reduce the computational time, we can use a smaller compositional model formed by the 12 chemical classes. We can approximate the total decomposition by applying the initial mass fractions as a constant weight for each reaction rate. This way, each decomposition of the type defined by Eq. 20 can be described by one chemical reaction with constant $r = \sum p_k r_k$ where p_k are the initial weight fractions defined in column labeled P of Table 3. Since the transport properties are constant in each chemical class, the operator A is approximated accurately with this lumped model. However, the chemical rates can be very inaccurate. This can be demonstrated by comparison with the experimental result obtained by Kumar et al. [3].

The objective of the experiment was to demonstrate the potential of ISU process through electrical heating of bitumen at 375 °C. A core consisting of unconsolidated sand saturated with bitumen was mounted in a steel core holder which was divided into four equal zones for heating in order to mimic the thermal front propagation of the reservoir in

the core. The core dimensions were 151-mm long and 50-mm diameter. Fluid were produced from the top using an outlet pressure of 15 bars and back-pressure control. The produced liquid was sampled at regular intervals and was analysed for its composition at various time.

The rock properties are identical to those of test case 2 (Table 4). The kinetic model is proprietary and cannot be published. It is of the same form as the one in Table 3. It contains 11 chemical classes than need 30 components to describe the chemical reactions accurately. Figures 7 and 8 compare the experimental results and the numerical results obtained using a one-dimensional grid of 50 cells. The simulation using the full compositional model is very accurate with an error of approximately 3 %. The run time is approximately 5 min. This is very long considering it is a model with only 50 cells. The simulation using the lumped model is faster (approximately 1 min) but with an error of approximately 10 %.

The simulation with the full compositional model was very slow for three reasons:

- The CPU time needed to solve the set of fully implicit equations with a large number of variables (pressure, temperature and compositions of chemical entity for each cell) is large (about 50 % of the total CPU time)

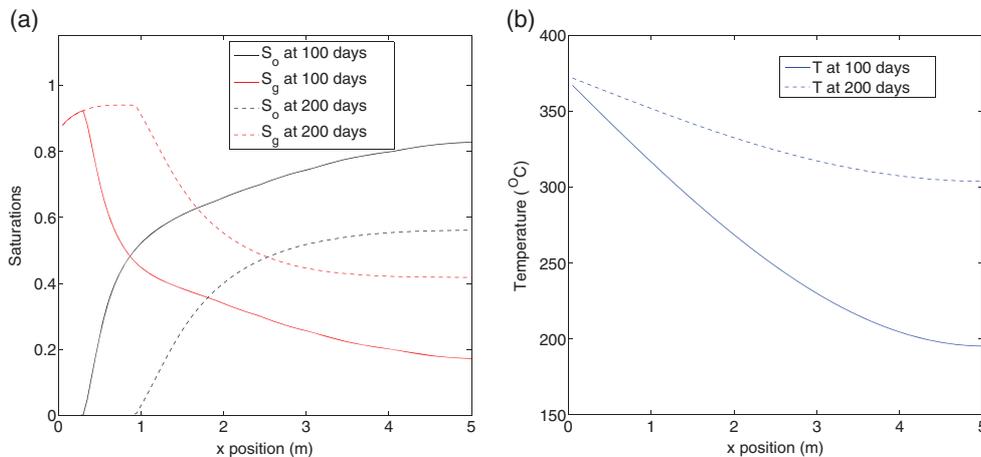


Fig. 4 a Saturation profile and b temperature profile for the ISU of bitumen (test case 2) after 100 and 200 days. The saturation front is progressing through the domain as the temperature increases. The time scale of the heat conduction in the domain is approximately 200 days

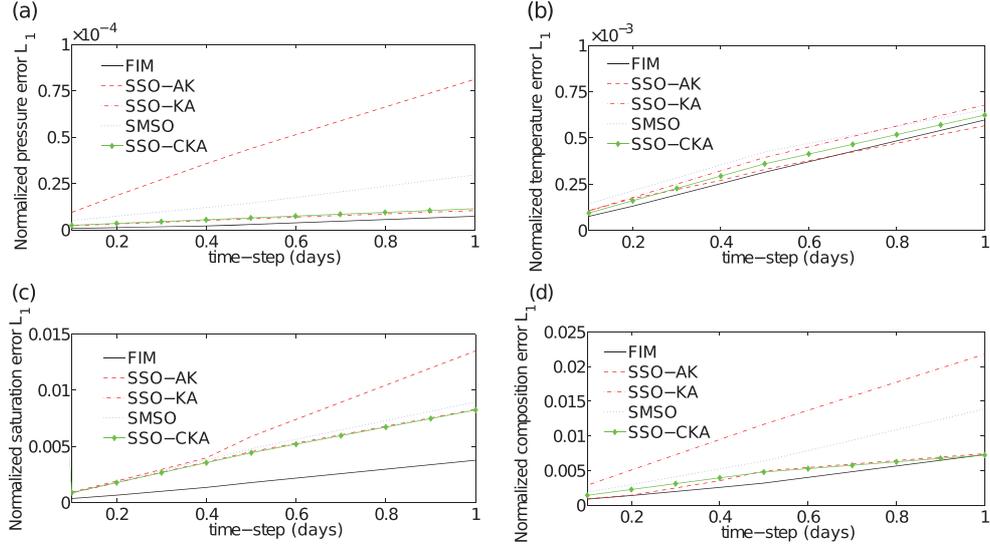


Fig. 5 Normalized error in **a** pressure, **b** temperature, **c** saturation and **d** composition with respect to the time-step size for test case 2. We observe that SSO-CKA gives the lowest discretization error of the splitting methods

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

One can obtain a large speed-up when splitting the advection-conduction and the chemical reactions. The advection and conduction operators can be solved with the same level of accuracy 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 (13 variables 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 . This is fully local, so the chemical rates do not need to be computed for each cell at each Newton step but only for those which have not converged yet. For Kumar's experiment, 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. Computational effort is thus focused on the remaining 10 % of cells which require 3 or more iterations to obtain a converged solution.

We compared the simulation time between FIM and SSO-CKA for Kumar's experiment with grid size from 10 to 100 cells. To obtain the same precision between the two methods, we used the a-posteriori error control algorithm

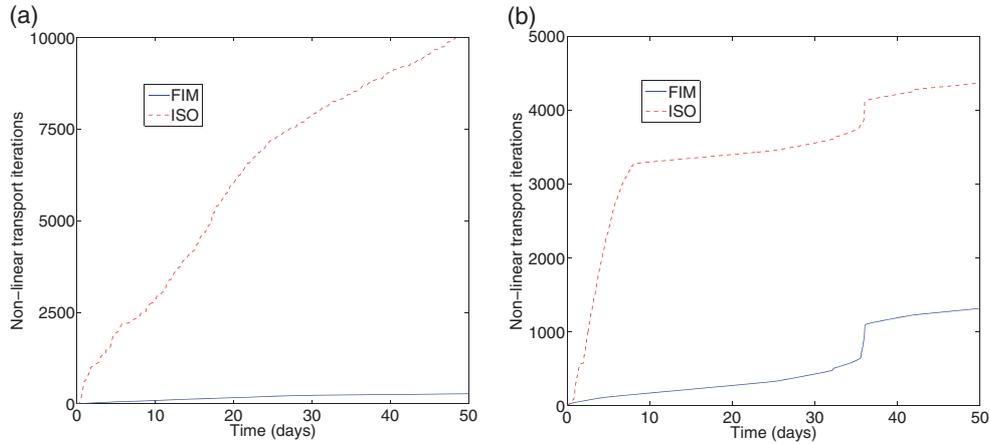


Fig. 6 Number of non-linear transport iterations for **a** the ISU of oil shale (test case 1) and **b** the ISU of bitumen (test case 2) for both FIM and ISO methods. We observe a large difference between the two methods, which is due to convergence failures for ISO

Table 3 Overall kinetic scheme for the thermal cracking of the C_{14+} Safaniya oil (data from [27])

	H_2S	C_1	C_2	C_{3-4}	C_{6-14}		C_{14+}				E (kJ/mol)	P (%)	A (s^{-1})
					Sat	Aro	Sat	Aro 1	Aro 2	Aro 3			
NSO	0.9	1.3	1.3	1.8	7.2	4.7	6.7	49.1			209	37.4	$3.2e12$
										218	4.1		
										226	52.8		
										243	5.7		
										Total	100		
C_{14+} Aro1	1.3	2.3	1.9	4.7	6.4	3.2	17.8	47.5			218	20.8	$3.0e13$
										226	79.2		
										Total	100		
C_{14+} Aro2		4.9							63.2	197	100	$4.6e10$	
C_{14+} Sat		3.8	4.9	17.2	53.9	5.8			14.4	268	55.4	$3.8e10$	
										276	25.2		
										285	17.2		
										293	1.8		
										301	0.4		
										Total	100		
C_{6-14} Sat		1.7	27.8	38.3		32.2				2	100	$3.8e10$	

defined in [29]. The relative difference in pressure, temperature and saturations between the two methods is smaller than 10^{-6} . SSO-CKA performs more time iterations, but since the splitting error is limited, the difference is not significant. For example, we used 262 steps for FIM and 289 steps for SSO-CKA on a grid with 50 cells. The evolution of the time-step for both methods is plotted in Fig. 9. Figure 10 shows the CPU time for both methods. We obtain

a speed-up of between 3 and 5. This speed-up can potentially be further improved by applying dedicated solvers to each operator. For example, AIM can be used for the advection step. Moreover, the precision and performance of the chemical reaction operator could be improved by using smaller local time-steps or higher order non-linear methods such as Runge-Kutta [8]. This will be investigated in future work.

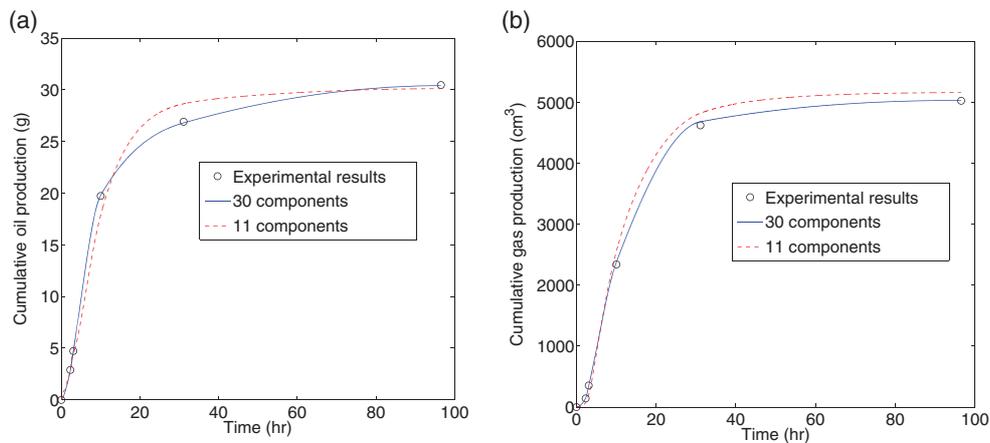


Fig. 7 Results of Kumar's experiment [3] for **a** oil production and **b** gas production and comparison with numerical simulation results obtained with a 30 component kinetic model and a 11 component

lumped model. The error obtained with the full model is approximately 3 % and the error with the lumped model approximately 10 %

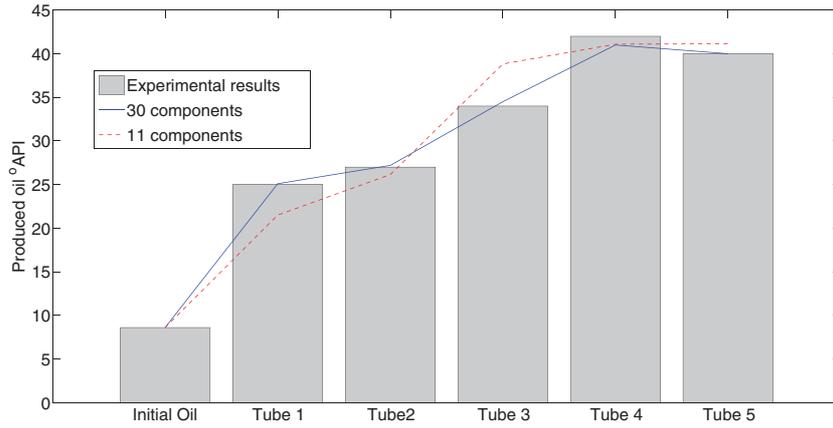


Fig. 8 Results of Kumar's experiment [3] for API degree of produced oil and comparison with numerical simulation results obtained with a 30 components kinetic model and a 11 components lumped model. The error obtained with the full model is approximately 3 % and the error with the lumped model approximately 10 %

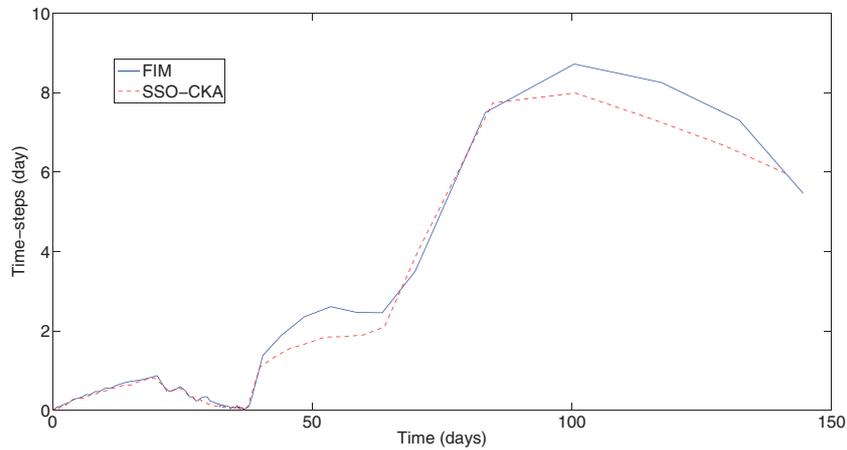


Fig. 9 Comparison of time-step size for FIM and SSO-CKA for Kumar's experiment with 50 cells. SSO-CKA performed more time iterations, but since the splitting error is limited, the difference is not significant

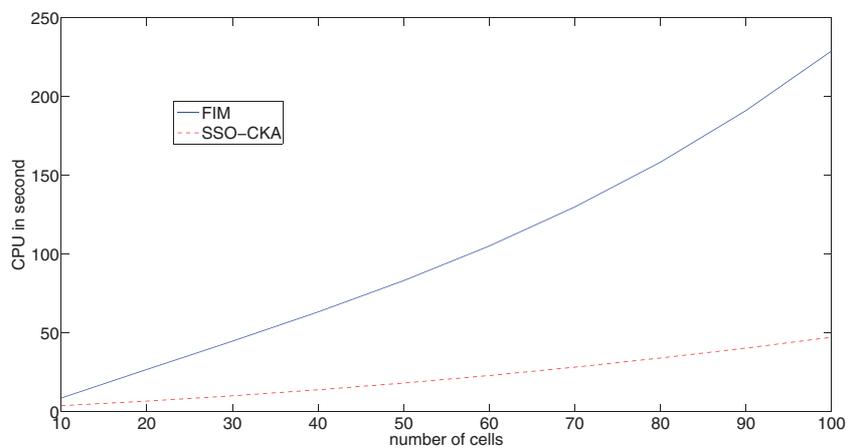


Fig. 10 Comparison of CPU time using FIM and SSO-CKA for Kumar's experiment as a function of number of grid cells. We obtain a speed-up of between 3 and 5

Table 4 Rock and initial properties for test case 1, 2 and 3

	Test case 1	Test cases 2 and 3	
Porosity (%)		30	36
Initial Permeability (mD)		2	4158
Coefficient a		20.0	20.0
Initial solid saturation		85.0	0.0
Rock volumetric heat capacity (kJ/m ³ /K)		1680	1800
Heat conductivity (W/(mK))		2.0	1.7
Rock compressibility (1/bar)		4.3e-5	5e-4
Initial pressure (bar)		7	15
Initial temperature (°C)		21.1	28
Heater temperature (°C)		370	395
Composition (wt %)	CO_2	0.1	0
	IC ₂	0	0
	IC ₁₃	0	2
	IC ₃₇	0	40.5
	NSO	0	57.5
	Kerogen	99.9	0
	Prechar	0	0

These data are adapted from [20] and [3]

Table 5 Fluid properties for test cases 1, 2 and 3

	NSO	IC ₃₇	IC ₁₃	IC ₂	CO ₂	KER	Prechar
Molecular weight (kg/kmol)	515	465.83	169.52	30.07	44.01	15	12
Critical pressure (bar)	6	9.36	24.05	46.09	73.80	NA	NA
Critical temperature (K)	1200	962.28	715.36	288.74	298.53	NA	NA
Accentric factor (no unit)	1.6	0.818	0.365	0.008	0.239	NA	NA
Liquid reference pressure (bar)	1	1	1	1	1	NA	NA
Liquid reference temperature (°C)	20	20	20	20	-78.1	NA	NA
Density at reference condition (kg/m ³)	1070	1013	760	460	1560	2000	2000
Liquid compressibility (1/bar)	2e-5	5e-5	1e-4	1.5e-4	2e-4	NA	NA
Liquid thermal expansion (1/K)	3e-4	6e-4	1e-3	1.6e-3	4e-3	NA	NA

Liquid compressibility and thermal expansion have been obtained using linear regression and the Peng-Robinson equation of state

7 Conclusions

This work has investigated the application of operator splitting methods to the numerical modelling of in-situ upgrading of heavy oil, where heat is applied to the reservoir to make the heavier oil components decompose into lighter, more mobile and more valuable liquid and gas components. The modelling of in-situ upgrading is both complex because of the non-linearity of the equations, and computationally intensive. The aim of this study was to determine whether operator splitting methods (which have been shown to reduce computational effort when used in the modelling of linear systems) have the potential to reduce CPU time for this application. Results from sequential split operator, alternating split operator and iterative split operator were compared against those obtained from a fully implicit model of the process for three different test cases taken from the literature [3, 20, 25].

Initially, the process was divided into two operators (chemical reaction and advection/heat transport). We found that using simple sequential split operator resulted in large errors in pressure and either saturation or composition, depending upon whether the chemical reaction or advection/heat transport step was calculated first. These errors were not improved by using an alternating scheme (the Strang-Marchuk split operator). Moreover, we observed that the iterative split operator was not stable and showed many convergence failures for our test cases.

Dividing the process into three operators (heat transport, chemical reaction, advection with no heat transport) and using a sequential split operator in the order given resulted in a much reduced splitting error for all variables. We note that these results were obtained for a system in which most of the reactant was in the solid or liquid phase. Also, the reaction enthalpies which generate further coupling between temperature and chemical reactions were neglected. Further work is needed to evaluate the impact of a very mobile gas phase and large reaction enthalpy which may alter the accuracy of this scheme. The impact of gravity also needs to be considered in future studies.

This scheme also resulted in a speed up of between 3 and 5 over the fully implicit model for an 30 component test case in 1D. This was obtained by using a lumped compositional model for the advection step only, with no loss of accuracy. This speed-up can be potentially further improved by using dedicated solvers to each operator. This will be investigated in future work.

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