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Reinventing Oil Reservoirs: A Subsurface Pathway to Hydrogen and Cleaner Hydrocarbons

Aysylu Askarova[1,*], **Alexey Cheremisin**[1], **Renbao Zhao**[2] and **Chengdong Yuan**[1]

[1] Skolkovo Institute of Science and Technology, Moscow 143026, Russia
[2] College of Petroleum Engineering, China University of Petroleum, Beijing 102249, China

Abstract

This article explores the emerging concept of in situ hydrogen generation (ISHG) within oil reservoirs as a transformative pathway toward clean energy and hydrocarbon upgrading. With the global energy sector facing decarbonization pressures and limitations of conventional hydrogen production, ISHG offers a promising alternative by turning mature or depleted oil fields into subsurface reactors for hydrogen and upgraded oil co-production. Through thermochemical processes such as in situ combustion (ISC), steam methane reforming (SMR), coke gasification and water-gas shift reactions (WGSR), hydrogen is produced underground while carbon dioxide and by-products remain trapped, minimizing surface emissions. Drawing on recent experimental, modeling, and pilot studies, we discuss advances in reaction mechanisms, numerical simulation, and techno-economic assessments, highlighting both technical opportunities and outstanding challenges. The article provides a forward-looking perspective on how ISHG can repurpose legacy oil infrastructure for a cleaner energy future.

Keywords: in situ hydrogen generation, heavy oil, steam methane reforming, oil upgrading.

1 Introduction

The global energy landscape is undergoing a profound transformation driven by climate commitments, net-zero targets, and the urgent need for sustainable alternatives to fossil fuels [1–3]. Among the emerging solutions, hydrogen has gained increasing attention as a clean energy vector capable of decarbonizing hard-to-abate sectors such as industry, heavy transport, and power generation [4]. Yet, the current methods of hydrogen production—primarily steam methane reforming (SMR) and electrolysis—are constrained by energy intensity, infrastructure demands, and carbon emissions. In response, researchers have proposed a transformative idea: in situ hydrogen generation (ISHG) from oil reservoirs, a process that reimagines depleted or mature fields not as relics of the fossil fuel era, but as assets for clean energy production [5, 6].

ISHG addresses many of these challenges by enabling hydrogen production directly within the reservoir, turning the subsurface formation into a chemical reservoir rather than transporting hydrocarbons to the surface for processing. Through thermochemical processes such as in situ combustion (ISC), steam

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***Corresponding author:**
✉ Aysylu Askarova
a.askarova@skoltech.ru

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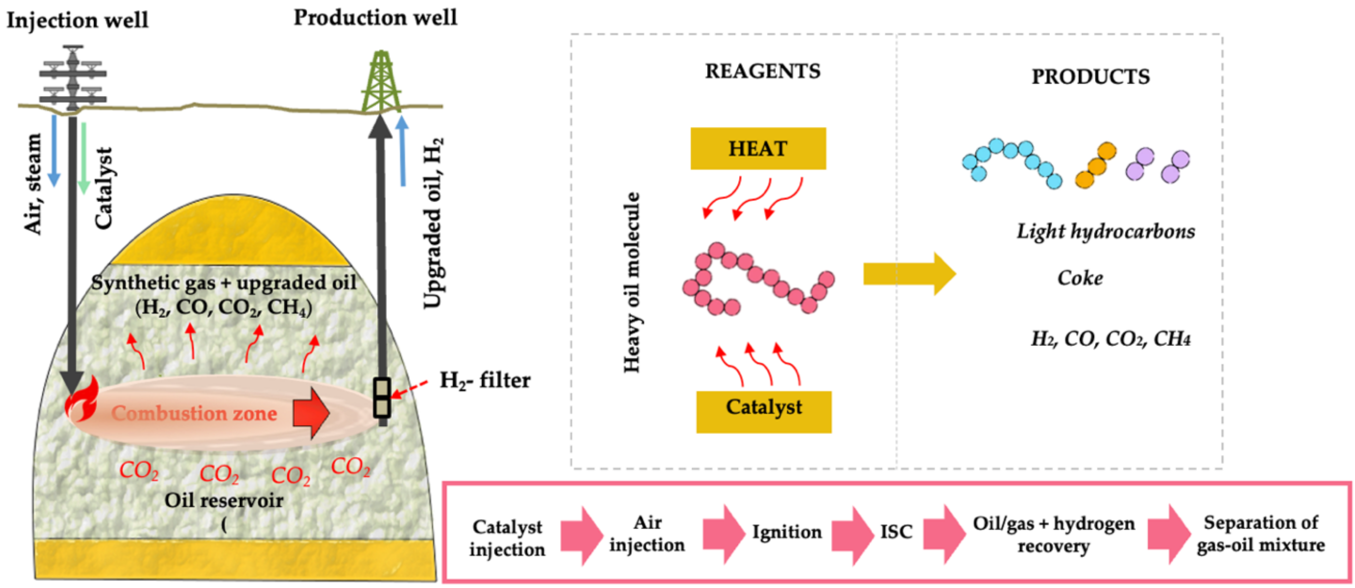

Figure 1. Conceptual scheme of ISHG and oil upgrading process [4].

methane reforming (SMR), and water-gas shift reactions (WGSR), hydrogen and upgraded oil can be co-produced [4]. Crucially, carbon dioxide (CO_2) and other by-products remain trapped in the formation, reducing surface emissions and simplifying processing infrastructure (see Figure 1).

The process starts with injecting oxidants to trigger low-temperature oxidation and combustion, heating the reservoir to 400–600°C. Catalyst precursors like nickel salts are then activated in situ, enabling coke gasification (1) and WGSR (2) that generate hydrogen and upgrade the oil. Concurrently, hydrogen reacts with heavy hydrocarbons, promoting in situ upgrading through hydrocracking and hydrogenation.

$$C + H_2O \longrightarrow CO + H_2 \qquad (1)$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \qquad (2)$$

This thermochemical sequence creates a reactive zone where hydrogen and light hydrocarbons are formed, and heavier fractions are cracked and desulfurized. These reactions, when properly managed, yield hydrogen concentrations of up to 5 vol.% in the produced gas, along with partially upgraded oil with lower viscosity, reduced asphaltenes, and increased light hydrocarbon fractions (C_5–C_{20}).

2 Experimental Case Studies

The concept of ISHG from oil reservoirs has gained momentum through a series of experimental, modeling, and early commercial studies. Article [5] work was among the first to combine combustion tube experiments with field-scale modeling, demonstrating that hydrogen concentrations could yield up to 15-30 vol.%. His findings revealed key reaction pathways—steam reforming, water–gas shift, and coke gasification—contributing to both hydrogen production and oil upgrading, with increased API gravity and reduced viscosity.

Further validation by [7], who used medium pressure combustion tube (MPCT) experiments on a depleted gas reservoir with 10% residual oil. Hydrogen concentrations reached 1 vol.%, with 35–40% methane conversion. Oil upgrading was also significant, with viscosity dropping from 2439 to 4.2 mPa·s and a notable increase in lighter hydrocarbons. Authors in [8] extended this work to heavy oil reservoirs with 60% oil saturation. Catalytic ISC using nano-nickel achieved hydrogen yields up to 5 vol.% and 398.2 mL/g. The catalyst promoted coke oxidation and aquathermolysis, leading to substantial oil upgrading.

A study by [9, 10] focused on the impact of different atmospheric conditions, showing that nitrogen-rich environments enhanced hydrogen formation via coke dehydrogenation, while oxidative atmospheres reduced yields. Mixed gas systems with clay and water improved both hydrogen concentration (1.29%) and conversion (179.4 mL/g), reinforcing the importance of ambient composition.

These studies demonstrate that ISHG is a technically viable and flexible approach for hydrogen production and in situ oil upgrading across a range of reservoir types and saturation levels.

3 Numerical Studies

Numerical modeling has played a pivotal role in understanding and optimizing ISHG and oil upgrading processes. These simulations complement experimental data by allowing reaction mechanisms to be tested under various reservoir conditions and scaled to field applications.

A research by [5] investigated hydrogen generation from Athabasca bitumen using ISC. Their numerical model, validated by experimental data, showed hydrogen yields over 16 vol.%, primarily from coke gasification and steam reforming. Optimal hydrogen production occurred at temperatures of 320–380 °C and 4 MPa pressure, emphasizing controlled reaction conditions for effective hydrogen generation. The work [11] presented a practical in situ gasification (ISG) process for bitumen reservoirs, using cyclic steam-oxygen injection with SAGD wells. Their model, validated against field data, showed efficient hydrogen production (up to 20 mole %) and bitumen upgrading. The proposed approach provided higher energy efficiency, reduced water use, and slightly lower CO_2 emissions compared to conventional thermal methods. The article by [12] develops a laboratory-scale simulation model to study hydrogen generation via ISC gasification of heavy oil. Their results show that hydrogen concentrations up to 34 mol.% can be produced at 800°C, with coke gasification and water-gas shift reactions dominating the process, and that higher temperatures and optimized water injection are critical for maximizing hydrogen yields.

The article by [13] presents a numerical study on ISHG from hydrocarbon reservoirs. Using chemical equilibrium calculations and CMG STARS reservoir simulations, the authors analyzed key thermochemical reactions including steam reforming and partial oxidation. They found that hydrogen yields increased with higher steam-carbon ratios but decreased with excessive oxygen injection, highlighting the importance of carefully controlling reactant ratios to optimize hydrogen production.

In a separate study, [7] combined experimental MPCT results with CMG STARS simulations to evaluate the kinetics and scalability of ISHG in depleted gas reservoirs with low residual oil saturation (~10%). The numerical models incorporated key thermochemical reactions such as coke gasification and steam reforming, and were validated against core-scale combustion and injection data. The simulations showed that even with limited oil content, sufficient heat and coke formation could drive hydrogen production, especially when followed by methane and steam injection. Simultaneously, the model predicted significant viscosity reduction and compositional shifts in the oil phase, confirming the feasibility of coupling hydrogen generation with oil upgrading.

Collectively, these numerical studies provide robust tools for designing and optimizing ISHG strategies. By integrating complex reaction networks with reservoir-scale models, they enable researchers and industry practitioners to predict system performance, reduce experimental uncertainty, and guide future pilot implementations.

4 From Pilot to Production: Commercial Outlook

Building on the foundational modeling and experimental work by [5, 11], researchers at the University of Calgary and Proton Technologies advanced integrated numerical models—including partial oxidation and reforming reactions—using CMG STARS to assess the field-scale feasibility of ISHG. These modeling efforts directly supported the launch of commercial pilot projects focused on hydrogen production from depleted oil and gas reservoirs, with the added benefit of CO_2 sequestration.

Today, several companies are piloting ISHG strategies worldwide, signaling growing industry confidence in this transitional pathway. For example, Proton Technologies has implemented a field demonstration in Alberta, Canada, utilizing pure oxygen injection and palladium membrane technology for hydrogen separation at the wellhead. Similarly, JX Nippon in Japan and Oxy in the USA have announced plans to repurpose legacy reservoirs for hydrogen production and CO_2 storage. Other notable pilots include C2CNT in Canada and PetroHunt in North America, each exploring various combinations of thermal cracking, catalytic reforming, and enhanced oil recovery. The Table 1 summarizes key pilot projects, highlighting their technology, reservoir type, environmental strategy, and main challenges.

Recent techno-economic reviews provide insight into the feasibility and costs of ISHG. Authors in [14] highlight that subsurface combustion and

Table 1. Overview of Current ISHG Pilot Projects and Key Parameters.

Parameter	Proton Technologies	JX Nippon	C2CNT	PetroHunt	Oxy
Country / Region	Canada (Alberta)	Japan	Canada (Vancouver, BC)	USA / Canada	USA (Texas, Permian Basin)
Technology	*In situ* H_2 generation (combustion front + membrane)	*In situ* H_2 and NH_3 generation (R&D, steam stimulation + catalysts)	Thermal cracking / reforming of bitumen	*In situ* H_2 via steam stimulation + catalytic hydrocarbon cracking	Thermochemical H_2 generation + CCS + carbon management
TRL	~6–7	~5	~4–5	~4	~5–6
Reservoir Type	Depleted oil gas reservoirs	Depleted oil reservoirs	Oil sands	Depleted oil gas reservoirs	Depleted active oil gas reservoirs
Temperature Range	500–800°C	300–600°C	400–700°C	400–600°C	500–700°C
CAPEX	Low	Medium	High	Medium	Medium–High
Environmental Aspect	CO_2 storage	Carbon reduction with CCS potential	CCS required	Carbon reduction during EOR + H_2	Full CCS cycle, DAC integration
Key Challenges	Membrane, combustion stability	Catalysis efficiency control	High energy demand	Temperature control uniformity	Integration of CCS and H_2 systems
Scalability	High	Medium	Limited	Medium	High
Pilot Locations	Saskatchewan, Canada	Pilot in Japan, RD facilities	USA, Canada	Permian Basin, Texas	Permian Basin, Texas

gasification can reduce CO_2 emissions and capital costs by using existing wells and storing byproducts underground, but economic success depends largely on membrane and oxygen costs and site-specific factors. Similarly, article [15] highlights that ISHG can be cost-competitive, with production costs as low as \$0.68/kg when leveraging existing infrastructure and hydrogen-selective membranes, but emphasizes that oxygen and membrane expenses, along with site characteristics, are key to economic viability.

Beyond technical feasibility and economics, ISHG offers strategic advantages, including a minimal surface footprint, the repurposing of stranded or aging assets, and strong alignment with national hydrogen strategies. For oil-exporting countries facing uncertain future demand, ISHG represents a practical bridge between current fossil operations and the emerging clean energy landscape, helping to future-proof energy sectors in the face of global decarbonization.

5 Outlook

The path to commercial ISHG deployment demands urgent advances in the following several aspects:

- Technologically, breakthroughs in catalyst resilience under extreme reservoir conditions and efficient hydrogen-separation membranes are non-negotiable—complemented by real-time monitoring tools and innovations like AI-managed reservoirs or hybrid geothermal coupling.
- Economically, reducing oxygen purity demands and slashing membrane costs through modular wellhead systems will dictate competitiveness, accelerated by carbon pricing and targeted pilot incentives.
- Strategically, establishing robust regulations for subsurface hydrogen storage and CO_2 sequestration enables fossil-dependent economies to repurpose infrastructure, retain expertise, and synchronize with national hydrogen agendas through cross-border demonstration projects.

6 Conclusion

Reinventing oil reservoirs as platforms for subsurface hydrogen generation and oil upgrading marks a fundamental shift in energy and decarbonization strategies. This article has reviewed the main objectives and findings in the field, showing that ISHG can effectively produce hydrogen and upgraded oil across a range of reservoir types, leveraging both experimental and modeling advances. Case studies confirm that ISHG is technically viable, delivering significant hydrogen yields and oil quality improvement, while numerical simulations offer guidance for optimizing field applications. Although challenges remain—such as catalyst durability, efficient monitoring, and policy adaptation—the expanding body of research and commercial pilot projects signals growing confidence in ISHG's future. Continued interdisciplinary collaboration, pilot demonstration, and supportive regulatory frameworks will be essential for realizing the potential of ISHG, transforming oil reservoirs from climate liabilities into foundational assets for a hydrogen-powered, low-carbon world.

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Conflicts of Interest

The authors declare no conflicts of interest.

Ethical Approval and Consent to Participate

Not applicable.

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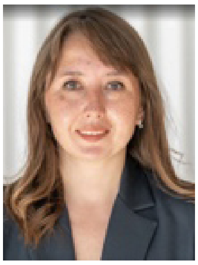

Aysylu Askarova is a senior research scientist at the Skolkovo Institute of Science and Technology's Center for Petroleum Science & Engineering, specializing in numerical modeling of thermal EOR methods including in situ combustion (ISC), high-pressure air injection (HPAI), and steam/hot water/scCO_2 processes. Her research integrates both laboratory experiments and reservoir-scale simulations, with a primary focus on heavy oil fields. Askarova also contributes to the development of in situ hydrogen generation technologies and carbon capture, utilization, and storage (CCUS) strategies. (Email: a.askarova@skoltech.ru)

Alexey Cheremisin is a full professor and deputy director at Skolkovo Institute of Science and Technology's Center for Petroleum Science and Engineering. He specializes in enhanced oil recovery and in situ combustion, leading research on experimental and numerical modeling of catalytic hydrogen generation in reservoirs. Cheremisin's work bridges laboratory studies and field-scale applications for low-carbon energy solutions. (Email: A.Cheremisin@skoltech.ru)

Renbao Zhao is a full professor at China University of Petroleum (Beijing), specializing in thermal enhanced oil recovery and catalytic in situ gasification. His work focuses on nanoscale nickel catalysts for hydrogen generation and oil upgrading in heavy oil reservoirs, achieving high hydrogen yields under reservoir conditions. Zhao also studies the effects of different atmospheric environments and develops numerical models to optimize in situ syngas production. (Email: zhaorenbao@vip.sina.com)

Chengdong Yuan is a professor and deputy director at the Skolkovo Institute of Science and Technology's Center for Petroleum Science and Engineering. He specializes in reservoir engineering, enhanced oil recovery, and catalytic upgrading of hydrocarbons, with a focus on in situ combustion and hydrogen generation. Yuan has published widely in these areas and is recognized for advancing innovative subsurface energy technologies. (Email: C.Yuan@skoltech.ru)