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MASTER THESIS

Hierarchical coarsening of simulation model for in-situ upgrading process

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Abstract

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Oil shales are sedimentary rocks containing organic matter in the form of kerogen which accounts for more than 5 trillion barrels of oil in place according to Birol, 2010; therefore, oil shales represents a plausible solution for the constantly increasing demand for hydrocarbons. Oil shale production is currently done using two different techniques, surface retorting and in-situ retorting. The last one being the focus of this study. During this process, the sedimentary rock containing the kerogen is brought into a high-temperature environment with oxygen deficit. At this stage, the organic matter is subject to a thermo-chemical decomposition that finally releases the hydrocarbon in liquid and gas forms. This process is also known as pyrolysis. During this process, solid and fluid components experience compositional and physical changes, which requires complex chemical models represented by multiple species and several governing relations.

In this work, we first developed a numerical solver for closed systems with simple kinetics models. This initial work allowed us to analyze the dynamic behavior of each component during the chemical decomposition of the kerogen and its impact in the porosity of the system. Then, we described an accurate base model for chemical decomposition of kerogen. This model was then implemented in our in-house simulator ADGPRS. The model is based on the most recent understanding of pyrolysis process, and it incorporates coupling of chemical kinetics to heat and mass transport. Due to the high number of species, variations of porosity as consequence of the transformation of solid species into fluid products and complex multi-scale structure of porous media, the simulation performance of the high-fidelity model is limited. Therefore, in the second step of this work, we introduce a hierarchy of coarser models to improve the run-time of forward solution without significant reduction in accuracy. We applied coarsening in time, space, and chemical representation, and quantify errors introduced at each coarsening level. In conclusion, we provided recommendations for large-scale modeling of in-situ upgrading process.

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Chapter 1

Introduction

1.1 Introduction to oil shale

1.1.1 Definition

Oil shales are commonly defined as diverse fine-grained sedimentary rocks, rich in organic matter that can be transformed or refined into fuels. A more technical definition provided by Gavin, 1924 states that oil shale is a compact, laminated rock of sedimentary origin, yielding over 33 % of ash and containing organic matter that yields oil when distilled, but not appreciable when extracted with ordinary solvents for petroleum. According to Dyni, 2006 oil shales can be found in a great diversity of depositional environments, from fresh-water to high salinity lakes, epicontinental marine basins, subtidal shelves and in limnic and coastal swamps. A very common mistake is confusing oil shale with coal. However, both of them are very different regarding mineral content and the precursors of their organic matter.

FIGURE 1.1: High-grade oil shale sample from Mahogany zone, Utah.
Adopted from Beckwith, 2012

The origin of oil shale according to Shale, 1976 results from continuous deposition and accumulation of inorganic and organic material content. The entire bibliographic reference documented for this work coincides that the organic content found in most of the oil shales have biological origins from marine algae and remains of spores, pollen, woody plants and some other cellular remains of marine and land plants. The following step in this process is the continuous burying of this organic material under anaerobic conditions and lack of destructive organism. Under this conditions, we can treat these type of formations as source rocks for petroleum and natural gas reservoirs. In fact, Dyni, 2006 mention that it is assumed that the Green River oil shale formation located in the United States is believed to be the source of oil in the Red Wash field in northeastern Utah. However, not all oil shale deposits achieve the required thermal maturity to become in oil or natural gas rock source.

Therefore those immature deposits have the potential to become economically exploitable by either surface mining or in-situ methods depending on the depth of the oil shale formation.

FIGURE 1.2: Oil sand containing oil from the Green River formation.
Adopted from Beckwith, 2012

1.1.2 Oil shale classification

From the literature studied for this work, we found different methodologies for oil shale classification. Among the different methods, we decided to present the most practical and useful from our perspective. It was developed by Hutton, 1991 and presents a classification primarily based on the origin of the organic matter and subsequently the depositional environment of the sediments.

FIGURE 1.3: Oil shale classification. Adopted from Dyni, 2006

1.1.3 Oil shale distribution in the world

This type of source rock is present in different parts of the world and based on information published by Dyni, 2006 a conservative estimation of the total resources adds up to 2.8 trillion U.S barrels of oil shale. In a most recent publication Biglarbigi et al., 2010, it is mention that oil shale are found in nearly 100 major deposits, on which they estimate up to 8 trillion barrels of oil equivalent. Therefore, oil shale represents a promising option for energy production. Table 1.1 summarizes the estimated global oil reserves per region.

World Region	Known Resources (Billion Barrels)	World Region	Known Resources (Billion Barrels)
North America	6,016	MENA	153
South America	82	Asia	292
Europe	120	Oceania	32
		South Africa	1002

TABLE 1.1: Global Oil Shale Resources. Table obtained from Biglarbigi et al., 2010

1.1.4 Methods of exploitation

To exploit this unconventional resources. First, we need to understand how oil shale is distributed in the rock and how it can be extracted. Every single oil shale formation has a unique composition. The percentage of organic material that is soluble in organic solvents heavily depends on the type of kerogen and solvent used for this purpose. For example for Green River shale, this percentage is around 5-10 % but for Type II-S kerogen this percentage can be 2-3 times higher Jarvie and Lundell, 2001. The remainder exists as insoluble kerogen, which requires a heating process, also known as pyrolysis, to transform kerogen and produce oil and gas sub-products.

In natural conditions, this maturation process requires a considerable amount of time (millions of years) for a complete thermal decomposition of the kerogen into hydrocarbon species. However, it can be accelerated by implementing two different extraction strategies. The first one is called *surface retorting*. In this approach, oil shale is mined, conveyed to the surface, and further processed under surface pyrolysis. In this process, oil shale is subjected to temperatures ranging from 500-550 °C. The obtained sub-products are collected and further upgraded in proper surface facilities. Among the several limiting factors of this strategy, one of them is the large volumes of expanded shale that later must be properly disposed. From the economic and operational point of view, this technique is only suitable for shallow formations under restrictive market conditions. The second strategy is called *in-situ retorting*. From this second strategy, we are interested only in *the in-situ upgrading process*. This technique does not require the extraction of oil shale rock from the ground. By contrast, it takes the maturation process directly to the reservoir by using down-hole heating devices, capable of supplying the energy required to produce light oil from the bitumen. This study is focused on an understanding and accurate representation of kinetically driven transformation of kerogen and mostly related to in-situ upgrading process.

The fact that mining is not required does not necessarily mean that in-situ upgrading is a less complex process. To implement this approach, we need to fully understand the process that will take place in the subsurface media. Kerogen pyrolysis is a complex process in which solid kerogen components will be converted into various types of fluid and solid species. Additionally, parallel reactions will take place in the cracking of the hydrocarbon components that are produced from the continuous kerogen decomposition. Therefore, from the modeling perspective, this process involves constant changes in fluids properties, phase transformations, fluids-solids chemical interactions and changes in effective porosity and permeability.

1.2 Literature review of in-situ upgrading numerical models

Among the several previous studies relevant to this research we highlight the work conducted by Burnham and Braun, 1984. In this work, authors presented a first general mathematical model for pyrolysis of the Green River oil shale. A reaction model including 5 gas species, oil, water, and kerogen was suggested for modeling pyrolysis. In a subsequent work, Braun and Burnham, 1987 investigated the general applicability of using activation energies distribution and simpler models for the description of the chemical kinetics reactions. In later work, Braun and Burnham, 1990, presented a complete mathematical model for simulating of oil generation, degradation and expulsion occurring during pyrolysis of petroleum source rocks over a specific history of temperatures and hydrostatic pressure. The model consisted of 32 vapor species, 32 liquid species, 19 solid species and 100 reactions. Additionally, a modified Redlich-Kwong-Soave equation of state was used for calculating the vapor-liquid equilibrium and PVT behavior of the fluid species. Later, Braun and Burnham, 1992, published a flexible model of oil and gas generation, cracking and expulsion (PMOD). For this last work, they developed a code, capable of simulating a wide variety of global models with different grades of complexity for the generation, cracking and expulsion of hydrocarbon from kerogen source rocks.

In a more recent study, Fan et al., 2010, developed a simulator capable of modeling in-situ upgrading process. This model presented a chemical kinetic model fully coupled with a thermal/compositional formulation. The results of its simulations showed reasonable agreement with data from a field test conducted by Shell (Sandberg et al., 2009). In another work, Lee et al., 2014 investigates the efficiency of oil shale in-situ upgrading by steam flowing. The objective of this work was to find an effective way of heating oil shale reservoirs by steam flowing in horizontal wells and natural vertical fractures. They expected that this method would be favorable for deep oil shale reservoirs. In a subsequent work, Lee et al., 2016 developed a comprehensive simulation model for kerogen in-situ upgrading. They also presented a chemical kinetic model fully coupled with a thermal/compositional formulation, but they account for the dynamic changes in porosity and permeability. They also analyzed the effect of reservoir parameters such as initial matrix effective porosity, oil shale grade and spacing of fracture network.

1.3 Work description and research objectives

This study is divided into two parts. In the first part, we developed a simple non-linear numerical solver for closed systems using two different kinetics models. This initial simulator was developed in MATLAB and it allowed us to understand better the dynamics behind the chemical decompositions of the different species involved in the reactions. In this part of the work, we were focused on understanding the interaction between solid kerogen disappearance and its impact on the porosity of the system. The following step on the first part of this work was the incorporation of this thermal chemical reaction model into the Automatic Differentiation General Purpose Research Simulator (ADGPRS) (Voskov and Tchelepi, 2012; Zaydullin, 2015; Garipov et al., 2016). We introduced and validate a high-fidelity multi-component multiphase fully coupled model for an in-situ upgrading of oil shales. The description of kerogen pyrolysis and subsequent oil cracking kinetic reaction model is adapted from Braun and Burnham, 1992. The reaction module is fully coupled with the mass and energy balance of the system using an extension of natural formulation for a solid phase treatment (Voskov et al., 2016). Fluid properties and phase equilibrium are modeled using Peng-Robinson equation of state (EOS) (Peng and Robinson, 1976). The model is capable of accurately describing the transformation of different species in the process. We also demonstrate that the same model can be used to predict diagenetic processes in subsurface sediments at the geological time-scale. The model also accounts for the dynamics changes of porosity and permeability due to the transformation of solid components. Finally, we propose and study simplified (coarser) models capable of capturing the dynamics of the high-fidelity model with fewer degrees of freedom.

Chapter 2

Mathematical formulation

In this section, we describe the mathematical model used for simulation of diagenetic and in-situ upgrading processes. We use a modification of the ADGPRS code describing the energy and mass transport phenomena, alongside to the thermodynamic relations used to compute fluid properties and phase equilibrium in the system. Additionally, we present the general mathematical description of the kinetic reaction model and the strategy used for porosity and permeability update.

2.1 Mass balance equation

The general mass balance conservation equation for a system containing n_c fluid components is following description by Forugh, 2016. For the purpose of this work, a fluid component will represent a hydrocarbon in liquid or gas phase, and a solid component refers to mineral species such as kerogen or coke.

$$F_i = \frac{\partial}{\partial t} \left[\left(\sum_{j=1}^{n_p} \phi X_{ij} \rho_j S_j \right) \right] + \nabla \cdot \sum_{j=1}^{n_p} \left(X_{ij} \rho_j \mathbf{u}_j - \rho_j \phi S_j D_{ij} \nabla X_{ij} \right) + q_i^W = \sum_{k=1}^{n_k} v_{i,k} \mathbf{r}_k \quad i = 1, \dots, n_c \quad (2.1)$$

Here n_p is the total number of fluid phases, n_k is the total number of kinetic reactions, X_{ij} represents molar fractions of fluid component i in phase j , ρ_j is the phase molar density, ϕ is the porosity, S_j is the saturation of phase j , v_{ik} are the stoichiometric coefficients of fluid component i in the kinetic reaction in reaction k , $\mathbf{r}_k$ are the rates of reaction, $\mathbf{u}_j$ is the Darcy velocity for phase j , D_{ij} is the dispersion tensor for component i in fluid phase j , and finally q_i^W is the well rate of component i .

Darcy velocity is obtained using the following expression:

$$\mathbf{u}_j = -\mathbf{K} \frac{k_{rj}}{\mu_j} \left(\nabla P_j - \rho_j g \nabla D \right), \quad j = 1, \dots, n_p \quad (2.2)$$

Here $\mathbf{K}$ is the permeability tensor, k_{rj} is the phase relative permeability, μ_j is the phase viscosity, P_j is the phase pressure, g is the gravitational acceleration and D is the vertical depth vector.

With respect to the solid components of the system, the current implementation does not consider the transport of solid particles in suspension. Therefore, the mass balance equation used for n_s solid components is adapted from Forugh, 2016 and it

is expressed in its residual form as follows:

$$F_i = \frac{\partial C_i}{\partial t} - \sum_{k=1}^{n_k} v_{i,k} r_k = 0, \quad i = 1, \dots, n_s \quad (2.3)$$

Where C_i represents the molar concentration for solid component i , $v_{i,k}$ are stoichiometric coefficients for the solid component i in the kinetic reaction k , and finally, r_k are the rates of reaction.

2.2 Energy balance equation

The next step is declaring the energy balance conservation equation. In our work the implementation is adapted from Zaydullin et al., 2014 and is written in residual form as:

$$F_e = \frac{\partial}{\partial t} \left[\Phi \left(\sum_j U_j \rho_j S_j \right) + (1 - \Phi) U_R \right] + \nabla \cdot \sum_j \left(H_j \rho_j \mathbf{u}_j \right) - \nabla \cdot (\kappa \nabla T) + \sum_j \left(H_j \rho_j Q_j^W \right) + Q^h = 0, \quad (2.4)$$

Where U_j is the phase internal energy, H_j is the enthalpy for phase j , H_R is the rock internal energy, κ is the thermal conductivity and Q^H is a heat loss in wells. No energy changes due to chemical reactions is included.

2.3 Phase equilibrium, fluids properties and local constraints

To close the previous system of conservation equations (2.1), (2.4), the assumption of instantaneous thermodynamic equilibrium is applied. Also, the conventional assumptions of compositional formulation were utilized in the model. The equations describing the phase partitioning in compositional model are adapted from Iranshahr et al., 2013:

$$f_{io}(p, T, y_i) - f_{ig}(p, T, x_i) = 0, \quad i = 1, \dots, n_h \quad (2.5)$$

$$z_k - V y_i - (1 - V) x_i = 0, \quad i = 1, \dots, n_h \quad (2.6)$$

$$\sum_{i=1}^{n_h} (x_i - y_i) = 0. \quad (2.7)$$

Here f_{io} and f_{ig} are the fugacity coefficients for component i in oil and gas phase, respectively. n_h is the total number of hydrocarbon components, z_i is the overall mole fraction of component i in system, x_i is the mole fraction of component i in the oil phase, y_i is the mole fraction of component i in the gas phase, L is oil phase mole fraction and V is the gas phase mole fraction. The phase molar densities are computed based on the Peng-Robinson EoS (Peng and Robinson, 1976) and viscosity is computed using the correlation described by Lohrenz et al., 1964. For simplicity we assumed that no connate water is present in porous media.

2.4 Kinetic reactions

The mathematical model used for the description of the kinetic reaction is based on the methodology presented by Braun and Burnham, 1992. Our implementation is capable of handling a diverse type of chemical reactions including multiple activation energy levels. The examples of the different types of reactions handled by the model are presented in the following table:

Parallel Mechanism:		Simple Examples:	
precursor 1	————→	product type 1	heavy oil potential —————→ heavy oil
precursor 2	————→	product type 2	light oil potential —————→ light oil
precursor 3	————→	product type 3	gas potential —————→ gas
Parallel Mechanism:		Simple Examples:	
starting material	————→	prim products	kerogen —————→ oil + gas + resid
prim products	————→	second products	oil —————→ gas + residue
second products	————→	tertiary products	residue —————→ gas + carbon
Synthesis mechanism:		Simple Examples:	
$\sum$ kerogen	————→	product j	kerog C + kerog O —————→ CO_2
element i			
etc			kerog C + kerog H —————→ CH_4
			kerog H + kerog S —————→ H_2S
Competing pathways:		Simple Examples:	
starting material	————→	intermediate	kerogen —————→ bitumen
products			oil+gas+residue

TABLE 2.1: Schematic chemical reactions for pyrolysis description (Braun and Burnham, 1992)

We considered all reactions to be independent of pressure. Temperature dependence is described by the Arrhenius equation as follow:

$$K_k = A.e^{(-E_a/RT)}, \quad (2.8)$$

Where A is the frequency factor, E_a is the activation energy level, R is the ideal gas constant and T is the temperature. In the described implementation, all species can be handled at multiple-energy levels which helps for accurate representation of kerogen transformation. Finally, the rate of reaction r_k (term used in equations 2.1 and 2.3) is assumed to be a first-order with respect to the concentration of the reactant and it is computed as:

$$r_k = K_k.min(C_i/v_{i,k}) \quad (2.9)$$

Where C_i is the concentration of the reactant i acting in the reaction k , K_k is the rate coefficient computed with previous equation, and $v_{i,k}$ is the stoichiometric coefficient of the reactant i acting in the reaction k .

2.5 Porosity and permeability changes

As mentioned before, one of the important capabilities implemented in this thermal chemical model is on accurate quantitative description of the constant changes

in porosity and permeability across the reservoir. Porosity changes take place in the reservoir as a consequence of the thermal decomposition and formation of the solid species of the reactive model. When a solid specie is decomposed into fluid sub-products, space previously occupied by the solid mineral is left behind to be occupied by the fluid components being generated and transported inside the reservoir. The result of this decomposition is the increase in the porosity of the system. A similar process occurs but with opposite effect in porosity when fluid components are transformed in solid species. These changes are computed using the following equation.

$$\Phi_b = 1 - \frac{\sum_i (C_i \cdot V_b \cdot MV_j) - VR_b}{V_b}, \quad b = 1, \dots, n_c \quad (2.10)$$

Where Φ_b is the porosity for the cell b , b is the block cell index, n_c represents the total number of cell blocks in the model, C_i is the mineral molar concentration of solid components, i represents the number solid components, and VR_b is the non reactive rock volume for cell block b .

In addition, permeability is affected due to the changes in the porosity of the reservoir. Therefore our model account for those changes based Carman-Kozeny relation.

Chapter 3

Development of high fidelity model

In this section, we first introduce the initial step of developing our first numerical model for a closed in-situ upgrading system. Once the two initial trial kinetic models have been tested, then we proceed with the final implementation of the thermal chemical model into the ADGPRS. In order to check our implementation, we run a reference kinetic cell model adapted from Behar et al., 2008. The results are later compared with those obtained using the PMOD2 code (Braun and Burnham, 1992).

3.1 Development of non linear solver for closed system

In this section, we first build the simplest non linear solver capable of modeling the production of oil and gas from the chemical decomposition of the kerogen inside a kinetic cell. The main objective of this initial model was to study the changes in moles distribution of each one of the species involved in the chemical reaction. As a secondary objective, we wanted to understand the changes in volumetric distributions inside the kinetic cell due to the appearance and disappearance of solid species. It is important to establish that for this model, neither thermodynamic phase changes nor thermal equilibrium analysis was taken into consideration. This initial model was restricted only to mass balance analysis for solid and fluid components (equations 2.1 & 2.3), kinetic reactions dynamics (equations 2.8 & 2.9) and porosity changes (equation 2.10).

The numerical model first takes as an input the properties of each species involved in the model. Then it requires the input of boundaries and initial conditions for the model. After that, it solves equations 2.1, 2.3, 2.8, 2.9 & 2.10 using backward Euler discretization. Once these equations have been written in residual form, the algorithm will solve the non linear system of equations using the Newton-Raphson method. The Jacobian is computed using numerical derivation, then the system of linear equations is solved at every non linear iteration. This procedure is further illustrated in figure 3.1.

Two models were used to test this numerical solver. However, only one will be discussed. The second model with corresponding results are presented in appendix A.

3.1.1 Simulation test Model A type II kerogen

Model description.

FIGURE 3.1: Flow chart for initial numerical model

The model is treated as a kinetic cell with closed boundaries. Rock, oil, coke and kerogen are assumed to be incompressible. Only one level of energy will be considered per reaction. No phase changes are taken into account. Information regarding the chemical reaction properties, reservoir and fluid properties are presented in tables 3.1, 3.2, 3.3 and 3.4.

Reaction	Chemical formula	
kerogen decomposition	Kerogen	→ Oil + Gas + Coke
cracking oil	Oil	→ Gas + Coke

TABLE 3.1: Model A Type II Kerogen. Data obtained from Braun and Burnham, 1993a

Component name	Energy level	Frequency factor (A)	Activation energy (E_a)
Kerogen	1	3.0e13	49
Oil	1	1.0e12	54

Pyrolysis model with $A[s^{-1}]$ and $E_a[\text{kcal/mol}]$.

TABLE 3.2: Frequency factors and activation energy levels for Model A Type II Kerogen. Data adapted from Braun and Burnham, 1993a

Kerogen	Oil	Gas	Coke
-1	3.21125e-01	5.89375e-02	6.19937e-1
0	-1	6.04583e-01	3.95417e-01

TABLE 3.3: Mass stoichiometric coefficients for Model A Type II Kerogen. Data adapted from Braun and Burnham, 1993a

Properties	<i>Kerogen</i>	<i>Oil</i>	Gas	Coke	Rock
Density [kg/m^3]	1180	980	6.71	1400	NA
MW [kg/mol]	2.5	0.2	0.016	2	NA
Comp [$1/bar$]	0	0	1e-03	0	0
Min Con [$kmol/m^3$]	0.025	NA	NA	2e-20	NA
Saturation [—]	NA	0.3	0.7	NA	NA
Init Volume [m^3]	0.1059	0.12	0.28	0	1.4941
Res Volume [m^3]			2		
Int porosity [m^3]			0.2		
Int press [bar]			10		

TABLE 3.4: Components and reservoir properties for model A type II kerogen

Results.

From figure 3.2 we can observe how kerogen is degraded as expected from the chemical reaction model. On the other hand, oil molar mass increases (due to kerogen decomposition), but later it starts decreasing due to the cracking to coke and gas. The other two species show a continuous increase in moles along the process as expected. With respect to volume distribution, it is clear to see how gas volume reacts to the changes of the other components. Gas volume expands when approaching 600 k because it is the only compressible phase. Therefore, it has to occupy the volume left behind by the kerogen that is being decomposed. However, as temperature increases, gas volume start to shrink due to the increasing volume of coke. Finally, we can observe that porosity follows a similar trend to the volume of gas.

FIGURE 3.2: Test results for model A type II kerogen

3.2 Implementation of chemical reactions in ADGPRS

After studying and understanding the dynamics involved in the kinetic reaction models, we implement this kinetic reaction functionality into the Automatic Differentiation General Purpose Research Simulator (ADGPRS).

To check the accuracy of our implementation, we first perform a validation test. The kinetic reaction model used for this purpose was adapted from Behar et al., 2008. It is important to note that this kerogen model is originally designed to describe a natural maturation process. Therefore, this validation test was performed for a real geological maturation process rather than an in-situ upgrading process. A kinetic cell simulation was performed using the PMOD2 code (Braun and Burnham, 1992) and compared with simulation results of the modified ADGPRS.

3.2.1 Test case description

The kinetic model involves five fluid species, two solid species and 15 kinetic reactions describing pyrolysis process. Kerogen converts into an immobile fluid phase (HO_3 – dichloromethane soluble NSO_s), volatile components (MO_3 – pentane soluble NSO_s and MO_1 – volatile liquid hydrocarbons), gas component (CO_2) and solid component (*Coke*). The significant number of reactions can be explained by the multiple energy activation levels of the kerogen and two of the fluid species (medium and heavy oils, MO_3 and HO_3 respectively). The simulation representing a diagenetic process in a closed system was run for 100 million years with a step-wise temperature increase by 2 K per each million years. Kerogen was homogeneously distributed in the system, and no fluid species were present initially. Specific details of the reaction model are described in tables 3.5, 3.6 and 3.7. Complete thermal description of the properties of the fluid species involved in the simulation can be found in table 3.8.

Reaction	Chemical formula
kerogen decomposition	$Kerogen \longrightarrow MO_1 + CO_2 + MO_3 + HO_3 + Coke$
cracking of heavy oil (3)	$HO_3 \longrightarrow CO_2 + MO_1 + MO_3 + Coke$
cracking of medium oil (3)	$MO_3 \longrightarrow MO_1 + Coke$
cracking of medium oil (1)	$MO_1 \longrightarrow CHX + Coke$

TABLE 3.5: High-fidelity chemical reaction model

3.2.2 Kinetic cell simulation with high-fidelity model

Base on the model described above; the simulation was performed using a modified version of ADGPRS. Comparisons between the results of two simulations is presented in Fig. 3.3. The small discrepancy in the dynamic behavior of this reaction can be explained by the difference in the heating models in two codes. While PMOD2 applies a constant temperature increase of 2 degrees (Kelvin) per million years across the oil shale sample, ADGPRS represent the heating by the injection of the constant enthalpy (heat) using the in-situ heater model. That explains the difference in dynamics between the results of two simulations. To avoid this discrepancy, we perform another simulation with ADGPRS using an identical temperature input in the simulation cell. These results are presented in Fig. 3.4 and validate the correctness of the implementation of kinetic reaction in the modified ADGPRS code. As one can see, matching temperature dynamic removes the difference in kinetic cell simulation results.

Component name	Energy level	Frequency factor (A)	Activation energy (E_a)	Mass fraction reacted
Kerogen	1	1.35e13	43.8	0.022
	2		46.5	0.285
	3		48.3	0.308
	4		50	0.346
	5		54	0.005
	6		56	0.034
HO ₃	1	1.35e13	44.8	0.594
	2		47.7	0.001
	3		49.5	0.237
	4		53.2	0.168
MO ₃	1	1.35e13	46	0.011
	2		49.5	0.468
	3		52.9	0.52
	4		54.7	0.001
MO ₁	1	1.35e13	53	1

Pyrolysis model with $A[s^{-1}]$ and $E_a[\text{kcal/mol}]$.

TABLE 3.6: Major parameter describing the high-fidelity chemical reaction model

Kerogen	MO ₁	CO ₂	MO ₃	HO ₃	CHX	Coke
-1	0.004	0.06	0.01	0.72	0	0.17
0	0.13	0.06	0.28	-1	0	0.53
0	0.65	0	-1	0	0	0.35
0	-1	0	0	0	0.85	0.15

TABLE 3.7: Mass stoichiometric coefficients of the high-fidelity reaction model

Species	MOl_{wt}	$T_c(k)$	$P_c(MPa)$	Acentric	Rackett
HO ₃	561.1	996	0.64	0.941	0.2232
MO ₁	378.7	930	1.20	0.664	0.2303
MO ₃	378.7	930	1.20	0.664	0.2303
CHX	45.1	370	4.25	0.153	0.2767
CO ₂	44.0	304	7.38	0.239	0.2944

TABLE 3.8: Mole weights and critical properties for the high-fidelity fluid components (based on Braun and Burnham, 1993b)

3.2.3 Kinetic cell simulation with coarser chemical model

Here we presented results corresponding to the coarsening in chemical representation. For the reference solution, we used the high-fidelity simulation model with 15 reactions, 11 fluid species (3 gas and 2 oils with 4 energy levels each) and 7 solid species (6 energy levels for kerogen and coke), see details in tables 3.5, 3.6, 3.7 and 3.8. For the simplified model, we reduced the activation energy levels to one per reaction. As a result of this changes, the coarser model has only 4 reactions involved in the process, 5 fluid species and 2 solid species. We used an averaged activation energy as an input for the model. The kinetic reactions parameters for the model are summarized in table 3.9.

All simulations were performed using ADGPRS in a one gridblock model with the heat rate corresponding to the average temperature changes by 13 K per day. It

FIGURE 3.3: Test Results using PMOD2 and ADGPRS using different heating process

Component name	Energy level	Frequency factor (A)	Activation energy (E_a)
Kerogen	1	1.35e13	48.5643
HO ₃	1	1.35e13	47.328
MO ₃	1	1.35e13	51.2347
MO ₁	1	1.35e13	53

Pyrolysis model with $A[s^{-1}]$ and $E_a[\text{kcal/mol}]$.

TABLE 3.9: Frequency factors and activation energy levels for a simplified model

can be seen that the coarser representation changes the dynamic of species transformation quite insignificantly. The comparison of the simulation results for the two models are shown in Fig. 3.5.

FIGURE 3.4: Test Results using PMOD2 and ADGPRS Test Results using PMOD2 and ADGPRS using identical heating process

FIGURE 3.5: Test Results ADGPRS with high fidelity model and coarser chemical model

Chapter 4

Reservoir test case

Here we perform the simulation of in-situ upgrading process. We describe a realistic 2D test case and present simulation results. Three different studies are performed. The analysis of coarsening in time, space, and chemical representation of the species will be presented in this chapter.

4.1 Description of the reservoir model

The simulation was performed in 2D cross-section of the subsurface reservoir with a layer-based heterogeneous distribution of kerogen. The reservoir contains three distinguishing layers: the cap-rock from 0 to 260 m, the payzone from 260 m to 674 m, and finally the bed-rock from 674 m to 874 m. The kerogen and corresponding porosity and permeability are vertically distributed based on the grade function adapted from Garipov et al., 2016. It is important to clarify that this kerogen distribution does not correspond to the same type of kerogen describe by the model adapted from Behar et al., 2008. Here we implement this distribution as an illustrative example of a real geologic variability of kerogen concentrations. The production setup involves an electrical heater located at the left boundary between 500 and 550 m, and a production well located on the opposite side with perforation interval between 450 and 550 m. The simulation model contains 4080 active gridblocks with 40 blocks in the x-direction by 0.5 m each and 102 blocks in the z-direction including over- and under-burden and payzone with 4.12 m block size. Initial porosity and kerogen distribution are shown in Fig. 4.1.

4.2 Reference solution

Here we present the results of simulation in the reference model as dynamic changes of temperature, porosity, and oil phase saturation. In Fig 4.2 you can see two different times in the simulation: 200 days, soon after oil bank breakthrough and 600 days when oil production begin to decline. The maximal oil saturation reach in payzone is $S_o = 0.25$ with the maximal temperature near the heater is around 1000 K.

It is clear from the results that the kerogen transformation is happening mostly in the layers connected to the heater which is consistent with previous observations by Garipov et al., 2016. The effect of solid decomposition can be observed as well in the dynamic behavior of porosity in areas exposed to the kerogen transformation. The results of this simulation provide a better understanding of the complex mechanism behind the in-situ upgrading process.

FIGURE 4.1: Kerogen grade, initial distribution and initial porosity in reservoir

FIGURE 4.2: Solution based on high-fidelity model description

4.3 Coarsening in time

In the next study performed here, we look at a sensitivity of the simulation results to the timestep size. We run the reference model with a larger timestep $\Delta t = 5$ days, which is the largest timestep supported by the nonlinear solver without cuts, and a smaller timestep $\Delta t = 0.1$ days. The simulation results are present in Fig 4.3.

FIGURE 4.3: Production rates for simulation at different timesteps

As you can see, the sensitivity to the timestep size is very small. The three results basically overlay on top of each other.

4.4 Coarsening in space

In the next simulations, we study a sensitivity of the solution to the grid resolution. The high-fidelity reference model was run at two levels of a coarser grid with 1040 grid blocks and 270 grid blocks. The simulation results are present in Fig. 4.4. As you can see, the spatial distributions look quite similar to the reference solution even in the case of the coarsest grid. However, after the inspection of Fig. 4.5, it is clear that the production dynamic for the 270 grid blocks model starts deviating from the fine grid simulation. Here, chemical interactions at a coarser scale of representation increase the mismatch in the simulation results usually associated with a coarser thermodynamic representation (Iranshahr et al., 2014).

4.5 Coarsening in chemical species

In this final section, we will present two different approaches for the lumping of the species. First, we will present a chemical model with all kerogen species and all oil species lumped. This model will present only one energy level per each reaction. Then we will study the effect on lumping all species except for HO_3 components.

4.5.1 Coarsening in kerogen and oil species

In Fig 4.6 you can see the results of the simulation. It is clear that the lower fidelity models cannot reproduce the dynamic of the reference system with the same level of accuracy. It is clear that the oil front propagates much faster in the coarser models. However, while fluid dynamics is not captured accurately enough, the porosity transformation and temperature distribution remain quite close.

FIGURE 4.4: Simulation based on a coarser simulation grid with 20×52 and 10×27 gridblocks

FIGURE 4.5: Production rates for simulation with different grid size

FIGURE 4.6: Solution for kerogen and oil lumped model

Similar conclusions can be derived based on dynamics of production rates presented in Fig. 4.7. The coarse model captured the rate of production gas quite well,

while the difference in oil rate prediction is more significant.

FIGURE 4.7: Production rates for kerogen and oil lumped model

4.5.2 Full description for HO3 and coarsening of kerogen and MO3

For this simulation we will require the properties of the lumped species (table 3.9) and the properties from the high fidelity model (table 3.6).

FIGURE 4.8: Solution for a full description of HO3 and coarsening of kerogen and MO3

FIGURE 4.9: Production rates for a full description of HO3 and coarsening of kerogen and MO3

If we compare the results of this simulation (figures 4.8 and 4.9) with the results of previous simulation (figures 4.6 and 4.7), we can observe that the largest error

is introduced by lumping HO3 species. As can be observed from the results, this model does reproduce the dynamic behavior of the reference system.

4.6 Run time and error quantification

On the first part of this section we present a quantitative error of all previous simulations. Here we used the L_2 error method to compute the error in oil and gas production. Results are showed in figure 4.11.

FIGURE 4.10: Error calculation

It can be seen that the largest error in the gas production is introduced by an aggressive coarsening in space. However, the oil dynamic is mostly affected by the lumping of the species involved into the heavy oil description. At the same time, time resolution almost have no impact on the results.

Regarding the run time we have the following results showed in figure 4.11.

FIGURE 4.11: Run time

As we can observe from figure 4.11, coarsening in space and physics show that run time can be reduced in large percentages. The 4 simulations (two coarsening in space and two coarsening in chemical species) showed that run time can be reduced in more than half. Additionally we can observe that coarsening in time shows the best balance between run time reduction and error quantification (Δt : 5 days).

Chapter 5

Conclusions

This thesis presents the first attempt to systematically quantify the errors introduced by different types of coarsening in reservoir simulation of in-situ upgrading of kerogen. We started by first studying the dynamics of the chemical reactions in kinetic cells for closed systems. Based on these simulation results, we understood how components reacted to the increments in temperature of the kinetic cell. Results of this study indicates that chemical model react differently depending on the heating process implemented in the simulation. In addition we also studied the effect of chemical transformations to the porosity of the system. Next, we design a high-fidelity model based on an accurate description of kerogen decomposition process and detailed 2D model of in-situ upgrading setup with heterogeneous kerogen distribution. The high number of species describing reaction and complex multiscale interactions related to the process requires a coarser representation to perform simulation study at the reservoir scale which often includes different types of inversion and requires many forward simulation runs. We studied a coarsening in chemical, spatial, and temporal representation to improve the run-time. Based on our findings, the coarsening in chemical representation introduce the most significant error to the simulation results. For this study, we proposed an initial coarser model in which we lumped all components individually. Therefore, the lumped model will present only one energy level per reaction. This model was run to the kinetic cell and reservoir level. When comparing both results, we can conclude that our proposed model works well at the kinetic cell level, while at reservoir level, the results are considerably different when compared to the high-resolution model. This behavior is associated with a coarser representation of the lumped species. In a further attempt to isolate the problem with the coarser model, we performed additional simulations, and found that problems were mainly associated with the coarser representation of the component HO_3 . On the other hand, we found that coarsening in time introduce the lowest error to the results of in-situ upgrading simulation. While coarsening in time looks the most attractive for the improvement of forward model efficiency, it still requires a robust nonlinear solver to guarantee the nonlinear convergence of the simulation.

Appendix A

Simulation test Model E type II kerogen

Model description.

The model treated as a kinetic cell with closed boundaries. Only gas species will be assumed to be compressible. Only one level of energy will be considered per reaction. No phase thermodynamic changes are taken into account. Information regarding the chemical reaction properties, reservoir and fluid properties are presented in tables A.1, A.2, A.3 and A.4.

Reaction	Chemical formula
1 Kerogen $\longrightarrow$	HO1+LO1+CHX+CH4+RESC+RESH
2 HO1 $\longrightarrow$	LO1+CHX+CH4+RESC+RESH
3 LO1 $\longrightarrow$	CHX+CH4+RESC+RESH
4 CHX $\longrightarrow$	CH4+RESC+RESH
5 RESC+RESH $\longrightarrow$	CHX + CH4
6 RESC+RESH $\longrightarrow$	CHX + CH4
7 RESC+RESH $\longrightarrow$	CH4

TABLE A.1: Model E Type II Kerogen. Data obtained from Braun and Burnham, 1993a

Reactants	Frequency factor (A)	Activation energy (E_a)
Ker	3.0e13	49
HO1	1.0e13	54
LO1	5.0e11	54
CHX	1.2e12	57
RESC + RESH (Reaction # 5)	1.0e13	54
RESC + RESH (Reaction # 6)	5.0e11	54
RESC + RESH (Reaction # 7)	1.2e12	57

Pyrolysis model with $A[s^{-1}]$ and $E_a[\text{kcal/mol}]$.

TABLE A.2: Frequency factors and activation energy levels for Model E Type II Kerogen. Data adapted from Braun and Burnham, 1993a

Results.

Ker	HO1	LO1	CHX	CH4	RESC	RESH
-1	0.278	0.143	0.018	0.005	0.528	0.027
0	-1	0.373	0.157	0.0301	0.425	0.016
0	0	-1	0.595	0.115	0.282	0.008
0	0	0	-1.0	0.681	0.311	0.008
0	0	0	0.609	0.668	-1.0	-0.277
0	0	0	0.122	1.202	-1.0	-0.324
0	0	0	0	1.336	-1.0	-0.336

TABLE A.3: Mass stoichiometric coefficients for Model E Type II Kerogen. Data adapted from Braun and Burnham, 1993a

Properties	Ker	HO1	LO1	CHX	CH4	RESC	RESH	Rock
Density [kg/m^3]	1180	980	960	8.71	6.71	1600	1600	NA
MW [kg/mol]	2.5	0.2	0.18	0.016	0.014	2	2	NA
Comp [$1/bar$]	0	0	0	1e-3	1e-3	0	0	0
Initial Moles $kmol$	2.2	31.5	31.5	4.55	4.55	2.575	2.575	NA
Init Volume [m^3]	4.66	6.43	5.91	8.36	9.49	3.22	3.22	58.72
Res Volume [m^3]					100			
Int press [bar]					10			

TABLE A.4: Components and reservoir properties for model E type II kerogen

FIGURE A.1: Test results for model E type II kerogen

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