UNRAVELING THE POTENTIAL OF IN-SITU HYDROGEN PRODUCTION VIA CYCLIC AIR-STEAM INJECTION IN HEAVY OIL AND BITUMEN RESERVOIRS

Mohamed Amine Ifticene and Qingwang Yuan

Bob L. Herd Department of Petroleum Engineering, Texas Tech University

ABSTRACT

Cyclic air-steam injection (CASI) is gaining attention as a promising approach for producing hydrogen (H_2) directly from heavy oil and bitumen reservoirs, presenting a potentially cost-effective and low-emission alternative to conventional hydrogen production methods. This study simulated in-situ hydrogen production using a Lloydminster heavy oil reservoir model with a single horizontal well pair, where air and steam were injected in cycles over a 20-year operational period. To determine key engineering designs and optimal operation parameters, a sector model optimization was performed using a genetic algorithm, and the optimal injection parameters were subsequently scaled up for field-scale simulation. The results indicated an average hydrogen production rate of approximately 998 kg/day, leading to a total hydrogen production of about 7.28×10^6 kg over 20 years. The oil-to-hydrogen conversion factor reached 77% with a hydrogen yield of 14.33 kg/bbl. These findings underscore CASI's potential as a viable hydrogen production method, providing a strong foundation for future development and field deployment in heavy oil and bitumen reservoirs.

1. INTRODUCTION

The growing demand for sustainable energy solutions has accelerated in recent years, largely due to the urgent need to mitigate climate change and reduce reliance on finite fossil fuel reserves. Among various alternatives, hydrogen stands out as a promising clean energy source, offering versatility, high energy density, and minimal environmental impact when utilized as a fuel (Ishaq et al., 2022; McLellan et al., 2005; Pathak et al., 2023). Steam methane reforming (SMR), which involves reacting methane with steam at high temperatures to produce hydrogen and carbon oxides, is the predominant hydrogen production method, supplying 95% of the hydrogen in the United States (US) (Sun et al., 2019). However, SMR is highly energy-intensive and is associated with high carbon emissions ranging between 9-10 eCO_2/kg H_2 produced (Cho et al., 2022). While carbon capture, utilization, and storage (CCUS) can help reduce emissions, integrating it with SMR significantly increases costs and energy requirements. Achieving sustainable hydrogen production calls for the development of cleaner and more energy-efficient alternatives to conventional technologies.

Among the multiple innovative hydrogen production technologies under development, cyclic air-steam injection (CASI) has gained significant attention as a promising approach to producing hydrogen directly from heavy oil and bitumen reservoirs. Heavy oil and bitumen are abundant fossil fuel resources and collectively account for approximately 70% of the world's crude oil reserves (Meyer et al., 2007), with estimated global reserves of 991.18 billion and 501.26 billion tons, respectively (Liu et al., 2019). Despite their vast potential, these resources pose substantial challenges due to their high viscosity. Currently, these resources are extracted via thermal recovery methods, the most common being steam injection methods such as steam-assisted gravity drainage (SAGD). However, SAGD in addition to heavy oil upgrading post-production, is associated with large greenhouse gas emissions, ranging from 99-176 kg of eCO_2/bbl of crude oil extracted (Charpentier et al., 2009). Meanwhile, CASI offers the possibility to repurpose these abundant resources for clean hydrogen production, offering a pathway to significantly reduce the carbon footprint of heavy oil and bitumen exploitation while contributing to the global clean hydrogen demand.

CASI is an in-situ hydrogen production technique applied in heavy oil and bitumen reservoirs, during which air and steam injections are alternated over multiple cycles (Gates and Wang, 2017). Air, which contains oxygen, is initially injected into the heavy oil or bitumen formation to oxidize a portion of the crude oil in situ and establish a combustion zone that heats the reservoir. When the reservoir achieves sufficiently high temperatures, steam injection is initiated to trigger gasification reactions, namely coke gasification and water-gas shift (Hajdo et al., 1985), to produce hydrogen. As hydrogen production diminishes due to a drop in reservoir temperature, air injection is resumed to restore the necessary thermal conditions, followed by another round of steam injection. This cycle is repeated multiple times. The produced hydrogen is subsequently brought to the surface and separated from other gases, including carbon oxides and methane. CASI presents numerous advantages over conventional hydrogen production methods. The energy required to produce hydrogen is generated directly inside the reservoir making it more energy efficient. Furthermore, existing heavy oil and oil sands field infrastructure can be repurposed, eliminating the need to build costly new hydrogen production plants.

In-situ hydrogen production from heavy oil and bitumen reservoirs via air and steam injections has shown to be technically achievable a multitude of times. BP Resources Canada conducted the in-situ combustion projects in Marguerite Lake in 1979 and Wolf Lake in 1985 targeted at bitumen recovery from oil sands in Alberta (Canada), during which the company tested simultaneous and alternating air and water injections. It was observed from gas analysis that the production wells had produced gas mixtures containing up to 33 mol.% hydrogen (Hajdo et al., 1985; Hallam et al., 1989). After analyzing the Marguerite Lake project data, Hajdo et al. (1985) observed that hydrogen was significantly generated when water was injected into the formation. They concluded that hydrogen was the product of bitumen combustion and gasification reactions. They hypothesized that hydrogen was mainly generated by coke gasification followed and the water-gas shift reaction during water injection into the formation. Later, Petrobank Energy and Resources conducted the Whitesands project in 2006 and the Kerrobert project in 2009, both employing the toe-to-heel air injection (THAI) techniques for heavy oil recovery in Alberta. These projects explored the co-injection of air with steam (Ayasse et al., 2005; Wei et al., 2020). Gas analysis from the production wells revealed hydrogen concentrations of up to 10 mol.% and 7 mol.% in the produced gas mixtures for the Whitesands and Kerrobert projects, respectively (Petrobank Energy and Resources Ltd., 2011, 2023). While originally designed for bitumen recovery, these projects demonstrated the potential for in-situ hydrogen production via air and steam injection into heavy oil and bitumen reservoirs.

Currently, in-situ hydrogen production via CASI is undergoing pilot testing in Canada (Hand, 2020). While this technology shows great promise, several challenges must be addressed for successful commercial deployment. The field-scale production potential of hydrogen through CASI has yet to be thoroughly evaluated. Key uncertainties remain, including the total hydrogen output from a single reservoir, the fraction of in-situ oil that can be converted into hydrogen, and the hydrogen yield per barrel of oil. Therefore, in this work, we assessed the potential of in-situ hydrogen production via CASI in a Lloydminster heavy oil reservoir from Saskatchewan, Canada. Reservoir simulations were conducted in CMG-STARS using a reliable reaction model that has been developed and experimentally validated for hydrogen production from Lloydminster heavy oil. Optimal engineering decisions and process designs were determined by combining numerical simulations with a genetic optimization algorithm. Potential total hydrogen production, in-situ oil conversion factor, and hydrogen yield were quantified. This study provides a solid framework for assessing the potential of clean and sustainable in-situ hydrogen production from heavy oil and bitumen reservoirs via the CASI process paving the way for its field deployment.

2. METHODOLOGY

2.1. Reservoir model

In this study, a representative model of a Lloydminster heavy oil reservoir was developed to simulate in-situ hydrogen production via CASI. The reservoir model was constructed using cartesian grids in the CMG-Builder software. Three-dimensional (3-D) and cross-sectional views of the model are illustrated in Fig. 1. The model spans 500 m in length and 50 m in width, has a 20 m thick pay zone, and is situated at an 800 m depth. As depicted in Fig. 1, the model is discretized into 25, 50, and 20 grid blocks along the I, J, and K directions, respectively.

The reservoir model features two horizontal wells: an injector (blue in Fig. 1) and a producer (green in Fig. 1). The wells in this model were arranged in a reversed SAGD layout, with the injector positioned below the producer. The wells were placed at the center of the corresponding grid blocks, with the horizontal injector located at a depth of 817.5 m and the producer positioned 5 m above it at 812.5 m. Both wells were perforated along their entire lateral sections. The production well was set to operate at a minimum bottom-hole pressure of 2 MPa.

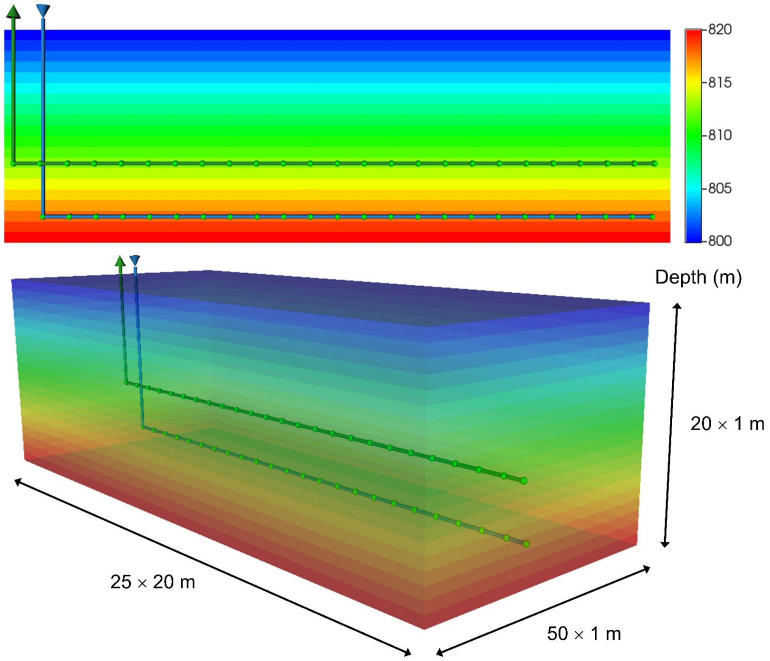


Figure 1 - Cross-sectional and 3-D views of the Lloydminster heavy oil reservoir model.

Due to the absence of detailed reservoir data, the model was assumed to be homogeneous, with no geological complexities incorporated. The reservoir properties were based on typical Lloydminster field values reported by Dusseault and El-Sayed (2000), with additional data sourced from AccuMap. Table 1 summarizes the key properties of the grid blocks. The reservoir model has a porosity of 30%, a horizontal permeability of 2000 mD, and a vertical permeability of 200 mD. The initial reservoir conditions were set at a pressure of 6 MPa and a temperature of 30°C. The reservoir was originally saturated with 70% heavy oil and 30% water, with no initial free gas present. To account for vertical heat conduction losses, the model included typical overburden and underburden shale layers. To ensure realistic thermal and mechanical behavior in the simulations, the compressibility and thermal properties of the Lloydminster reservoir rock were adopted from Bai et al. (2022).

Table 1 - Lloydminster reservoir model properties.

Property	Value
Depth (m)	800
Thickness (m)	20
Porosity (%)	30
Horizontal permeability (mD)	2,000
Vertical permeability (mD)	200
Initial pressure (kPa)	6,000
Initial temperature (°C)	30
Initial oil saturation (%)	70
Initial water saturation (%)	30

Rock compressibility (kPa^{-1})	4.9×10^{-7}
Rock heat capacity (J·m^{-3}·C^{-1})	2.28×10^{6}
Overburden & underburden heat capacity (J·m^{-3}·C^{-1})	1.89×10^{6}
Overburden & underburden thermal conductivity (J·m^{-1}·day^{-1}·C^{-1})	1.6×10^{5}
Rock thermal conductivity (J·m^{-1}·day^{-1}·C^{-1})	6.04×10^{5}
Water thermal conductivity (J·m^{-1}·day^{-1}·C^{-1})	5.81×10^{4}
Oil thermal conductivity (J·m^{-1}·day^{-1}·C^{-1})	1.33×10^{4}
Gas thermal conductivity (J·m^{-1}·day^{-1}·C^{-1})	4.32×10^{3}

The Lloydminster reservoir rock was assumed to be water-wet. The relative permeability values for Lloydminster heavy oil used in this study were adopted from Bai et al. (2022). For computational efficiency, the temperature dependence of relative permeability endpoints was disregarded. Three-phase relative permeabilities were calculated using Stone's second model in CMG-STARS.

2.2. Compositional model

The compositional model used in this study consists of four phases and nine components: an oleic phase (heavy oil), a water phase, a gas phase, and a solid phase (coke). Among these, the liquid and gas phases are mobile, while the solid coke phase is considered immobile. Lloydminster heavy oil (oleic phase) was modeled as a single-component fluid, while coke was represented as pure carbon.

The molecular weight and critical pressure/temperature of Lloydminster heavy oil were obtained from Shi and Yang (2017), while the properties of the other fluid components were characterized using CMG-WinProp. Viscosity data for Lloydminster heavy oil were taken from Mohebati et al. (2010).

2.3. Reaction model

CASI is a complex process governed by multiple chemical reactions occurring alongside fluid flow in the reservoir. Predicting, controlling, and monitoring this process is challenging, making reservoir simulation a crucial tool for evaluating its performance under various conditions. A reliable chemical reaction kinetics model is essential, as reaction kinetics dictate the rates of subsurface reactive transport. In this study, we employed a simple yet reliable reaction kinetics model for in-situ hydrogen generation during CASI. This reaction kinetics model was developed by our research group specifically for Lloydminster heavy oil and was experimentally validated through history-matching of numerical simulations with kinetic cell experimental results (Ifticene et al., 2024b, 2024a). The reaction model consists of two Lloydminster heavy oil oxidation reactions, two hydrogen generation reactions, and two hydrogen consumption reactions. The frequency factors, activation energies, and enthalpies of the reactions are given in Table 2.

Table 2 - Kinetic parameters and reaction enthalpies.

Reaction No.	Frequency factor ($day^{-1}\cdot kPa^{-1}$)	Activation energy ($J\cdot mol^{-1}$)	Enthalpy ($J\cdot mol^{-1}$)
1	1.2×10^7	7.6×10^4	3.8×10^6
2	9.7×10^6	1×10^5	2.6×10^5
3	4.3×10^{11}	1×10^5	-1.3×10^5
4	2.8×10^{13}	7.5×10^4	4.1×10^4
5	1×10^{17}	2×10^5	7.4×10^4
6	3×10^6	1.6×10^5	4.2×10^5

The first reaction is the low-temperature oxidation, known as LTO. The LTO reaction for Lloydminster heavy oil can be written as follows (Ifticene et al., 2024b):

$$Oil + 0.5\,O_2 \rightarrow 0.8\,CO_2 + CO + 12.15\,H_2O + 18\,Coke \qquad \text{(R1)}$$

During air injection, the injected oxygen reacts with the heavy oil in the reservoir at temperatures below 350 °C through LTO reactions to form oxygen-rich compounds. The formed oxygen-rich compounds together with heavy compounds in the crude oil subsequently go through oxidative cracking and pyrolysis reactions. During this process, coke (also known as fuel) is deposited in the pore space, and CO_2, CO, and H_2O are released (Freitag, 2016; Yuan et al., 2022). Subsequently, the deposited coke from LTO reactions serves as fuel for the high-temperature oxidation reaction, which is known as HTO. During HTO, the deposited coke reacts with the injected oxygen at high temperatures (usually above 350 °C) and is combusted to generate heat and release CO_2 and CO as follows (Ifticene al., 2024b):

$$Coke + 0.78\,O_2 \rightarrow 0.56\,CO_2 + 0.44\,CO \qquad \text{(R2)}$$

LTO and HTO play a substantial role during CASI. The deposited coke during LTO serves as a feedstock for the gasification process. During CASI, steam reacts with the deposited coke (either injected steam or in-situ generated due to high reservoir temperatures) to generate H_2 and CO (Hajdo et al., 1985; Ifticene et al., 2024). This reaction is known as coke gasification and is the main in-situ hydrogen generation mechanism during the CASI process (Ifticene et al., 2023). Coke gasification is an endothermic reaction and requires high enough in-situ temperatures to occur, which are achieved during HTO in the reservoir. This highlights the role of HTO in the CASI process. The coke gasification reaction is written as follows (Ifticene et al., 2024b):

$$Coke + H_2O \rightarrow CO + H_2 \qquad \text{(R3)}$$

Steam can further react with CO released from either heavy oil oxidation or coke gasification in the reservoir to generate H_2 and CO_2 through the water-gas shift reaction as follows (Ifticene al., 2024b):

$$CO + H_2O \rightarrow CO_2 + H_2 \qquad \text{(R4)}$$

Simultaneously, the generated hydrogen from Reactions 4 and 5 can be consumed by the methanation reaction (Hajdo et al., 1985; Ifticene et al., 2024). Hydrogen can react with the deposited coke in situ and release CH_4 as follows (Ifticene al., 2024b):

$$Coke + 2\,H_2 \rightarrow CH_4 \tag{R5}$$

Furthermore, hydrogen can also be consumed by unreacted oxygen in the reservoir through the hydrogen oxidation reaction as follows (Hajdo et al., 1985; Ifticene et al., 2024):

$$O_2 + \frac{1}{2}\,H_2 \rightarrow H_2O \tag{R6}$$

2.4. Operations design and optimization

To model hydrogen production through the CASI process, air and steam were alternately injected into the reservoir in four-month cycles, consisting of 60 days of air injection followed by 60 days of steam injection. The simulations, performed using CMG-STARS, spanned 20 years from January 2024 to December 2044, totaling 60 alternating air-steam injection cycles. To initiate crude oil ignition, a heater was placed at the injector well and operated for 24 hours before injection began.

Before conducting field-scale simulations, we first determine the optimal engineering design to maximize hydrogen production throughout the life of the CASI project. This task is framed as an optimization problem by defining an objective function that incorporates optimization parameters. To address this challenge, the Storn-Price differential evolution algorithm (Storn and Price, 1997) was utilized. This algorithm is widely recognized for its robustness and effectiveness in handling complex optimization problems.

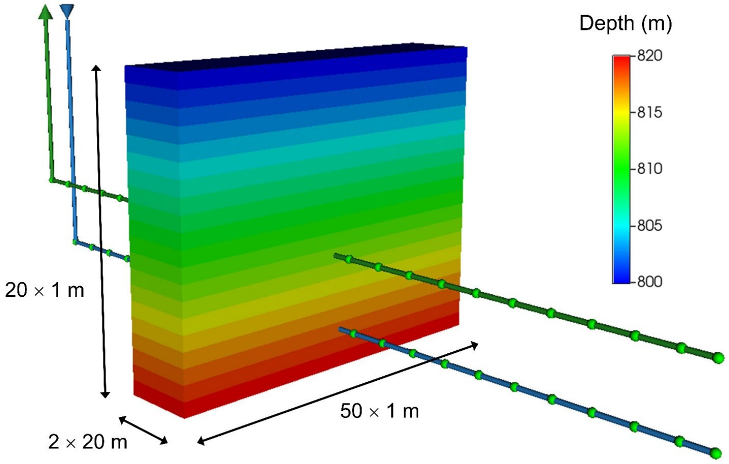


Figure 2 - 3-D view of the Lloydminster heavy oil reservoir sub-model used for the sector optimization.

To maximize cumulative hydrogen production, which is set to be the objective function, four injection parameters were selected as optimization variables: air injection rate, injected oxygen concentration, steam injection rate, and injected steam temperature. The goal was to identify the optimal combination of these parameters that would yield the highest hydrogen production. Hence, we solve the following optimization problem:

$$\begin{array}{ll} \underset{Q_{air},\, C_{oxygen},\, Q_{steam},\, T_{steam}}{Maximize:} & H_2\ production \\ Subject\ to: & Q_{air\ min} < Q_{air} < Q_{air\ max} \\ & C_{oxygen\ min} < C_{oxygen} < C_{oxygen\ max} \\ & Q_{steam\ min} < Q_{steam} < Q_{steam\ max} \\ & T_{steam\ min} < T_{steam} < T_{steam\ max} \end{array} \tag{1}$$

where Q_{air} is the air injection rate, C_{oxygen} is the injected air oxygen concentration, Q_{steam} is the steam injection rate, T_{steam} is the injected steam temperature, and *min* and *max* are the parameter sampling range boundaries.

Reservoir-scale simulations are highly computationally intensive and time-consuming. To improve efficiency, a sector optimization approach was implemented using a reservoir sub-model, as shown in Fig. 2. This sub-model was extracted from the center of the full-field model by selecting two slabs along the I direction. The sector model consists of 2, 50, and 20 Cartesian grid blocks in the I, J, and K directions, respectively. Optimization simulations were first performed on this sub-model to identify the optimal injection parameters. The parameter values were then volumetrically upscaled to the full-field reservoir model. This approach ensures that a sufficient number of optimization cases can be evaluated within a reasonable timeframe as the optimizer was set to conduct 1,000 simulation cases. The sampling ranges of the optimization parameters are given in Table 3. Note that the steam injection rate is given in cold water equivalent (CWE) volume at standard conditions.

Table 3 - Injection parameters and their respective sampling ranges.

Parameter	Range
Air injection rate (m^3/day)	[1,000, 15,000]
Water injection rate (m^3/day)	[1, 15]
Oxygen concentration (%)	[21, 95]
Steam temperature (°C)	[100, 300]

A schematic of the optimization algorithm's workflow is shown in Fig. 3. The algorithm optimizes the injection parameters by iteratively exploring and refining potential solutions. It begins by initializing a population of candidate parameter sets. These candidates are evolved over successive generations using mutation, crossover, and selection operations. Mutation introduces diversity by combining weighted differences between randomly selected parameter sets, while crossover ensures that offspring inherit traits from both parent solutions. The optimizer evaluates each candidate set based on the objective function. The highest hydrogen-producing solutions are retained, guiding the algorithm toward an optimal set of parameters. Once the 1,000 optimization simulation cases are concluded, the optimal injection parameter combination is volumetrically upscaled to conduct the reservoir-scale simulation.

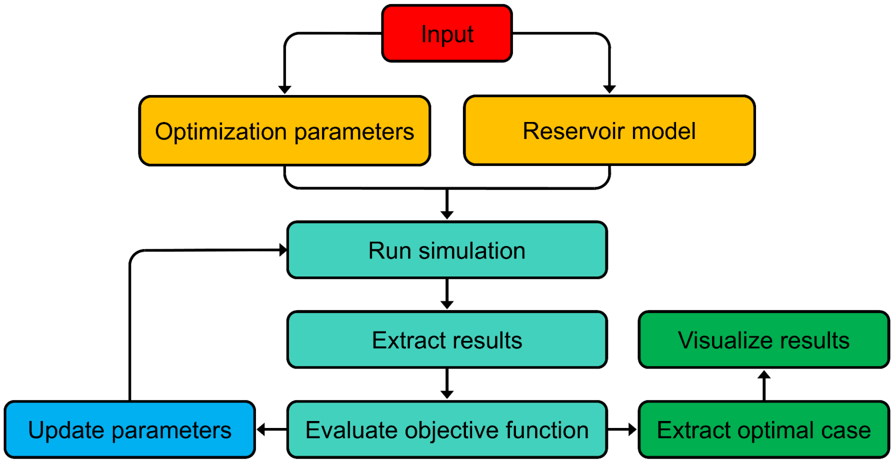


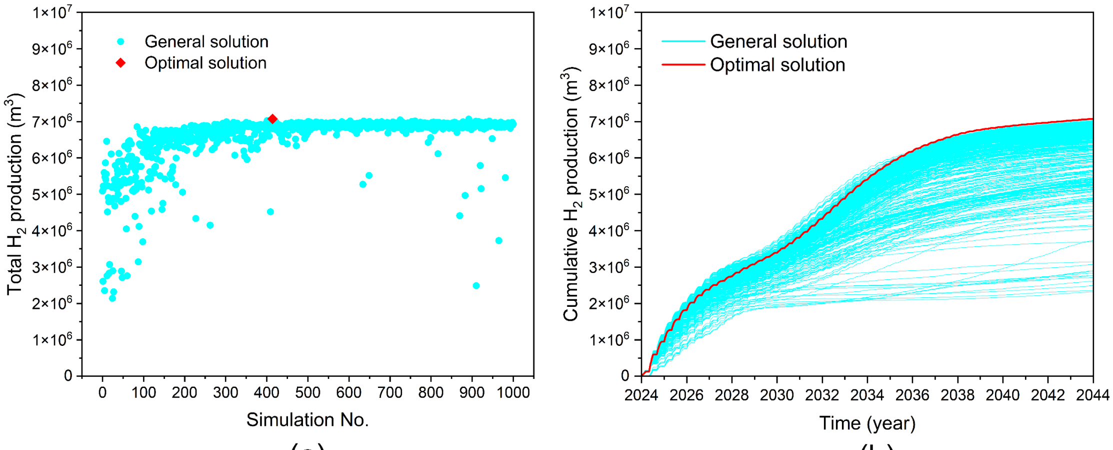
Figure 3 - Optimization algorithm workflow.

3. RESULTS AND DISCUSSION

3.1. Sector optimization results

The sector optimization results, shown in Fig. 4, depict hydrogen production across all 1,000 simulated cases, including the optimal scenario. Hydrogen production varied significantly, ranging from 2.1×10^6 to 7×10^6 m^3, highlighting the strong dependence of hydrogen yield on injection parameters. This variation underscores the necessity of precise control over injection rates, steam temperature, and oxygen concentration in CASI operations, as suboptimal choices can drastically reduce production. The results emphasize the importance of a systematic optimization approach, demonstrating that carefully tuned injection parameters can lead to substantial improvements in hydrogen output. Ultimately, these findings highlight the critical role of engineering design optimization in maximizing the efficiency and economic viability of the CASI process.

The optimal parameter combination values obtained from the sector optimization and parameter combination values used for the full-field scale simulation are given in Table 4. In order to conduct the full-field reservoir scale simulation, the sector model optimal parameter values were volumetrically upscaled by multiplying by 12. This value was chosen based on the volume ratio of the sector model to the volume of the full-field model.



(a) (b)

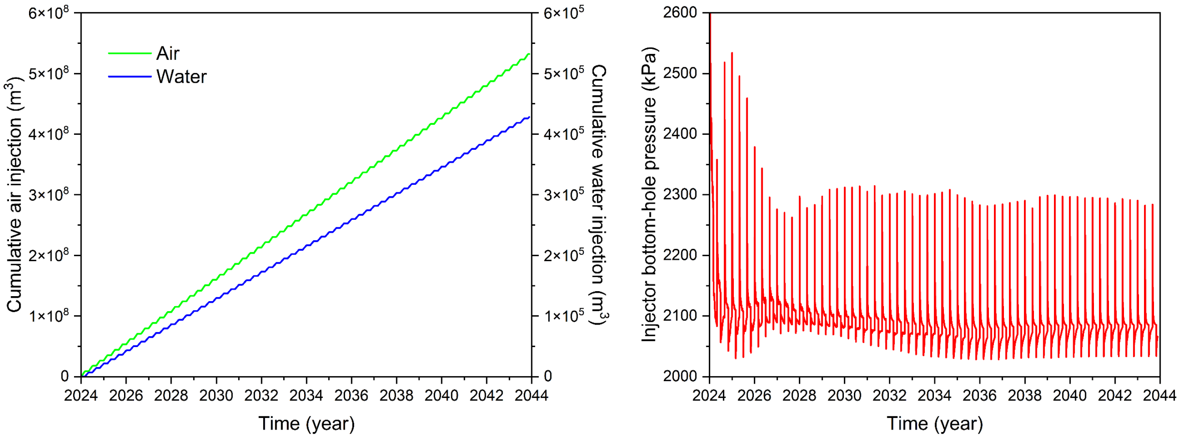
Figure 4 - Sector optimization results: (a) total H_2 production per simulation case and (b) cumulative H_2 production.

Table 4 - Optimal parameter values obtained from the sector optimization and upscaled values used in the full-field reservoir simulation.

Parameter	Sector model	Full-field model
Air injection rate (m^3/day)	12,230	146,760
Water injection rate (m^3/day)	9.8	117.7
Oxygen concentration (%)	21	21
Steam temperature (°C)	234	234

3.2. Reservoir simulation results

The full-field reservoir simulation results are shown in Figs. 5 and 6. Figure 5(a) depicts the cumulative air and steam injections for 20 years of operation, during which air was injected for 60 days followed by steam for 60 days at rates of 146,760 m^3/day and 117.7 m^3/day, respectively. Note that the cumulative steam injection is given in CWE volume at standard conditions. The total air and water volumes injected into the reservoir after 20 years are 5.32×10^8 and 4.28×10^5 m^3, respectively. Figure 5(b) shows the injector well's bottom-hole pressure variation over time. The injection pressure was about 2.1 MPa for most of the injection time with some sudden increases reaching up to approximately 2.5 MPa during the first 2 years of injection and 2.3 MPa for the rest of the injection time. These pressure peaks are mainly due to the steam volume expansion during steam injection periods.

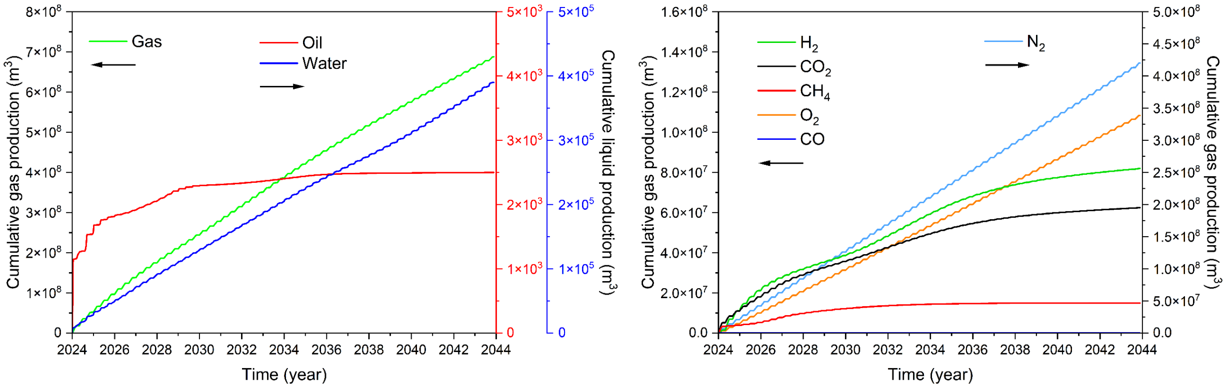


(a) (b)

Figure 5 - Reservoir simulation results: (a) cumulative fluid injection and (b) injection bottom-hole pressure.

Figure 6(a) illustrates the cumulative produced volumes of oil, water, and gas. The results show that gas and water were continuously produced at almost constant rates throughout the 20 years of injection time. The continuous water production was mainly due to the injection of steam into the reservoir. Most of the injected steam was condensed into water and produced to the surface. The total water production reached approximately 3.89×10^3 m^3, which is about 90% of the injected CWE volume as steam (4.28×10^3 m^3). This means that a significant fraction of the water used for steam injection can be recycled and re-injected into the reservoir. CASI is a process that requires high amounts of fresh water for steam generation. By treating and re-injecting produced water, the environmental impact of CASI can be significantly reduced. Heavy oil was produced rapidly during the first five years of injection after which it significantly slowed down and hit a plateau after approximately 12 years. The total crude oil production reached 2498 m^3 (15,716 bbl) after 20 years, achieving an oil recovery factor of approximately 2.4%. The rapid crude oil production in the first 5 years is mainly attributed to the viscosity reduction effect due to high in situ reservoir temperatures during the CASI process. This effect allows the heavy oil surrounding the production well to flow more easily after the well is opened for production. Subsequently, the remaining in situ oil will tend to migrate downward inside the reservoir due to the gravity segregation and viscosity reduction effects, which explain the plateau exhibited by the oil production curve. As a result, a significant portion of the oil remains in the reservoir, where it participates in combustion and gasification reactions to generate hydrogen. This behavior underscores the dual benefit of the gravity segregation effect, which not only retains oil for hydrogen production but also facilitates the upward migration of the generated hydrogen toward the production well. It also highlights the suitability of the reversed SAGD well configuration for the CASI process.

Figure 6(b) displays the cumulative production of individual gases within the produced gas mixture. The highest-produced gases in the mixture were N_2 and O_2, primarily resulting from air injection. The highest produced gas from the chemical reactions occurring during the CASI process was H_2 reaching approximately 8.19×10^7 m^3 after 20 years, followed by CO_2 and CH_4 reaching approximately 6.23×10^7 m^3 and 1.5×10^7 m^3, respectively. The hydrogen production curve showed a drop in production rates after 2035. As depicted in Fig. 6(b), the average rate of H_2 production was approximately 15,514 m^3/day (1,380 kg/day) during the first 12 years after which it decreased to approximately 4,777 m^3/day (425 kg/day) for the remaining 6 years. This drastic decrease in the H_2 production rate coincides with the oil production plateau, which could be an indication that the reservoir starting to reach a depletion state. Overall, the average rate of H_2 production for the 20 years of injection was approximately 11,219 m^3/day (998 kg/day).



(a) (b)

Figure 6 - Reservoir simulation results: (a) cumulative fluid production and (b) gas cumulative productions.

3.3. Hydrogen generation mechanisms

Analyzing the composition of the produced gases offers valuable insights into the mechanisms driving hydrogen generation within the reservoir during CASI. Figure 7 presents the gas composition of the produced gas mixture versus time. Hydrogen concentrations in the produced gas mixture reached peaks of approximately 65 mol.%. These peaks of high H_2 concentrations appeared during the steam injection stages. This highlights the crucial role of steam in driving in-situ hydrogen generation by triggering coke gasification and water-gas shift (Reactions 3 and 4). The high H_2 concentrations in the produced gas during steam injection are the result of alternating air and steam injections instead of co-injecting them. During CASI, when air injection is stopped, nitrogen is no longer introduced into the reservoir, eliminating its dilution effect on the produced gas mixture. Additionally, the absence of air injection mitigates the consumption of hydrogen by oxygen through Reaction 6. Similar observations were reported by Abu et al. (2015) and Fassihi et al. (2024), where the co-injection of air and steam during heavy oil combustion tube experiments showed a rapid increase in hydrogen concentration when air injection was stopped while maintaining steam injection. This underscores the benefit of alternating air and steam injection cycles in enhancing hydrogen production.

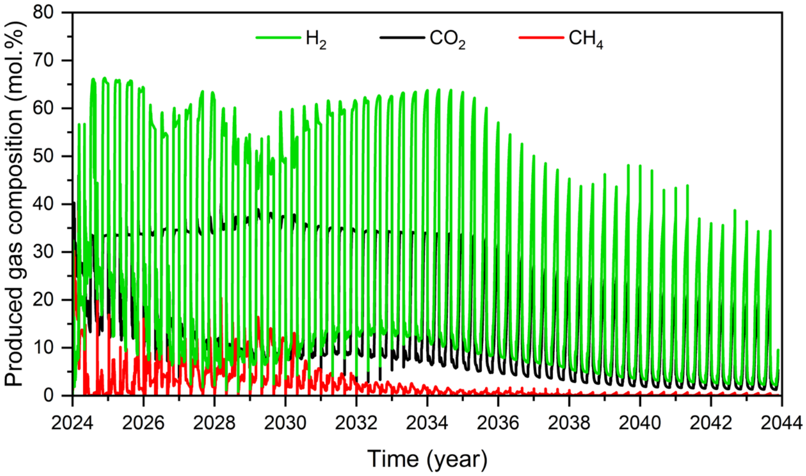


Figure 7 - Composition of the produced gas mixture.

To gain a deeper understanding of the in-situ hydrogen generation process during CASI, we analyzed the in-situ temperature and hydrogen concentration distributions in the reservoir during the simulation. Figure 8 illustrates the comparison of in-situ temperature and hydrogen concentration distributions in the reservoir model during the air (left side) and steam (right side) injection stages. During the air injection stage, when combustion reactions dominate the process, the in-situ reservoir temperatures are high. This is mainly due to the exothermic nature of the heavy oil combustion reactions that release enough heat to raise the temperature of the reservoir. During this stage, the hydrogen concentrations in the reservoir are significantly low (almost no hydrogen is present in the model). Although coke (from Reaction 1) and steam (from in-situ water evaporation due to high temperatures) are present in the reservoir during this stage, very little to no hydrogen is generated. This is because coke tends to react much faster with oxygen than steam. Therefore, most of the deposited coke during this stage will be combusted. Some hydrogen may be generated through the water-gas shift reaction (Reaction 4) of the released CO during this stage. However, due to the presence of oxygen, most of this hydrogen will be consumed through Reaction 6. During the steam injection stage, the process is dominated by gasification reactions. The reservoir temperature decreases during this stage mainly due to the endothermic nature of the gasification process. The heat generated during the combustion process is absorbed to trigger gasification reactions (Reactions 3 and 4) and drive in-situ hydrogen generation. The hydrogen concentration in the reservoir during this stage is high, indicating that hydrogen is mainly generated during the steam injection stage.

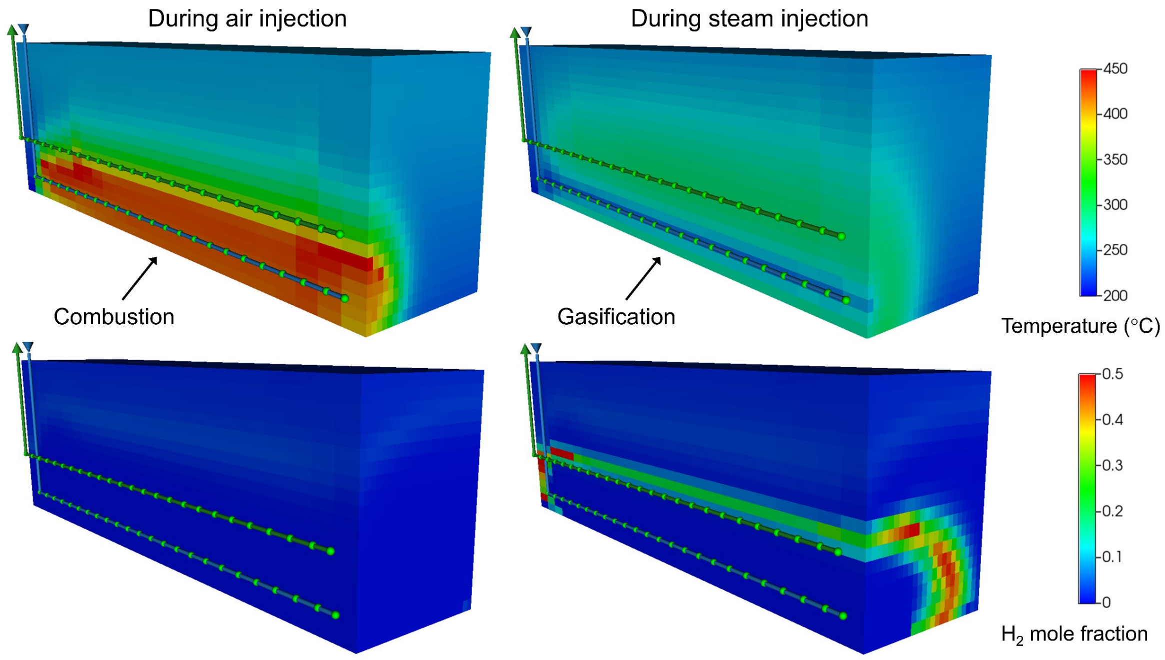


Figure 8 - 3-D view of the reservoir model showing the comparison of temperature and hydrogen concentration distributions between air and steam injection periods.

3.4. Hydrogen production potential

Evaluating the hydrogen yield during the CASI process is essential for assessing its efficiency and feasibility. This requires estimating the amount of hydrogen generated from a given volume of crude oil and determining the fraction of the original oil in place that undergoes conversion into hydrogen, referred to as the oil conversion factor (CF). The oil CF can be calculated using the following formula:

$$\boldsymbol{CF = \frac{Original\ oil\ in\ place - Produced\ oil - Residual\ oil}{Original\ oil\ in\ place} \times 100} \tag{2}$$

where the *original oil in place* is the volume of oil present in the reservoir before any production, the *produced oil* is the volume of oil recovered to the surface, and the *residual oil* is the volume of oil remaining in the reservoir after production. Equation 2 can also be written as follows:

$$\boldsymbol{CF = \frac{Converted\ oil}{Original\ oil\ in\ place} \times 100} \tag{3}$$

where the *converted oil* is the volume of oil that undergoes combustion and gasification reactions in the reservoir to produce hydrogen. All volumes are reported at standard conditions to ensure consistency in calculations.

Figure 9 illustrates the cumulative hydrogen production alongside the variations in converted oil volume and oil CF over time. The results indicate that after 20 years of CASI, 77% of the original oil in place (equivalent to 508,579 barrels of oil) was converted through combustion and gasification reactions to produce hydrogen. This demonstrates that a substantial portion of in-situ oil can be effectively utilized for hydrogen generation. The estimated hydrogen yield reached approximately 14.33 kg H_2 per barrel of converted oil, highlighting the process's potential for large-scale hydrogen production.

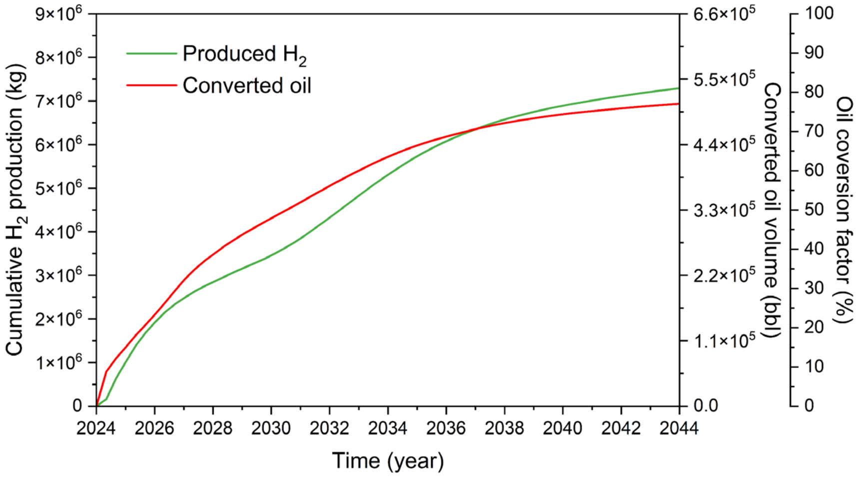


Figure 9 - Cumulative hydrogen production, converted oil volume, and oil conversion factor as a function of time.

4. CONCLUSIONS

This study assesses the potential of in-situ hydrogen production from heavy oil and bitumen reservoirs via CASI. Reservoir simulations, combined with a genetic optimization algorithm, were employed to determine optimal engineering designs for field operations and to evaluate hydrogen production. The results demonstrated that CASI can achieve an average hydrogen production rate of 998 kg/day, leading to a total hydrogen output of approximately 7.28×10^6 kg over 20 years from one production well. Around 77% of the original oil in place was converted to hydrogen, with a yield of 14.33 kg per barrel of heavy oil. These findings indicate that CASI has the potential to be a key player in the transition to cleaner hydrogen production.

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