REVIEW ARTICLE

In-situ Hydrogen Production in Natural Gas Reservoirs: From Methane Conversion Mechanisms to Techno-economic and Environmental Feasibility

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Abstract

In-situ hydrogen production from natural gas reservoirs (IHP-NG) is an emerging pathway for low-carbon hydrogen by converting methane-rich subsurface resources while retaining carbon-bearing byproducts underground. This review critically evaluates the reaction mechanisms, experimental and modelling evidence, techno-economic position, life-cycle implications, and deployment challenges of IHP-NG. Unlike heavy-oil in-situ combustion gasification, IHP-NG is governed mainly by methane conversion reactions, including steam methane reforming, partial oxidation, autothermal reforming, methane cracking, dry reforming, and water–gas shift, alongside competing pathways such as methanation, reverse water–gas shift, and coking. Existing studies show that high temperature, adequate steam supply, controlled oxidant dosage, effective catalysis, and selective H_2 recovery are essential for meaningful hydrogen generation. However, uncertainties remain around reservoir heterogeneity, heat management, catalyst stability, well integrity, H_2 separation, and carbon retention. Techno-economic and life-cycle assessment indicates that IHP-NG is a process-integration concept, not an inherently cheaper or cleaner hydrogen route. Its competitiveness and carbon advantage depend on high H_2 yield, reliable separation, infrastructure reuse, verifiable CO_2 retention, low methane and H_2 losses, and manageable monitoring and liability costs. Field-scale validation is therefore essential before IHP-NG can be deemed a credible low-carbon hydrogen pathway.

Keywords: sustainability, climate action, in-situ hydrogen production, techno-economic analysis, energy transition, risk assessment.

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1 Introduction

Hydrogen is increasingly regarded as a strategic energy carrier for decarbonizing sectors where direct electrification is technically difficult or economically inefficient, including refining, ammonia synthesis, steel production, long-distance transport, and high-temperature industrial heat [1, 2]. However, the climate value of hydrogen depends strongly on how it is produced. Global hydrogen demand reached almost 100 Mt in 2024, but production remains dominated by fossil-fuel-based routes, consuming large quantities of natural gas and coal, while low-emissions hydrogen still accounts for less than 1% of global output [3]. Conventional hydrogen production is therefore not yet aligned with deep decarbonization goals. Steam methane reforming (SMR), partial oxidation (POX), autothermal reforming (ATR), and coal gasification are commercially mature, but they generate large volumes of CO_2 unless coupled with carbon capture, utilization, and storage (CCUS) [4]. Blue hydrogen partially addresses this limitation, yet its overall effectiveness is constrained by capture efficiency, methane leakage, CO_2 transport and storage requirements, cost, and long-term monitoring obligations [5–7].

In situ hydrogen production (IHP) has emerged as a potentially transformative alternative because it relocates part of the hydrogen-generation process from surface facilities to the subsurface [8]. In this concept, hydrocarbons are converted into hydrogen directly within geological formations or wellbore–reservoir systems, while carbon-bearing byproducts such as CO_2, CO, coke, or solid carbon are retained underground [9, 10]. The reservoir therefore functions simultaneously as a feedstock source, a high-pressure reactor, and a carbon-retention medium. This integration could reduce the need for surface reformers, external CO_2 capture plants, long-distance CO_2 transport, and new large-scale storage sites, while also allowing existing wells, surface facilities, and subsurface infrastructure to be repurposed for low-carbon energy production [11, 12]. Nevertheless, IHP remains an early-stage technology, and its feasibility depends on reaction control, heat management, catalyst stability, hydrogen selectivity, reservoir integrity, and reliable field-scale monitoring [13].

Most IHP research to date has been motivated by observations from thermal enhanced oil recovery, particularly in-situ combustion (ISC) and heavy oil upgrading processes [14]. In heavy oil and bitumen reservoirs, air or oxygen injection generates a combustion front that oxidizes part of the hydrocarbon, raises the reservoir temperature, and promotes thermolysis, aquathermolysis, coke gasification, reforming, and water–gas shift reactions [10]. Several historical ISC projects unintentionally produced hydrogen-rich gases, demonstrating that hydrogen can be generated under reservoir conditions even when it is not the target product. Reported examples include LERC TS-2C, Marguerite Lake, Wolf Lake, Whitesands, and Kerrobert, where hydrogen appeared in produced gases during heavy oil or bitumen recovery operations [9]. These observations have led to the concept of in-situ combustion gasification (ISCG), in which hydrogen is intentionally generated and selectively recovered while CO_2 and other undesired gases remain underground.

Natural gas reservoirs represent a particularly important but underexplored target for IHP. Unlike heavy oil reservoirs, gas reservoirs contain methane-rich hydrocarbons with high hydrogen-to-carbon (H/C) ratios, which makes them attractive feedstocks for hydrogen generation [15]. Mukhina et al. [16] emphasized that gaseous reservoirs contain substantial energy resources and that their high H/C ratio creates the potential for greater hydrogen generation than lower-H/C hydrocarbon systems. The concept is especially relevant for depleted, mature, or late-life gas fields, where conventional gas recovery has already extracted part of the resource but residual methane, existing wells, pipelines, and surface facilities may still be available for repurposing. In this context, natural gas reservoirs could be transformed from declining hydrocarbon assets into subsurface hydrogen-generation and carbon-retention systems, extending field life while reducing the need for new surface reforming and CO_2-handling infrastructure [8]. Recent gas-reservoir studies have therefore shifted attention from incidental hydrogen formation in oil combustion projects toward deliberate methane conversion in porous media through steam reforming, partial oxidation, autothermal reforming, methane cracking, and water–gas shift reactions [17, 18].

Despite these opportunities, direct extrapolation from heavy oil ISCG to natural gas reservoirs is not sufficient [14]. Heavy oil ISCG is controlled by oxidation and gasification of liquid hydrocarbons, resins, asphaltenes, and coke, whereas natural gas reservoirs are dominated by methane and light hydrocarbons with different reaction pathways [19,

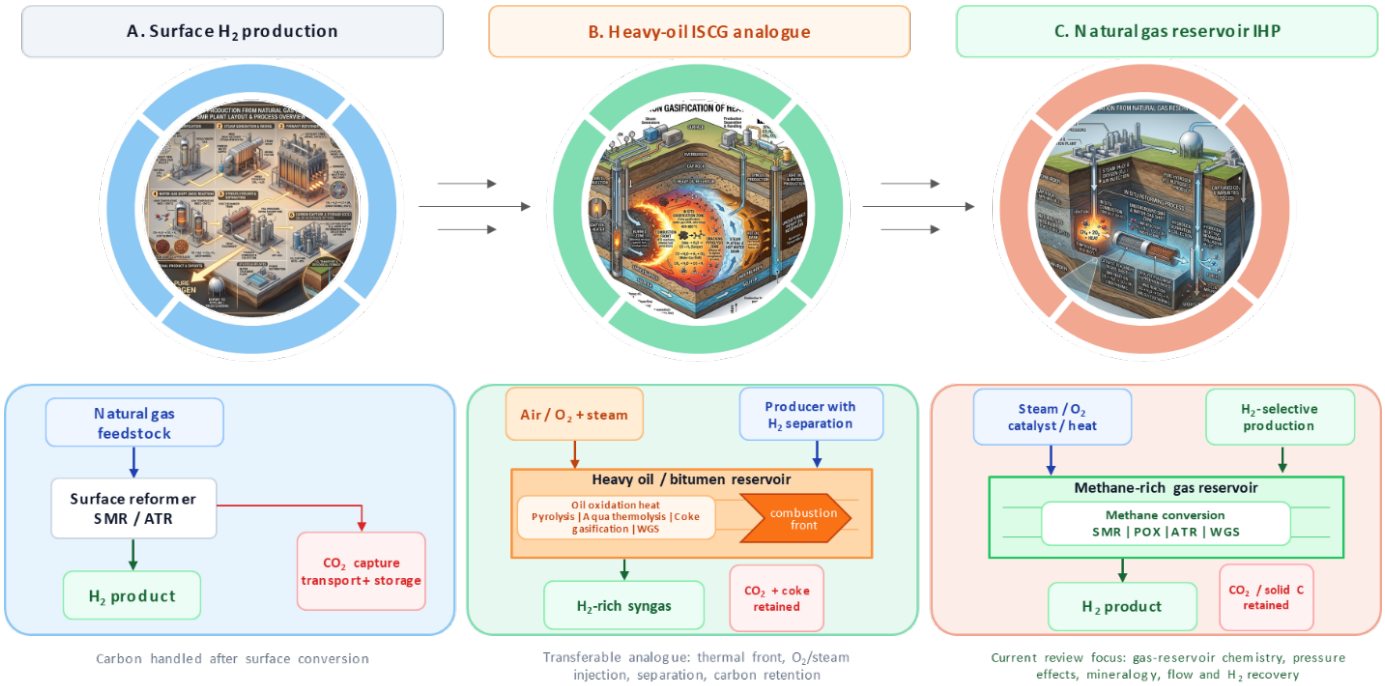

Figure 1. Conceptual distinction between surface hydrogen production, heavy oil in-situ combustion gasification, and IHP from natural gas reservoirs.

20]. In gas reservoirs, hydrogen generation is expected to occur mainly through SMR, POX, ATR, dry reforming of methane (DRM), methane cracking, and water–gas shift (WGS) reactions [16]. The relative importance of these pathways depends on reservoir and operating conditions. Key controls include temperature, pressure, steam-to-carbon (S/C) ratio, oxygen availability, residence time, mineralogy, catalyst distribution, and gas composition [18]. Unlike heavy oil reservoirs, gas reservoirs generally contain limited liquid fuel or coke-forming material; in conventional in-situ combustion processes, such liquid fuel and coke inventories are central to sustaining the combustion front, generating heat, and providing in-situ reducing agents [21]. Therefore, while heavy oil ISCG provides valuable analogues for thermal-front propagation, oxygen/steam injection, downhole separation, and carbon retention, it cannot fully represent the chemistry, flow behavior, and engineering constraints of IHP in natural gas reservoirs (Figure 1).

Existing reviews have established important foundations for IHP as summarized in Table 1. Nevertheless, these reviews are broader in scope or are centered on oil reservoirs rather than natural gas reservoirs. Salahshoor and Afzal [8] reviewed IHP from fossil fuel resources and included a preliminary techno-economic assessment, but their discussion was not dedicated to natural gas reservoirs. Ifticene et al. [9] focused on ISCG from petroleum reservoirs, with strong emphasis on heavy oil and bitumen systems. Okere and Sheng [10] reviewed clean hydrogen generation from petroleum reservoirs by discussing reaction mechanisms, field applications, membranes, and economic challenges, but the dominant framework remained oil reservoir conversion. Smith et al. [12] examined subsurface combustion and gasification with techno-economic and life-cycle perspectives, while Hassanpouryouzband et al. [11] provided a broad future-energy perspective on in-situ hydrogen generation from underground fossil hydrocarbons. More recently, Ozyurtkan et al. [13] reviewed in-situ hydrogen generation in hydrocarbon reservoirs, including production methods, membranes, facility requirements, shale applications, technology readiness, and underground hydrogen storage. However, the review remained a broad hydrocarbon-reservoir synthesis rather than a critical assessment dedicated to natural gas reservoir applications.

These reviews collectively demonstrate the growing importance of in-situ hydrogen generation, but they also reveal a clear gap. Natural gas reservoirs have not yet been treated as a distinct primary system, despite their methane-rich composition, high H/C ratio, widespread infrastructure, and potential use as subsurface reactors with integrated carbon

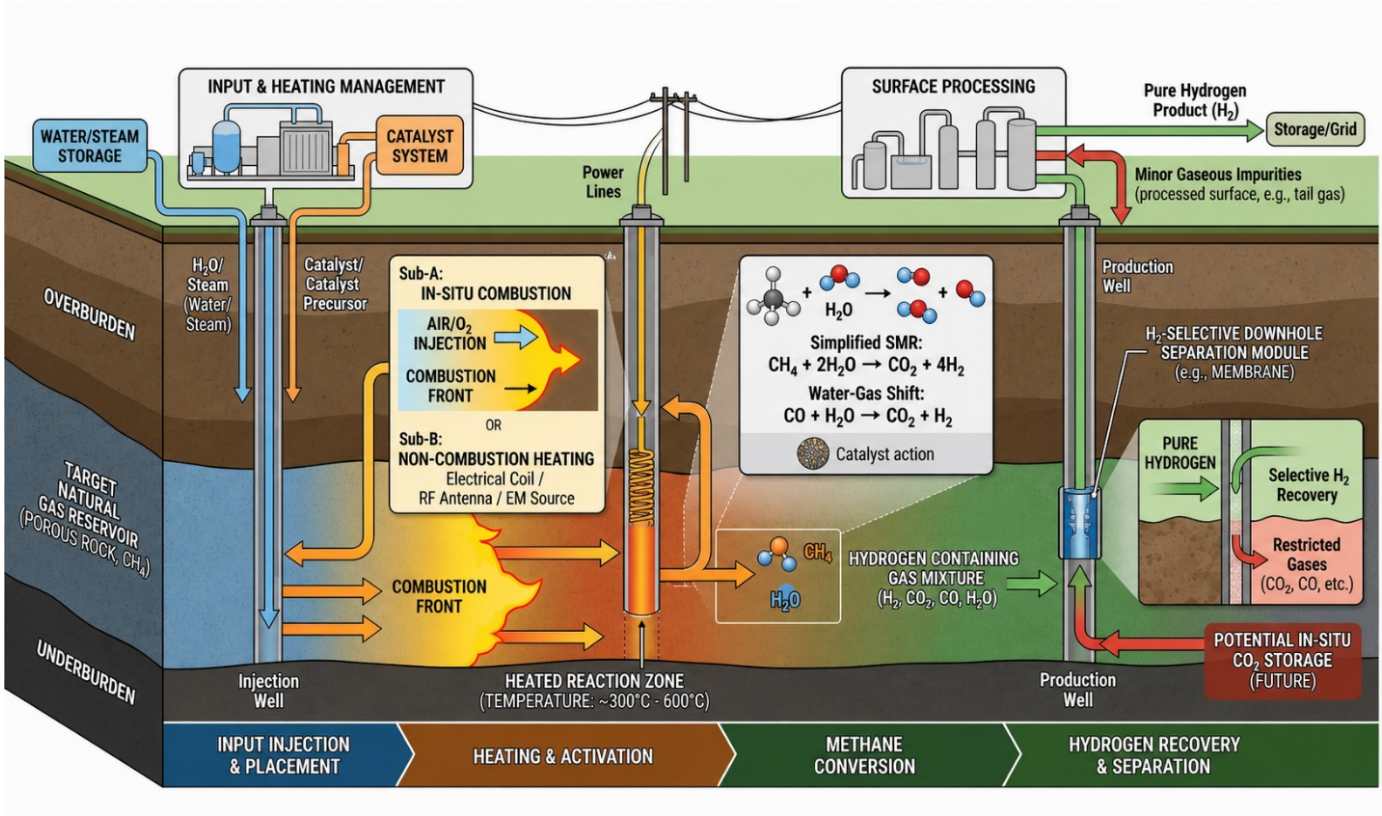

Figure 2. Schematic representation of IHP in natural gas reservoirs.

Table 1. Comparison of previous reviews on in-situ hydrogen production.

Author(s)	Main focus	Resource/reservoir type	Main contribution	Limitation
Salahshoor and Afzal [8]	In-situ hydrogen production and techno-economic analysis	Broad fossil-fuel resources	Evaluated IHP concepts and key economic drivers	Not dedicated to methane-rich natural gas reservoirs
Ifticene et al. [9]	In-situ combustion gasification for hydrogen production	Petroleum reservoirs, especially heavy oil/bitumen	Detailed ISCG principles, reaction chemistry, field evidence, and technical challenges	Strongly centered on heavy oil/bitumen systems rather than gas reservoirs
Okere and Sheng [10]	Clean hydrogen generation from petroleum reservoirs	Petroleum reservoirs	Reviewed reaction mechanisms, field applications, membranes, and economic/technical barriers	Broad petroleum-reservoir focus; gas-reservoir IHP is not treated as the central system
Smith et al. [12]	Subsurface combustion and gasification for hydrogen production	Hydrocarbon and coal resources	Integrated reaction mechanisms with techno-economic and life-cycle assessment	Broader ISC/ISG focus; limited gas-reservoir-specific analysis
Hassanpouryouzband et al. [11]	In-situ hydrogen generation from underground fossil hydrocarbons	Broad fossil hydrocarbon systems	Provided a future-energy perspective on thermochemical and biological IHP pathways	Broad conceptual review; not dedicated to natural gas reservoirs
Ozyurtkan et al. [13]	In-situ hydrogen generation in hydrocarbon reservoirs	Hydrocarbon reservoirs, including oil, gas, shale, and storage systems	Reviewed ISHG methods, membranes, well/facility requirements, TRL, shale applications, UHS, and safety issues	Broad hydrocarbon-reservoir synthesis; natural gas reservoir IHP is included but not critically isolated as the primary focus

retention. The current review addresses this gap by focusing specifically on IHP from natural gas reservoirs. Heavy oil ISCG studies are considered only as analogues where they provide transferable insights into thermal-front propagation, oxygen and steam injection, downhole separation, carbon retention,

and field-scale operational risks. This distinction is important because gas reservoir IHP is governed by methane conversion, gas transport, pressure-sensitive equilibria, catalyst–rock interactions, and hydrogen separation challenges that differ substantially from coke and liquid hydrocarbons (especially heavy oil) systems.

Accordingly, this review aims to critically evaluate the current status, controlling mechanisms, technical barriers, and deployment outlook for IHP from natural gas reservoirs. The specific objectives are to: (i) define the thermochemical pathways relevant to natural gas reservoirs; (ii) synthesize the experimental, simulation, and process-modeling evidence for gas reservoir IHP; (iii) identify the operating and reservoir parameters that control hydrogen yield, methane conversion, carbon retention, and hydrogen selectivity; (iv) assess catalyst, mineralogical, heat-management, and well-integrity constraints; (v) evaluate hydrogen recovery and CO_2 retention strategies; and (vi) develop a research roadmap for laboratory validation, reservoir-scale modeling, pilot testing, monitoring, and regulation. By separating natural gas reservoir IHP from broader subsurface hydrogen and heavy oil ISCG reviews, this paper provides a focused framework for assessing whether depleted or active gas reservoirs can be repurposed as low-carbon hydrogen generation systems.

2 Conceptual basis of IHP in natural gas reservoirs

2.1 Process configuration for natural gas reservoir IHP

IHP from natural gas reservoirs is governed by the coupling of heat generation, methane conversion, porous-media transport, catalyst–rock interactions, and selective gas recovery. Unlike surface reforming, where feed composition, catalyst loading, heat supply, and residence time are controlled in engineered reactors, gas reservoir IHP must operate within a heterogeneous porous medium under elevated pressure. The reservoir therefore acts as a reactive flow system in which thermodynamics, kinetics, heat transfer, and gas separation occur simultaneously.

A simplified gas reservoir IHP configuration can be described as a sequence of linked operations as shown in Figure 2. Steam or water and, where required, a catalyst or catalyst precursor are introduced into the target interval. Heat is then supplied to activate methane conversion. This heat may be generated by in-situ combustion after air or oxygen injection, or by non-combustion methods such as electrical, radio-frequency, or electromagnetic heating. The heated reaction zone promotes conversion of methane or natural gas into a hydrogen-containing gas mixture. Hydrogen is then recovered through a production well, ideally through selective separation that restricts CO_2 and other non-target gases from reaching the surface. This concept is described as a four-stage process involving catalyst/steam injection, oxygen or air injection and ignition, methane conversion in porous media, and hydrogen recovery through a selective membrane while CO_2 remains confined in the formation [16].

2.2 Reaction pathways during IHP in gas reservoirs

IHP from natural gas reservoirs invokes a suite of thermochemical reactions whose relative contributions depend on temperature, pressure, oxidant availability, and catalytic environment. About eleven reaction families define the chemistry which can be organized into three functional groups. These include heat-supplying reactions, hydrogen-forming reactions, and hydrogen-consuming or selectivity-limiting reactions. These reactions are reviewed below and summarized in Table 2.

Steam Methane Reforming: SMR is the primary endothermic reaction converting methane and steam into hydrogen and carbon monoxide:

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2 \quad \Delta H^{\circ}_{298} = +206\ kJ/mol \tag{1}$$

The reaction is thermodynamically favoured only at elevated temperatures, typically above 700–800 °C, and is suppressed by elevated pressure due to the increase in molar volume; thermodynamic optimisation studies confirm that these constraints govern methane conversion and hydrogen yield across a wide range of operating conditions [22]. On nickel catalysts (i.e. the industrial standard), a study by Blaylock et al. [23] identifies CH_4 adsorption and subsequent C–H bond activation as rate-limiting steps. The most important carbon-bearing surface intermediate is CH*, which can proceed toward CO via CHO* or CH–OH* intermediates, or deposit as solid carbon. In the subsurface context, the steam source must be injected or generated by combustion of a fraction of the hydrocarbon feed (as in ATR) since reservoir formation water alone rarely provides sufficient vapour at the required partial

Table 2. Major reaction pathways relevant to in-situ hydrogen production.

Reaction pathway	Thermal nature	Role in IHP	Main concern
Steam methane reforming	Endothermic	Primary H_2-forming pathway	Requires high heat and catalyst
Water–gas shift	Mildly exothermic	Increases H_2 and converts CO to CO_2	Sensitive to temperature and equilibrium
Overall SMR + WGS	Endothermic overall	Produces high H_2 with CO_2 retention	Needs steam and heat
Partial oxidation	Exothermic	Provides syngas and heat	Excess O_2 causes full combustion
Autothermal reforming	Thermally balanced	Couples heat generation and H_2 formation	Requires precise O_2/steam control
Dry reforming	Endothermic	Converts methane and CO_2 to syngas	Produces lower H_2/CO ratio
Methane cracking	Endothermic	Produces H_2 without CO_2 formation	Carbon deposition and pore/catalyst blockage
Methanation	Exothermic	Competing H_2-consuming pathway	Favored by high pressure and low temperature
Reverse WGS	Endothermic	Alters CO/CO_2 balance	Consumes H_2 at high temperature
Combustion	Exothermic	Heat generation	Consumes methane without producing H_2
Carbon deposition / coking	Pathway dependent	Governs whether carbon is retained as solid phase	Catalyst fouling, pore blockage, and permeability impairment

pressure. Microkinetic modelling at representative industrial conditions (800 °C, 10 bar, H_2O/CH_4 = 2.5) confirms that the rate-limiting character of CH_4 activation means that surface catalytic properties like rock mineralogy, transition-metal content etc, will strongly modulate hydrogen yield in subsurface applications [23].

Partial Oxidation of Methane: POX converts methane and a sub-stoichiometric oxygen supply into syngas:

$$CH_4 + \frac{1}{2}O_2 \rightleftharpoons CO + 2H_2 \quad \Delta H^{\circ}_{298} = -38\,kJ/mol \quad (2)$$

Unlike SMR, POX is exothermic, providing the heat required to drive reforming reactions. The literature contains a long-standing mechanistic debate. An older hypothesis—the indirect mechanism—proposed that POX proceeds in two sequential stages: first, complete combustion of a fraction of methane to CO_2 and H_2O in an oxygen-rich inlet zone, followed by steam and dry reforming of the remaining methane using those combustion products [24]. However, Lapszewicz and Jiang [25] presented experimental evidence directly refuting this model, showing that the previously proposed mechanism does not explain the observed reaction rates and product selectivity. The mechanism they and others favour instead involves direct methane dissociation on the metal surface, forming strongly adsorbed carbonaceous intermediates (CH_x*), which are subsequently oxidized by adsorbed oxygen to yield CO and H_2 as primary products [25, 26]. At the elevated temperatures typical of IHP, this direct pathway is generally regarded as the more relevant mechanism for catalytic POX, although its contribution depends on the catalyst and local reaction conditions. The O_2/CH_4 ratio at the reaction front is therefore a critical selectivity control: a ratio of approximately 0.5 corresponds to the stoichiometric requirement for POX, whereas greater oxygen availability increasingly promotes complete oxidation and reduces H_2 and CO yields [27].

Complete Oxidation of Methane: Methane combustion is the most exothermic reaction in the system, releasing approximately 803 kJ/mol at standard conditions (Equation 3). It is the dominant pathway whenever O/C $\geq$ 2 or when the gas mixture burns under fuel-lean conditions [28]. All the carbon ends up as CO_2 and all the hydrogen as H_2O, making it the reaction most hostile to hydrogen yield.

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$
$$\Delta H^{\circ}_{298} = -803\ \text{kJ/mol (LHV, gaseous } H_2O) \quad (3)$$

Kinetically, complete oxidation is favoured over partial oxidation at low temperatures and long residence times, because the surface oxidation of adsorbed CH_x species to CO_2 and H_2O is kinetically competitive with the desorption of CO and H_2 [29]. M. Wang et al. [30] studied complete methane oxidation kinetics over a $PtPd/Al_2O_3$ catalyst and found that H_2O competes with CH_4 for the same active sites, resulting in severe inhibition, and that a CH_4 activation energy of 96.7 kJ/mol governs the catalytic rate under practical conditions. The inhibitory role of H_2O is directly relevant to subsurface environments where steam is present. At higher temperatures (above approximately 800 °C) and reduced oxygen levels, selectivity shifts toward partial oxidation and the POX products CO and H_2 dominate, as discussed in the POX section. In the IHP context, complete combustion serves a dual function. It is the primary heat source that drives the endothermic reforming reactions [16], and it is simultaneously the competing reaction that consumes CH_4 without producing H_2. Managing the O/C ratio at the reaction front to maximise POX while supplying sufficient heat for downstream reforming is therefore the central operational trade-off.

Autothermal Reforming: ATR combines POX and SMR in a single reactor zone, using the heat released by the exothermic partial oxidation to drive the endothermic steam reforming:

$$CH_4+\frac{1}{2}O_2+H_2O \rightleftharpoons CO_2+3H_2 \quad \Delta H^{\circ}_{298} = -79\,kJ/mol \tag{4}$$

The net thermal balance is adjustable by varying the O/C and S/C ratios. Thermodynamic modelling indicates that optimal H_2 fractions exceeding 68% (dry basis) are achievable at approximately 715–730 °C, 0.7–1.0 MPa, with O/C ratio ~0.6–0.7 and S/C ratio ~3.2 [31]. In ATR, two mechanistically distinct stages are identifiable: rapid combustion at the inlet (generating H_2O and CO_2), followed by catalytic steam reforming and WGS reactions downstream [32]. Adding steam reduces the temperature hot-spot and suppresses CO formation relative to POX alone. For IHP, ATR offers a practical advantage: it is thermally self-sustaining and does not require external heat input, making it more compatible with a subsurface environment where heat management is constrained.

Water-Gas Shift: The WGS reaction converts CO produced during reforming or combustion into additional H_2 by reaction with steam:

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \quad \Delta H^{\circ}_{298} = -41.1\,kJ/mol \tag{5}$$

The reaction is exothermic and thermodynamically limited: equilibrium strongly favours the forward (H_2-producing) direction at low temperatures but decreases with temperature. At 298 K with stoichiometric feed, the degree of conversion approaches 99.7%; by 1500 K it falls to ~38% [33]. This means that for maximum H_2 recovery, the gas stream should be cooled to promote WGS, or the CO_2 product should be removed to shift equilibrium (sorption-enhanced WGS). However, such processes are not feasible in the context of IHP. Chen and Chen [34] provide a comprehensive review of WGS thermodynamics, kinetics, and catalyst types, confirming that CO conversion beyond the thermodynamic limit is achievable through membrane-assisted or sorption-enhanced variants. In natural gas reservoirs, WGS may proceed autocatalytically on mineral surfaces and is likely thermally activated by heat from the combustion/POX front, making it a secondary but important source of H_2.

Overall Steam Reforming: This combined reaction represents the net outcome when the primary SMR reaction (Equation 1) is followed by the WGS reaction (Equation 5):

$$CH_4 + 2H_2O \rightleftharpoons CO_2 + 4H_2 \quad \Delta H^{\circ}_{298} = +165\,kJ/mol \tag{6}$$

The net stoichiometry delivers a maximum theoretical yield of 4 mol H_2 per mol CH_4, with CO_2 rather than CO as the final carbon-containing product. Pashchenko [35] described industrial SMR in this sequential framework, where SMR is followed by WGS at the same outlet temperature. The WGS step is important not only because it increases H_2 yield, but also because it shifts the product distribution toward H_2 while generating a more concentrated CO_2 stream that is suitable for capture [34]. In the IHP context, the combined reaction is the target for any steam-injected subsurface reforming process. The strongly endothermic net enthalpy (+165 kJ/mol) means that external or in-situ heat supply is required, and the equilibrium is sensitive to operating conditions.

Dry Reforming of Methane: DRM is the most strongly endothermic of the methane reforming

reactions. Unlike SMR, which uses steam as the oxidant, DRM uses CO_2, converting two greenhouse gases simultaneously into syngas (Equation 7) with an H_2/CO ratio of 1:1, which is lower than that of SMR (~3:1) and better suited for Fischer-Tropsch synthesis or dimethyl ether production [36].

$$CH_4 + CO_2 \rightleftharpoons 2CO + 2H_2 \quad \Delta H^{\circ}_{298} = +247\ kJ/mol \tag{7}$$

Thermodynamically, DRM is negligible below about 600 °C and generally requires temperatures above 700–800 °C at atmospheric pressure to achieve meaningful conversion [37]. The reaction is also highly susceptible to carbon deposition. Coke formation is favored at low temperatures and high CH_4/CO_2 ratios, mainly through the Boudouard reaction and methane decomposition [38]. Using a CO_2-rich feed of 70% CO_2 and 30% CH_4 to represent the Natuna gas field, Sophiana et al. [39] found that increasing the CO_2/CH_4 ratio reduced carbon formation. Under optimized conditions, they reported carbon deposition of 7.1 mg C/gcat. DRM has direct relevance to IHP in gas reservoirs because CO_2 may be naturally present in reservoir gas and can also be generated in situ through combustion or oxidation reactions. Where CO_2 contacts hot CH_4 near the reaction front, particularly at temperatures above approximately 700 °C, DRM may contribute to additional syngas formation while simultaneously consuming part of the available CO_2. In this way, subsurface DRM can provide a partial CO_2-utilization pathway, although its effectiveness will depend on local temperature, CH_4/CO_2 ratio, catalyst or mineral activity, residence time, and the extent of carbon deposition.

Methane Thermal Cracking (Pyrolysis): At sufficiently high temperatures (>900 °C), methane undergoes direct thermal decomposition without requiring an oxidant or steam:

$$CH_4 \rightleftharpoons C + 2H_2 \quad \Delta H^{\circ}_{298} = +75\ kJ/mol \tag{8}$$

This reaction produces CO_2-free hydrogen and solid carbon. The mechanism proceeds through sequential C–H bond cleavage [40]. Density functional theory calculations of the methane pyrolysis mechanism show that the first C–H bond cleavage (dehydrogenation) step has an activation energy of ~272 kJ/mol at 1200 K, and that hydrogen radical attack on adsorbed carbonaceous intermediates is kinetically preferred over homogeneous thermal decomposition, a distinction relevant to both surface pyrolysis carbon formation and subsurface cracking conditions [41]. The equilibrium analysis confirms that above 900 °C the reverse reaction (methanation of carbon) becomes negligible, meaning high temperatures drive near-complete conversion [42]. Metal-based catalysts can reduce the apparent activation energy substantially (from 147 – 421 kJ/mol to 29.5 – 88 kJ/mol), but catalyst deactivation by coking is a major challenge [43]. In subsurface IHP, pyrolysis is deployed with electromagnetic-assisted heating [44]. The solid carbon product accumulates in the rock matrix, which unlike a surface reactor, cannot be easily cleared, with implications for pore plugging and permeability reduction.

Methanation: Methanation is the reverse of reforming: CO_2 (or CO) reacts with H_2 to produce methane and water:

$$CO + 3H_2 \rightleftharpoons CH_4 + H_2O \quad \Delta H^{\circ}_{298} = -206\ kJ/mol \tag{9}$$

$$2CO + 2H_2 \rightleftharpoons CH_4 + CO_2 \quad \Delta H^{\circ}_{298} = -247\ kJ/mol \tag{10}$$

$$CO_2 + 4H_2 \rightleftharpoons CH_4 + 2H_2O \quad \Delta H^{\circ}_{298} = -165\ kJ/mol \tag{11}$$

The reaction is strongly exothermic and thermodynamically favoured at temperatures below ~450 °C and elevated pressure [45, 46]. Thermodynamic analysis at 400 °C and 10 bar yields equilibrium mole fractions of approximately 0.30 CH_4, with near-complete CO_2 conversion [47]. Under subsurface confinement conditions, nanopore geometry can shift the methanation equilibrium toward CH_4 relative to bulk-phase predictions, an effect demonstrated through Monte Carlo simulation of CO_2 methanation in confined pores [48]. For IHP, methanation is a critical parasitic reaction: it consumes the H_2 produced by reforming and cracking, reducing net yield. Tackie-Otoo et al. [14] confirm that methanation is a primary H_2-loss pathway in subsurface gasification simulations, particularly as reformed gases cool below 500 °C moving away from the reaction front. Suppressing methanation requires maintaining sufficient temperature throughout the

reactive zone, rapid H_2 extraction via downhole membranes before the gas cools, or minimising CO_2 partial pressure in the product stream.

Reverse Water-Gas Shift: RWGS is the thermodynamic reverse of the WGS reaction and is mildly endothermic (Equation 12). It is favoured at elevated temperatures (above approximately 400–500 °C) where the equilibrium constant shifts toward CO and H_2O formation. At lower temperatures the forward WGS direction dominates; at higher temperatures RWGS competes increasingly with DRM and SMR.

$$CO_2 + H_2 \rightleftharpoons CO + H_2O \quad \Delta H^{\circ}_{298} = +41\, kJ/mol \quad (12)$$

Jadhav and Vaidya [49] measured RWGS kinetics over a ZnO/Al_2O_3 catalyst from 673–973 K and found an activation energy of 68 kJ/mol, with the redox mechanism (CO_2 adsorption, C–O bond scission, then H_2 hydrogenation of the surface oxygen) being dominant at the temperatures tested. Lalinde et al. [50] measured spatially resolved RWGS and methanation kinetics over Ni/Al_2O_3 between 320–420 °C and found that the rate-determining step involved an oxygenated surface intermediate (COH* or HCOO*), consistent with an associative mechanism at lower temperatures. High-temperature, high-pressure RWGS kinetics relevant to gasification conditions have also been studied in homogeneous systems, confirming that the reaction proceeds without catalyst above approximately 700 °C [51]. In the IHP context, RWGS is a significant secondary reaction: wherever H_2 and CO_2 coexist at high temperature, RWGS will consume some H_2 and regenerate CO and H_2O. This moderates net H_2 yield, and the H_2O produced can in turn drive SMR or shift equilibria downstream. The reaction is easily overlooked but represents a meaningful redistribution pathway in the multireaction gas-phase environment of a high-temperature reservoir.

Carbon Deposition: Solid carbon can form via three principal pathways, each with distinct temperature regimes and products. These include methane decomposition (Equation 8), Boudouard reaction (CO disproportionation) shown in Equation 13 and CO reduction in Equation 14.

$$2CO \longrightarrow C(s) + CO_2 \quad \Delta H^{\circ}_{298} < 0 \text{ (exothermic)} \quad (13)$$

$$CO + H_2 \rightarrow C(s) + H_2O \quad (14)$$

Bartholomew [52] remains a foundational reference on carbon deposition in reforming and methanation systems. The study showed that catalyst deactivation can occur through metal-surface fouling, pore blockage, and physical disintegration of catalyst supports. These mechanisms are directly relevant to subsurface IHP, where carbon deposition may impair catalyst activity, reduce pore connectivity, and alter flow pathways within the reservoir. The Boudouard and methane-decomposition pathways deposit morphologically distinct carbons (amorphous, filamentous, or graphitic) depending on temperature and catalyst metal [53]. Studies on Boudouard reaction carbon formation over Ni catalysts show that graphite-like deposits form preferentially at ~700 °C and are controlled by weakly interacting surface nickel particles [54]. For IHP in gas reservoirs, carbon deposition is a dual concern: it can plug pore throats and reduce permeability (damaging reservoir deliverability), but solid carbon retained underground is also the carbon-negative product of the turquoise pathway. The net effect depends on the spatial location of deposition relative to the production well.

2.3 Reservoir controls on reaction selectivity

As emphasized earlier, the reactions involved in gas-reservoir IHP do not operate in isolation. The thermodynamic landscape in a gas reservoir undergoing IHP will produce a temperature gradient from a high-temperature combustion core to a cooler periphery [18] (Figure 3). Near the high-temperature combustion zone, complete oxidation supplies heat [16], while POX and ATR can generate syngas and sustain endothermic conversion [55]. In oxygen-limited regions, SMR, DRM, and methane cracking become prominent, producing H_2 while distributing carbon among CO, CO_2, and solid carbon. At the cooler periphery, secondary reactions modify the produced gas composition: the WGS reaction can increase H_2 yield and convert CO to CO_2, whereas RWGS and methanation can consume H_2 and reduce hydrogen selectivity [14]. Carbon-forming and carbon-converting reactions, including methane decomposition, the Boudouard reaction, and carbon gasification by steam or CO_2, determine whether carbon is retained as solid deposits, converted to CO, or shifted toward CO_2; these competing pathways have been characterised

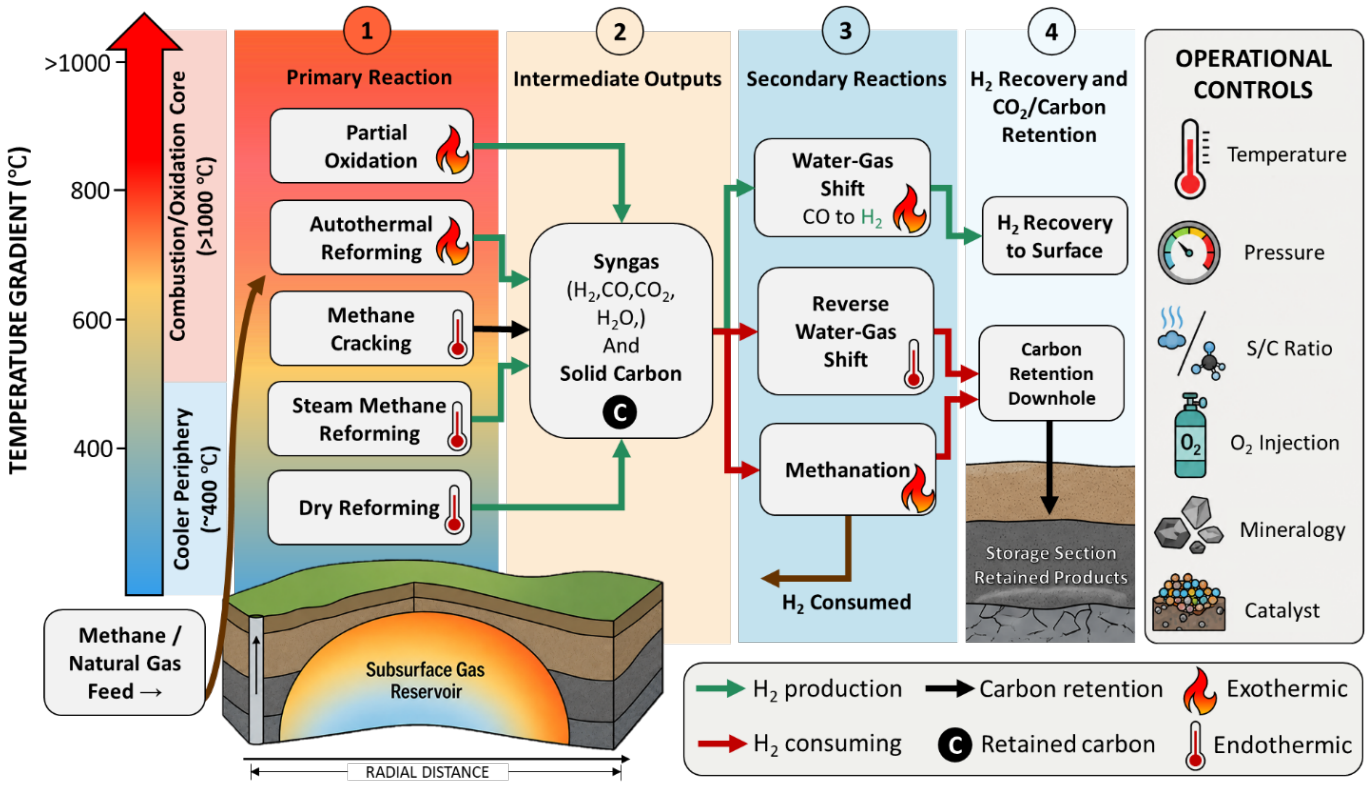

Figure 3. Reaction network for IHP from natural gas reservoirs

in high-temperature reforming environments where carbon management poses analogous challenges to those anticipated in subsurface IHP [56]. The net H_2 yield is therefore controlled by kinetic competition among these reaction pathways.

The central design challenge is not simply to activate methane conversion, but to direct the reaction network toward hydrogen selectivity. Steam-rich conditions favor reforming and WGS reactions, increasing H_2 production and shifting carbon into CO_2. Oxygen-rich conditions generate heat but may over-oxidize methane to CO_2 and water. Steam-deficient conditions may promote methane cracking, producing H_2 and solid carbon, but excessive carbon deposition can block pore throats, foul catalysts, and reduce permeability. Therefore, the reaction pathway selected for gas reservoir IHP must balance hydrogen yield, carbon-retention mode, heat demand, and long-term reservoir deliverability. In surface reactors, these interactions are managed through engineered catalyst beds, controlled heat input, and product separation. However, for subsurface IHP, control is indirect through injection strategy, reservoir characterization, catalyst placement or mineral activation, production management, and real-time monitoring.

3 Transferable concepts from heavy oil IHP to natural gas reservoirs

Heavy oil and bitumen reservoirs provide the most developed analogue for IHP because there are observations that various ISC field pilots in the 1970s to early 2000s accidentally produced hydrogen in produced gas [57]. A summary of these observations is provided by Ifticene et al. [9]. These include reported peak hydrogen concentrations of approximately 14 mol% in the LERC TS-2C project [58], up to 33 mol% in Marguerite Lake [59], about 25 mol% in Wolf Lake [60], 10 mol% in Whitesands [61], and up to 7 mol% in Kerrobert [62]. Consequently, a growing number of laboratory and modelling studies have since deliberately targeted IHP from heavy oil through ISCG, making this one of the most developed sub-domain of subsurface IHP [20, 63, 64]. The body of work on IHP from heavy oil and bitumen reservoirs is now substantial. This accumulated experience contains genuine insights transferable to natural gas reservoirs, but also embeds system-specific concepts that cannot be applicable without modification. This knowledge transfer requires decomposing the heavy oil IHP process into its constituent mechanisms. Therefore, the various insights and how they transfer to application in natural gas are discussed in this section and summarized in Table 3.

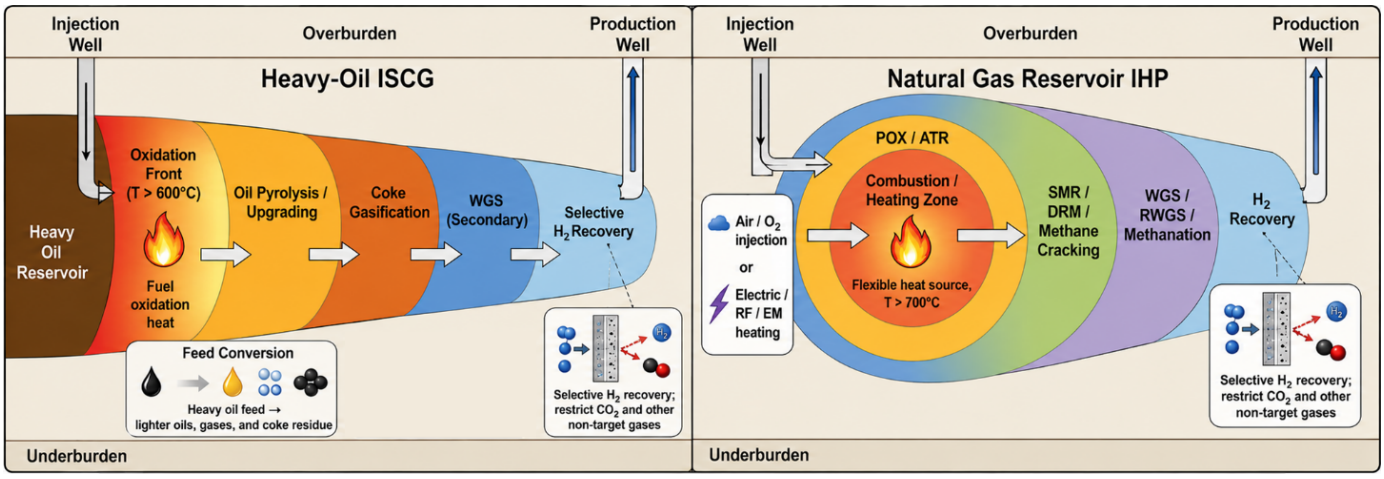

Figure 4. Schematic representation of comparative reaction zones in heavy oil ISCG (left panel) and natural gas reservoir IHP (right panel).

Table 3. Transferability of heavy-oil ISCG lessons to natural gas reservoirs.

Heavy oil IHP lesson	Evidence from heavy oil ISCG	Transferability to gas reservoirs	Required adaptation
Heat-front control	ISC/ISCG generates high-temperature zones	Partly transferable	Gas reservoirs may need alternative heating or limited oxidation
Oxidant management	Wet combustion improves heat transfer and WGS	Highly transferable	Optimize S/C and O/C ratios
Reaction zoning	Oxidation, pyrolysis, gasification, WGS zones	Highly transferable conceptually	Replace oil/coke reactions with methane reforming/cracking pathways
Well configuration	SAGD, THAI, CAGD, horizontal/vertical patterns	Partly transferable	Re-design for H_2 buoyancy and breakthrough risk; dry gas systems have higher flow rates because gas is less viscous and more mobile than heavy oil.
H_2 separation	Downhole membrane or surface separation with reinjection	Highly transferable	Must handle $H_2/CH_4/CO_2/CO/H_2S$ mixtures
Carbon retention	CO_2/coke retained or reinjected underground	Highly transferable	Need gas-reservoir trapping and leakage assessment
Catalyst use	Metal additives and catalytic upgrading	Partly transferable	Catalyst delivery and deactivation differ in gas reservoirs
Oil upgrading	Hydrogen may upgrade heavy oil	Low transferability	Not relevant to dry methane-rich gas reservoirs

3.1 Transferable concepts

The core thermochemical logic of IHP is the same in both settings: an oxidant front generates heat, which drives endothermic reforming reactions, and the combination of steam injection with elevated temperature enables WGS to increase H_2 yield. Okere and Sheng [10] categorise the hydrogen-generating reactions in petroleum reservoirs as primary (aquathermolysis, pyrolysis, and reforming) and secondary (coke gasification and WGS). It is worth noting that the WGS reaction is a universal feature of all IHP settings wherever CO and steam coexist at suitable temperatures. This hierarchy applies equally in a gas reservoir, where SMR followed by WGS remains the dominant H_2-producing sequence once temperatures exceed ~600 °C [17]. This temperature threshold is also consistent with the heavy oil experience.

Additionally, reaction zoning as described in subsection 2.3 is consistent with heavy oil IHP. In

heavy oil ISCG, a sequence of thermal and chemical zones, including oxidation, pyrolysis, cracking, coke formation, coke gasification, steam reforming, and WGS zones is created. Smith et al. [12] describe ISCG as processes involving low-temperature oxidation, pyrolysis, steam gasification, WGS, reforming, and tar cracking, with combustion-front temperatures that can reach approximately 800 °C. This zonal concept is directly useful for natural gas reservoir IHP as illustrated in Figure 4. This is because methane conversion will also occur across spatial gradients rather than at a single uniform temperature [18].

Secondly, operational lessons on oxidant control transfer directly. Oxygen and steam injection must be managed as selectivity controls rather than only as operational inputs. Okere and Sheng [20] showed in SARA-based modelling that oxygen injection yields less hydrogen than air injection in heavy oil ISCG, because excess oxygen drives complete combustion at the expense of partial oxidation and reforming. Hamdy et al. [65] similarly found that increasing steam injection rate from 0.005 to 0.012 m^3/day raised H_2 mole fraction from 0.1% to 42% in heavy oil ISCG simulations, identifying the steam rate as the single most sensitive control variable. The underlying principle—that steam supply governs reforming yield, while O/C ratio governs the combustion–reforming balance—is general and applies to natural gas reservoirs. IHP in natural gas reservoirs, therefore requires careful optimization of O/C ratio and S/C ratios to balance heat generation, hydrogen yield, carbon retention, and hydrogen-consuming reactions.

Furthermore, the role of catalysis as a productivity lever also transfers. Fassihi et al. [66] demonstrated in combustion tube tests with Ni/Mo catalysts that in-situ upgrading of heavy oil produced significant hydrogen volumes through aquathermolysis, thermal cracking, and WGS, and that methanation reactions subsequently consumed a fraction of the H_2 produced. The same catalytic pathway; Ni-based catalyst enabling SMR in the subsurface, is the basis for the natural gas reservoir IHP concept demonstrated by Mukhina et al. [16]. The authors showed that a water-soluble Ni catalyst precursor injected into methane-saturated rock cores produced measurable H_2 at 600–800 °C. The lesson that cheap, earth-abundant catalysts can be delivered in soluble precursor form and activated in situ by thermal conditions is a direct import from the heavy oil catalyst literature.

Pore-scale and wellbore engineering experience also transfers in principle. The observation that coke deposition reduces average porosity by ~22% in oxidised cores, as measured through NMR by Li et al. [67], flags formation damage as a credible risk in any subsurface combustion process. The less severe but analogous risk in gas reservoirs is carbon deposition from methane cracking or Boudouard reactions, which also causes pore-throat occlusion if temperatures and S/C ratios are not controlled [68]. The heavy oil literature's framework for tracking formation damage as a function of mineralogy (clay catalysis of coke deposition, feldspar dissolution) provides a conceptual template, even if the specific mineral – reaction interactions differ.

Moreover, heavy oil ISCG concepts have drawn from Steam-Assisted Gravity Drainage (SAGD), Toe-to-Heel Air Injection (THAI), Combustion-Assisted Gravity Drainage (CAGD), and other thermal recovery configurations. Ifticene et al. [9] discuss reversed SAGD configurations in which injection is placed lower and hydrogen production higher, exploiting hydrogen buoyancy and pressure gradients. The authors further note that THAI configurations can be adapted so that a combustion front advances along a horizontal injector and generated gases migrate toward a producer [9]. These concepts are relevant to natural gas reservoirs because hydrogen is highly mobile and buoyant, and selective recovery will depend on well placement, pressure drawdown, gas segregation, and breakthrough control; experience from underground hydrogen operations shows that these parameters are equally critical for managing hydrogen migration and containment in porous formations [69, 70]. However, in gas reservoirs, mobility ratios, gas-phase mixing, and the risk of oxygen or steam breakthrough may differ substantially from heavy oil systems. Therefore, heavy oil well configurations can be used as design analogues, not direct templates.

Finally, simultaneous H_2 recovery and carbon retention in heavy oil ISCG is achieved in two possible ways. This is achieved either by surface separation and reinjection of undesired gases on-site, or by selective production through downhole membranes [9]. For natural gas reservoirs, this lesson is critical because hydrogen generation alone is not sufficient; the technology must also prevent excessive production of CO_2, CO, residual methane, H_2S, and steam if the product is to meet downstream requirements.

3.2 Concepts that require modification

The single most important structural difference between heavy oil and gas-reservoir IHP is the nature and availability of the solid fuel that sustains the combustion front. In heavy oil ISCG, the process depends critically on the deposition of coke from thermally cracked asphaltenes, resins, and aromatic fractions ahead of the combustion front. Lin et al. [71] established through combustion tube simulation that fuel deposition mechanism, fuel composition, and the locations of transient zones depend directly on crude oil and reservoir rock properties. The K-values of light oil components and cracking kinetics are the dominant parameters controlling fuel availability [71]. None of these parameters exist in a gas reservoir: methane has no distillation K-values and does not crack to coke at practical ISC temperatures. Furthermore, Hascakir et al. [72] showed through CT-imaging and post-mortem XPS analysis of 9–12 °API crudes that the quantity, reactivity, and spatial distribution of this coke, shaped by API gravity, clay mineralogy, and cracking kinetics, determines whether the front is stable and self-sustaining. Therefore, a gas reservoir has no analogue of the coke-banking mechanism that is central to heavy oil ISC front propagation and H_2 yield. Additionally, the front-stability models developed for heavy oil ISC and the kinetic parameters calibrated against ramped-temperature oxidation (RTO) tests of bitumen and heavy crude [73–75], cannot be transferred to natural gas systems without comprehensive re-parameterization.

The thermal budget also differs fundamentally. In heavy oil ISCG, the heat released by coke combustion is large and spatially concentrated, generating peak front temperatures often exceeding 600–700 °C from the exothermic coke oxidation alone [57]. Kapadia et al. [76], simulating Athabasca bitumen ISC, identified temperature as the primary lever for H_2 yield, with a maximum of ~28 mol% H_2 achievable at ~735 °C. In a dry natural gas reservoir, no coke inventory is pre-deposited; the heat must come entirely from the combustion of methane itself. This is a gaseous oxidation with very different flame stability and spatial distribution of generated heat. Sustaining the >600 °C front temperatures required for SMR in a gas reservoir demands continuous methane combustion, which competes directly with the reforming reactions. This type of competition does not arise in the same way in heavy oil because the coke provides heat independently of the hydrocarbon fraction undergoing reforming.

It is also worth highlighting that, due to compositional differences, some reaction pathways are unique to heavy oil and bitumen. Song et al. [57] confirmed that in bitumen ISCG, H_2 generation is dominated by coke gasification and WGS reactions at low and high temperatures, respectively. Coke acts as both a stored fuel inventory and a direct H_2 precursor via gasification. Furthermore, aquathermolysis, is a reaction pathway unique to heavy oil. In this pathway, steam hydrolyses sulphide bonds and cleaves C–S and C–C linkages in asphaltenes at relatively low temperatures (200–300 °C) to produce H_2 and lighter hydrocarbons [10], yet has no analogue in methane. This implies that practical modelling frameworks developed for heavy-oil IHP are also not transferable without restructuring. For example, Okere and Sheng [20] developed a novel numerical model based on SARA saturates, aromatics, resins, asphaltenes (SARA) hydrocarbon characterization for ISCG in heavy oil. The SARA framework is not applicable to a single-component methane system. Gas reservoir IHP models must instead be built around gas phase combustion kinetics, SMR/DRM/WGS equilibria, and methane cracking, as demonstrated by Askarova et al. [77].

4 State of the art: Experimental and Simulation studies

Inspired by the progress in research on IHP from heavy oil and bitumen, various studies have been conducted to extend this concept to natural gas reservoirs. These studies include experimental investigations and modeling studies. In this section these studies are critically reviewed to draw insight on common trends and contradictions reported and identify existing knowledge gaps. A summary of these studies is presented in Table 5.

4.1 Experimental studies

The experimental designs used across recent studies on IHP vary substantially depending on the process objective, operational scale, and intended field representation. These setups include customized autoclaves or combustion tubes used as the reactor with other accessories depending on mode of operation. These setups are operated in either static or dynamic mode. Each configuration and mode of operation offers specific insights into the thermal, catalytic, and geological aspects of hydrogen generation but also comes with trade-offs in control precision, realism, and scalability.

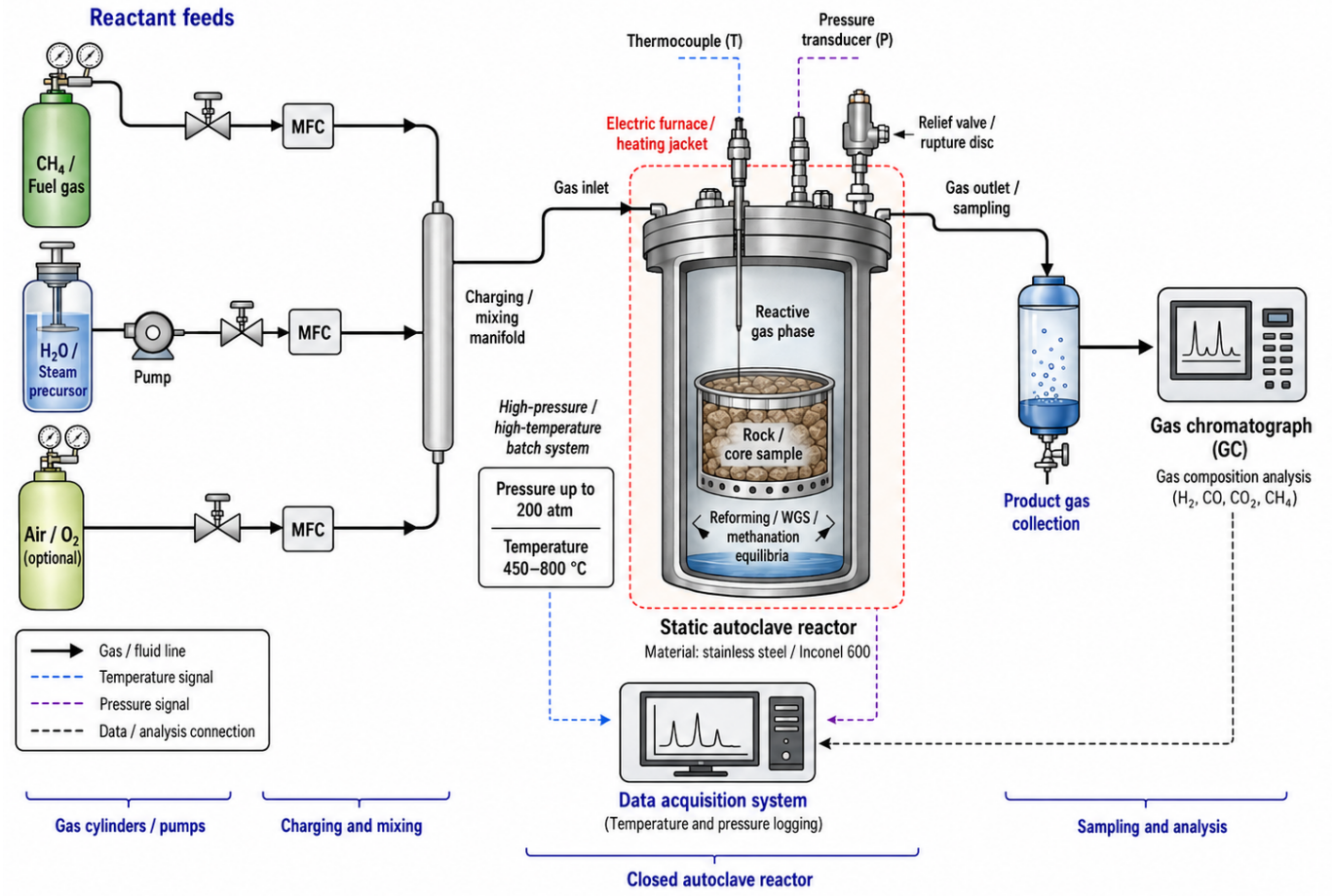

Figure 5. Schematic diagram of static experimental setup for IHP in gas reservoirs.

Static autoclave systems were employed in several foundational studies [14, 19, 55, 78], designed primarily to replicate the closed high-pressure and high-temperature environment of a subsurface gas reservoir. These reactors, example shown in Figure 5, are typically made of different materials (like stainless steel, Inconel 600 alloy etc.) depending on the required pressure and temperature rating. They are equipped with gas inlets and outlets, thermocouples, and pressure transducers to simulate reservoir pressures (up to 200 atm) and temperatures (450–800 °C). They enable precise control of reactant composition (CH_4, H_2O, O_2/air) and S/C ratios, allowing detailed evaluation of reforming, WGS, and methanation equilibria.

The reported studies that used static experimental setups focused on replicating reservoir confinement and reaction equilibria for hydrogen synthesis under controlled high-pressure and temperature conditions. Afanasev et al. [19] employed an Inconel autoclave reactor to perform catalytic methane conversion tests using real core and inert materials at 300–450 °C and up to 207 atm. They demonstrated H_2 generation onset at $\geq$ 450 °C and confirmed the feasibility of catalytic methane conversion in static gas–liquid environments. Afanasev et al. [78] used the same autoclave in a batch configuration at 450 °C and 9 MPa. They reported H_2 production of 0.7 mol% in natural cores with high CO_2 concentration. Rui et al. [55] used a high-pressure static reactor (max 400 bar, 600 °C) packed with field debris to simulate gas-reservoir conditions under pseudo-static operation. They reported a H_2 fraction of 26.6 % at 600 °C and showed that debris minerals promote POX and ATR. Recently, Tackie-Otoo et al. [14] used a custom static autoclave reactor (1200 psi, 200 °C) with natural-gas mixtures to validate in-situ H_2 generation under realistic reservoir compositions.

Dynamic systems (example shown in Figure 6) such as combustion tubes, flow reactors, and reforming furnaces replicate continuous subsurface gas flow and reactive transport conditions, allowing realistic assessment of H_2 synthesis through SMR and ISC mechanisms. Various studies used such setups to investigate coupled thermal oxidation and reforming mechanisms in core packs or synthetic rock media [16, 17, 77–79]. These reactors generally include injection

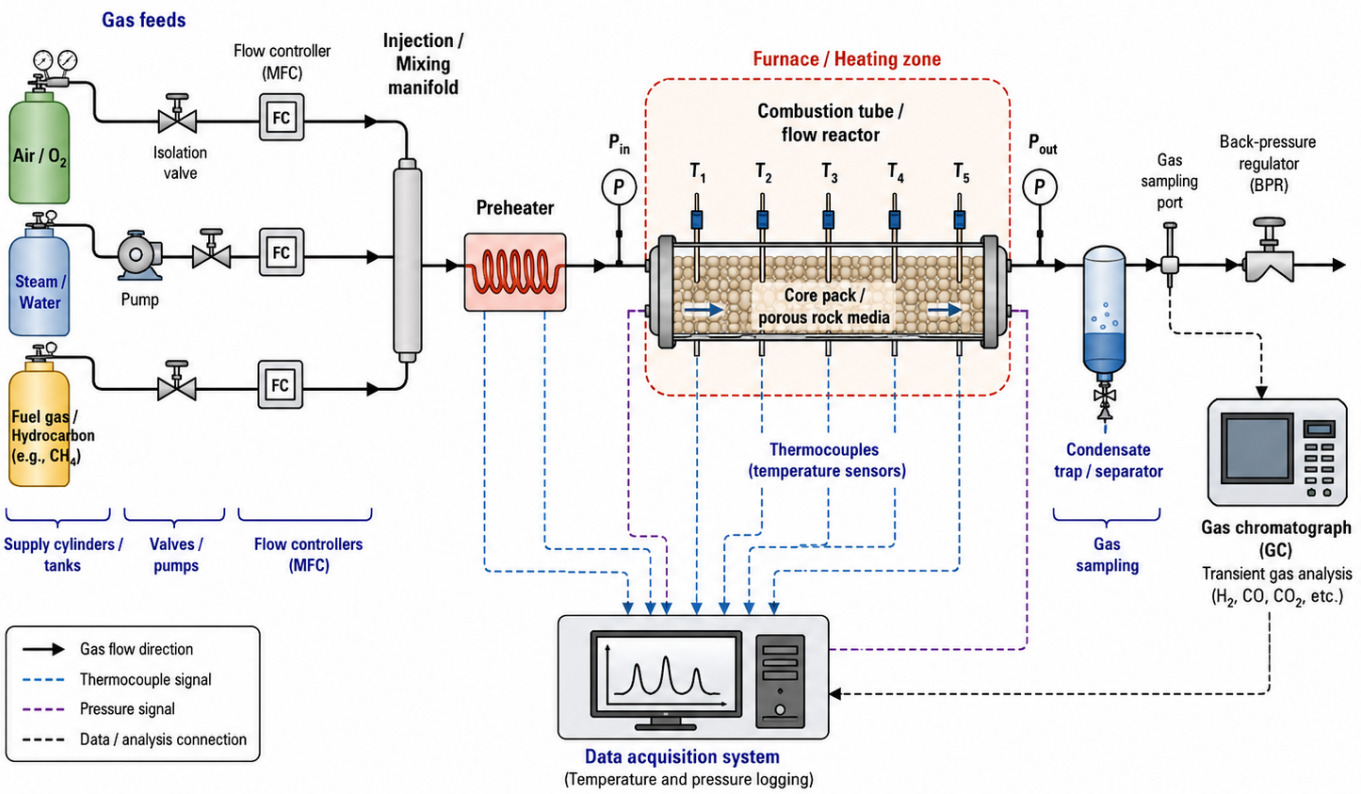

Figure 6. A schematic diagram of dynamic experimental setup for IHP studies.

Table 4. Comparison of experimental setups for in-situ hydrogen production studies.

Setup type	Strengths	Limitations
Static autoclave	Enables precise control of process variables (temperature, pressure, S/C ratio). Allows direct simulation of reservoir confinement and compositional equilibria. Suitable for screening catalyst performance and assessing thermodynamic feasibility. Safe and relatively low-cost for early-stage studies.	Lacks flow dynamics, limiting its representation of actual reservoir displacement processes. The reaction is batch-type, making it difficult to simulate continuous feed and product withdrawal. Heat and mass transfer gradients within the reactor can result in non-uniform temperature fields. Scale-up to reservoir conditions requires additional validation in dynamic systems.
Dynamic flow reactor and combustion tube	Provides continuous flow conditions, closely representing reservoir displacement and ISC phenomena. Captures temperature and reaction fronts relevant to large-scale in-situ combustion or steam flooding. Enables real-time gas monitoring and transient analysis of product distribution. Better suited for scale-up and kinetic model validation.	More complex and costly than batch systems, requiring multiple safety and control elements. Limited to short experimental durations due to heating element and reactor material constraints. Difficult to achieve uniform temperature control across the reactor length. Experimental reproducibility is lower due to natural heterogeneity in rock or catalyst packing.

manifolds for air, oxygen, or steam; temperature sensors distributed along the length; and gas sampling outlets for analyzing transient H_2, CO, and CO_2 compositions. The dynamic setup offers the most realistic representation of reservoir processes, allowing detailed observation and detection of fluctuations or instabilities in gas composition [16].

Afanasev et al. [17, 78] deployed flow-reactor to

study H_2 synthesis under reservoir-like conditions ($\geq$ 800 °C, 3 – 9 MPa), initially focusing on reservoir pressure regime and rock mineral impact, then on temperature, S/C ratio and rock–catalyst interactions. Similarly, Mukhina et al. [16] used this dynamic flow reactor operating up to 800 °C and 8 MPa with real and inert porous media to simulate methane–steam interaction in gas reservoirs. This configuration provided direct control over S/C ratios and enabled continuous monitoring of gas composition through gas chromatography. The setup simulated the migration of combustion fronts and gas-phase reforming dynamics in porous media. Askarova et al. [77] extended the approach by employing a medium-pressure combustion tube (MPCT) that allowed simultaneous injection of methane, air, steam, and catalysts to reproduce ISC-assisted SMR, capturing transient reaction fronts and validating the process through coupled kinetic and numerical models. Alekhina et al. [79] further integrated dual-stage flow and combustion experiments, comparing industrial Ni/Al_2O_3 and in-situ synthesized Ni catalysts under dynamic conditions, confirming superior H_2 yield (~ 48 vol%) and better stability for in-situ-synthesized catalysts.

The absence of flow in static setups limits their ability to capture reaction front propagation, mass transfer, and transient gas evolution. Dynamic systems address these limitations but are more complex, costly, and difficult to stabilize or reproduce because of heterogeneous flow paths and thermal variations. The strengths and limitations of both configurations are presented in Table 4.

4.2 Modeling and simulation studies

IHP in natural gas reservoirs is a complex, multi-phase process that requires careful consideration of numerous factors, including reservoir selection, well configuration, injection strategy, and the composition and rate of oxidant injection. An effective IHP model should be capable of predicting critical aspects of the process, such as:

- the composition and yield of the produced syngas,
- the temperature and pressure distribution within the reservoir,
- the advancement of the combustion or reforming front,
- the interaction between gaseous products and the rock matrix, and
- the extent of subsurface CO_2 retention and associated geochemical transformations.

Given the wide range of physicochemical phenomena occurring during IHP; combustion, reforming, heat transfer, diffusion, and mineral interactions, no single model can fully capture all processes with complete fidelity. Each modeling approach represents an approximation of reality that focuses on specific elements of the system. It is well recognized that IHP must be optimized to achieve high hydrogen purity while minimizing undesirable by-products such as CO, CO_2, and CH_4. Achieving this balance is challenging because product composition depends on multiple interrelated parameters: the O/C and S/C ratios, reservoir temperature and pressure, the catalytic properties of the formation, and the flow behavior of injected gases. Assessing the relative importance of these parameters is particularly difficult, as a condition that enhances one reaction pathway (e.g., steam reforming) may suppress another (e.g., WGS or methanation). Various modeling approaches have therefore been developed to analyze different facets of the IHP process. These models differ in their level of physical detail, computational demand, and the type of data required. Broadly, they can be classified into equilibrium models, kinetic models, and computational fluid dynamics (CFD) models. More recent developments have incorporated coupled frameworks that integrate multiple modeling strategies to provide a holistic representation of the IHP process [80–82].

4.2.1 Equilibrium models

Equilibrium models use chemical thermodynamics to predict reaction outcomes assuming all reactions proceed to an equilibrium state. This means either the chemical reactions occur at an infinitely fast rate or the reaction time is sufficiently long for equilibrium to be established [82]. Therefore, equilibrium models do not track time-dependent behavior; instead, they predict the ultimate yields of hydrogen and other products if the system reaches thermodynamic equilibrium. These models typically fall into two broad classes, distinguished by how the equilibrium state is formulated and by the inputs they require. There is a stoichiometric (reaction-set) approach that specifies a set of reactions and uses the law of mass action with equilibrium constants to compute the final composition. Then there is the non-stoichiometric (Gibbs minimization) approach that does not predefine reactions; instead, it determines the stable mixture by minimizing the

system's total Gibbs free energy subject to elemental balance constraints. The details on these models and equations that define the hydrogen production process can be found in [81, 82].

Equilibrium models offer several advantages for simulating IHP in natural gas reservoirs. They enable a rapid estimation of the maximum theoretical hydrogen yield and the thermodynamic feasibility of reactions under reservoir conditions [80]. Therefore, they are particularly useful for preliminary screening of operational parameters such as temperature, pressure, and S/C ratio. Computationally, these models are relatively simple since they rely on algebraic equations derived from thermodynamic relationships rather than on complex, time-dependent differential equations [83]. Since kinetic models rely on system-specific parameters, equilibrium models provide a more universal approach, requiring only basic thermodynamic data like enthalpy and entropy and avoiding uncertainties tied to reactor design or kinetic assumptions [81, 83].

However, equilibrium models possess notable limitations when applied to IHP in natural gas reservoirs. These models are zero-dimensional, do not consider reactor geometry, and typically disregard heat losses, assuming the system to be perfectly adiabatic and thermally isolated from its surroundings [82]. They provide no information on reaction kinetics or rates, as they inherently assume infinitely fast reactions and complete mixing [81]. Moreover, equilibrium models disregard transport phenomena and spatial gradients such as variations in temperature, pressure, reactant flow, and catalyst distribution which are intrinsic to heterogeneous reservoir environments [18]. They provide only a single steady-state solution and cannot capture time-dependent processes like combustion followed by reforming unless each stage is modeled separately [80]. Furthermore, thermodynamic equilibrium analysis of methanation reactions has demonstrated that equilibrium composition is strongly sensitive to temperature and pressure—a sensitivity that makes CO and CO_2 methanation particularly difficult to suppress under subsurface confinement conditions [84].

Equilibrium models have been deployed in the investigation of IHP in natural gas reservoir for various purposes. Afanasev et al. [19] employed equilibrium modeling as a thermodynamic foundation to guide and interpret the experimental study on IHP within natural gas reservoirs. The equilibrium model, based on SMR and the WGS reactions, was used to calculate the theoretical limits of methane conversion and product gas composition. The authors reported that the model overestimated methane conversion. Similarly, Rui et al. [55] applied thermodynamic equilibrium calculations to a depleted gas reservoir scenario to estimate hydrogen generation potential. Using the principle of minimum Gibbs energy, they computed methane conversion and hydrogen yield for reactions like POX and ATR at various operating parameters. Their findings identified the thermodynamic requirements (high temperature, sufficient steam) for IHP before any kinetic or field modeling. Ikpeka and Ugwu [85] developed an equilibrium-based model by solving a set of nonlinear equations for four key hydrogen-forming reactions (SMR, POX, ATR, and pyrolysis). The equilibrium analysis (via Gibbs free energy minimization) was used to screen reaction feasibility and optimal conditions. The equilibrium results then guided the implementation of a numerical reservoir model in that study.

4.2.2 *Kinetic model*

Kinetic models incorporate the rates of chemical reactions and are typically formulated as ordinary or partial differential equations coupling reaction kinetics with mass and heat balance [80]. They define a network of reactions (with rate laws and parameters like activation energies and frequency factors) to simulate how hydrogen is generated over time in the reservoir [77]. In the context of IHP, kinetic models often include reactions for fuel combustion (to provide heat) and reactions for hydrogen generation (SMR, WGS, methane cracking, etc.), each with specific rate equations [77, 80]. These models can be implemented in reservoir simulators as reported by Askarova et al. [77, 86] or process simulations, solving transient changes in species concentrations, temperature, and flows. The mathematical approach involves integrating coupled differential equations representing conservation of mass and energy along with Arrhenius kinetic rate expressions [80].

Kinetic models offer a dynamic and realistic framework for simulating IHP in natural gas reservoirs. Unlike equilibrium models, they capture the temporal evolution of chemical reactions, thereby providing information on reaction mechanisms, intermediate states and impacts of various reaction conditions; such time-resolved modelling approaches have proven essential in subsurface gasification contexts where

transient reaction fronts and coupled transport phenomena cannot be represented by equilibrium assumptions [87]. By explicitly accounting for reaction rates, they naturally incorporate incomplete conversions and competing side reactions such as methanation or coking, thereby aligning closely with experimental observations [86]. Integrated within reservoir simulators or CFD tools, kinetic models also couple chemical reactions with transport processes like heat and mass flow through porous media, reflecting the influence of heterogeneity and well configurations on hydrogen yield [88]. Once validated, they serve as powerful sensitivity tools, allowing systematic assessment of how operational parameters such as injection rate, steam fraction, and oxygen dosage affect overall hydrogen production efficiency and reservoir performance.

Despite their strengths, kinetic models present several challenges when applied to IHP. They rely on detailed reaction mechanisms and rate constants, making them computationally expensive [81]. There is also large variability in kinetic parameters reported across different studies, and these parameters are often poorly defined under reservoir conditions such as high pressures, mineral interactions, and heterogeneous pore structures; this challenge is well documented in subsurface reactive systems where kinetic data calibrated under one set of conditions frequently fail to transfer to different geological settings [18, 87]. Developing and calibrating these models requires extensive experimental data, and each kinetic framework must often be revalidated for different catalysts or reservoir types. Finally, translating laboratory-calibrated kinetics to field-scale applications remains difficult due to scaling effects, heat and mass transfer limitations, and uneven catalyst distribution, all of which can reduce predictive accuracy unless transport processes are carefully integrated into the modeling framework.

Various studies on IHP in natural gas reservoirs have been based on kinetic models mostly coupled with reservoir simulation [77, 86, 88, 89]. Askarova et al. [86] developed a detailed kinetic reaction model to simulate IHP in a gas reservoir context. Their model included ISC reactions for liquid hydrocarbon (to generate heat) coupled with methane conversion reactions (SMR and related reactions to produce H_2). Using a thermal reservoir simulator, they numerically replicated a laboratory combustion-tube experiment, capturing hydrogen production during the combustion stage. The kinetic simulation was able to reproduce key features of the experiment, and it helped identify that secondary reactions were consuming hydrogen (leading to lower yields than ideal), validating the principle of the IHP process and providing a tool to optimize hydrogen generation conditions. Ikpeka et al. [88] applied a kinetic ISC model (based on their earlier equilibrium study [85]) in a series of parametric reservoir simulations. By integrating their reaction network into a reservoir model, they studied the effect of various reservoir and well parameters on hydrogen output. This kinetic-based simulation approach enabled optimization of conditions, demonstrating how certain reservoir properties and operational strategies improve hydrogen yields.

4.2.3 Process simulation versus CFD models

Once a mathematical model for a specific hydrogen production system has been developed and validated, it can be employed to predict, simulate, or optimize the system's performance under various operating conditions. However, when modeling an entire process flowsheet, often comprising hundreds of variables and equations, the complexity can become prohibitive [80]. In such cases, process simulators offer an efficient alternative, allowing rapid evaluation of process behavior across different scenarios with minimal computational effort. These simulators are built upon embedded mathematical frameworks; the user's role is primarily to construct the process flowsheet, define interconnections among unit operations, and supply the necessary input data for simulation and performance analysis.

Process simulation can be carried out under either steady-state or transient conditions. In steady-state simulation, temporal variations in process variables are neglected, assuming that the system has reached equilibrium, whereas transient simulation incorporates time-dependent behavior by including accumulation terms in the mass, energy, and momentum balance equations. The dynamic approach provides a more realistic representation of process behavior over time, making it particularly valuable for analyzing transient phenomena and developing effective process control strategies. A range of steady-state simulators such as Aspen Plus, HYSYS, and ChemCAD are widely used for modeling hydrogen production processes. Tackie-Otoo et al. [14] deployed HYSYS to study IHP in natural gas reservoirs, and further deployed equilibrium and kinetic models using Aspen Plus [18]. These models gave acceptable predictions of produced

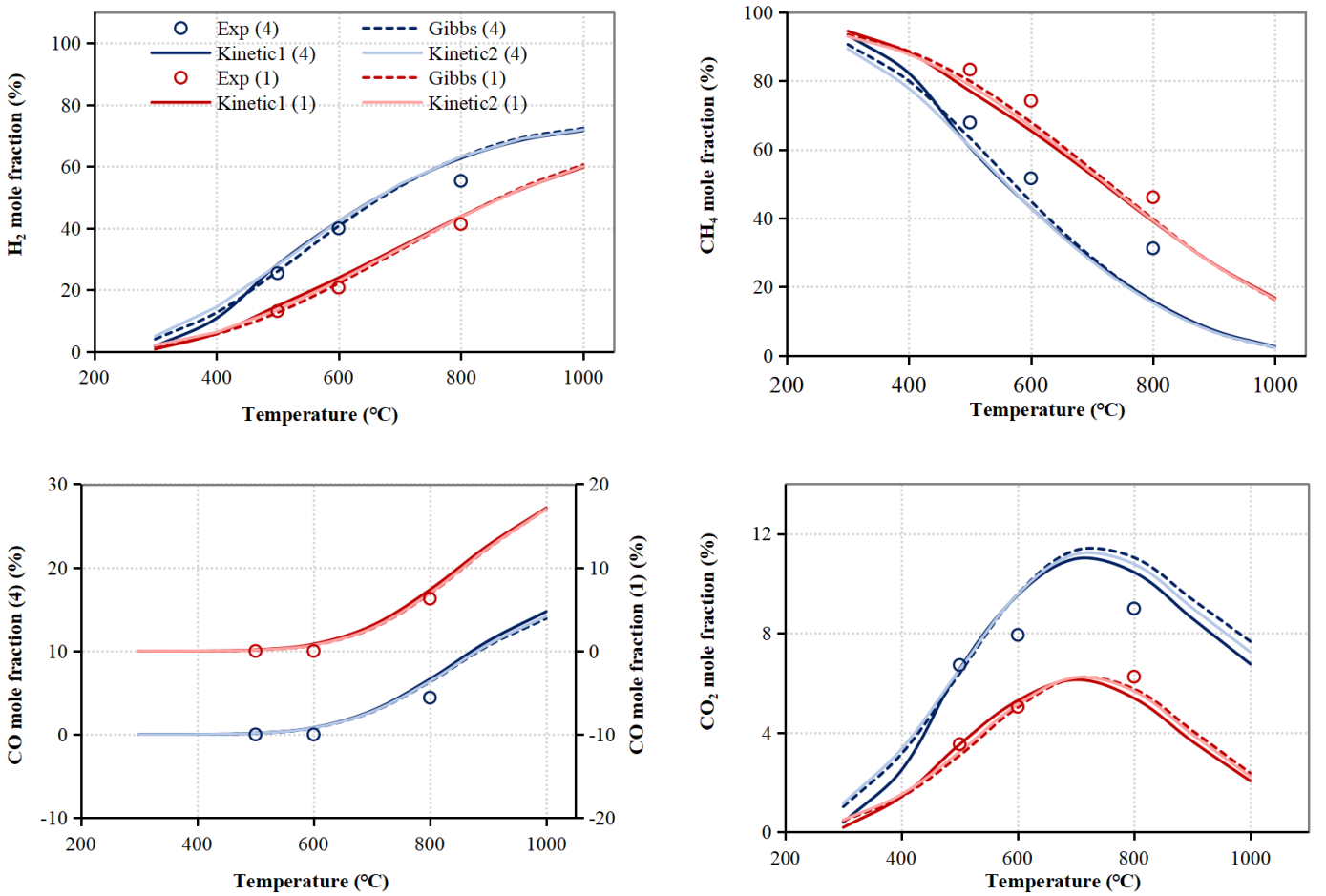

Figure 7. Produced gas mole percentages (dry basis) match for process simulation (Gibbs and Kinetic) by Tackie-Otoo et al. [18] and experimental data (Exp) from Mukhina et al. [16].

gas composition from experiments conducted by Mukhina et al. [16] as shown in Figure 7. For transient simulations, tools like MATLAB, ANSYS Fluent, ANSYS CFX, and CFD2000 are commonly employed to capture the real-time response and interactions within complex reacting systems [80].

On the other hand, CFD models solve the detailed transport equations for fluid flow, heat transfer, and chemical reactions in a continuum. In the context of IHP, CFD can refer to high-fidelity simulations of the reacting flow either in the porous reservoir (using a Darcy-flow based approach) or in experimental reactors (using Navier–Stokes equations for flow in reactors or near-well regions). These models discretize the spatial domain into a fine grid and compute profiles of velocity, pressure, temperature, and species concentrations by solving the governing partial differential equations (conservation of mass, momentum, energy, and species) coupled with reaction kinetics; this computational framework has been applied to model reactive flow in porous geological media, providing a structural template for the CFD representation of subsurface conversion processes [87]. In practice, reservoir simulators like CMG STARS or Eclipse are specialized forms of CFD for porous media (using Darcy's law for flow), solving multi-component fluid flow and heat transport with reactions on a grid representing the reservoir [88]. Alternatively, general CFD software (ANSYS Fluent, COMSOL, etc.) can be used to simulate smaller-scale processes (e.g. flow through a catalyst-packed reactor or near-wellbore combustion) with detailed physics [80].

Various IHP studies used reservoir simulation (a form of CFD for porous flow) to model the process. Ikpeka and Ugwu [85] validated their hydrogen production model by implementing it in CMG STARS, a commercial thermal reservoir simulator. STARS solved the coupled 1D flow of fluids, heat, and reaction kinetics along a reservoir grid, effectively acting as a CFD tool to predict hydrogen output, and the simulator's results closely matched the custom equilibrium model's predictions when run under the same conditions. Similarly, Askarova et al. [86]

used a 1D reactor model in a simulator to reproduce their combustion tube experiment, calculating detailed temperature profiles and gas compositions along the core length. This shows how CFD modeling in porous media can be used to design and interpret in-situ combustion and reforming processes.

While currently not used in IHP studies, validated CFD models of methane–steam reactive flow through catalyst-packed beds demonstrate that such tools can resolve local temperature gradients, species concentration profiles, and mass transfer limitations at the reactor scale [90, 91]. For instance, one could use Fluent or COMSOL to model the flow of methane, steam, and oxygen through a catalyst-packed core plug to investigate mixing and reaction at the pore-to-core scale. Such an approach would capture effects like local heat spots or mass transfer limitations around catalyst particles that bulk reservoir models might average out. The insights from these CFD studies complement reservoir-scale models by identifying, for example, regions that may run cooler or flow paths that bypass certain zones, which can then be addressed by adjusting the field design (injector placement, injection rate, etc.).

4.3 Effect of operating conditions

As established already, the suite of thermochemical reactions that occur during IHP in natural gas reservoirs proceed differently depending on the prevailing reservoir conditions. Therefore, reaction selectivity can be controlled by managing these conditions. The various works reported in the literature have investigated the impacts of these operating conditions to identify thresholds and optimal conditions to improve selectivity towards hydrogen production. The various findings reported are discussed in this subsection.

4.3.1 Temperature effect on IHP process

Temperature is the main control on H_2 production. The various endothermic H_2 production reactions require high temperatures to proceed at meaningful rates. Experimental works under simulated gas reservoir conditions have confirmed this trend though their identified thresholds vary (Figure 8). Afanasev et al. [19] found little to no H_2 generated below 450 °C, with experiments at 300 °C yielding only trace hydrogen. Hydrogen generation became observable only at 450 °C or above (e.g. ~5.8% CH_4 conversion at 450 °C) [19]. Subsequent works raised this minimum: Afanasev et al. [78] concluded that "temperature higher than 550 °C" is required to convert meaningful amounts of methane. Rui et al. [55] likewise determined the reservoir temperature should not be lower than 600 °C for IHP. Consistently, Afanasev et al. [17] observed effectively no hydrogen at 500 °C, but substantial yields once $\geq$ 600 °C; in their tests. Raising the temperature from 600 °C to 800 °C boosted the H_2 concentration to ~40% [17]. Mukhina et al. [16] explicitly recommend avoiding low temperatures, noting that optimal yields occur at ~800 °C, whereas 400 °C was insufficient.

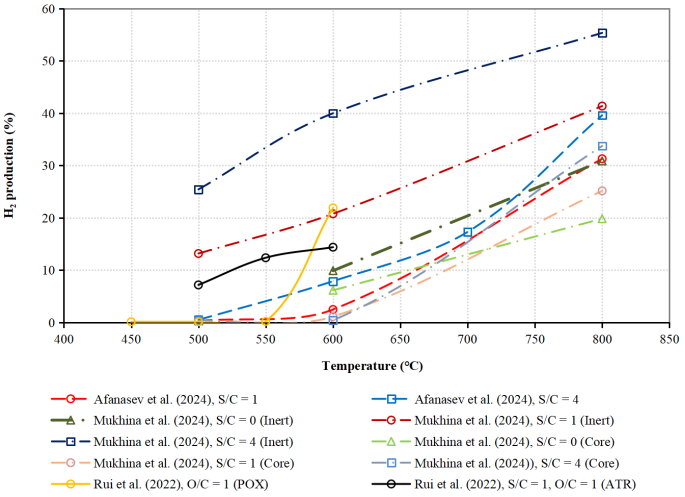

Figure 8. H_2 production against temperature for various IHP in natural gas studies. Data from [16, 17, 55]

While higher temperatures drive the endothermic SMR and methane cracking reactions to the right, low-temperature operation can limit conversion and favor hydrogen-consuming side reactions. A clear example is reported by Tackie-Otoo et al. [14], where process simulations predicted substantial H_2 generation through SMR and WGS at a reservoir temperature of 200 °C. However, experiments conducted under similar conditions produced only trace amounts of H_2. This discrepancy is mainly due to the use of a stoichiometric equilibrium model that excluded the methanation reaction. The observed increase in methane mole fraction in the experimental produced gas suggests that limited H_2 formation at low temperature was further offset by H_2 consumption via methanation Tackie-Otoo et al. [14]. This interpretation was later confirmed by the authors using a non-stoichiometric equilibrium model [18]. In general, H_2 fraction and methane conversion rise steeply with temperature. Afanasev et al. [78] reported H_2 concentrations reaching 70.8% in an inert porous medium at 800 °C. Similarly, Mukhina et al. [16] saw H_2 increase from ~0% at 400 °C to >40% at 800 °C.

The optimal temperature range identified across these works is broadly 600 – 800 °C, with some authors suggesting that even higher temperatures, if achievable in situ, could further enhance H_2 yield [16, 19]. Nevertheless, it is worth noting that higher temperatures also favour RWGS which consumes produced H_2 [68]. Furthermore, lower temperatures not only gave low conversions, but also led to unfavorable reaction pathways. For instance, Askarova et al. [77] observed that a 450 °C wet-combustion stage produced only ~0.2% H_2 (dry gas) while releasing an "abnormally high" CO_2 fraction from carbonate breakdown. This observation indicates that at insufficient temperature the rock/mineral reactions (CO_2 release) and H_2-consuming side reactions dominate. These studies therefore show that attaining very high reservoir temperatures through superheated steam injection, ISC, or related methods is a key design criterion for IHP.

4.3.2 *Pressure effect on IHP process*

Pressure introduces an important thermodynamic constraint. Many hydrogen-forming reforming reactions increase the total number of gas moles – conditions which Le Chatelier's principle disfavors at high pressure [92]. Therefore, H_2 production is less favored at high pressure as reported by various studies. Afanasev et al. [19] explicitly showed via equilibrium calculations that highest methane conversions are attainable at low pressures (Figure 9(a)). Similar Tackie-Otoo et al. [18] also reported decreasing H_2 purity with pressure for different natural gas compositions (Figure 9(b)). Afanasev et al. [19] reported that at 800 °C the CH_4 conversion drops from ~100% at 1 atm (0.1 MPa) to <60% at 100 atm (10 MPa). They noted, however, that such low-pressure conditions are *not* practically achievable in situ. Gas reservoirs are inherently high-pressure systems, and steam injections tend to pressurize the formation [19]. Consequently, their experiments were conducted at pressures up to 100–200 atm, where conversion was much lower.

In a subsequent study, the effect of pressure reduction in depleted gas reservoirs was investigated. Afanasev et al. [78] compared experiments conducted at 9 MPa and 3 MPa. However, because temperature was varied in the opposite direction, the isolated effect of pressure may have been masked. Askarova et al. [86], however, directly demonstrated this trend within a single experiment by depressurizing the system from 8.9 MPa to 2.2 MPa while maintaining a constant temperature of 550 °C. Methane conversion increased

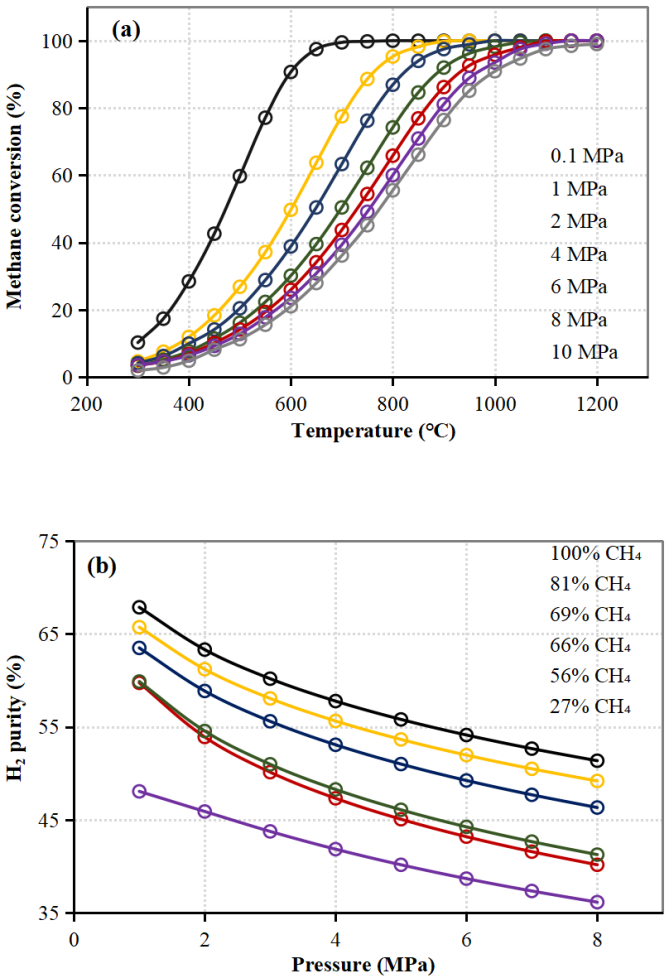

Figure 9. (a) Methane conversion at different temperature and pressure [19] and (b) H_2 purity variation with pressure for various natural gas compositions [18].

from ~21.6% to 35.3%, resulting in a corresponding increase in hydrogen generation, as shown in Figure 10. These findings agree that high reservoir pressure inhibits the forward H_2-producing reactions, and that utilizing a depleted reservoir (with lower pressure) or creating pressure drawdown in situ can boost H_2 yields.

Pressure also influences the product composition and reaction pathways. Several studies found that at high pressure, certain side reactions become more prominent. Afanasev et al. [19] observed that in their highest-pressure runs (up to 207 atm in a core-filled reactor), a considerable amount of CO_2 and heavier hydrocarbons (C_2–C_5) were produced alongside H_2. In one core experiment, the CO_2 fraction reached 47.7 mol% – notably higher than the equilibrium CO_2 predicted by SMR chemistry alone [19]. Ethane, ethylene and propane appeared in other high-pressure runs (trace ~0.5–1 %) – an "interesting" finding since pure methane was used. This is attributed

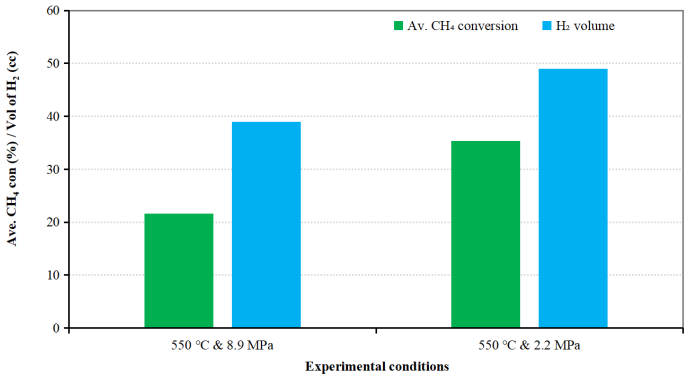

Figure 10. Methane conversion at different experimental conditions showing the impact of pressure. Data extracted from Askarova et al. [86].

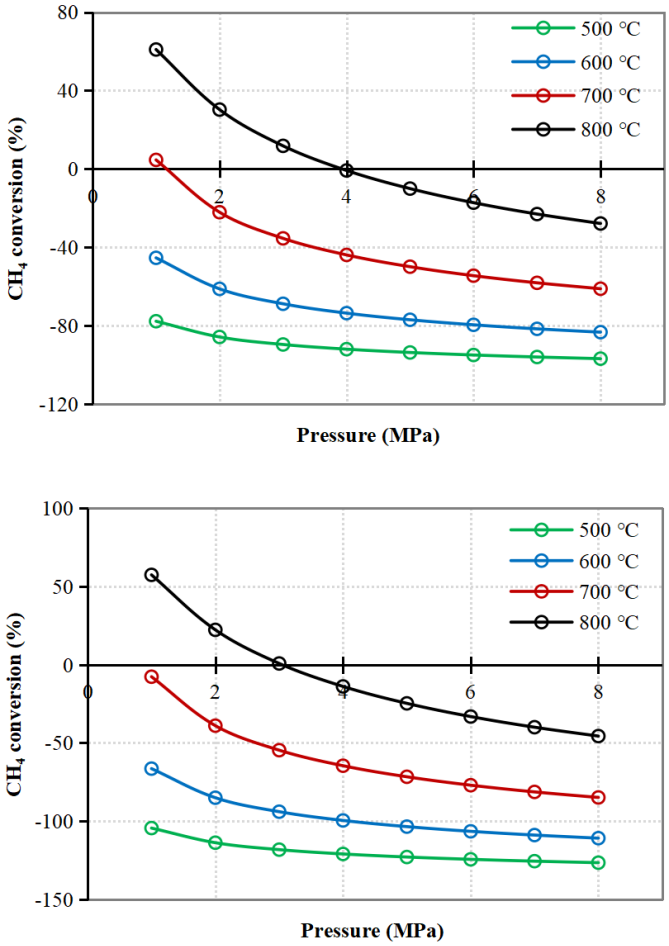

Figure 11. Impact of pressure on methane conversion at various temperatures for (a) 8.5% ethane and 14.5% propane composition and (b) 18% ethane and 9.8% propane composition. Data from [18].

to pyrolysis with subsequent hydrogenation to yield light hydrocarbons promoted by catalyst at high pressure. Askarova et al. [86] found that at 8.9 MPa, oil-driven combustion produced by-products and secondary reactions (hydrogenation of cracked oil, reverse WGS) that consumed H_2, leaving a low H_2 yield despite appreciable methane conversion. High pressure also promotes methanation [18]. At 600 °C, increasing pressure from 2 to 10 MPa raises the equilibrium product-to-reactant mole fraction ratio for CO methanation by a factor of 25 under ideal gas conditions. Consistent with this effect, simulations showed negative methane conversion only at elevated ethane and propane fractions, with the effect becoming stronger at higher pressure and lower temperature (Figure 11; see Section 4.4).

In summary, high pressure tends to shift the system toward methane and heavier molecules, unless temperature is high enough to overcome this. One silver lining is that high pressure helps retain CO_2 in the reservoir (as a supercritical phase, for sequestration). Several studies note that CO_2 produced in situ will stay downhole under pressure, while H_2 (being light) will preferentially migrate to producers [55]. This means that although high pressure adversely affects H_2 generation, it aids the sequestration of the undesirable byproduct (CO_2), which is a goal of the IHP concept. The consensus is that for maximizing H_2, if operating at high pressure, then other parameters (temperature, steam, catalyst) must be optimized to counteract the equilibrium shift. Employing catalysts tailored to high-pressure conditions (to avoid methanation catalysis) could mitigate H_2 losses at high pressure [14].

4.3.3 S/C ratio effect on IHP process

The S/C ratio controls both reforming capacity and carbon management. It is a critical leverage point for IHP as highlighted in the various studies. Steam availability promotes steam reforming and WGS reactions; therefore, increasing the S/C ratio consistently drives the reactions toward greater H_2 production as shown in Figure 12. Afanasev et al. [19] observed the impact of S/C ratio in both modeling and experiments. Their equilibrium calculations showed methane conversion rising with steam addition – e.g. at 450 °C, raising S/C from 1 to 5 doubles the theoretical H_2 yield [19]. Experimentally, they found that injecting additional steam pulses dramatically increased hydrogen output: in one trial, each steam injection caused a spike in H_2 concentration, from ~18% up to a peak 33.9 mol% H_2 [19]. Rui et al. [55] similarly reported that higher S/C ratio generated more H_2, based on pseudo-dynamic experiments where S/C was varied. Their ATR experiment showed

H_2 production rise steadily as S/C increased from 1 up to 15 at constant O/C ratio as shown in Figure 12 [55].

The magnitude of S/C ratio effect is clearer in reports by Afanasev et al. [17]. As shown in Figure 12 at 800 °C, a change from S/C = 1 to S/C = 4 raised the H_2 fraction from ~31% to ~40% [17]. Conversely, with no steam (S/C = 0, pure methane), only methane cracking can produce H_2 – which gave much lower yields (~9.6% H_2). Mukhina et al. [16] directly compared multiple S/C ratios in inert and real-rock systems. They reported the highest H_2 yields at the highest S/C ratios tested. In the inert pack, the maximum H_2 yield was obtained at S/C = 4 and 800 °C, whereas the core-rock system required S/C = 10 at 800 °C to achieve its highest H_2 output. This suggests that, in real reservoir cores, a higher steam fraction is required to suppress side reactions and approach the performance observed in inert media. This is consistent with their observation that steam mitigated some adverse core-rock effects [16]. Tackie-Otoo et al. [14] also underscores the importance of S/C ratio. Their experiment had a "low S/C ratio", which led to very poor H_2 yields at 200 °C. The low steam availability not only limited SMR but also aggravated methanation – with insufficient H_2O, the WGS reaction is inhibited and the excess H_2 is consumed by CO and CO_2 [14]. They conclude that much higher S/C would be needed to realize the high H_2 yields that their simulations predicted [14].

The S/C ratio also has important implications for catalyst stability. Excess steam generally reduces the tendency for carbon deposition on catalyst surface [68]. In agreement with this, Mukhina et al. [16] observed more pronounced carbon-fiber/coke formation under low-steam conditions and recommended high S/C ratios, together with sufficiently high temperatures, to minimize methane decomposition and catalyst coking. Despite the clear benefits of increasing the S/C ratio, practical constraints must be considered when translating laboratory observations to field-scale IHP. Excessively high S/C ratios may be difficult to sustain because of the additional energy required for steam generation and the potential effects on reservoir pressure and thermal balance [93]. Some studies reported investigating S/C ratio as high as ~17 – 21 [19] yet the optimum S/C ratio is reported ~3.5 – 4 and could be around 10 to combat adverse effect of rock minerals [16]. Therefore, the optimum S/C ratio for IHP should not be defined solely by maximum H_2 yield, but by a balance between enhanced reforming performance, coke formation suppression, steam-generation energy demand, and reservoir pressure/thermal management.

4.4 Effect of natural gas composition

Feed gas composition is another important distinction between idealized methane experiments and field scale natural gas applications. Most of the reported studies on IHP in natural gas reservoirs, especially experimental studies, used pure methane to simplify the analysis process. However, actual gas reservoirs may contain ethane, propane, CO_2, N_2, H_2S, and trace contaminants and the composition has significant impact on H_2 production. Rui et al. [55] acknowledged that though they only considered methane in their experimental investigation and thermodynamic models, other gas components can be impactful. The use of natural gas more accurately represents conditions within a depleted gas reservoir, whereas employing pure methane tends to produce overly optimistic hydrogen yields. In industrial SMR operations, such results are achievable because the feedstock typically consists of nearly pure methane, either obtained through cryogenic separation or derived from natural gas with an exceptionally high methane concentration [92]. However, in natural gas reservoirs, methane composition varies widely (approximately 30–98%) [94], and implementing cryogenic separation for IHP is not feasible in practice.

Although methane is the predominant constituent of natural gas, heavier hydrocarbons can significantly alter syngas composition and overall reaction behavior. Their presence generally reduces the H_2/CO ratio [95] and increases the tendency for thermal cracking and carbon deposition, which may foul catalysts or obstruct pore spaces. Tackie-Otoo et al. [14] used natural gas in their investigation, although the effect of composition was not quantified. A subsequent process simulation study showed that H_2 production generally increased with methane mole fraction and further quantified the influence of ethane and propane [18]. When these components were varied independently in two representative natural gas compositions, methane conversion decreased progressively with increasing mole fraction. The transition to negative conversion occurred at approximately 3–5 mol% ethane and 2–3 mol% propane, depending on the background gas composition (Figure 13). Propane produced a more pronounced decline in methane conversion than ethane. The negative values indicate that methane formation through secondary reactions

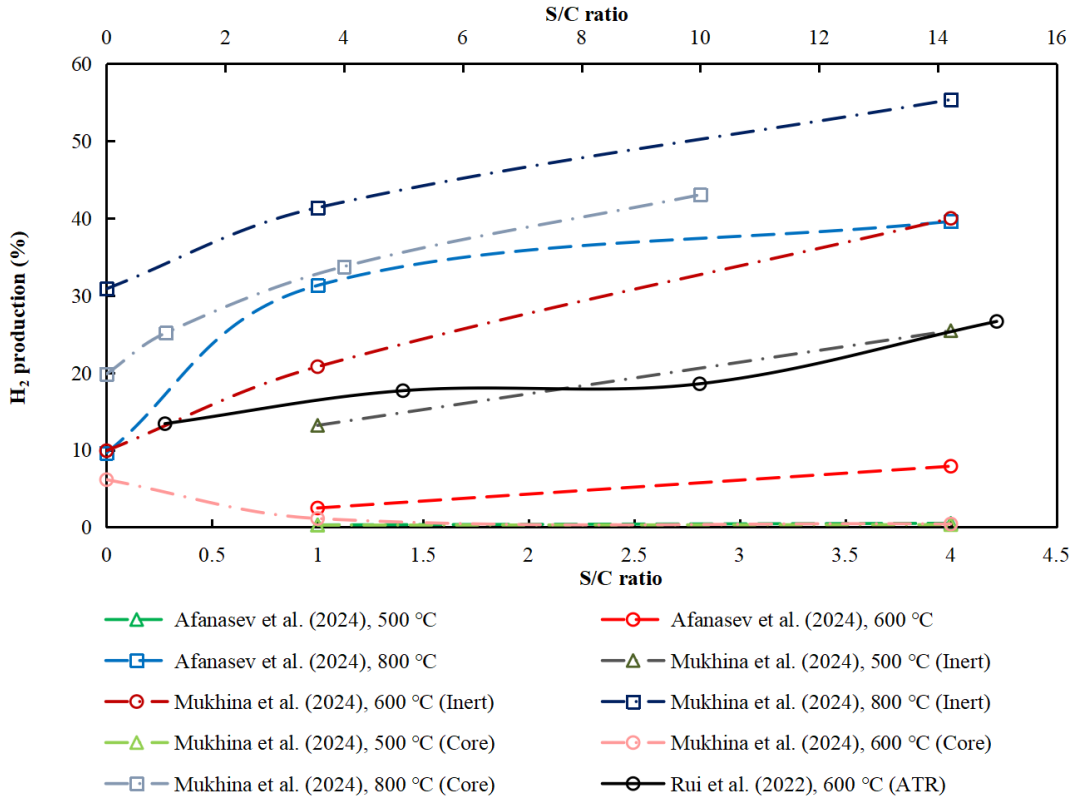

Figure 12. H_2 production against S/C ratio for various IHP in natural gas studies. Data from [16, 17, 55]

exceeded methane consumption, an effect that was suppressed by reducing the pressure or increasing the temperature [18].

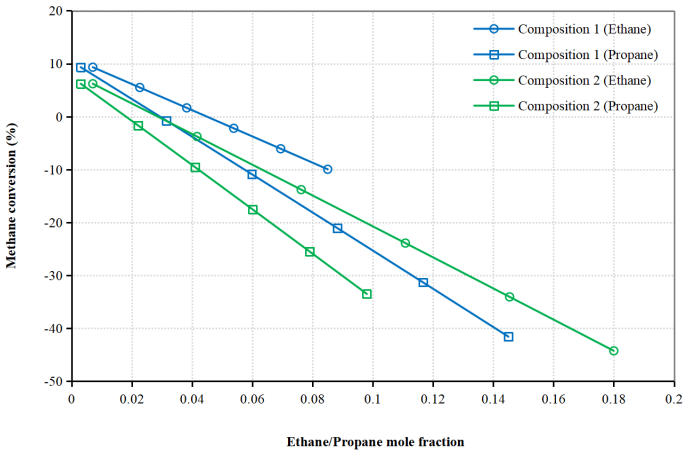

Figure 13. Impact of heavier hydrocarbon component on methane conversion for two natural gas compositions. Data from [18].

4.5 Effect of rock minerals

Reservoir mineralogy is a key control on IHP because rock minerals can either suppress or promote hydrogen forming reactions depending on the dominant reaction pathway. For SMR/WGS-based IHP, reported experimental studies generally show lower H_2 yield in real reservoir cores than in inert porous media (Figure 8 and 12). Afanasev et al. [78] reported that, at 800 °C, H_2 concentration reached 70.8 mol% in crushed alumina but only 34.0 mol% in the original core, indicating that natural core can reduce catalyst effectiveness. Similarly, Mukhina et al. [16] observed consistently lower H_2 production in real core than in α-Al_2O_3; at 800 °C and S/C = 4, H_2 yield decreased from 55.36 vol% in the inert model to 33.75 vol% in the real core.

This inhibitory effect is attributed to both physical and chemical factors. Real cores may provide lower effective surface area than inert Al_2O_3, while reactive minerals and residual organic matter can introduce competing reactions or catalyst deactivating species. Carbonates such as calcite and dolomite may decompose within the IHP temperature range, releasing additional CO_2, although the resulting CaO/MgO may also re-sorb CO_2 under favorable conditions. Residual organic matter can also decompose at elevated temperature, contributing to CO_2 release and coke formation. In addition, sulfur-bearing minerals such as pyrite are undesirable because sulfur species can poison Ni-based catalysts; hence, low organic content and the absence of sulfur-bearing minerals have been identified as favorable reservoir characteristics.

However, the effect of rock minerals is not universally negative. Yan et al. [44] showed that sandstone can promote CH_4 cracking under electromagnetic heating, with H_2 generation beginning at ~394 °C. The catalytic effect was attributed to Fe-bearing minerals, and the addition of Fe_2O_3 to sandstone increased H_2 concentration and CH_4 conversion to 91 mol% and 80%, respectively, at 666 °C. This contrasts with quartz-rich or carbonate/sulfur/organic-bearing rocks, which tend to inhibit SMR-based IHP. Therefore, mineralogy should be treated as an active process variable in reservoir screening: low-sulfur, low-organic rocks are preferred for SMR/WGS-based IHP, whereas Fe-bearing sandstones may be particularly favorable for methane-cracking or EM-assisted IHP concepts. Furthermore, the impact of specific rock minerals on SMR/WGS needs to be investigated. Though Tackie-Otoo et al. [18] provided this investigation through process simulation, experimental validation is still required.

4.6 Studies on Catalyst used

Catalysts are central to IHP from natural gas reservoirs because the dominant hydrogen forming reactions, particularly SMR and WGS, require sufficient catalytic activity under high-pressure, high-temperature, and mineralogically complex reservoir conditions. Unlike surface reformers, where catalyst loading, regeneration, and replacement can be directly controlled, subsurface catalysts must be delivered as solid particles, generated in situ from soluble precursors, or supplemented by naturally catalytic minerals [96, 97]. This makes catalyst deployment, distribution, stability, and resistance to poisoning key design considerations. Reported studies have mainly used Ni-based systems, either as industrial Ni/Al_2O_3 catalysts or water-soluble Ni precursors that form active Ni/NiO phases under reservoir conditions [16, 17, 79].

Afanasev et al. [17] demonstrated that a water-soluble Ni-based precursor could activate hydrogen generation reactions in natural core at 8 MPa and 500–800 °C, with significant methane conversion requiring temperatures of at least 600 °C and higher S/C ratios. This is important for field application because soluble precursors are easier to inject and distribute through porous media than pre-formed solid catalysts. However, catalyst performance remains strongly coupled to reservoir conditions. Askarova et al. [96] further highlighted the practical importance of catalyst delivery mode during combustion-assisted IHP. Their experiments showed that dry and wet methane combustion without catalyst produced very low H_2 yields, whereas adding a Ni/Al_2O_3 catalyst followed by an SMR stage increased H_2 production sharply, reaching up to 68% in sand-packed tests. However, when sandstone core was used, H_2 yields were lower because of the inhibiting effect of the natural rock as discussed earlier. Importantly, continuous delivery of a water-soluble $Ni(NO_3)_2{\cdot}6H_2O$ precursor in the core-packed combustion tube sustained catalyst availability and produced up to 49% H_2, confirming the feasibility of in situ catalyst delivery under reservoir conditions.

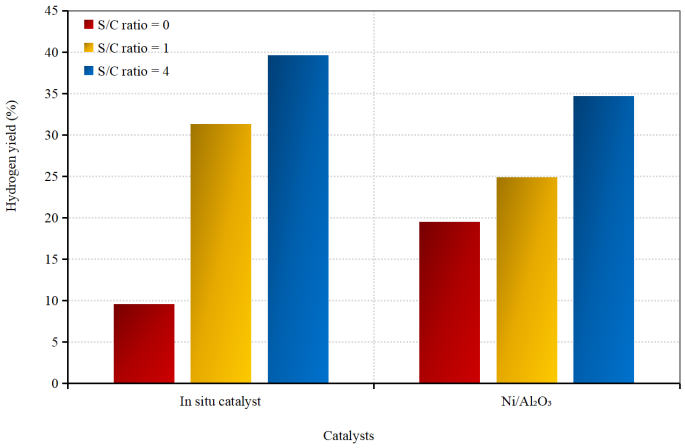

Figure 14. Hydrogen yield obtained with different catalysts at 800 °C. Data extracted from Alekhina et al. [79].

Alekhina et al. [79] provided the most detailed comparison of catalyst type and delivery method for IHP in gas reservoirs. They evaluated commercial Ni/Al_2O_3 and in situ synthesized Ni-based catalysts under simulated reservoir conditions. Although both catalysts promoted H_2 generation, the in situ synthesized Ni catalyst showed the most favorable performance under steam-containing conditions (Figure 14). It achieved 39.6% H_2 in flow-reactor tests and 48.4 vol% H_2 in combustion-tube experiments. In comparison, commercial Ni/Al_2O_3 produced 24.1 vol% H_2 in the corresponding combustion-tube test, an outcome attributed to better catalyst distribution within the rock matrix and lower carbon contamination with the in situ variant, whereas solid catalysts were more susceptible to localized coking and delivery limitations. Therefore, the current evidence suggests that field-scale IHP will require catalysts that are not only active for SMR/WGS but also injectable, well distributed, sulfur- and coke-tolerant, and compatible with reservoir mineralogy and steam availability.

Table 5. Experimental and simulation studies on in-situ hydrogen production from natural gas and hydrocarbon reservoirs.

Reference	Equipment / Model Type	Study variables	Main Findings
Tackie-Otoo et al. [18]	Simulation: non-stoichiometric equilibrium model and kinetic model.	- Temperature: 100–1500 °C - Pressure: 1–8 MPa - S/C: 1–4 - Residence time: ∼0.5–11 s - Catalyst loading: 0–1000 kg - Natural gas composition - Reservoir minerals	- Higher temperature and S/C ratio improved H_2 yield and purity. - High pressure favored methanation and reduced H_2 yield. - Residence time and catalyst loading improved conversion up to an optimum. - Quartz-rich rocks inhibited steam-reforming-based H_2 generation.
Tackie-Otoo et al. [14]	Experimental: autoclave reactor (static) Simulation: stoichiometric equilibrium model	- Temperature: 100–1000 °C (simulation) and 200 °C (experimental) - S/C ratio: 1–6 (simulation) and < 1 (uncontrolled in experiment)	- Process simulation predicted high H_2 yields due to the dominant water-gas shift reaction at 200 °C. - Experimental results confirmed H_2 production but were significantly low due to the low S/C ratio and inadequate temperature. - The presence of rock samples improved H_2 yield through mechanochemical reactions.
Alekhina et al. [79]	Experimental: flow reactor & combustion tube (dynamic)	- Temperature: 800 °C - Pressure: 8 MPa - Catalyst amount: 1 g dry equivalent - S/C ratio: 0, 1 and 4 - Type of catalyst	- The highest hydrogen yield was 48.4 vol% in combustion-tube experiments and 39.6% in flow-reactor tests, both achieved using the in situ synthesized catalyst at S/C = 4. - Elevated temperatures and increased S/C ratios are crucial for higher methane conversion and hydrogen yield. - The in situ catalyst enhances H_2 generation while minimizing carbon contamination, without significantly altering the core's properties.
Askarova et al. [96]	Experimental: combustion tube reactor Simulation: CMG STARS 3D radial combustion-tube model	- Catalyst type/delivery - Water saturation: 0 or 20% - Methane-air combustion - Cyclic combustion/SMR operation - Porous medium type - Gas injection rate: 95–1000 L/h (experimental) and 300–9000 L/h (simulations) - Pressure: 1 atm (experimental) and 1 or 7 MPa (simulations)	- Catalyst and water/steam presence were essential for significant H_2 generation. - Combustion followed by SMR increased H_2 yield, reaching up to 68% in sand-packed tests. - Sandstone core reduced H_2 yield compared with sand-packed systems. - In situ delivery of $Ni(NO_3)_2{\cdot}6H_2O$ sustained catalytic activity and produced up to 49% H_2. - Numerical simulations matched experimental trends and supported scale-up assessment.
Mukhina et al. [16]	Experimental: lab reactor (dynamic)	- Temperature: 500, 600, and 800 °C - S/C ratio: 0, 1, 4 and 10 - Porous media models	- Demonstrates the potential for IHP in natural gas reservoirs using SMR initiated by in situ gas combustion. - H_2 yield is significantly influenced by temperature and S/C ratio, with higher values leading to higher yields. - Porous media type and catalyst selection strongly influenced process efficiency.
Ikpeka et al. [88]	Simulation: full-field compositional model (kinetic & stoichiometric equilibrium model)	- Porosity: 10–30% - Permeability: 20–200 mD - Well location (I-location): 1–9 - Well location (J-location): 2–9 - Injection rate: 500–1000 m^3/day - Injection pressure: 24,131.66–41,368.51 kPa	- Lower permeability and porosity reservoirs support higher hydrogen yields. - Injection pressure has a negligible effect on hydrogen yield, while oxygen injection rates above 1200 m^3/day negatively impact production. - Permeability has a stronger influence on cumulative hydrogen production than porosity.
Yan et al. [44]	Experimental: microwave reactor (dynamic)	- Materials: San Saba sandstone, quartz, silicon carbide (SiC), Fe_2O_3 particles - Sandstone particle size: 38–100 μm - Gas flow rates: 30 sccm CH_4 - Temperature: 650–680 °C - Microwave power: ∼0.1–1.2 kW - Iron catalysts: 0 or 5 wt% Fe_2O_3	- Sandstone demonstrates a natural catalytic effect for methane conversion to hydrogen, starting at 394 °C. - Adding iron catalysts enhances hydrogen production and methane conversion to 91 mol.% and 80%, respectively, at 666 °C. - The process generates negligible carbon oxides, suggesting a carbon-zero technology.
Askarova et al. [77]	Experimental: combustion tube (dynamic) Simulation: kinetic model & reservoir simulation	- Pressure: 8.9 MPa - Temperature: 450–500 °C wet combustion, 540–580 °C dry combustion, and up to 600 °C in field simulation - Presence or absence of a catalyst - Injection rate of air: 29.35 $m^3(ST)/(m^2{\cdot}h)$; field air injection: 26,500–56,500 m^3/day - Water/oil-injection stage: 10 m^3/day	- Confirmed ISHG feasibility from methane using ISC, steam, and catalyst under reservoir conditions. - H_2 generation was observed but remained low, with maximum released H_2 conversion of 4.43% during ISC. - Methane conversion was active, reaching 14–35% across different experimental stages. - Numerical simulation successfully matched temperature profiles, gas production, and gas composition. - The validated kinetic model was upscaled to field-scale reservoir simulation. - H_2 production can be optimized through air-injection rate, injection duration, and well-pattern design.

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Table 5 – continued from previous page

Reference	Equipment / Model Type	Study variables	Main Findings
S. R. Gillick and Babaei [89]	Simulation: kinetic model	- Volume of the reformer/reactor chamber - Operating temperature: 600 °C - Pressure: 40–100 bar - Overall molar flow rate: 2×10^4 kmol/h - Reaction energy input: 1×10^9 kJ/h - S/C ratio: 1.5	- Proposed a wellbore-based IHP process for low-carbon hydrogen production from natural gas wells. - Uses the wellbore as the reaction zone, reducing surface processing needs and environmental risks. - Integrates in situ carbon capture, avoiding downstream CO_2 capture requirements. - Improves economic potential through lower capture costs and possible CO_2-EOR benefits.
Afanasev et al. [17]	Experimental: autoclave reactor with natural cores (dynamic)	- Temperature: 500–800 °C - S/C ratio: 0, 1, and 4 - Reagent exposure time: ∼3.5–4.5 h	- Significant methane to H_2 conversion required temperatures of at least 600 °C. - Higher temperature and S/C ratio increased H_2 concentration. - The highest H_2 concentration was obtained at 800 °C, alongside increased CO_2 formation. - Water-soluble Ni-based catalyst precursor effectively enhanced H_2 generation under reservoir conditions.
Afanasev et al. [78]	Experimental: autoclave reactor (static & dynamic)	- Temperature: 450, 550, and 800 °C - Pressure: 3 and 9 MPa - Core model type (inert vs. natural core)	- High temperatures above 550 °C are necessary for significant methane conversion to hydrogen. - H_2 concentrations up to 70.8% and 34.0% were achieved at 800 °C with inert and natural core models, respectively. - The technology is promising when combined with catalyst treatment and ISC for high methane conversion rates.
Askarova et al. [86]	Experimental: combustion tube (dynamic) Simulation: kinetic model	- Temperature: 450 and 550 °C - Pressure: 2.2–8.9 MPa - Gas injection rate: 57.6 std L/h air, 2.4 std L/h CH_4 (ISC), and 10.62 std L/h CH_4 (SMR) - Water injection rate: 1–3.15 mL/min - Steam quality: 80% - Steam temperature: 302.5 °C	- Achieved up to 40% methane conversion during the combustion stage. - Actual H_2 yield remained low, likely due to secondary H_2-consuming reactions. - Reported significant oil upgrading, including reduced viscosity, density, sulfur, and asphaltene content.
Ikpeka and Ugwu [85]	Simulation: stoichiometric equilibrium model & reservoir simulation	- S/C ratio: 0–1.0 - O/C ratio: 0–1.0 - Initial reservoir pressure: 24,476.39 kPa - Initial reservoir temperature: 90 °C - Permeability of reservoir layers: 20–150 mD (horizontal) and 2–15 mD (vertical) - Oxygen injection rate: 1000 m^3/day	- H_2 yield increased with S/C ratio during in situ combustion. - Excess oxygen reduced H_2 yield, indicating the need to optimize the O/C ratio. - The developed model provides a basis for optimizing future IHP experiments and operating conditions.
Rui et al. [55]	Experimental: high-T/P reactor (static) Simulation: non-stoichiometric equilibrium model	- Temperature: 300–600 °C (experimental); 400–1000 °C (equilibrium calculations) - Reaction time: 1–10 h - O/C ratio: ∼0.2–1.0 - S/C ratio: 1–15 - Fluid flow rate: 2.8–4.2 std mL/min	- Higher temperature and S/C ratio are crucial for increased H_2 generation, with a minimum temperature of 600 °C. - Debris acts as a catalyst, enhancing H_2 production. - Maximum H_2 yield occurs at an O/C ratio of 0.5, with S/C optimized through alternating water and gas injection.
Afanasev et al. [19]	Experimental: autoclave reactor (static) Simulation: stoichiometric equilibrium model	- Type of catalyst - S/C ratio: 2–21 - Temperature: 300–450 °C - Pressure: 64–207 atm - Type of porous medium	- Demonstrated catalytic methane conversion in core material using an ex situ Ni-based catalyst at high pressure and temperatures ≥450 °C. - Achieved a maximum methane to H_2 conversion of 5.8%. - Ex situ Ni-based catalyst and packed core model enhanced catalytic activity and enabled H_2 generation.

5 Techno-economic and life-cycle assessment

5.1 Techno-economic prospects of IHP-NG within the natural gas-based hydrogen production landscape

The techno-economic case for IHP-NG is not that subsurface conversion is intrinsically less expensive than surface reforming. Its potential value lies in process integration: a suitable reservoir may supply methane, provide the reaction environment, accommodate part of the carbon-management function, and permit reuse of wells and surface infrastructure [8]. These potential savings must be weighed against costs that conventional surface plants either do not incur or manage under more mature conditions. In particular, well conversion, equipment replacement, and workovers are material cost assumptions in downhole conversion models [98]. For reservoir-scale electromagnetic heating configurations, membrane cost and heating electricity are reported as principal cost drivers [99]. IHP-NG should therefore be evaluated as a site-specific alternative to a defined natural gas hydrogen pathway, not as a generic substitute for grey or blue hydrogen.

A comparable techno-economic assessment (TEA) should report the levelized cost of hydrogen (LCOH) in a common currency year and per kilogram of hydrogen at a stated product specification and delivery point. Cross-study comparison is otherwise unreliable because differing assumptions and system boundaries can materially change reported hydrogen costs [100]. The assessment should identify the comparison cases; at minimum, unabated natural-gas reforming and natural gas reforming with capture, transport, and storage of CO_2 [101]. It should also state the project life, discount rate, capacity factor, natural gas and electricity prices, carbon management treatment, and whether CO_2 transport and storage, hydrogen compression, blending constraints, and monitoring liabilities are included. This level of disclosure is consistent with discounted cash flow hydrogen cost models, which explicitly incorporate capital cost, operating cost, capacity factor, financial inputs, and sensitivity analysis [102]. A coupled assessment of surface SMR and CCS illustrates why this definition matters: capture reduced carbon intensity but increased LCOH, while CCS cost, electricity demand, hydrogen sales price, and rate-of-return assumptions materially influenced the modeled result [101].

Published estimates for IHP-NG remain preliminary and are not directly interchangeable. Yan et al. [99] modelled electromagnetic heating assisted, reservoir-scale IHP and reported a potential cost as low as USD 0.86 kg^{-1} H_2 when renewable electricity is integrated; membrane cost and electricity for electromagnetic heating were the principal modeled cost drivers. Gillick and Babaei [98] applied the H2A framework to a different configuration; a proposed methane gasification tool located in the wellbore rather than conversion within the reservoir. They reported modeled costs below USD 1 kg^{-1} H_2 in a multiwell case and near USD 2 kg^{-1} H_2 in other scenarios. This latter study is useful as a sensitivity and infrastructure reuse analogue, but it should not be presented as direct validation of reservoir-scale IHP-NG. Its lower cost cases assume, among other inputs, 100% methane conversion, a 100% operating capacity factor, a five-year tool lifetime, and hydrogen blending below 20 vol% to avoid major surface upgrades. The model also excludes reservoir-specific CO_2 sequestration revenues because sequestration capacity is uncertain, underscoring that both upside and liability remain site-dependent [98].

The appropriate interpretation of the available studies is not a single cost estimate for IHP-NG, but a structured set of conditions under which the concept might be competitive [100]. The numerator of LCOH includes (i) capital for well conversion, downhole equipment, injectant or heating systems, and separation facilities [98]; (ii) operating costs for energy, oxygen or steam where required, catalyst replacement, compression, maintenance, and measurement and verification [99]; and (iii) end-of-life costs for plugging, remediation, and post-operation monitoring [103]. The denominator depends on methane conversion, hydrogen selectivity and purity, separation recovery, uptime, well productivity, and the productive life of the conversion system [98]. Carbon credits avoided CO_2 transport and storage costs, and revenues associated with residual methane or other co-products should be reported separately as scenario-specific value streams rather than embedded as universal savings [98, 101].

Three comparisons are particularly important. First, IHP-NG may reduce surface-reforming and CO_2 transport and storage requirements [89], but this benefit should be credited only where reservoir retention is demonstrated and recognized within the relevant carbon-accounting framework [100, 104]. Second, reusing a mature field's wells, gathering system, and compression assets may reduce upfront expenditure, but integrity remediation, hydrogen

Table 6. Comparison of major cost components for IHP-NG, grey hydrogen, and blue hydrogen.

Cost component	IHP-NG	Grey Hydrogen	Blue Hydrogen	Economic implication
Hydrocarbon feedstock	Reservoir gas consumed in situ	Purchased natural gas feedstock	Purchased natural gas feedstock plus energy penalty from CCS	IHP-NG is favored when low-value gas can be converted without major new infrastructure.
Main reactor system	Reservoir acts as reaction medium	Surface reformer and shift reactors	Surface reformer/ATR plus shift and capture units	IHP-NG avoids part of the surface reactor train but requires reliable subsurface reaction control.
Carbon management	Intended in-reservoir CO_2 retention	No capture	Capture, compression, transport, and storage	IHP-NG advantage depends on verified carbon retention and regulatory recognition.
Hydrogen separation	Downhole or surface separation required	Mature PSA/membrane systems	PSA plus CO_2 capture train	Downhole separation is potentially cost saving but remains one of the least mature components.
Wells and completions	Major cost block; existing wells may be reused	Not central	Not central unless linked to CO_2 storage	Infrastructure reuse can reduce CAPEX, but well integrity upgrades may erode savings.
Steam/oxygen supply	Required for SMR/WGS and combustion-assisted heating	Steam required; oxygen usually not central	Steam plus possible oxygen for ATR-based systems	IHP-NG economics depend strongly on injectant cost and energy source.
Catalyst management	Catalyst must be injected, generated, or retained in situ	Catalyst replacement is controlled in surface reactors	Like SMR plus capture solvents/sorbents	Subsurface catalyst deployment adds uncertainty and replacement difficulty.
Monitoring and liability	High importance for H_2/CO_2 containment, leakage, and well integrity	Standard plant HSE	CCS monitoring and storage liability	IHP-NG shifts part of CCS cost into subsurface monitoring and long-term stewardship.

compatible upgrades, and additional monitoring can erode or potentially offset that benefit [105, 106]. The wellbore tool analysis illustrates this sensitivity: its higher H_2 blending scenario assumed major surface equipment upgrades, whereas its baseline cases assumed that H_2 remained below 20 vol% in the export stream [98]. Third, integrating hydrogen production from natural gas with CO_2 capture may improve the overall process economics through heat recovery and reduced carbon management costs, but such benefits must be substantiated by rigorous process-specific mass and energy balances rather than inferred from qualitative arguments alone; integrated process designs for natural gas reforming with carbon capture illustrate that claimed heat-recovery and cost-reduction benefits are highly sensitive to the specific process configuration and operating assumptions [88, 107]. Taken together, these comparisons show that IHP-NG redistributes rather than simply eliminates costs; the corresponding cost architecture is summarized in Table 6.

Accordingly, this review does not assign a point LCOH to IHP-NG. Instead, the evidence supports a sensitivity-based TEA in which the base case and scenario range transparently vary as summarized in Figure 15. The variables that should be defined include methane conversion and hydrogen recovery; product purity and separation performance; well productivity and retrofit scope; catalyst and downhole-equipment life; heat, electricity, oxygen, and steam requirements; CO_2 retention and monitoring obligations; infrastructure compatibility; and financing, carbon-price, and regulatory assumptions. Under a favorable brownfield case, high sustained hydrogen recovery, limited upgrade scope, durable equipment, low-carbon energy supply where needed, and verifiable carbon retention, IHP-NG could reduce costs associated with surface processing and carbon management. Under a less favorable case, separation losses, low conversion, equipment replacement, integrity work, or monitoring and liability costs may remove that advantage. Pilot data should therefore

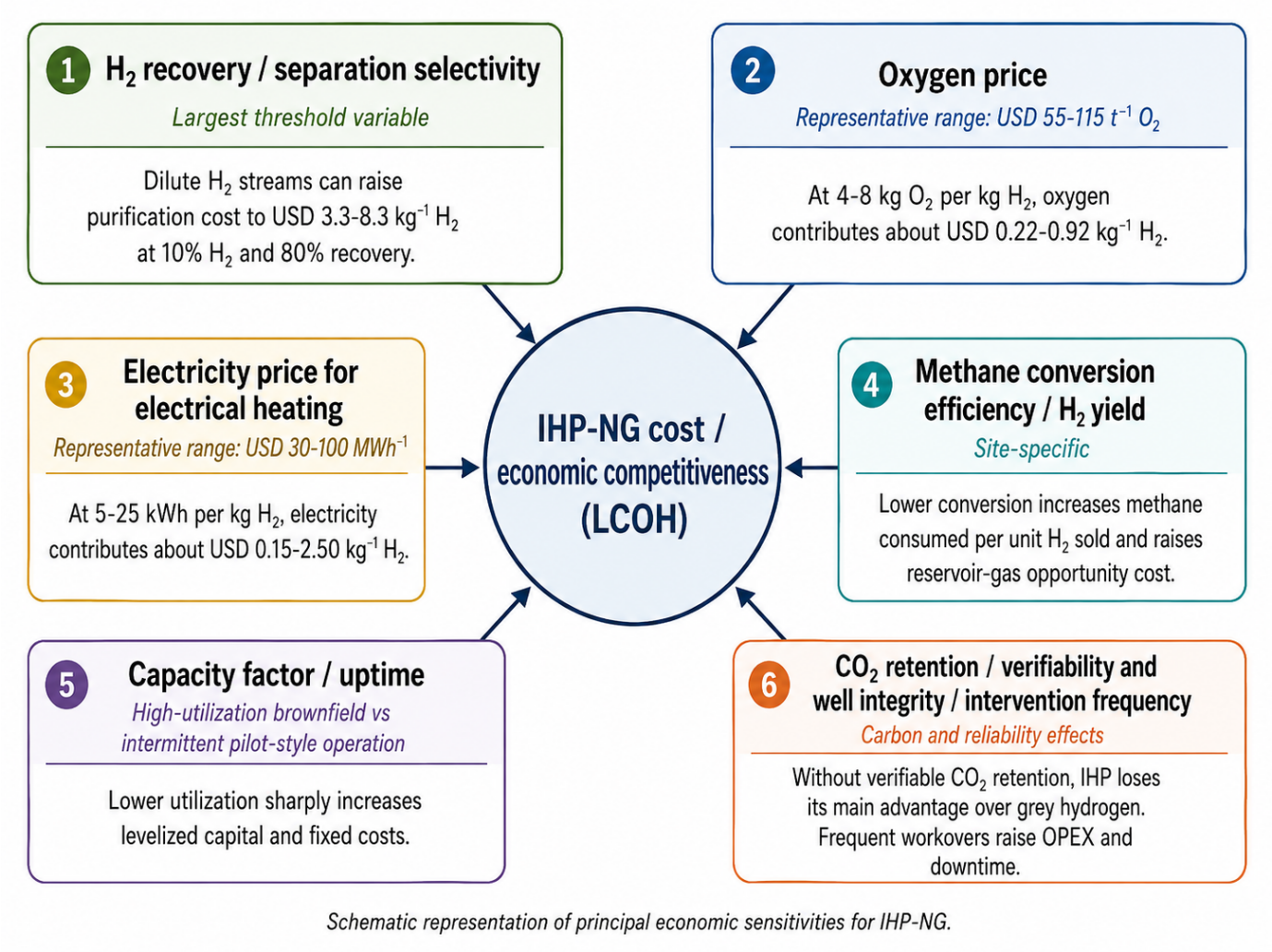

Figure 15. Schematic representation of principal economic sensitivities for IHP-NG.

be used to update these ranges before commercial comparisons with established hydrogen pathways are made.

5.2 Life-cycle assessment of IHP-NG

The potential environmental advantage of IHP-NG arises only if carbon-bearing products remain securely contained while the emissions associated with energy, materials, gas losses, and long-term stewardship remain sufficiently low. This is a hypothesis to be tested by life-cycle assessment (LCA), not a property conferred by locating methane conversion underground. LCA comparisons of hydrogen pathways are highly sensitive to the selected system boundary, functional unit, treatment of co-products, energy supply, and geographic setting [108]. Therefore, inconsistent choices can change the resulting carbon-intensity estimate and, in some cases, reverse pathway rankings [109].

The purpose of an IHP-NG LCA is therefore to estimate the cradle-to-gate climate intensity of producing one kilogram of hydrogen at a stated purity and pressure at the defined delivery point, and to compare that result with explicitly defined natural gas-based alternatives. The assessment should identify the global warming characterization method and time horizon; geographical setting; electricity, oxygen, and steam supply; treatment of any residual methane, CO_2, or other co-products; and the method used to quantify hydrogen and methane losses. This explicit goal and scope statement is needed before numerical comparisons are made, because hydrogen LCA studies differ materially in functional unit, production, storage, transport, end-use, and boundary choices [108, 110].

Figure 16 presents the proposed IHP-NG inventory as four connected boundaries: (1) upstream inputs; (2) subsurface conversion and carbon retention; (3) hydrogen recovery and delivery; and (4) post-operation stewardship. Figure 16 is an accounting framework, not evidence that a particular IHP-NG

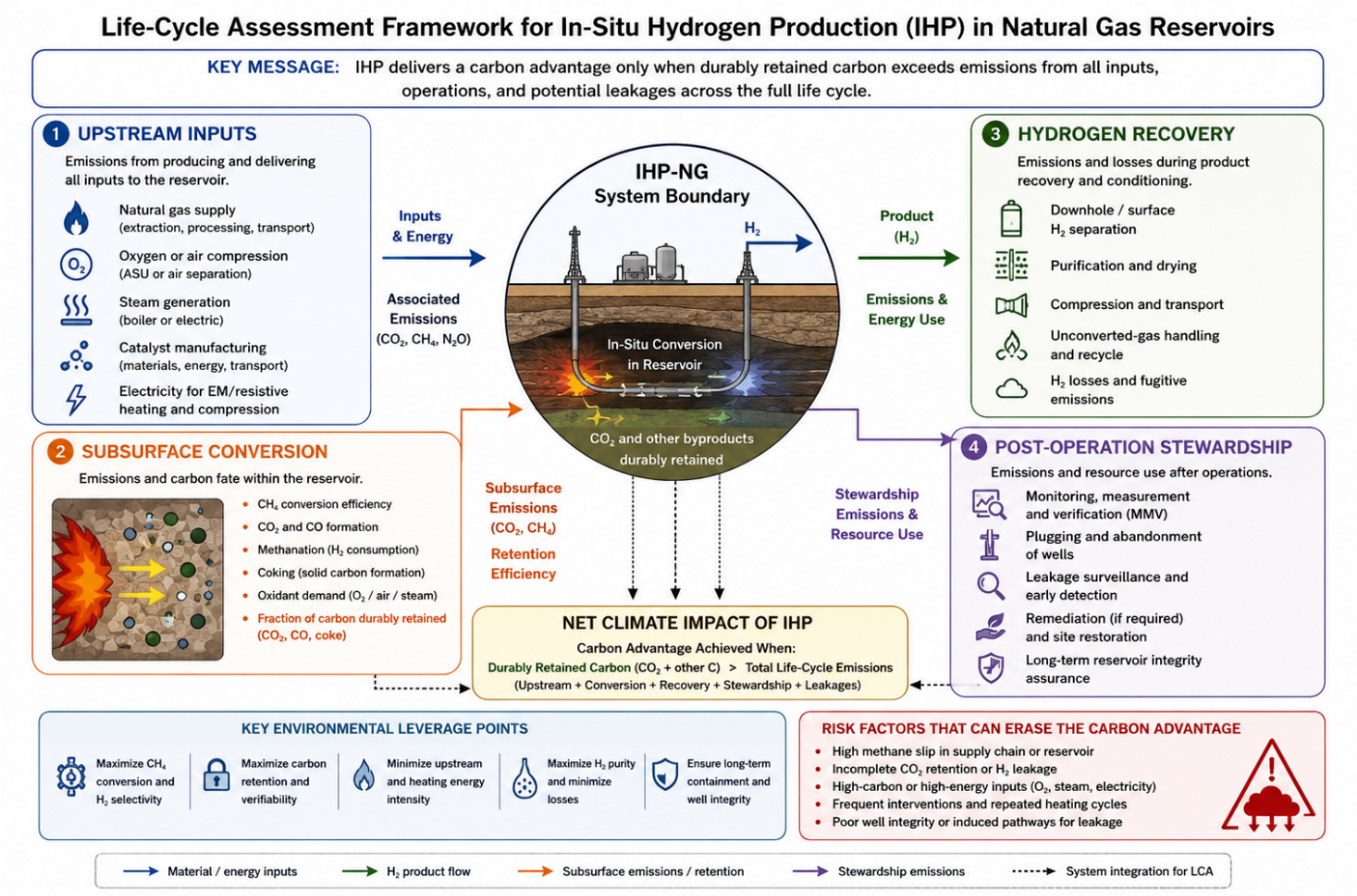

Figure 16. Life-cycle assessment framework for IHP-NG.

configuration has achieved low carbon intensity. Each boundary should be populated with measured field data when available and otherwise with transparent, scenario-specific assumptions.

Upstream inputs. The inventory should include methane supplied to the conversion system; electricity for compression, electromagnetic heating, separation, and other surface equipment; oxygen or enriched air; water and energy for steam generation; catalysts and their delivery; and construction or retrofit materials. The electricity mix deserves explicit treatment, rather than being represented by a generic grid factor. In the only reservoir-scale electromagnetic-heating IHP study identified in this review, the reported greenhouse gas result and eligibility for a clean hydrogen credit depended on the electricity source and its renewable share; membrane cost and heating electricity were also central process variables [99].

Subsurface conversion and carbon retention. The conversion boundary should quantify injected materials and energy, methane conversion, hydrogen yield, carbon-containing product formation, unconverted methane, and the fate of carbon dioxide [99]. Carbon retained in the reservoir should not be credited simply because it is not produced at the wellhead [111]. The inventory should distinguish CO_2 dissolved in formation water, residually or structurally trapped CO_2, mineralized carbon where demonstrated, CO_2 reinjected into a storage interval, and CO_2 that is co-produced or leaked [112]. Site-specific reservoir modeling and monitoring should establish the mass balance and the durability of each retained fraction [113]. This distinction is necessary because system boundary selection critically affects hydrogen carbon intensity results [109], while available reservoir-scale environmental assessments of IHP-NG remain model-based and dependent on assumptions that have not been validated at field scale [99, 114].

Hydrogen recovery and delivery. This boundary should include downhole or surface separation, hydrogen recovery fraction and purity, compression to the delivery specification, any additional purification, and emissions associated with handling residual gas. Methane and hydrogen losses should be reported separately by source, including incomplete

conversion, bypass during separation, routine venting, and well or surface leakage, then characterized with the selected climate metric [115]. If hydrogen is transported as a blend with natural gas, the blend level, required infrastructure modifications, and allocation of common compression and pipeline energy should be stated [116]. In the wellbore-tool model of Gillick and Babaei [98], the assumed hydrogen blend limit and surface upgrade requirement materially affected estimated cost; the same design choice also changes the appropriate LCA inventory.

Post-operation stewardship. The LCA boundary should extend beyond active hydrogen production to include monitoring, measurement and verification of CO_2 and H_2 containment; plugging and abandonment; corrective action or remediation where required; and post-closure data management. The duration of monitoring and its associated resource requirements should be defined according to the applicable regulatory framework and site-specific evidence of containment. For example, projects regulated as geologic CO_2 sequestration under the United States Class VI framework are subject to a default post-injection site care period of at least 50 years, unless an alternative timeframe or earlier closure is approved on the basis of site-specific monitoring and modeling demonstrating that underground sources of drinking water are not endangered [117]. Accordingly, jurisdiction-specific monitoring, closure, and liability requirements should be incorporated into the LCA rather than represented by a generic duration. Monitoring costs should not be treated as negligible: CCS techno-economic assessments include capture, transport, injection, storage, and monitoring within the connected project boundary [103], while recurring monitoring can represent a substantial proportion of geological storage costs [118].

This four-boundary framework does not establish that IHP-NG is lower carbon than grey or blue hydrogen. It specifies the evidence needed to make that determination. A credible future assessment must report its carbon-intensity result together with its methane and hydrogen loss assumptions, electricity and injectant sources, separation and compression energy, carbon-retention evidence, monitoring period, and sensitivity analysis. Until pilot-scale projects provide these data, LCA results should be presented as scenarios rather than as verified technology-level performance claims.

5.3 Containment, leakage, and permitting sensitivities

Containment performance is central to the environmental and economic viability of IHP-NG. Leakage of hydrogen, methane, or carbon dioxide through caprock, faults, fractures, or wells could reduce product recovery, increase life-cycle emissions, undermine subsurface carbon retention, and introduce permitting constraints. Because reservoir-scale evidence for IHP-NG remains limited, the relevant failure mechanisms are assessed primarily using evidence from underground hydrogen storage, CCS, and related in-situ hydrogen concepts. These analogues provide a useful basis for identifying potential risks and their consequences, although they cannot establish failure probabilities for a specific IHP-NG configuration.

Hydrogen leakage and caprock containment. Hydrogen can be lost through caprock, faults, fractures, and legacy wells. Such losses directly reduce the recoverable hydrogen output used in the LCOH calculation and may add to the life-cycle climate burden [115]. Leakage pathways that cannot be adequately characterized or monitored would also weaken the project's permitting case. Caprock sealing depends on wettability, interfacial tension, permeability, pore structure, and diffusion, and these properties must remain suitable under the relevant pressure and temperature conditions [119]. Pore-scale analysis of shale caprocks yielded theoretical H_2 column heights of 59–667 m, compared with 20–500 m for CO_2, depending on caprock type [120]. Although this comparison suggests potentially favorable capillary sealing of hydrogen, the estimates are based on an intact, water-wet caprock that has not undergone thermal alteration. In IHP-NG systems, conversion-related heating may modify wettability, permeability, pore structure, and fracture behavior, while faults, legacy wells, and molecular diffusion provide additional leakage pathways not represented by the column height calculation. Site-specific containment assessment must therefore consider these thermal, geological, and well-integrity effects alongside capillary sealing capacity.

Well integrity and leakage pathways. The same wells that create a potential brownfield cost advantage can become conduits for hydrogen, methane, or carbon dioxide leakage. Underground hydrogen storage studies identify cement degradation, elastomer failure, microbial corrosion, hydrogen blistering, hydrogen-induced cracking, embrittlement, and

caprock-sealing failure as mechanisms that can compromise well integrity and cause leakage [121]. In a North Sea gas field reuse model, injection pressure strongly controlled leakage across a microannulus, and reducing the maximum pressure lowered the modeled leakage rate at the expense of storage capacity [122]. IHP-NG introduces additional uncertainty because wells and the near-wellbore region may be exposed simultaneously to elevated temperatures, pressure cycling, hydrogen, steam, oxygen, and other reactive gases during conversion. The resulting effects are likely to depend on the completion design and material properties and should therefore be evaluated under representative operating conditions. Well integrity failure would reduce hydrogen recovery, weaken confidence in carbon retention, increase remediation and workover costs, and complicate environmental approval.

CO_2 migration and groundwater protection. The proposed carbon management advantage of IHP-NG disappears if the carbon dioxide generated during conversion cannot be retained. Reservoir simulations of hydrogen generation involving SMR and CO_2 injection indicate that containment depends partly on the balance between injected fluids and produced gases, with poorly controlled injection potentially promoting displacement beyond the intended interval [104]. Migration through caprock, faults, or well pathways can reduce the carbon retention credit used in the LCA and create groundwater protection concerns, particularly where pressure changes or artificial penetrations connect the storage interval to shallower formations. CCS regulatory frameworks consequently treat site characterization, corrective action for artificial penetrations, monitoring, well plugging, site closure, and financial responsibility as connected elements of demonstrating storage security [117]. For IHP-NG, the carbon balance used in the environmental assessment must therefore be supported by site-specific geological characterization, well integrity evidence, pressure management analysis, and monitoring of potential gaseous and dissolved phase migration pathways.

Oxygen breakthrough and combustion control. In IHP-NG configurations that use air or oxygen injections, reservoir heterogeneity and preferential flow may carry oxidant beyond the intended reaction zone and toward the production well [12]. Breakthrough into the production system can interrupt the intended conversion and separation regime and expose wells and completion materials to oxidative conditions [123]. Mixing of hydrogen and oxygen within the production system would also create a combustion and explosion hazard [124]. These outcomes extend beyond operational safety because uncontrolled oxidation can change gas composition, methane conversion, hydrogen yield, and the distribution of carbon-bearing products. An inability to control or adequately characterize the reaction front would therefore undermine the mass balance and containment assumptions used in TEA, LCA, and permitting assessments.

Thermal and mechanical effects on long-term containment. Heating, cooling, pressure cycling, and reaction-induced changes in the near wellbore region can alter the properties of casing, cement, reservoir rock, and caprock. Thermal expansion and pressure changes may generate fractures or reactivate existing discontinuities, particularly in naturally fractured formations; field evidence and modelling of fluid injection into thermally stressed reservoirs confirm that such thermo-mechanical coupling can trigger slip on pre-existing faults and alter caprock permeability at conditions relevant to subsurface energy operations [125, 126]. Thermally induced microstructural damage may also reduce the sealing capacity required for long-term hydrogen and carbon dioxide containment [127]. The relevant concern is therefore not simply that IHP-NG operates at elevated temperature, but that conversion may alter the barriers relied upon after the reservoir has been heated. Thermal management is consequently linked to hydrogen recovery, carbon retention accounting, potential remediation liabilities, and the evidence required for environmental approval.

The practical implication is that containment performance must be evaluated as a condition of project viability. A credible pilot should integrate material qualification, well integrity assessment, pressure and thermal management, reaction-front control, baseline and repeat monitoring, gas-composition measurements, and complete carbon and hydrogen mass balances. These physical pathways connect reservoir behavior directly to project cost, life-cycle carbon intensity, and regulatory viability. Containment performance must therefore be demonstrated before infrastructure reuse, avoided carbon management costs, or low-emission performance can be treated as evidence-based project attributes.

6 Research gaps and future direction

Based on the various studies discussed earlier, IHP from natural gas reservoirs has transitioned from proof-of-concept to systematic investigation, yet several critical research gaps remain before field deployment is viable. Current studies agree that IHP is thermodynamically feasible through SMR, POX, ATR, and methane cracking reactions at reservoir temperatures between 600–900 °C and pressures up to 8 MPa. However, major uncertainties persist regarding reaction kinetics, heat and mass transfer in porous media, and multi-phase flow coupling under realistic reservoir heterogeneity. Most laboratory and numerical experiments rely on simplified models or crushed-core setups that neglect natural stratification, capillary barriers, and dynamic gas–water interactions. Furthermore, equilibrium and kinetic models often diverge significantly from experimental data due to incomplete mixing, uneven heating, and catalyst deactivation. The absence of validated, reactive-transport reservoir models integrating combustion fronts, steam dynamics, and catalytic behavior is a critical limitation for field-scale prediction and optimization [55, 77].

A second major gap concerns catalyst design, delivery, and stability under downhole conditions. While Ni-based catalysts remain dominant, their thermal sintering, sulfur poisoning, and carbon deposition reduce long-term activity. Studies by Alekhina et al. [79] demonstrated that in-situ synthesized Ni catalysts dispersed through water-soluble precursors outperform conventional Ni/Al_2O_3 in hydrogen yield and dispersion. Yet, scalability of catalyst transport through low-permeability formations, control of particle deposition, and regeneration mechanisms remain unresolved. Mineralogical effects further complicate this issue—iron-bearing phases in sandstone promote methane reforming, whereas pyrite and carbonates release H_2S and CO_2 that deactivate catalysts. Future research must focus on adaptive or self-activating catalytic systems, potentially multi-metallic (Ni–Fe–Ce or Ni–Nb hybrids), with engineered supports compatible with reservoir mineralogy. Kinetic data based on new catalysts, other natural gas components and specific rock minerals will be relevant for developing robust kinetic models [18].

Finally, field-scale validation and environmental integration remain nascent. While small-scale combustion-tube and autoclave experiments have achieved partial methane conversion, there are no pilot-scale demonstrations of stable hydrogen generation in natural gas reservoirs. The lack of thermal management strategies, safety protocols, and wellbore integrity assessments under cyclic heating pressures introduces major engineering and regulatory barriers. Future directions should emphasize (1) coupled electromagnetic or in-situ combustion heating systems to sustain the 700–900 °C reforming window; (2) reactive multiphase simulations incorporating kinetics, porosity evolution, and gas transport; and (3) techno-economic and life-cycle assessments to quantify carbon intensity relative to blue hydrogen routes. Integrating these dimensions will transform IHP from laboratory feasibility to an integrated reservoir-scale hydrogen production–storage system, bridging the fossil and renewable energy sectors through a carbon-constrained, infrastructure-leveraged pathway [14, 85].

7 Conclusion

This review critically assessed the current status, controlling mechanisms, research gaps, and deployment outlook for IHP-NG. Unlike broader subsurface hydrogen or heavy-oil ISCG reviews, the focus here was on natural gas reservoirs as distinct reactive systems, where hydrogen generation is governed by methane conversion, high-pressure equilibria, catalyst–rock interactions, heat management, hydrogen recovery, and carbon retention. The reviewed studies show that IHP-NG is technically plausible, but its performance is highly condition dependent. Substantial hydrogen generation generally requires high temperatures, adequate steam availability, controlled oxygen supply, suitable catalyst or mineral activity, and suppression of hydrogen-consuming side reactions such as methanation and RWGS. Existing laboratory studies have demonstrated hydrogen formation under reservoir conditions, but most remain limited by simplified reactor geometries, short durations, idealized core materials, and incomplete representation of reservoir heterogeneity.

The review further identifies that techno-economic and life-cycle assessments are limited in the literature. Therefore, the review provides information on critical areas that require attention to prove the economic viability and low carbon advantage over conventional methods. The study further clarifies that IHP-NG should not be presented as inherently cheaper or cleaner than conventional hydrogen pathways. Its value proposition lies in process integration: using

the reservoir as both a hydrogen-generation zone and a carbon-retention medium, while potentially reusing existing wells and surface infrastructure. However, the economic advantage over blue hydrogen is conditional on high H_2 yield, reliable downhole or near-well separation, verifiable CO_2 retention, manageable well retrofit costs, and limited monitoring and liability burdens. Similarly, the life-cycle carbon advantage depends not only on retaining carbon underground, but also on accounting for upstream gas emissions, oxygen or steam generation, heating energy, compression, H_2 losses, methane slip, leakage surveillance, and long-term stewardship. Thus, both TEA and LCA must be treated as sensitivity-based assessments.

Therefore, IHP-NG remains a promising but verification-limited low-carbon hydrogen pathway. The most urgent research needs are validated reactive-transport models, reservoir-specific catalyst systems, high-temperature well-integrity testing, durable H_2-selective separation, full carbon and hydrogen mass balances, and pilot-scale demonstrations under realistic gas reservoir conditions. Future work should move beyond proving that hydrogen can be generated in natural gas reservoirs toward demonstrating that it can be produced selectively, recovered efficiently, retained or separated safely, and certified as a low-carbon product. Satisfying these technical, economic, environmental, and regulatory conditions will move IHP-NG from an attractive subsurface concept to a credible component of the low-carbon hydrogen economy.

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Not applicable.

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Conflicts of Interest

Arshad Raza served as an Associate Editor of the *Reservoir Science* at the time of manuscript submission. To ensure the integrity of the peer-review process, Arshad Raza was not involved in the editorial handling, peer review, or decision-making process for this manuscript, which was handled independently by another editor. The remaining authors declare no conflicts of interest.

AI Use Statement

The authors declare that ChatGPT-5 was used for language editing of the manuscript. The authors have carefully reviewed, revised, and verified the AI-assisted output and take full responsibility for the content of the manuscript.

Ethical Approval and Consent to Participate

Not applicable.

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