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Enhanced Recovery of Heavy Oil Using A Catalytic Process

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Enhanced Recovery of Heavy Oil Using A Catalytic Process

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Abstract. Oil is a major source of energy around the world. With the decline of light conventional oil, more attention is being paid to heavy oil and bitumen, as a good alternative to light oil for energy supplies. Heavy crude oils have a tendency to have a higher concentration of metals and several other elements such as sulfur and nitrogen, and extraction of these heavy oils requires more effort and cost. Toe-to-Heel Air Injection (THAI) is a novel process of enhanced heavy oil and bitumen recovery and upgrading. In this technique, horizontal well concepts are integrated with the reactions of high temperature oxidation to achieve a potentially high recovery ratio. Since the process works through a short distance displacement technique, the produced oil flows easily toward the horizontal producer well. This direct mobilized oil production and short distance are the major features of this method which lead to robust operational stability and high oil recovery. This technique gives the possibility of a higher recovery percentage and lowers environmental effects compared to other technologies like steam based techniques. A novel well design consisting of two horizontal injectors and two horizontal producers was used in different well configurations, to investigate the potential for improved efficiency of the THAI process on the heavy oil recovery. A 3D dimensional model, employing the CMG-STARS simulator, was applied for this process. Two horizontal injectors and producers were utilised in this project, instead of the conventional horizontal injector and producer used in the Greaves model (the base case model), to investigate the effect of the extra injector and producer on the performance of the THAI process. It was found that the locations of the well injections and the well productions significantly affected the oil production. It was found that the amount of the produced oil rose up to about double of the amount of the oil produced by the original model. For the study of the effectiveness of the catalysts in the oil upgrading process, the CAPRI technique has been simulated to investigate the effect of several parameters, such as catalyst packing porosity, the thickness of the catalyst layer and hydrogen to air ratio, on the performance of the CAPRI process. The TC3 model used by Rabiu Ado [1], which was the same model utilised in the experimental study of Greaves et al. [2], was also employed in this study. The silica-alumina catalyst characterised by Hasan [3] was placed around the horizontal producer in this simulation.

1. Introduction

Thermal methods are used frequently for oil production from heavy oil reservoirs. The In-Situ combustion (ISC) technique is one of these methods; it has been used for over 80 years in a lot of fields around the world. ISC is considered the most commonly used of the valuable thermal processes because no external energy source for the process is required. Injected air, used in in-situ combustion, helps to burn part of the crude oil generating heat, which lowers oil viscosity and causes high cracking rates of heavy oil located in front of the combustion zone. The cracking of the crude oil leads to in-situ upgrading of heavy oil. This feature is considered the most important advantage of the in-situ technique compared to the other EOR techniques. However, this method has several disadvantages. One of these drawbacks is that the ignition inside the well can happen spontaneously. Because of this spontaneous ignition, the consumption of the oxygen will occur close to the injector, and the process will be changed by this feature into forwarding combustion [4]. Also, because the oxygen is exhausted near to the injection well, which causes a deficiency in the oxygen supply, it will be difficult to reach a high-temperature combustion mode, which makes it difficult to maintain the combustion [5,6].

In addition, the conventional ISC technique uses a vertical injector and a vertical producer in which hydrocarbons need a long time to travel from the injector well to the producer well. These operational patterns suffer from some considerable problems, such as gravity override of gas, and the production of heavy oil from the reservoir can be affected by these problems. The Toe-to-Heel air injection technique (THAI) is a process in which the heavy oil production rate can be increased dramatically. This method is an advanced ISC technique, which combines the conventional ISC technique with horizontal producer wells, instead of vertical producer wells as in the conventional methods. The reason for this is to avoid the long distance between the injection well and the production well, to keep combustion advanced ahead from the “toe” to the “heel” within the producer well. The THAI process is designed to operate in a way involving stabilization of the drainage by gravity, which is restricted to a narrow mobile oil zone, which will travel along the horizontal production section. This short distance between the injector and the producer causes direct transferring of the mobilized fluids to the production well [7].

The THAI process for enhanced oil recovery follows the same basic mechanism as for the in-situ combustion technique. Part of a heavy residue is burned by air introduced via the injection well, producing heat to increase the temperature of the heavy oil, which causes a high reduction in the oil viscosity; as a result, the mobility of the oil will be increased. The thermal cracking reaction of the heavy oil produces fuel (mainly coke) which will be generated ahead of the combustion advance. The amount of this coke cracked is a very significant parameter to sustain the combustion propagation [8]. Xia et al. [9] have conducted a set of 3D experimental evaluations of THAI for upgrading of Wolf Lake oil with API gravity of 10.5° and Athabasca Tar Sand Bitumen with API gravity of 8°, both originating from Canada, using different well configurations as follows: vertical injector/horizontal producer (VIHP) and horizontal injector/horizontal producer (HIHP) wells in direct line drive, and staggered line drive of vertical injector/two horizontal producer (VI2HP) and two vertical injector/horizontal producer (2VIHP). It was demonstrated that the horizontal injector/horizontal producer (HIHP) was the most effective for obtaining quick start-up, which means that the required time for commencing propagation of the combustion front is very short.

Further previous work using different well configurations includes simulation by Fatemi et al. [10] to evaluate the effects of several parameters regarding injector-producer wells arrangement, namely the distance between the positions of the wells, the depth of the injector and the length of the horizontal producer, on the performance of THAI technique in reservoirs including heavy crude oil. 3D combustion cell, employing the CMG-STARS simulator, has been applied in this study for the heavy oil carbonate reservoir in Iran named Kuh-E-Mond (KEM). It was noticed that significant parameters, such as depth of injection, horizontal producer length, and the distance between injectors, should be taken into account, in order to fulfil the highest performance in the THAT process. The findings revealed that the best configurations forfield scale are the 2VIHP and VIHP schemes.

Experimental work on in-situ combustion (ISC) was performed on the heavy oil of the Orinoco Belt in Venezuela using a combustion tube by Anaya et al. [11], to investigate the technique performance. The laboratory scale results, obtained from the combustion tube experiment, were simulated to scale the laboratory tests up to full field scale. Several different well configurations were considered for the numerical ISC simulation, taking into account distances between the injector and the producer, to

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determine the most favourable positions of injection and production wells. The tested distances between the injector and the producer were 50 m, 100 m and 200 m, with a constant rate of air injection of ~7063 m^3 min^{-1}. It was found that the suitable distance between the injector and the producer, to operate the experiment in the field, was 100 m. The findings revealed that the model, in which the distance between the injector and the producer was 100 m, gave a high recovery factor and delayed gas breakthrough.

Moreover, a catalytic reactor can be integrated into the THAI technique to be a very effective method to upgrade crude oils prior to the refinery. Catalytic-Processing In-Situ (CAPRI) upgrading of high molecular weight hydrocarbons using ISC provides the possibility of increasing the extent of the improvement process of the heavy oil in situ Abu et al. [12]. The way of using this technique is to attain further upgrading of heavy oil by covering a perforated horizontal producer by a layer of catalyst [8, 13].

In the THAI process, the cracking reaction, created due to the high temperature within the mobile oil zone (MOZ), generates the coke precursor for the CAPRI process [14]. The MOZ involves mobilized oil, water as steam, unconsumed oxygen and gases produced from the combustion process including a small amount of carbon monoxide at high temperatures in the range of 450-650 ℃ [15]. The gases produced from the combustion reaction operations are given by the following equations [16]:

Heavy oil → light oil + gas + coke + absorbed heat (1)

Coke + O_2 → H_2O + CO_2/CO + heat (2)

Heavy oil + O_2 → H_2O + CO_2/CO + heat (3)

Light oil + O_2 → H_2O + CO_2/CO + heat (4)

It is thought that heavy oil is upgraded by a hydroprocessing operation in which carbon-rejection reactions are integrated with the addition of hydrogen at the catalyst surface [14]. According to Hajdo et al. [17], the hydrogen used in the process could be provided via a gasification process and/or the water-gas-shift reaction. The THAI-CAPRI technique is considered environmentally friendly because it makes the heavy oil free of undesirable contaminants such as sulfur, vanadium and nickel. The method is a new technology which offers the significant feature of a combination of enhanced oil recovery process simultaneously with the catalytic upgrading of immobilized to mobilized oil [18].

Experimental THAI-CAPRI work has been conducted by Shah et al. [14], using different catalysts to optimize the catalyst type and to find the favourable conditions for use of this technique. A microreactor was employed to perform this experiment, utilizing different temperatures, pressures and various gas media. Alumina-supported CoMo, NiMo and ZnO/CuO catalysts have been tested. It was found that the improvements of the API gravity, and the reduced levels of the viscosity, are dependent upon the flow rate of the oil and the temperature. It was also noticed that, at high temperature, more upgrading could be achieved, but that led to reduction in the lifetime of the catalyst bed. On the other hand, decreasing the temperature has led to a longer catalyst-bed lifetime, but the upgrading levels of the produced oil went down. Therefore, a balance in the operating temperature, between upgrading performance and the lifetime of the catalyst, is required to achieve acceptable consequences.

Hart et al. [16] have experimentally tested a different type of gas in the THAI-CAPRI method to investigate the effects of the gas environment, using CoMo catalyst supported by γ alumina. Heavy oil has been utilized with API gravity of 14°. It has been found that the reactions of the hydrocracking and hydrogenation occurring in THAI process were promoted when hydrogen gas was used. Employing hydrogen gas gave rise to an API gravity of the produced oil 4° above the original value of the API of the feed, which was the highest number for the different gases level. Further, using hydrogen gas results in a higher reduction in the viscosity and higher conversion of heavier hydrocarbons, with a high boiling point, to lighter fractions, with a lower boiling point. Moreover, it was noticed that hydrogen media leads to convert unsaturated to saturated components as well as enhance the productivity of the saturated hydrocarbon.

A numerical THAI-CAPRI model has been simulated by Rabiu Ado [1] at laboratory scale to investigate the catalyst activity on the heavy oil upgrading, using the same dimensions of the 3D

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combustion cell used in Greaves model. The effect of the frequency factor of the reaction on several parameters, such as oil rate, cumulative oil production and the API gravity, has been demonstrated. It was found that slight differences in the peak temperature were observed between the various values of the frequency factor, where during the combustion period, the maximum variance in the temperature difference was 40 °C. It is also found that the increase in the frequency factor has led to the increase in the production rate.

Further studies are needed to further understand the THAI-CAPRI technique. In this study, more parameters, such as catalyst thickness, catalyst packing porosity, will be investigated. In addition, the effect of the ratio of hydrogen to air will be taken into account in this project. Additionally, this present work aims to simulate the effect of different well configurations on the performance of the THAI process applied at the laboratory scale. Two horizontal injectors and two horizontal producers (2HI2HP) were employed in different well configurations. Three different locations of the injectors and producers were simulated to look at the effects of the various places of the wells on the THAI process performance. Several parameters such as oil recovery factors, combustion front temperature, oxygen profile and solid phase (coke), have been tested on the THAI technique to choose the best configuration at laboratory scale.

2. Methodology

2.1. 3D combustion cell model

In this work, the Greaves model [2] was adopted, and a numerical CMG STARS model developed to carry out the simulations. A 30 × 19 × 7 (i, j, k) gridblocks experiment scale model was applied using Virgin Athabasca oil sand data, as reported by Greaves et al. [2]. The API of the oil was 8° with specific gravity 1.0143. The measurements of this 3D rectangular combustion cell are 0.6 m long, 0.4 m wide and 0.1m deep, using two horizontal injectors (2HI) and two horizontal producers (2HP) which were positioned in different schemes. Real reservoirs are continuous and all flow factors, which depend on the time, change constantly. Because of this continuous change of fluid properties, a reservoir simulator cannot solve these variables. Therefore, the continuous reservoir has to be divided into finite size elements and this division is indicated as the reservoir discretization. Each element of the group is called a reservoir grid or a cell. The STARS software includes the discretised wellbore (DW), which allows the fluid and the heat flow in the wellbore and between the wellbore and the reservoir to be accurately modelled. All types of equations, wellbore mass, energy conservation and chemical reactions equations are combined together and solved by the software in each wellbore part,using fully implicit finite difference method. However, to solve these equations, several reservoir input parameters are required. The original geological parameters used in this simulation (porosity, vertical permeability and horizontal permeability of the cell) are given in Table 1, and the relative permeability curve can be seen in Figure 1. PVT data used in the THAI process is reported in Table 2. The initial gas and oil saturation were 0.15 and 0.85, respectively, and the initial water content has not been considered. The air was used alone (known as dry combustion) with a flow rate for the air injection of 8000 $cm^3\ min^{-1}$, which corresponded to 12 $m^3\ m^{-2}\ h^{-1}$, at the beginning of the run, when pre-heating was finished. Then, depending on the pre-heating time, the air flow was increased to 10667 $cm^3\ min^{-1}$, which is equivalent to a flow rate of 16 $m^3\ m^{-2}\ h^{-1}$, and continued at this rate until the end of the simulation.

Table 1. Geological parameters of the rocks used in the simulation.

So (%)	Sw (%)	Porosity (%)	Vertical permeability (md)	Horizontal permeability (md)
85	15	34	2300	11500

Table 2. PVT data applied to this project.

Component	Mol fraction (%)	Molecular weight (g mol^{-1})	Critical pressure (kpa)	Critical temperature (°C)	Density (kg m^{-3})
Light component	36.47	170.0	2305.95	425.16	903.8
Heavy component	63.53	878.0	1031.29	780.0	1012.07

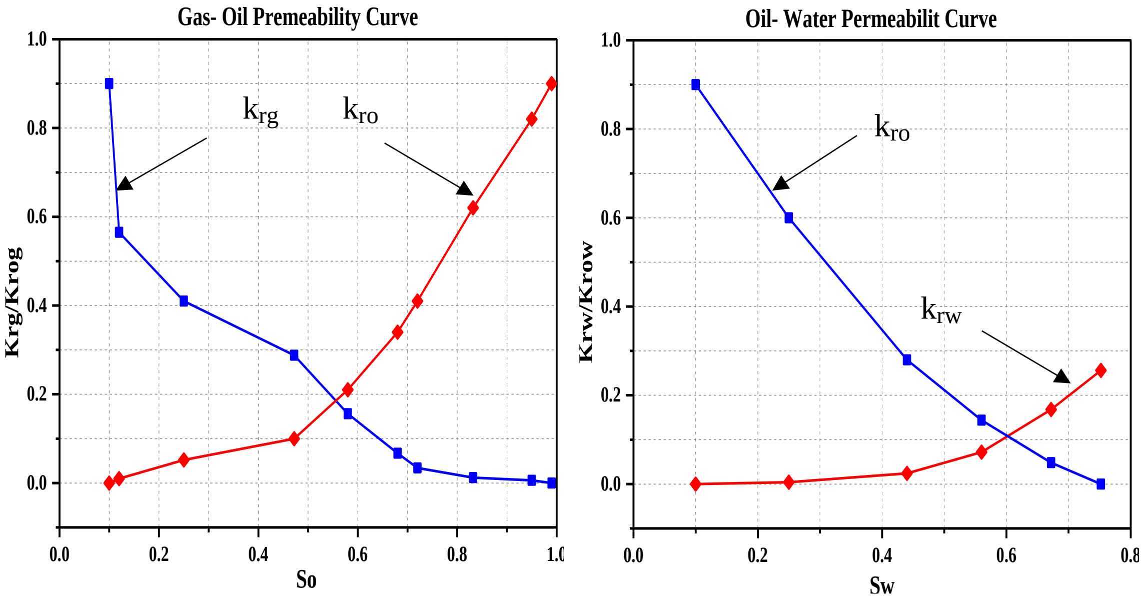

Figure 1. Relative permeability of Athabasca bitumen.

In order to make sure all parameters are consistent with the Greaves model (the original model), the total rate of the injected air for one injector in the Greaves model was equally divided between the two well injections in this study.

2.2 Different well arrangements

A numerical simulation has been carried out in this work using two horizontal injectors and two horizontal producers in different well configurations. In each well configuration, the injectors and the producers have been put in different locations, therefore the different designs of the injectors and the producer's positions are very important in this work. The configurations of the well were arranged as follows:

Greave's model (the original model) is represented, Ao, as shown in Figure 2a. The first well arrangement, A1, was that the first injector, I1, was placed on the top horizontal layer while the second injector, I2, was placed on horizontal layer two rows directly under I1, and the producers, P1 and P2, were positioned on the horizontal layers five and six rows perpendicular to the injectors as shown in Figure 2b. The second configuration, A2, was that the injector, I1, remained at the same position, and the second injector, I2, was moved to the other edge of the reservoir on the top horizontal layer, while the producer, P1 and P2 were centred at the middle of the reservoir as presented in Figure 2c. Finally, in configuration A3, the injectors, I1 and I2, were positioned on the top horizontal layers at the centre

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of the reservoir and the producers, P1 and P2, were fixed on both sides of the reservoir as shown in Figure 2d.

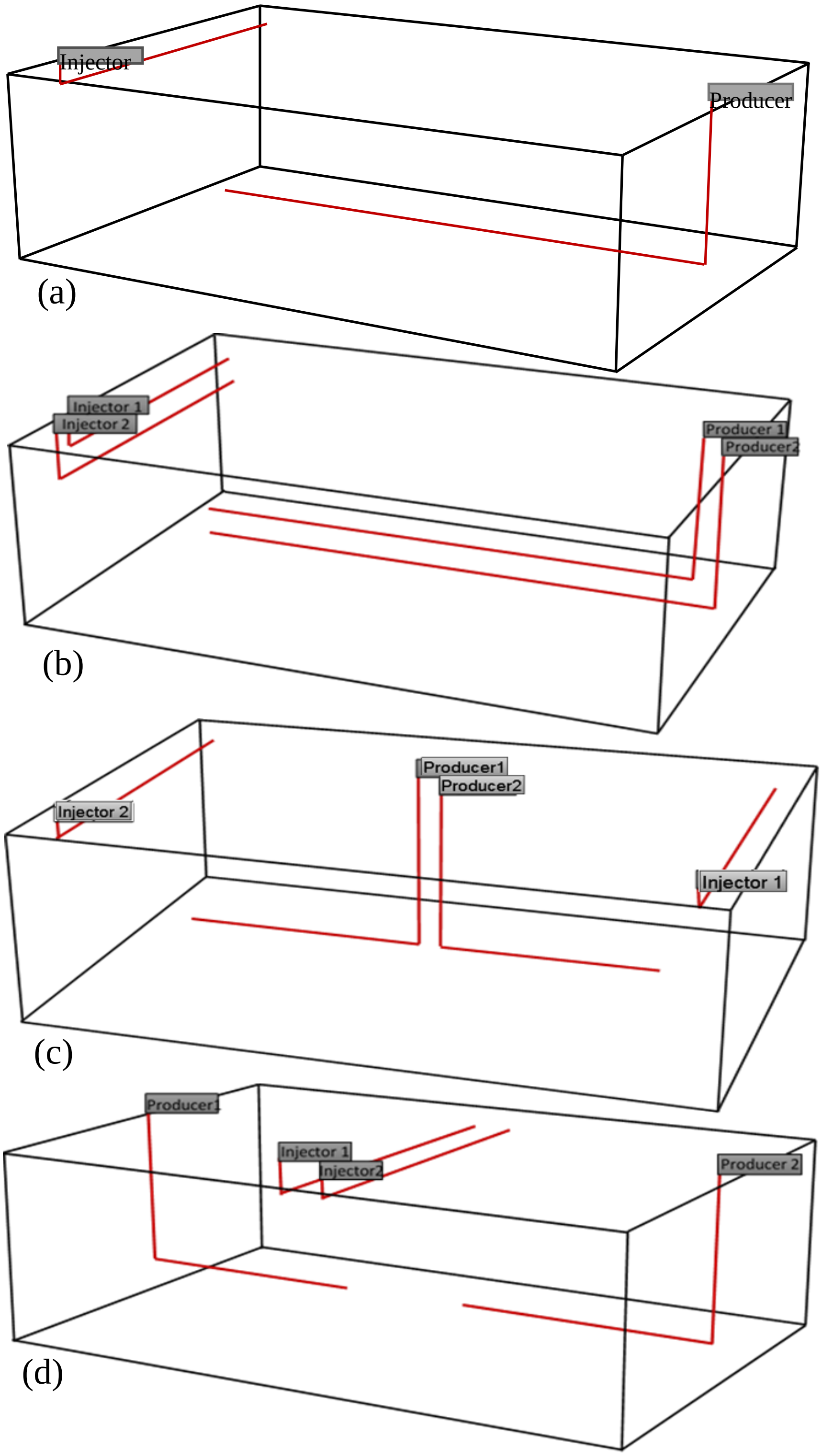

Figure 2. 3D reservoir well configurations in (a) original model, (b) model A1, (c) Model A2, (d) Model A3**.**

3. Results and Discussion

3.1 Effect of wells configuration on THAI process

Heavy oil of Virgin Athabasca was used in the THAI simulation runs. The oil specific gravity was 1.0143 with 8°API.

3.1.1. Oil rate and production

The oil rate and production are considered the most important indicators to assess the performance of THAI process. Figure 3 shows that no oil was produced during the ~13 minutes of the heating period. This is because no oil exists inside the production well before starting the air to be injected. It can be seen from Figure 3, for all models oil production started earlier in comparison with the Greaves model A0 (the original model). The reason is the presence of two well injectors in the models helps to increase the required amount of heat to pre-heat the inlet zone of the reservoir. As a consequence, it helps to establish a quick communication between the injector wells and the producer wells. It was also observed that, at the beginning, the rate of the oil production dramatically increased to create a high sharp peak. The reason for this is due to the high pressure generated near to the toe of the producer, which is caused by the gaseous and light hydrocarbons produced as a result of the thermal cracking occurring due to the heat provided at the inlet zone of the horizontal injectors. Based on the comparison between all the well configurations, it is obvious that A2 arrangement had the highest production rate and the A3 model then came second; however, the A0 and A1 configurations had the lowest oil production rates. From Figure 4, it can be observed that the cumulative oil recovery, for the A0 and A1 configurations, is almost the same. The highest amount of the produced oil was the A2 model and then the A3 model. It is suggested that the presence of the two well injectors in these models was behind the high amount of the oil production.

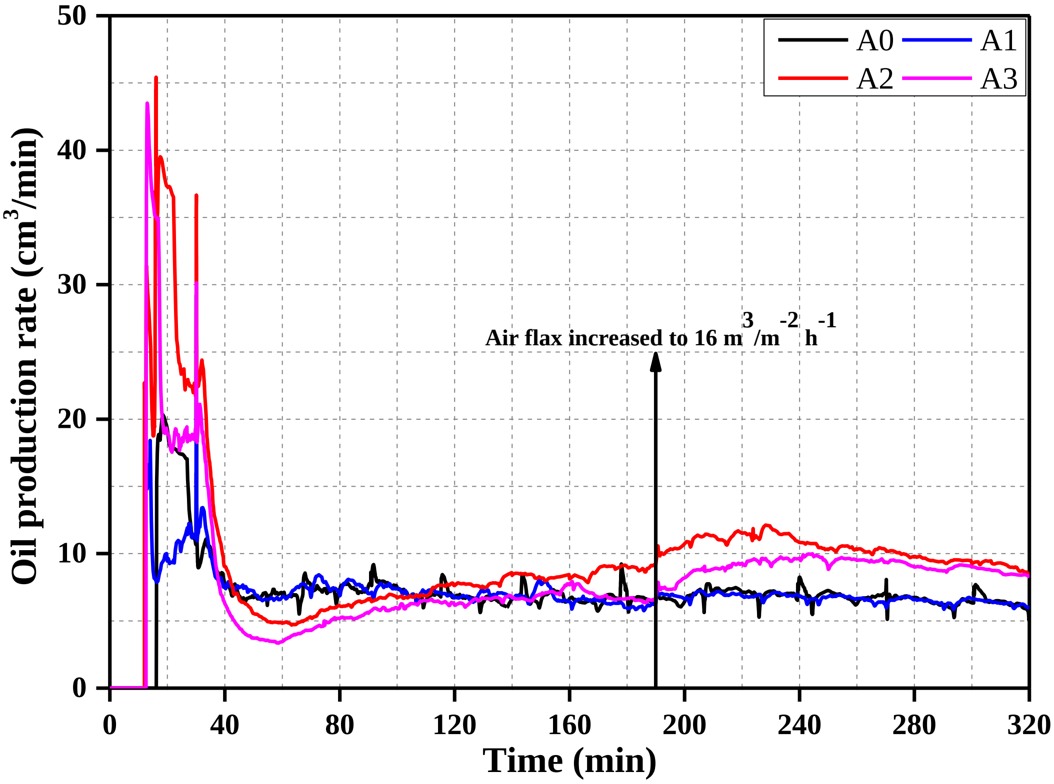

Figure 3. Oil production rates of different models.

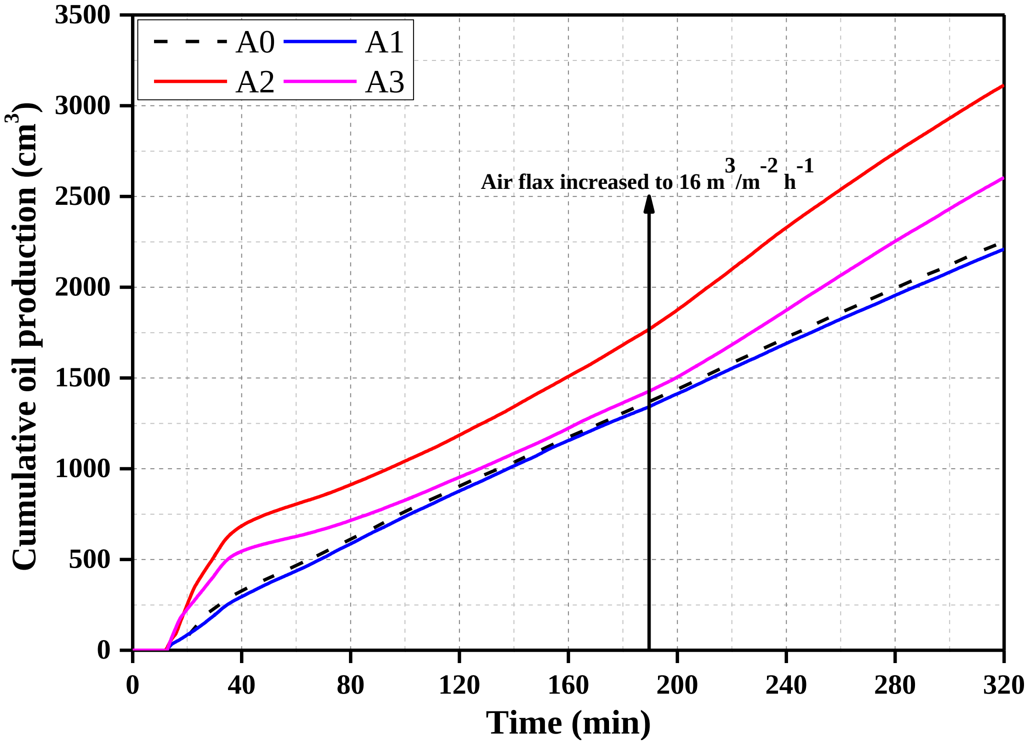

Figure 4. Cumulative oil production.

3.1.2 Combustion front temperature

The most significant feature in the THAI in-situ combustion process is that the advancing combustion front is propagated in a very stable way throughout the distance from the top to the bottom of the heavy oil reservoir. Oxygen is injected from the top of the reservoir to generate this combustion front, which can be sustained by the continued flow of the oxygen-containing gas at the reservoir's top, with low viscosity oil passing toward the production well. High-temperature reactions take place in this process. At the combustion front, most of the oxygen will be consumed by these reactions. From Figure 5, it can be seen that, during the pre-heating time period, the peak temperatures for all the models followed nearly the same trend, except the A3 model which was a little below the others. Then, after ignition is achieved, the A0 and A1 models exhibited almost the same behaviour until the end of the simulation. However, the behaviour of the A2 and A3 models were different, where the A2 model was more stable than the A3 model until the simulation end. As a consequence, the location of the injectors and producers has a significant effect on the stability performance of the THAI process. The small spikes on the more smooth tradition peak temperatures, which have different position depending on the well arrangement, are due to the combustion front reaching a high coke concentration at this point of the peak temperatures inside the producer.

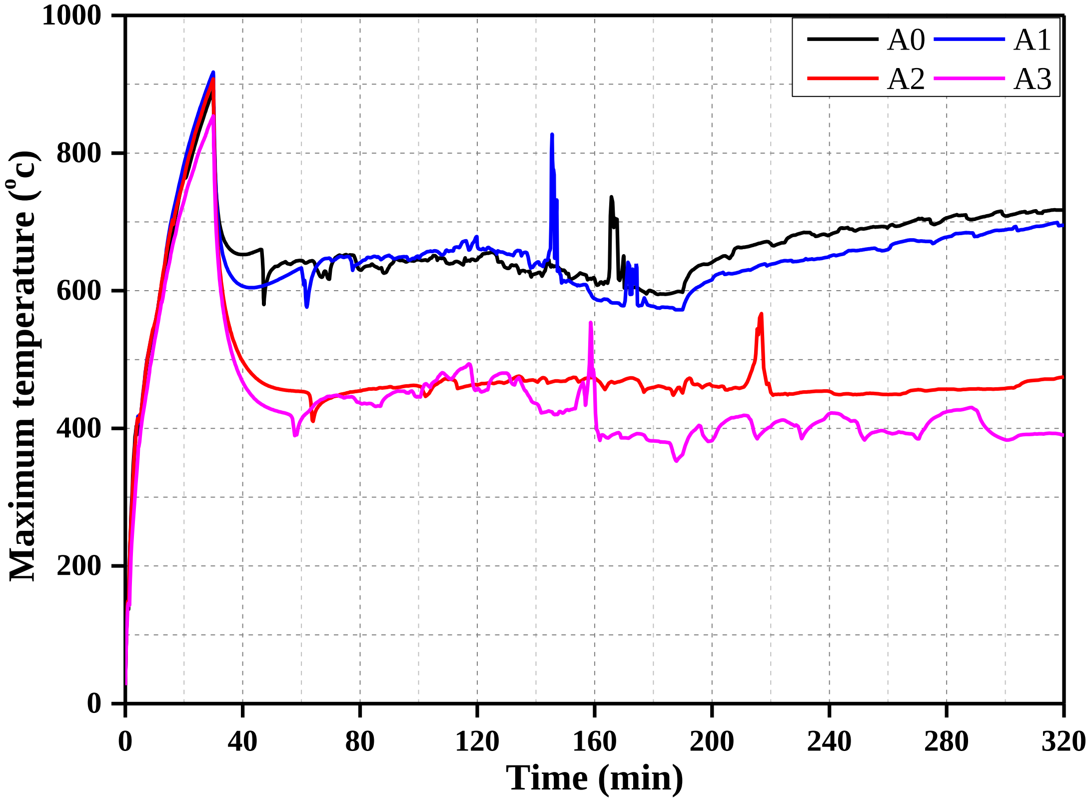

Figure 5. Peak temperatures for different Well Configurations.

3.1.3 Mole fraction of oxygen production

The amount of the oxygen used is one of the most important parameters in the THAI process for enhanced heavy oil recovery. It is considered a good indicator of the performance of the combustion propagation. Therefore, the amounts of consumed and produced oxygen are very significant for the sustainability and the stability of the combustion front. On the other hand, the amount of the consumed oxygen can be calculated from the oxidation process occurring in front of the combustion front because of the high temperature generated through the burning process of the heavy oil. Figure 6 shows the mole fraction of produced oxygen for the different models during the time period of the simulation. It is clear that the oxygen production started early in the A3 model at about 160 min, while it began late in the A1 and A2 configurations. Although the oxygen production commenced late in A2, it behaved more stable than the other models compared to the Greaves model, i.e., that well configuration affects stability. It can be also observed from Figure 7 that oxygen profile in model A2 showed close agreement with that for Greaves model (A0). The concentration of the deposited coke at the toe and the heel of the HP well has a direct effect on the amount of the produced oxygen. In the case of the model A3, where the fuel concentration was low,the oxygen breaks through earlier. In contrast, the concentration of the fuel was more in the A1 and A2 models.

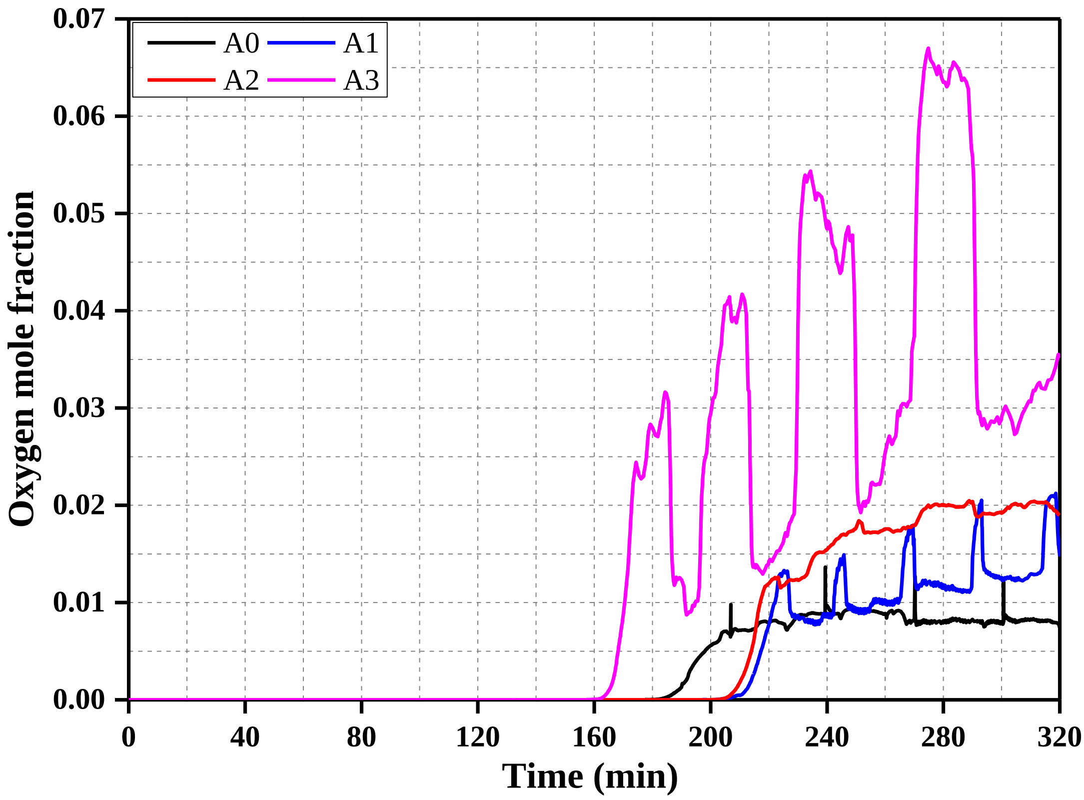

Figure 6. Mole fraction of produced oxygen in the 3D combustion cell.

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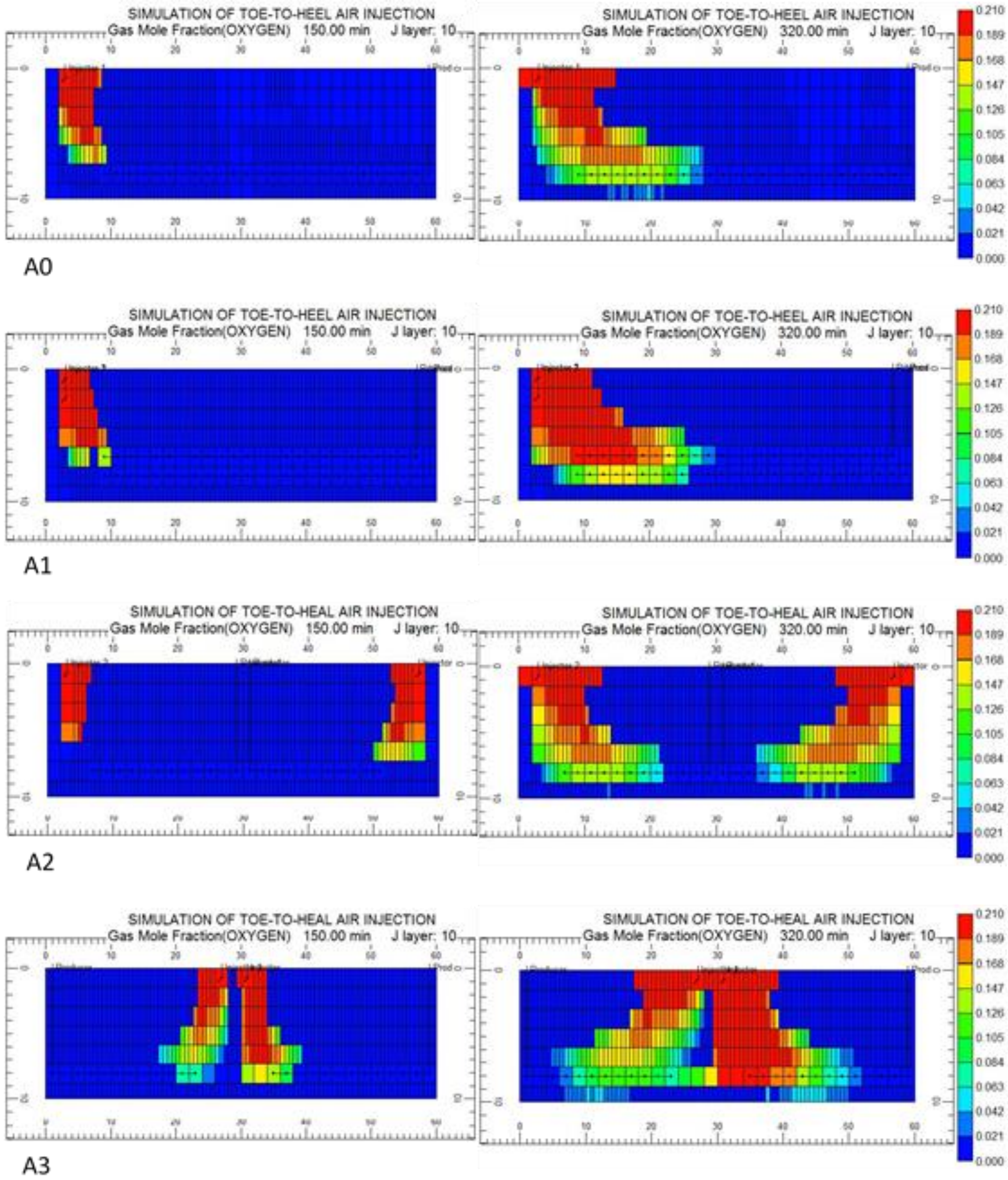

Figure 7. Oxygen profiles along the vertical plane for various configurations at 150 min and 320 min.

3.1.4. Solid Phase (Coke)

The solid phase (coke), which is a result of the heavy oil thermal cracking process, is created in front of the combustion zone in the oil reservoir. This provides the required fuel to sustain the combustion process for the THAI technique. The concentrations of the deposited coke in each of the configurations analysed at the same section and same time, gives a good indication of the efficiency of the volumetric sweep. From Figure 8, it can be seen that the shape of the volumetric sweep in all models is almost the same. It can be noticed that the deposited coke extends over a wide zone gradually from the low concentration at the top reaching the highest concentration at the base of the reservoir down near the horizontal production well. The blue area represents the shape of the propagated combustion front, through the cross-section, which is entirely burned because of the ready supply of oxygen.

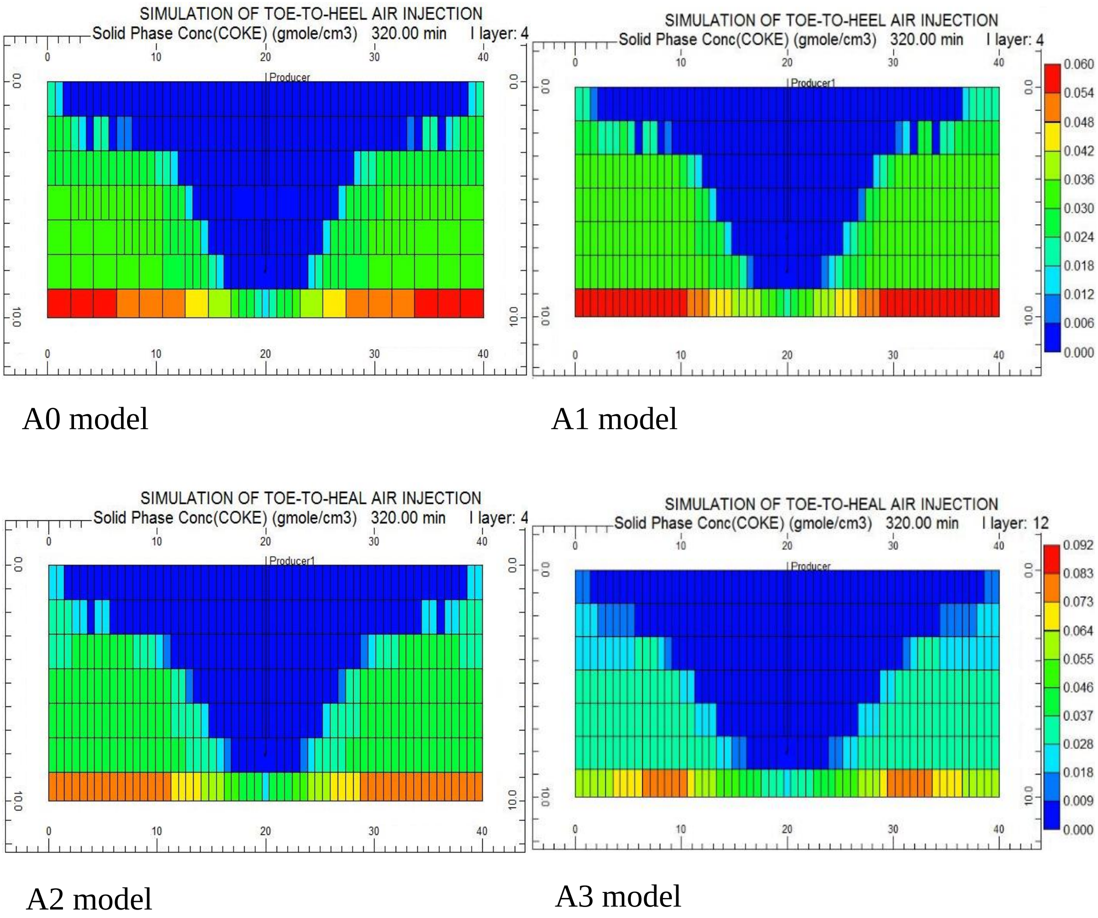

Figure 8. Solid Phase (Coke) concentrations for the various THAI well configurations.

To enhance the amount of the produced oil further, the model A2 was used to test the impact of the flow rate of the injected air on the performance of the THAI process. The results obtained from the model A2 were compared to the original model (A00 as shown in Figure 9 and Figure 10. Figure 9 shows the amount of the oil produced in the A0 and the A2 models through the combustion period, at different air flow rates. Quantitatively, it can be observed that oil produced in the model A2 was increased with increasing the flow rate of the injected air. It was clear that the amount of the oil produced in the model A2 had become about twice of that the oil produced by Greaves model (A0) when the air flow rate was increased about 50 % compared to what was injected in the model A0.

Figure 10 clarifies the behaviour of the peak temperatures of the model A2 at different air injection flow rates compared to the peak temperature obtained from the original model. It was noted that the temperature of the combustion cell was significantly affected by the flow rate of the injected air to the reservoir. As a consequence of increasing the flow rate of the air injection in the model A2, the amount of the produced oil doubled, compared to the original model A0. In addition, the temperature of the combustion zone was substantially raised to be very close to that temperature in the original model (A0) as can be noticed in Figure 10.

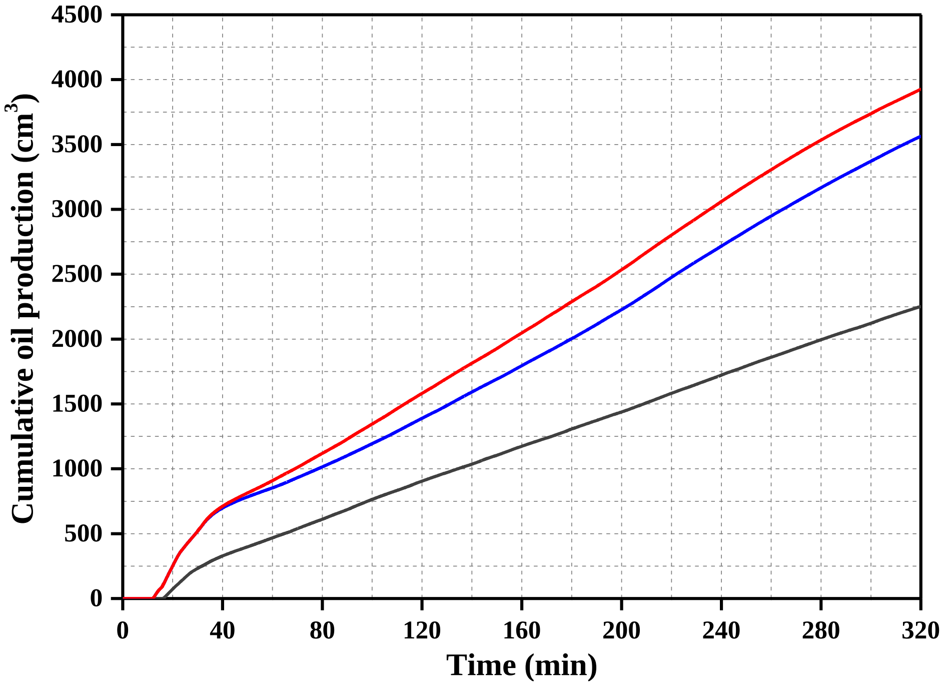

Figure 9. Cumulative oil production for two different well arrangements at different air flow rates, a grey line is the Greaves model at 12 and 16 m^3 m^{-2} h^{-1}, a blue line is the A2 model at 15 and 20 m^3 m^{-2} h^{-1} and a red line is the A2 model at 18 and 24 m^3 m^{-2} h^{-1} flow rates.

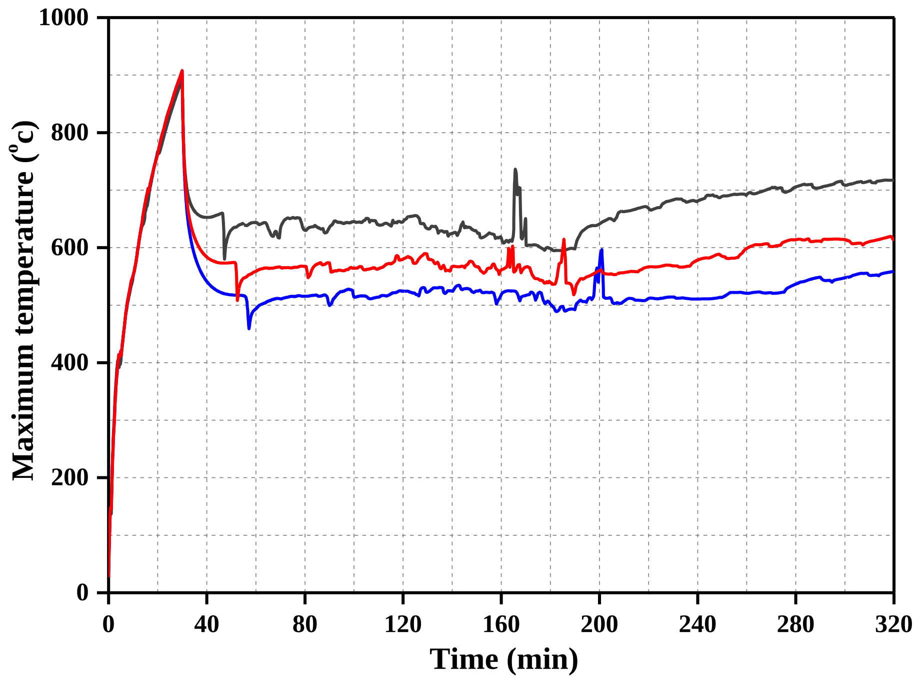

Figure 10. Peak temperatures for two different Well Configurations at different flow rates, a grey line is the Greaves model at 12 and 16 m^3 m^{-2} h^{-1}, a blue line is the A2 model at 15 and 20 m^3 m^{-2} h^{-1} and a red line is the A2 model at 18 and 24 m^3 m^{-2} h^{-1} flow rates.

3.2. THAI-CAPRI simulation results

The largest reserves of oil in the world are heavy oil and bitumen which represent about 80% of the World's reserves and are concentrated in Canada and Venezuela. These reserves could compensate for the depletion in conventional oil production [19]. Since heavy oil and bitumen have a high viscosity and are poorly transportable, they need to be subjected to an upgrading process to be transformed to light crude oils. The crude oils then become readily transportable and acceptable to be used as a refinery feedstock [20]. In addition, the upgrading technology adds a significant environmental advantage since it retains heavy metals, such as S, Ni and V, in the reservoir. Rabiu Ado [1] has generated the input parameters to simulate THAI-CAPRI process at laboratory scale. The frequency values of the hydrotreating reactions were adjusted, via trial and error, based on the API values illustrated by Xia and Greaves [8] and Xia et al. [9], until an average value of the API gravity was achieved about 6 points above the original oil. At the beginning of the study, the original frequency factors were applied, creating a base case model to be compared with others having different frequency factors. The models were denoted TC0 (which is a base case) TC1, TC2, TC3 and TC4. In each model, the original frequency value has been multiplied by a variable factor to study its effect on the simulated performance of the CAPRI process. Among these models, it was found that the TC3 model was the best one, in which the frequency factor of the kinetic reactions has been adjusted to give a high cumulative oil production, which has been subsequently adopted in this study. An electrical heater was used to pre-heat the sand pack for 30 minutes, and a gas mixture of air and hydrogen was then injected at a flow rate of 10000 $cm^3\ min^{-1}$, which corresponded to 15 $m^3\ m^{-2}\ h^{-1}$. The initial hydrogen to the air ratio (HAR) used was 1:4 as it was assumed in the study of Shah et al. [14] and Hart et al. [18]. As discussed concerning the standard THAI process, after 190 minutes, gas flow was increased to 13333.3 $cm^3\ min^{-1}$, which is equivalent to a flow rate of about 20 $m^3\ m^{-2}\ h^{-1}$, and it was maintained until the end of the simulation. In this project, the effect of the catalyst thickness has been investigated as well as the effect of hydrogen to the air ratio. In addition, the effect of the catalyst packing porosity has been taken into account.

3.2.1. Model configuration

The TC3 model used by Rabiu Do [1], which is the same model used in the experimental study of Greaves et al. [2], was also used in this study. The model has horizontal injector and producer (HIHP) wells which were configured in a staggered line drive (SLD). In addition, a catalyst layer was placed around the HP section in the CAPRI model as illustrated by the coloured part in Figure 11. Moreover, instead of using 30 × 19 × 7 grid blocks in the original model, the CAPRI model was discretised into 30 × 19 × 9 grid blocks to compensate the area lost due to the added catalyst.

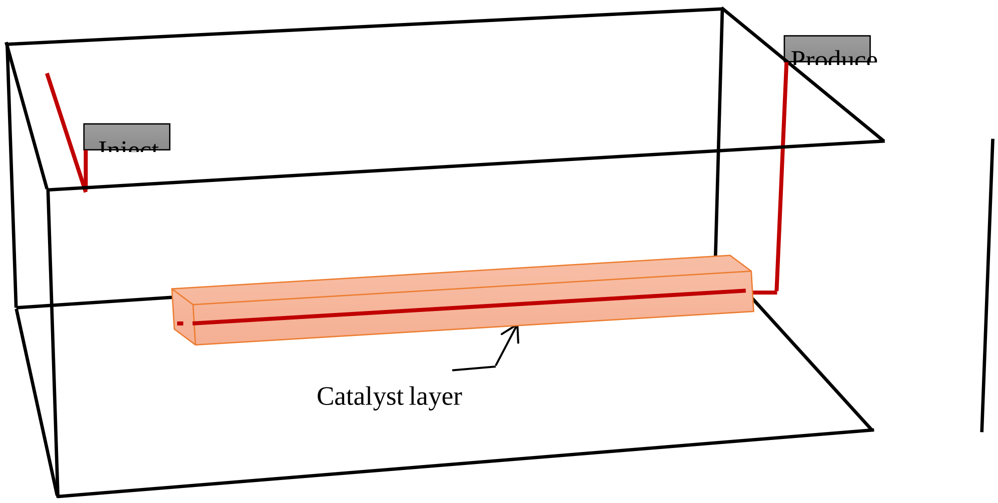

Figure 11. 3D schematic diagram of THAI-CAPRI technique with a catalyst layer placed around the producer.

3.2.2. Physical properties of the upgraded oil

Based on the distillation data obtained by Hart et al. [16] and Rabiu et al. [1] has computed the PVT data of the light and heavy upgraded oil using Aspen HYSYS software as presented in Table 3.

Table 3. Physical properties of the upgraded oil produced [1].

Components	Mole fraction (mol%)	Molecular weight (g/mol)	Density (Kg/m^3)	TC (℃)	PC (kPa)
LUO	20.31	128.01	776.53	353.12	2448.61
HOU	79.69	252.50	850.48	502.19	1523.46

In addition, during the THAI-CAPRI process, catalytic reactions occur beside the different pyrolysis reactions occurring when the THAI process has been tested alone. These catalytic reactions involve mostly hydrodesulfurization (HDS) and hydrodenitrogenation (HDN). Water/gas shift (WGS) and steam gasification (SG) reactions are also observed for the process. Therefore, to simulate the model, further calculations needed to determine the kinetic parameters, the stoichiometry of these reactions, the frequency factor and the activation energy and the fractions of sulphur and nitrogen atoms. All these requirements have been reported in detail by [1], as illustrated in Table 4 and Table 5.

Table 4. Balanced reactions of HDS and HDN with the kinetics parameters.

HDS and HDN reactions	Activation Energy (J/mol)	Frequency Factor (min^{-1})
Heavy oil + 19.932 H_2 $\longrightarrow$ 3.477 HUO + 0.585 H_2S	87×10^3	2.7×10^7
Light oil + 3.286 H_2 $\longrightarrow$ 1.328 LUO + 0.194 H_2S	87×10^3	2.7×10^7
Heavy oil + 1.593 H_2 $\longrightarrow$ 3.477 HUO + 0.189 NH_3	75×10^3	1.0×10^6
Light oil + 0.095 H_2 $\longrightarrow$ 1.328 LUO + 0.011 NH_3	75×10^3	1.0×10^6

Table 5. Elemental compositions of the pseudo-components.

Constituent	Bitumen	Heavy	Light	LUO	HUO
H (wt%)	10.687	10.430	13.005	16.764	12.866
C (wt%)	84.075	84.210	82.859	82.859	84.210
N (wt%)	0.414	0.447	0.112	0.019	0.147
S (wt%)	4.824	4.913	4.025	0.359	2.777

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3.2.3. Catalyst preparation

The catalyst used in this study was silica-alumina which has been tested, discussed in the experimental section, by different techniques such as mercury porosimetry, gas adsorption, NMR etc. The catalyst was placed around the producer well so that the produced oil entering the production well has to go through the catalyst first. The layer thickness for the catalyst as used by Rabiu Ado [1] has been adopted in this study with an initial thickness of 0.5 cm to commence with. The catalyst properties obtained from the experiments were used to compute the packing porosity and the concentration of the catalyst used to simulate the model. The elements, and their particular fractions, of the silica-alumina catalyst, can be seen in Table 6. The bulk density of the catalyst, 1361.7 kg m^{-3}, is taken from the empirical results in this study. This density is integrated with the void volume and the packing porosity to calculate the concentration of the catalyst loading, using the following equation taken from STARS manual.

$$\varphi_f = \varphi_v[1- C_c/\rho_c] \qquad (5)$$

where: φ_f is the packing porosity, φ_v is the void porosity, C_c is the catalyst concentration (kg m^{-3} pore volume), ρ_c is the catalyst bulk density (kg m^{-3}). The initial value of the catalyst packing porosity used was taken from Abu et al. [12], which was 45.1%. Two other values of the packing porosity have been investigated to simulate the effect of this feature on the performance of the CAPRI process. These values with the results obtained from the above equation were tabled in Table 7.

Table 6.: Element composition of silica-alumina catalyst.

Element	RMM (g/mol)	Amount/ wt%
Al_2O_3	101.96	40.54
SiO_2	60.08	48.44
Cl	35.45	6.20
TiO_2	79.866	3.03
Fe_2O_3	159.69	1.15
Total	76.89	100.00

Table 7. Calculated catalyst concentrations based on different fluid porosities.

Packing porosity (%)	Void porosity (%)	Bulk density (kg/m^3)	Catalyst loading (kg/m^3 pore volume)	Catalyst loading (mol/cm^3 pore volume)
44.0	0.99	1361.7	756.50	0.009912517
44.55	0.99	1361.7	748.93	0.009813392
45.1	0.99	1361.7	741.37	0.009714267

3.2.4. Effect of packing porosity

The initial porosity is likely the most important parameter, which can be affected by the particle packing. Spherical and cylindrical particles are the most predominantly used in the chemical engineering operations. For cylindrical particles, both the initial porosity and the packing size are dependent on the shape of the particle. Generally, sphericity is considered the most commonly utilized factor to describe the particle shape, which represents the ratio of the sphere's surface area to the surface area of the particle possessing the same volume as the sphere [21]. The packing formation has an effect on many parameters such as fluid behaviour, heat transfer and mass transfer, which affect the macroscopic process. Principally, a packing of cylindrical particles behaves differently from one of spherical particles because cylinders offer directional freedom, and their geometry involves a diversity of surface constituents such as a flat and curved surface in addition to corners [22]. An experimental study has been conducted by Abu et al. [12] to upgrade Athabasca bitumen using packing porosity values of 44 and 45.1 %, which were used in this study as well as 44.55 %.

3.2.4.1. Oil production

Figure 12 shows the amount of oil production at the time of the simulation for several various packing porosities. It can be observed that there is a slight difference in the amount of the produced oil during the CAPRI process. However, an increase in the oil production, with the increase in the value of the packing porosity, can be seen. This is because that the initial porosity of the catalyst increased as more space between the catalyst particles was increased, which allows for more fluid passing through the catalyst into the production well, i.e., the higher porosity has a lower pressure drop.

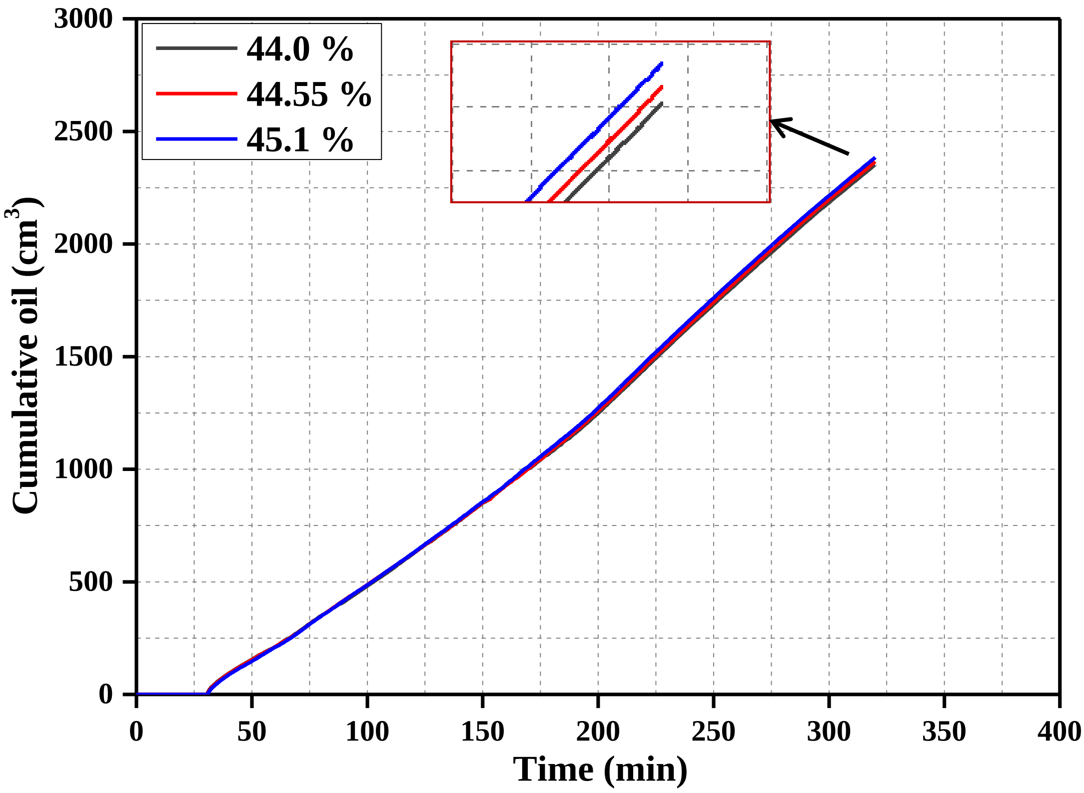

Figure 12. Cumulative oil for different values of packing porosity.

3.2.4.2. Temperature distribution

Figure 13 illustrates the effect of the several values of packing porosity on the temperature distribution with time during the THAI-CAPRI process. Despite the differences in the packing porosity, all models have nearly the same predicted temperature pathway along the combustion front until the simulation end, as can be seen from Figure 13. Therefore, based on the peak temperature characteristics, the change in the packing porosity value has no effect on the temperature distribution. This means that the combustion front propagation is stable, and all models have almost the same combustion front shape as can be noticed in Figure 14. Figure 14 showed that the shape of the combustion front, at 320 minutes, was forward leaning and swept in the upper portion of the reservoir, which is considered as one of the indication parameters of stability.

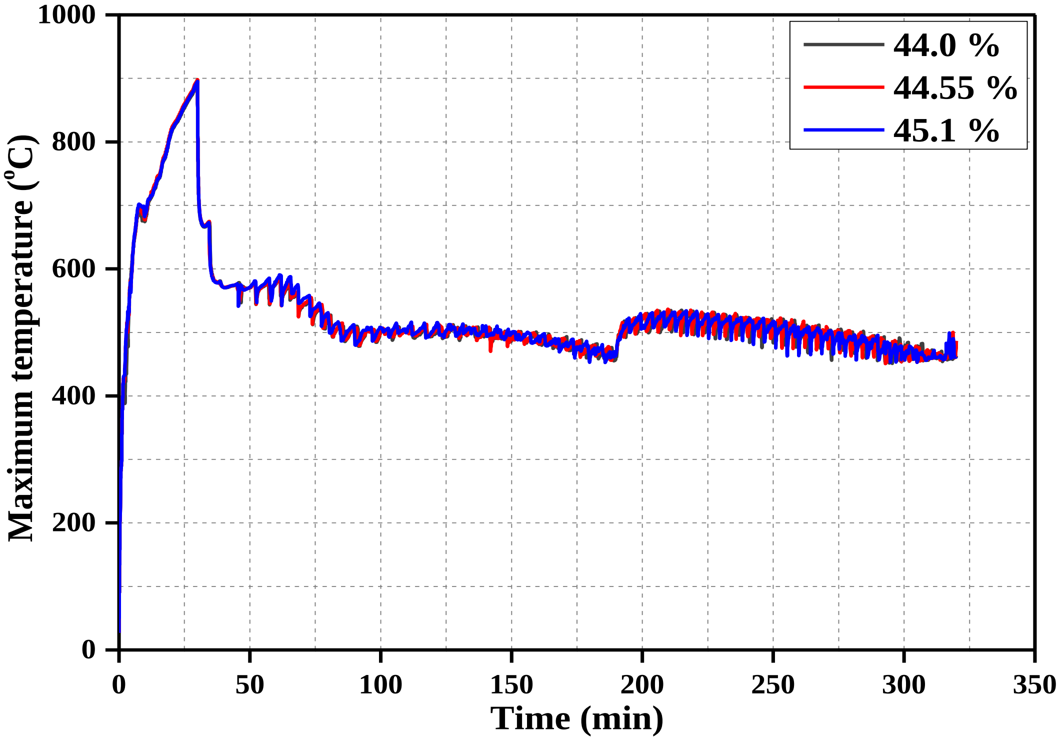

Figure 13. Peak temperature for several different packing porosities**.**

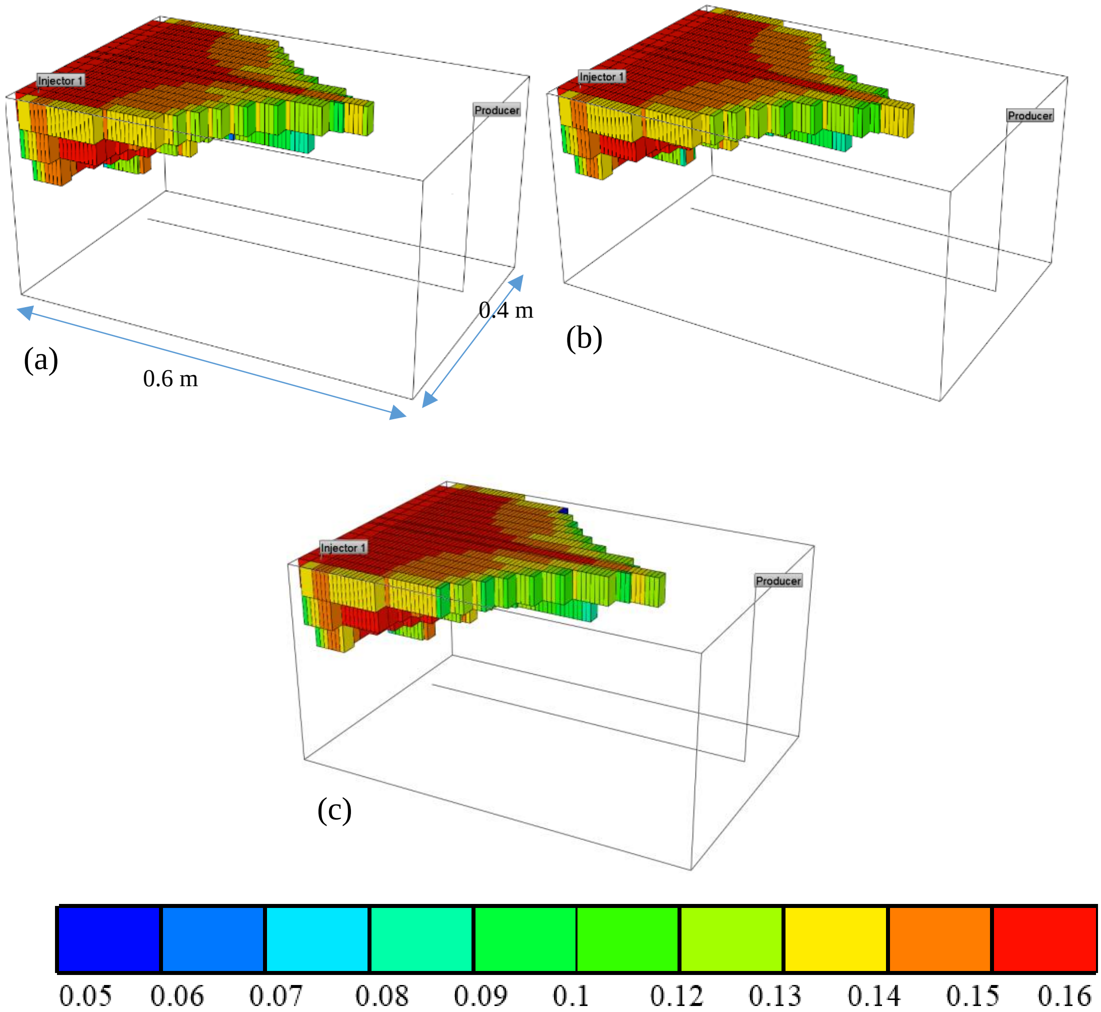

Figure 14. 3D combustion front propagation for CAPRI reactor porosities of (a) 44.0%, (b) 44.55%, (c) 45.1%.

3.2.5. Effect of hydrogen to air ratio

During the THAI-CAPRI process, the existence of hydrogen is a necessary requirement for in-situ catalytic cracking reactions. Hydrogen injected with air in the presence of the catalyst around the horizontal producer assists in the hydrogenation reaction. The hydrogenation process and asphaltene removal result in the upgrading of heavy oil in situ [23]. Another source of hydrogen can be provided by steam gasification (SG) and/or water-gas-shift reactions (WGS) [17], as presented in the following simple equations [1]:

$$\text{WGS: } CO + H_2O \longleftrightarrow CO_2 + H_2 \quad (6)$$

$$\text{SG: } C_iH_a + 2iH_2O \longrightarrow iCO_2 + (2i + a/2)\, H_2 \quad (7)$$

Hydrogen plays an important role in the HDN reaction in which the bond between the carbon atom and the nitrogen is broken and replaced with hydrogen atom, and combination process takes place between nitrogen and hydrogen to form ammonia [12]. Hart et al. [16] have been investigated several types of gas media on the performance of CAPRI upgrading using heavy oil and bitumen. It was found that the addition of hydrogen enhances the reactions of the hydrocracking and the hydrogenation processes, whereas, in the case of the other gas media, heavy coke formation was associated with the upgrading process. It is also noticed that hydrogen results in characteristically high API gravity, low viscosity and high distillables in the produced oil. In this study, three different ratios of hydrogen to air have been employed to investigate its effect on the performance of the CAPRI process. These ratios are 1/4, 2/4 and 2.5/4.

3.2.5.1. Oil production

The effect of the various ratios of hydrogen to air on the cumulative oil in the THAI-CAPRI technique has been illustrated in Figure 15. As can be seen from Figure 15, the amount of the produced oil was affected by the value of the injected hydrogen. Where the oil production decreased with increasing of the hydrogen to air ratio. 2366 cm^3 of oil was recovered when the ratio of hydrogen to air was low, and when the ratio was increased, the amount of the produced oil dropped to 2161 cm^3, and a further increase of the hydrogen to air ratio, the recovered oil declined to 2059 cm^3. The high ratio of hydrogen to air means the lower injected air, and this resulted in an increase in the amount of the coke deposited, which in turn led to drop in the oil production.

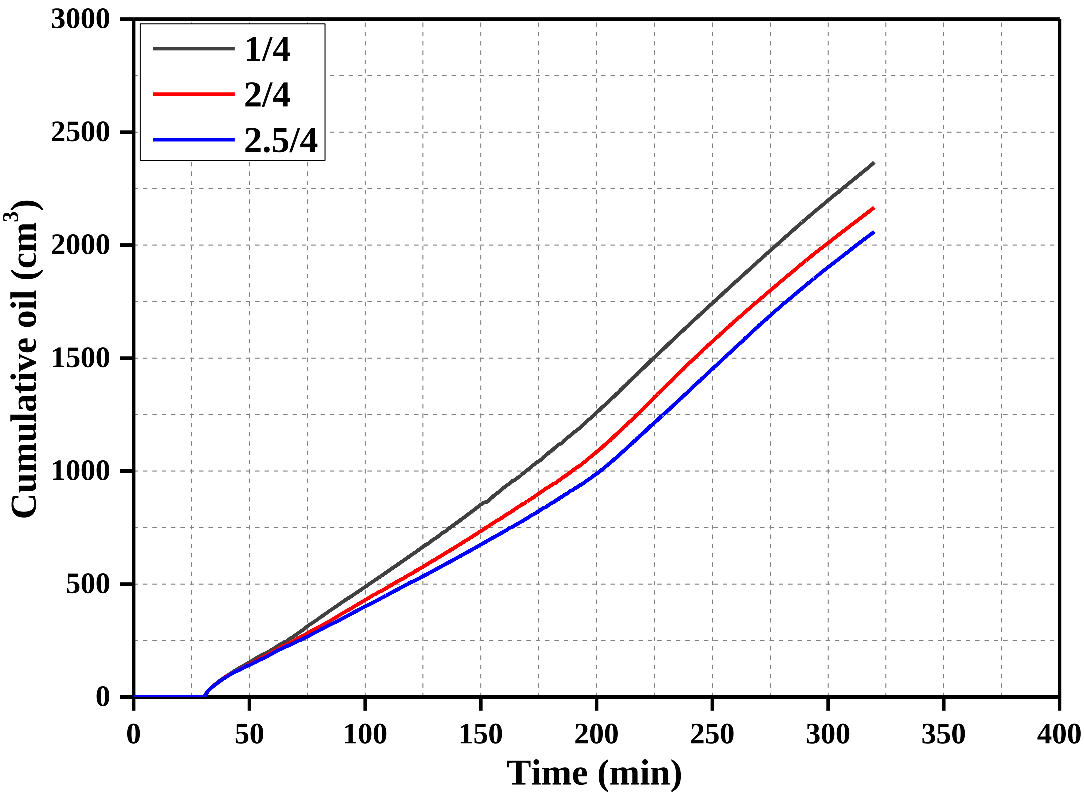

Figure 15. Cumulative volume of produced oil against time using different hydrogen to air ratios.

3.2.5.2. Peak temperature

Figure 16 shows the variation in maximum temperature of the produced oil along the reservoir as a function of time. It is noticed that the peak temperature having the lowest hydrogen to air ratio diverges first and continues to lie above all the other curves up to the end of the process, and then the second one with the middle value and following with the highest ratio of hydrogen to air. This is because of the produced oxygen which started very early in case of the highest ratio of hydrogen to air.

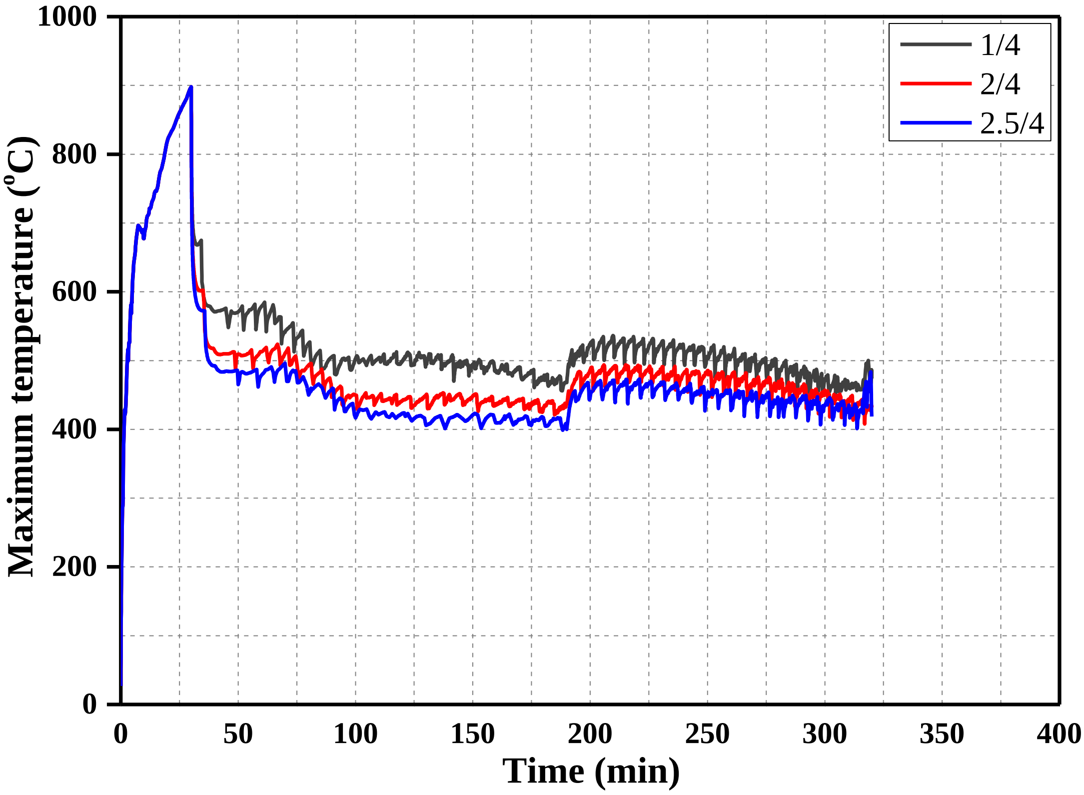

Figure 16. Peak temperature variation with time with different hydrogen to air ratios .

3.2.6. Effect of catalyst thickness

Catalysts are materials that can speed up chemical reactions and enhance the selectivity of the reaction without consumption themselves (Huang et al., 2012). The reaction can be described by the following equation:

$$\text{Heavy oil} + 19.932\ H_2 + \text{CAT} \longrightarrow 3.477\ \text{HUO} + 0.585\ H_2S + \text{CAT} \quad (8)$$

In this part, the effect of the catalyst thickness on the performance of the THAI-CAPRI process is illustrated. Three different thicknesses of catalyst have been investigated to study its effect on the cumulative oil production and the peak temperature. The thicknesses were 0.5, 0.75 and 1.0 cm.

3.2.6.1. Oil production

Figure 17 shows the effect of the catalyst thickness on the cumulative oil during the simulation period. As can be noticed from Figure 17, there is a slight difference in the amount of the produced oil. It is observed that the model having a catalyst with a thickness of 0.5 cm has the highest amount of the produced oil, and this amount decreased with an increase of the catalyst thickness. This is because that most of the thermal cracking has taken place on the surface of the catalyst in the presence of a high temperature, which resulted in a high concentration of the coke. However, as further of the catalyst thickness increased, more coke formed on the catalyst surface, and thereby, the amount of the produced oil reduced.

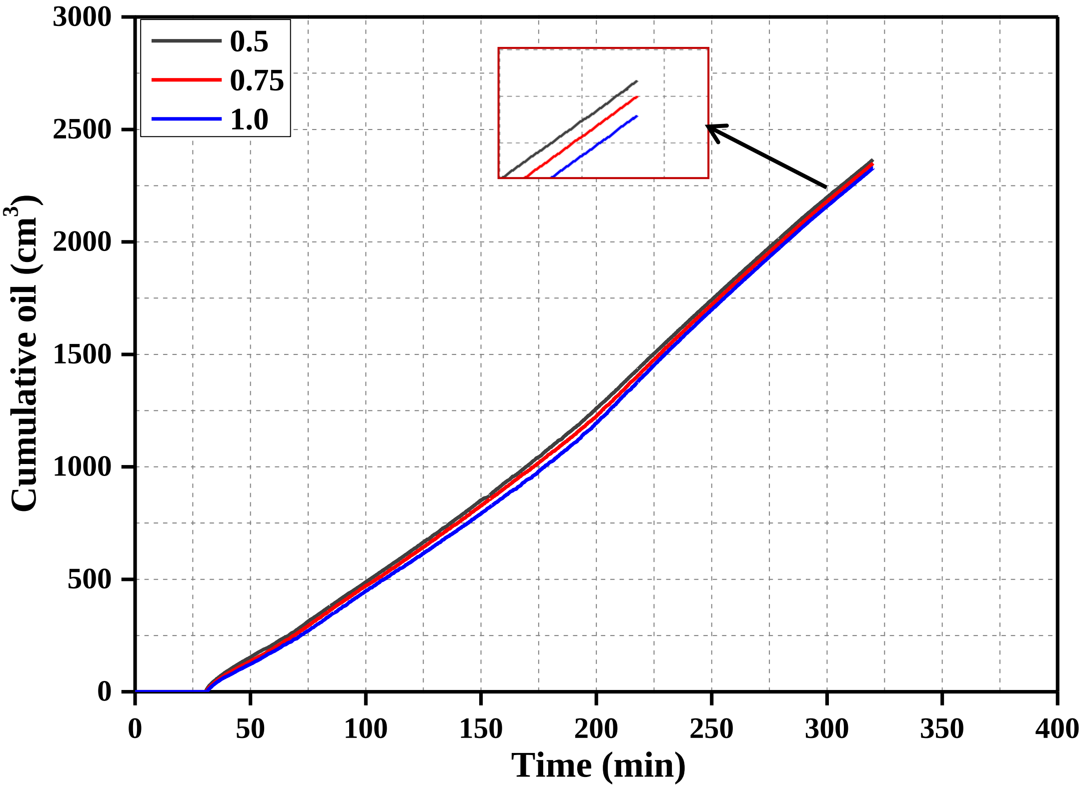

Figure 17. Cumulative oil vs time using different catalyst thickness.

3.2.6.2. Peak temperature

Figure 18 displays the change in the peak temperature along the reservoir with the time for diverse values of catalyst thicknesses. From Figure 18, the peak temperature, in the case of the catalyst thickness of 0.5 cm, rose up to about 900 ℃ with ~80 to 100 ℃ higher than that when the thicknesses of the catalyst are 0.75 and 1.0 cm respectively. This is due to the difference in the produced amount of the coke at the end of the preheating time. It is observed that during the lowest air flux from 30 to 190 minutes, the trend of all curves is almost the same.

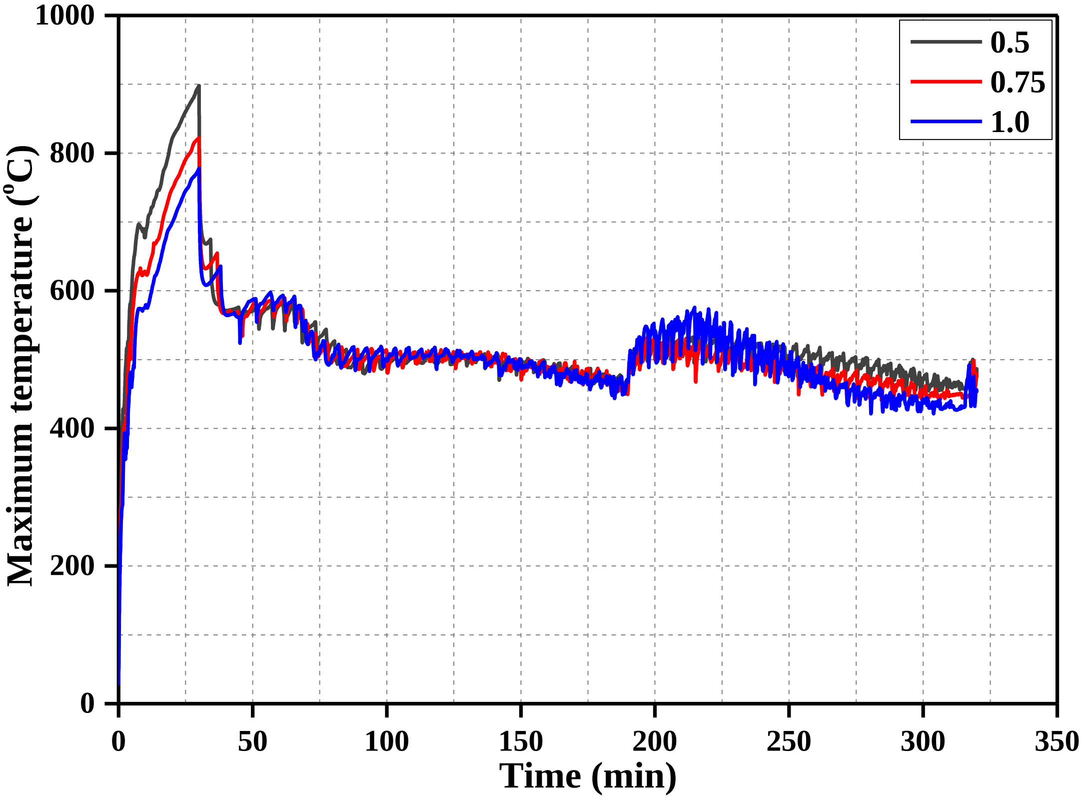

Figure 18. Peak temperature for different catalyst thickness.

However, after 190 minutes when the air flow increased, the curve for the model having a thickness of 1.0 cm was above the other curves up to about 230 minutes, and then they reordered depending on the thickness from the lowest one to the highest until the end of the combustion period. During the period between 190 to 230 minutes, when the flow rate of the injected air was increased, more oil flows through the catalyst layer, and due to the large catalyst thickness, the produced oil remains a longer time within the catalyst which leads to increase the temperature in this zone.

4. Discussions

It has been found that the best model was the A2 model in which the injectors were designed to be on both sides of the reservoir, and the producers were located in the centre of the reservoir. The findings revealed oxygen breakthrough, which is considered a most important parameter, acted in the same trend as the original model of Greaves (A0). This feature gives an indication that, in appropriate reservoir, THAI technique is stable and effective process. However, in the other models, the oxygen production followed an oscillating path to the end of the simulation period. It is also observed that model A2 gave high cumulative oil compared to the other models, at the same flow rate of the injected air used in the A0 model. The reason for this is that the symmetry of the combustion front achieved in A2 model has affected a larger volume of the reservoir and hence resulted in higher volumetric sweep of the reservoir.

Further, when the air injection flow rate was increased in the model A2 by about 50 % of that used first, the amount of the produced oil rose up to about double of the amount of the oil produced by the original model. As a result, about half reduced the time required in the A2 model to recover the same amount of the oil produced by the original model A0.

Moreover, catalytic upgrading using THAI-CAPRI process was simulated for the recovery of Athabasca Heavy Oil to investigate the effect of several parameters on the performance of the CAPRI technique. The change in the packing porosity values had a slight effect on the oil production, and no effect mention on the peak temperature. This small impact could be due to the difference in the particles arrangement from one to another. Similar, the effect of the catalyst thickness on the performance of the CAPRI process, where the amount of the cumulative oil increased with decreasing the thickness of the catalyst placed on the producer. This because of the coke deposited on the surface of the catalyst on which the thermal cracking occurred. Since the cracking reaction takes place on the solid surface, the high catalyst thickness obstructs the flowrate of the oil which leads to a high concentration of the coke on the catalyst surface.

However, the oil production was obviously affected by the ratio of hydrogen to air injected by the injectors to the reservoir. The low ratio of hydrogen to air produced the higher oil cumulative, compared to the high ratios. The high amount of hydrogen implies a low amount of injected oxygen and that resulted in an increase in fuel availability which substantially affects the recovery of the oil.

5. Conclusions

3D models using CMG-STARS have been employed for simulations of the THAI and THAI-CAPRI processes to investigate an effect of several parameters on the performance of the technique. The influence of variables such as different well configurations using two horizontal injectors and producers have been studied for the THAI technique. Moreover, the packing porosity, catalyst thickness and hydrogen to air ratio have been tested to illustrate its effect on the THAI-CAPRI process. Three different models, with varying locations for the injectors and producers, have been simulated for the THAI process, using Virgin Athabasca oil sand. Compared to the Greaves model (the original model), the second configuration, in which the injectors are located on both sides of the reservoir while the producers are centred in the middle of the reservoir, was the best scheme for the THAI technique, since it gave the highest cumulative oil, and, it also gave rise to the same behaviour as the Greaves model in terms of the temperature distribution and the oxygen breakthrough. In addition, the combustion front shape for the presented simulation was forward leaning, like the combustion shape in Greaves model, which indicates that the process was perfectly stable. However, in the other models in which the injectors are designed to be near to each other, and this could be the reason for that the amount of the produced oil was less than that in the case of the second model.

In terms of the THAI-CAPRI process, the model used by Rabiu Ado (2017) has been adopted in the present study, but using silica-alumina catalyst whose properties have been obtained from the practical part of this study. Several parameters such as packing porosity, hydrogen to air ratio, and catalyst thickness were investigated as an extension to the Rabiu Ado (2017) work. The CAPRI simulation presented here provides a new prediction of the required amount of the hydrogen used in the hydrotreating process during THAI-CAPRI technique for the upgrading of heavy oil and bitumen. The findings found that the amount of the produced oil was affected by the value of the hydrogen to air ratio. The simulation also displays that the combustion front propagation was entirely restricted to the upper portion of the sandpack, indicating that the process was completely stable. It is also that the results showed that the oil production was slightly influenced by the packing porosity and the thickness of the catalyst placed around the horizontal producer.

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