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Comprehensive Life Cycle Analysis of Methanol Production and Methanol-to-Diesel Conversion.

April | 2025

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EXECUTIVE SUMMARY

Methanol is a strategic chemical and intermediate in the manufacture of synthetic diesel, due to its versatility, diesel's compatibility with existing infrastructure, and their role in industrial and transport applications. Conventional production methods for methanol, primarily steam methane reforming (SMR), rely on natural gas and are subject to the price variability due to market conditions and geopolitical events. They are also associated with greenhouse gas (GHG) emissions. Methanol and synthetic diesel production could be integrated with nuclear energy to stabilize fuel prices and insulate pricing from outside geopolitical events due to the relative stability of nuclear fuel as compared to natural gas. This could lead to increased transportation fuel security, reliability and resilience. An added benefit is the abatement of emissions when substituting nuclear energy for conventional energy from natural gas.

This report presents a comprehensive life cycle analysis (LCA) framework which was developed to evaluate the GHG emissions reduction potential associated with nuclear integrated methanol production, methanol-to-diesel upgrading, and end-use combustion. Gate-to-gate methanol production and cradle-to-grave emissions were evaluated in the cases as shown in Table ES 1, starting with a business-as-usual (BAU) SMR-based methanol plant, and then considering stepwise nuclear integration. Methanol-to-diesel (MTD) conversion was evaluated accounting for nuclear energy integration and hydrogen production via high-temperature steam electrolysis (HTSE) using electricity either from the grid or from a dedicated nuclear power system. This multi-step process diverts stable and reliable nuclear energy into the transportation sector by upgrading low energy dense natural gas into liquid fuels fully compatible with existing infrastructure.

Table ES i. BAU conventional and nuclear integration cases with and without CCSU

Category	BAU	Nuclear Integration		Amine-Based CCSU		Oxy-fuel Combustion CCSU	
Case Number	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7
Case Description	Business-as-Usual	H_2 Fuel Switch	Electrified Reformer	NG-CHP Powered	Nuclear Powered	O_2 from Nuclear Powered Air Separation	O_2 from Nuclear HTSE

Each scenario was assessed using consistent system boundaries, with particular attention to the spatial layout of facilities (co-located vs. separate sites) and the source of external energy inputs, especially for hydrogen generation. The study reveals the following major findings. Figure ES 1 displays the gate-to-gate results with the wide bars showing the positive and negative lifecycle emissions from all subsystems and plant sections in the given case and the narrow bar displaying the net lifecycle emissions in grams of CO_2 equivalent per megajoule of methanol on a lower heating value basis. Figure ES 2 displays the cradle-to-grave results in a similar format.

1. **Gate-to-Gate Methanol Production:**

- BAU scenarios obviously present the highest emissions at 4.3 g CO_2 eq/MJ of methanol, due to reliance on natural gas for heat and for hydrogen production without carbon capture.
- CCSU integration alone (Case 4) reduces emissions to 0.2 g CO_2 eq/MJ.
- Hydrogen substitution using nuclear-powered HTSE (Case 2) reduces GHG emissions to -37.3 g CO_2 eq/MJ, surpassing electrified reformers with a result of -23.8 g CO_2 eq/MJ (Case 3). Each of these scenarios show a reduction in lifecycle emissions by reducing NG fuel consumption by substituting nuclear power.
- Case 7—an oxy-fuel SMR system with oxygen supplied via HTSE—achieves -89.7 g CO_2 eq/MJ. This results from high-purity oxygen, efficient combustion, and complete integration of nuclear with hydrogen production and carbon capture.

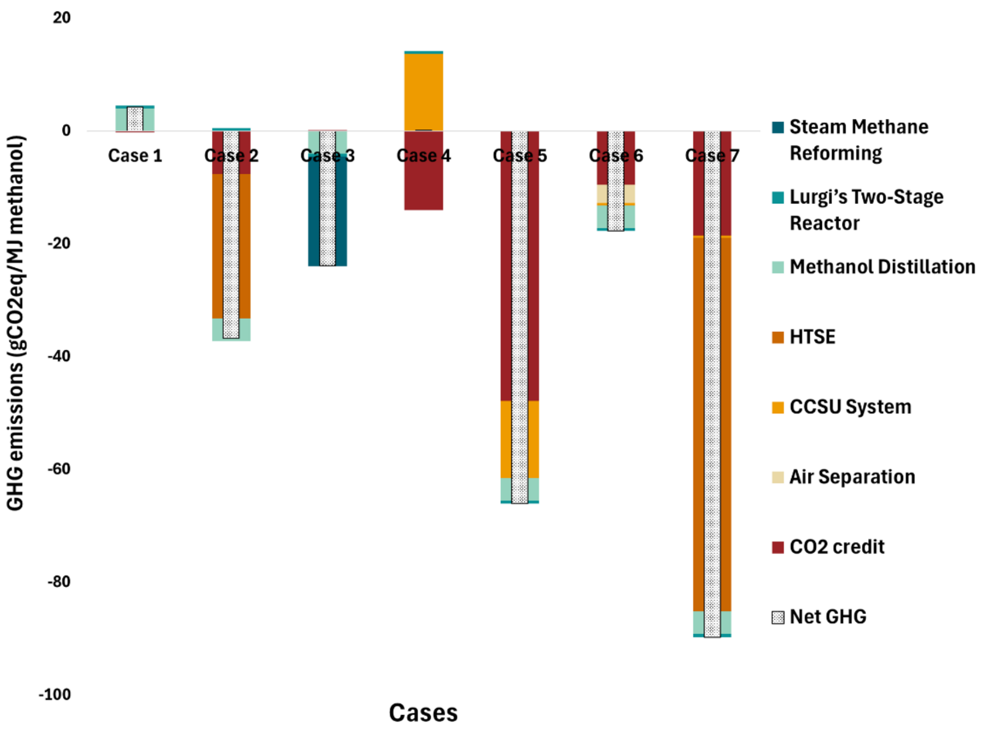

Figure ES i. GHG Emissions of Steam Methane Reforming Case Studies

2. Methanol-to-Diesel Conversion

- The process is internally energy-balanced, with the heat released by the exothermic oligomerization reactions being recovered for use in the distillation reboilers. Electricity for hydrogen production is the only major external energy requirement.
- Grid-powered HTSE results in 7.6 g CO_2 eq/MJ of methanol, reflecting the combustion-derived sources in typical electricity mixes.
- Dedicated nuclear energy enables HTSE to operate with high efficiency and no combustion-related emissions, resulting in -7.6 g CO_2 eq/MJ, showing potential for net GHG reductions through system integration.

3. Cradle-to-Grave Fuel Pathways

- BAU (Case 1) and non-nuclear integrated CCSU (Case 4) yield the highest full-cycle emissions, ranging from 74.3 to 105.3 g CO_2 eq/MJ.
- Hydrogen-based cases (Cases 2a–2c) without CCSU result in 31.1 to 57.1 g CO_2 eq/MJ, while electrified reformers (Cases 3a–3c) reach 52.5 to 77.4 g CO_2 eq/MJ.
- Best results are achieved with full integration of CCSU, hydrogen, and thermal power (Case 7c), delivering emissions as low as -17.1 g CO_2 eq/MJ.
- Co-located facilities consistently outperform separate setups, thanks to improved energy sharing, reduced transport emissions, and higher capture efficiency.

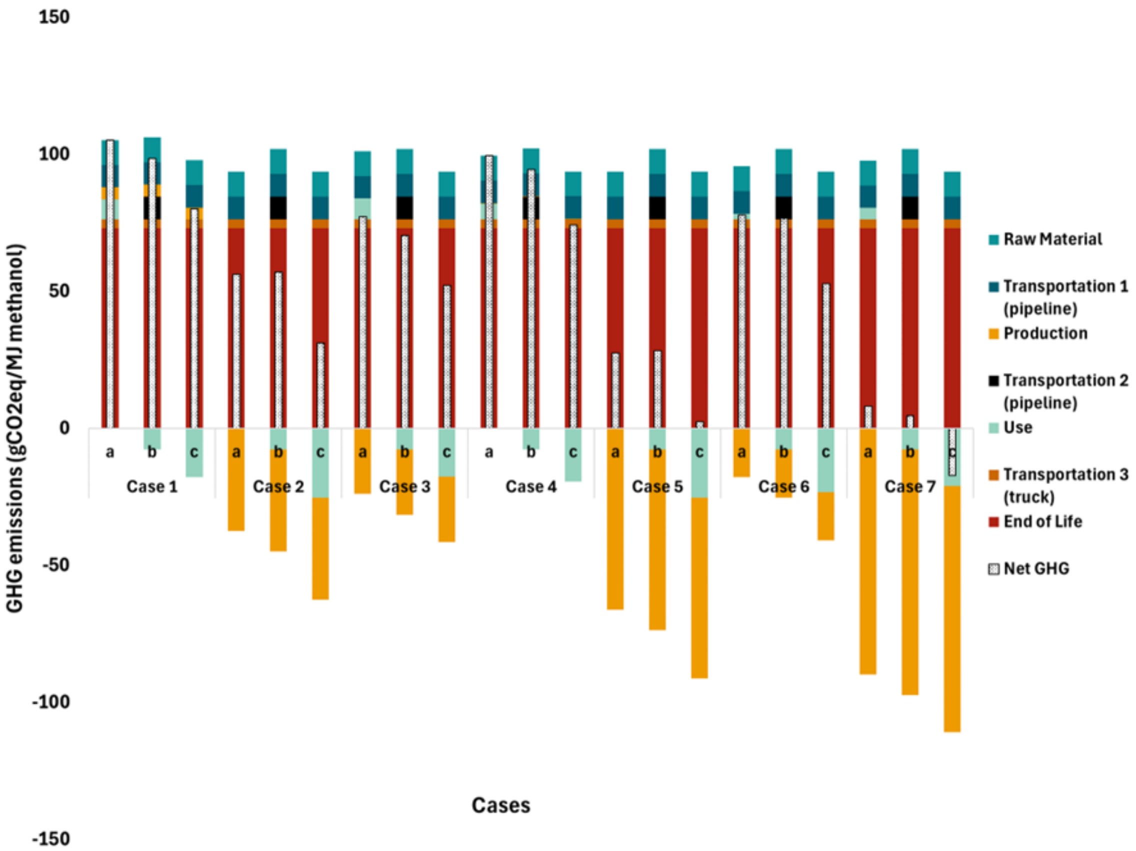

Figure ES ii. GHG Emissions from cradle-to-grave of Methanol Production: **a.** Co-located plants for methanol and diesel production using electricity from the grid **b.** Non-co-located plants for methanol production with nuclear integration for diesel production **c.** Co-located plants for methanol and diesel production integrated with nuclear energy

This study demonstrates that in reducing GHG emissions from methanol and methanol-to-diesel production, the most effective strategies involve combining high-efficiency hydrogen production using nuclear powered HTSE, advanced carbon capture methods like oxy-fuel combustion, co-location of production units for maximum integration, and substituting nuclear hydrogen for combustion-based heat and power sources. By aligning process design, carbon capture technologies, and energy supply sources, significant reductions, including net-negative emissions, are achievable. These approaches support strategic decisions for industrial operators looking to enhance environmental performance while maintaining reliability and compatibility with existing fuel markets.

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FIGURES

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ACRONYMS

ANL	Argonne National Laboratory
ASU	air separation unit
BAU	business-as-usual
BFD	block flow diagram
CCSU	carbon capture, sequestration, and utilization
CHP	combined heat and power
DOE-NE	Department of Energy, Office of Nuclear Energy
GHG	greenhouse gas
GREET	Greenhouse gases, Regulated Emissions, and Energy use in Technologies
GWP	global warming potential
HTGR	high-temperature gas reactor
HTSE	high-temperature steam electrolysis
IES	Integrated Energy Systems
INL	Idaho National Laboratory
IRA	Inflation Reduction Act
LCA	life cycle analysis
MTD	methanol-to-diesel
NG	natural gas
RWGS	reverse water-gas shift
SMNR	small modular nuclear reactor
SMR	steam-methane reforming
TEA	techno-economic assessment
WGS	water-gas shift
WHR	waste heat recovery

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1. INTRODUCTION

Methanol and diesel are crucial energy carriers with well-established infrastructure supporting modern industrial and transportation systems. These fuels serve as the backbone of energy supply chains, enabling a vast array of applications across industries ranging from manufacturing to logistics. Their importance is reflected in their widespread use for power generation, chemical processing, and mobility solutions. The global economy heavily depends on their availability, making them indispensable for sustaining modern industrial activities. As demand for energy continues to rise, ensuring the stability and sustainability of methanol and diesel supply chains is critical for economic resilience and energy security.

Methanol is a highly versatile chemical feedstock that plays a fundamental role in industrial production. It serves as a building block for various chemicals, plastics, and synthetic fuels, supporting key industries such as pharmaceuticals, agriculture, and construction. Additionally, methanol is increasingly being explored as a fuel for clean energy applications within the transportation industry, including its potential use in fuel cells and as a marine fuel alternative to conventional petroleum-based products. The demand for methanol continues to grow as industries seek more efficient and scalable chemical solutions to meet evolving market and regulatory requirements. Its adaptability and broad applicability make it a key contributor to industrial progress and energy innovation.

Diesel, on the other hand, is essential for powering critical sectors that require high-energy-density fuels. It is widely used in heavy-duty transportation, shipping, railways, and industrial machinery, where electrification is not yet a feasible alternative. The reliability and energy efficiency of diesel make it the preferred choice for commercial fleets, construction equipment, and emergency backup power systems. Its ability to provide uninterrupted energy supply for essential services, such as agriculture and public transportation, highlights its significance in maintaining social and economic stability. As industries and governments work toward reducing emissions, the need for sustainable diesel alternatives has become increasingly urgent.

Despite their widespread utility, conventional methods of producing methanol and diesel are heavily reliant on fossil fuels. This dependence introduces significant economic and environmental challenges, as fluctuations in crude oil and natural gas prices can lead to supply chain instability and market volatility. Additionally, geopolitical factors and resource depletion further contribute to concerns about long-term availability and affordability. The risks associated with fossil fuel dependency underscore the urgent need for alternative production pathways that can provide energy security while reducing environmental impact. Developing more sustainable and economically resilient fuel production methods is essential for future energy stability.

Methanol production is primarily based on steam-methane reforming, a highly energy-intensive process that generates substantial greenhouse gas (GHG) emissions. Similarly, diesel is predominantly derived from petroleum refining, which not only emits large amounts of carbon dioxide (CO_2) but also involves complex refining processes that require vast amounts of energy and raw materials. These conventional production methods contribute significantly to climate change, resource depletion, and environmental degradation. As global regulations tighten around carbon emissions and sustainability standards, industries must explore cleaner and more efficient production alternatives to remain viable in the evolving energy landscape.

To enhance energy security and environmental sustainability, it is crucial to develop alternative methods for producing methanol and diesel. Reducing reliance on fossil fuels can help stabilize energy markets, shield economies from price volatility, and lower carbon emissions. The search for viable alternatives has led to increased interest in advanced energy technologies capable of providing consistent and low-emission energy sources for industrial applications. Clean energy integration into fuel production systems is a key strategy for reducing the carbon footprint of essential fuels without compromising their accessibility or performance.

Advanced nuclear energy offers a transformative solution for methanol and synthetic diesel production by providing a stable and carbon-free power source. Through nuclear-assisted methanol-to-diesel (MTD) processes, industries can transition away from fossil-based energy while maintaining operational efficiency and economic competitiveness. Unlike intermittent renewable sources, nuclear reactors generate continuous, high-output energy that is essential for large-scale industrial applications. The integration of nuclear power into fuel synthesis pathways represents a strategic shift toward cleaner, more reliable, and cost-effective energy solutions.

Nuclear reactors produce consistent, low-emission electricity, heat, and – when coupled to high-temperature steam electrolysis (HTSE) – hydrogen, all of which are critical inputs for sustainable methanol production. The availability of high-temperature process heat from advanced nuclear systems can enhance the efficiency of methanol synthesis while reducing overall energy consumption. Additionally, nuclear-generated hydrogen offers a clean alternative to fossil fuel-based hydrogen, further improving the environmental performance of synthetic fuel production. By leveraging nuclear energy, industries can decarbonize fuel manufacturing processes while ensuring long-term economic and operational sustainability.

The integration of advanced nuclear systems with carbon capture, sequestration, and utilization (CCSU) technologies further enhance the potential for a circular carbon economy. Capturing carbon dioxide (CO_2) from industrial emissions and recycling it as a feedstock for methanol production can significantly reduce net carbon emissions. This approach minimizes the need for virgin carbon sources and helps close the carbon loop in fuel and chemical manufacturing. The ability to reuse captured CO_2 aligns with global efforts to develop more sustainable industrial processes while addressing climate change challenges.

Nuclear power's high energy density and minimal material requirements make it a highly efficient and sustainable alternative to fossil fuels. Unlike conventional energy sources, nuclear reactors provide reliable baseload power with minimal environmental impact, making them well-suited for large-scale industrial applications. Additionally, the ability to operate independently of weather conditions makes nuclear energy an attractive option for regions where renewable energy sources alone cannot meet industrial energy demands. As industries seek long-term solutions for clean energy integration, nuclear technology emerges as a key enabler of resilient and low-carbon fuel production systems.

As concerns over energy security, climate change, and resource sustainability continue to grow, advanced nuclear technologies offer a viable pathway for the future of fuel and chemical production. The integration of nuclear energy with methanol and diesel synthesis can help industries mitigate risks associated with fossil fuel dependency, market fluctuations, and regulatory pressures. By investing in nuclear-powered fuel production, industries can secure a stable and sustainable foundation for future energy systems. This strategic transition positions nuclear energy as a crucial component of a cleaner, more resilient, and economically competitive industrial landscape

This report presents a comprehensive cradle-to-grave life cycle analysis of methanol and methanol-to-diesel production systems, with a focus on configurations that incorporate advanced nuclear technologies. It begins with a high-level overview of the study objectives and provides relevant background context. The analysis defines the scope, system boundaries, and functional units, and it draws on consistent and transparent data sources for the life cycle inventory. Key process stages include raw material extraction, methanol production via steam methane reforming and CO_2-based pathways, conversion of methanol to diesel, and fuel use. Two detailed gate-to-gate analyses are developed for the methanol synthesis and methanol-to-diesel conversion stages, which serve as inputs to the overall cradle-to-grave analysis. The report examines energy flows and GHG emissions associated with each configuration, comparing results across different technological pathways. It concludes with a synthesis of key findings, supported by figures and tables that illustrate system boundaries, process flow diagrams, emissions data, and modeling assumptions.

The results of the life cycle analysis (LCA) will be interpreted in the context of industrial and research priorities. Interpretation will involve identifying key environmental hotspots in the production processes and opportunities for improvement. Trade-offs, such as the increased material use for advanced nuclear infrastructure versus the substantial reduction in emissions, will be analyzed. The results will offer recommendations, focusing on technologies and practices that maximize environmental benefits in the entire system. Additionally, the reduction of greenhouse gas (GHG) emissions plays a critical role in estimating the benefits provided by the Inflation Reduction Act (IRA) in the techno-economic assessment (TEA). By quantifying the decrease in GHG emissions, it is possible to determine the eligibility for various incentives, tax credits, and subsidies offered under the IRA, which are designed to encourage the adoption of cleaner technologies and sustainable practices. These financial incentives can significantly offset the costs associated with implementing environmentally friendly processes, thereby improving the overall economic feasibility and attractiveness of the project. Incorporating the GHG emission reductions into the TEA enables a more accurate assessment of the potential financial benefits, demonstrating how the alignment with the IRA's objectives can enhance the sustainability and profitability of the initiative.

2. METHODOLOGY

LCA is defined in Section 2.1, and the elements of the methodology relevant to synthetic fuels production are discussed. The plan for obtaining input data needed to conduct the LCA is established in Section 0. Then, the material and energy balances for the specific case studies are outlined in Sections 2.3 and 2.4. Together, the thermodynamic models designed in previous work [1, 2] and the methodology designed here are used to generate the results featured in Section 3.

2.1 Scope and Boundaries

The primary objective of this study is to evaluate and compare the environmental impacts of traditional fossil-based production pathways against emerging, sustainable alternatives that leverage advanced nuclear energy for heat and power. These pathways include processes using CCSU and hydrogen.

LCA is a systematic approach that calculates the environmental burdens of a product or system. Methanol production and MTD life cycle models will be a compilation of unit processes in which parameters are scaled to reflect a functional unit of methanol that accounts for uncertainty across multiple scenarios. An LCA requires a functional unit, boundaries, scenarios, and metrics.

2.1.1 Functional Unit

A functional unit is necessary to provide a common basis for scaling life cycle stages and, in some instances, to compare scenarios. The functional unit for this analysis is 1 MJ of methanol delivered to the consumer, on a lower heating value basis.

2.1.2 System Boundaries and Case Study Definitions

A gate-to-gate analysis within the context of an LCA focuses on evaluating the environmental impacts associated with a specific segment of a product's life cycle, typically from the point of entry into a particular process or production facility to the point of exit. This method provides a detailed examination of the inputs, outputs, and emissions directly related to the manufacturing processes, allowing for a more precise identification of opportunities for environmental improvements and efficiencies within that specific boundary. By narrowing the scope to a single stage in the product's life, gate-to-gate analysis offers a targeted approach for identifying and mitigating environmental impacts, thereby contributing to the overall sustainability of the product. This study will perform two different gate-to-gate analyses: one for methanol production through steam methane reforming and another for the process of converting methanol to diesel. These cases will be aligned with the case studies presented in the previous report and presented in Section 2.3 where nuclear integration and CCSU are included [1].

In this analysis, methanol production is considered as the *production* stage, while diesel production via methanol-to-diesel conversion is treated as the *use* stage within a comprehensive cradle-to-grave analysis. The system boundaries for the cradle-to-grave analysis are clearly defined in this study to capture all relevant upstream and downstream processes (Figure 1).

To support this full LCA, two detailed gate-to-gate analyses are conducted independently. The first focuses on methanol synthesis based on the steam methane reforming (SMR) process, encompassing feedstock inputs, hydrogen production, and methanol synthesis. The second gate-to-gate analysis evaluates the conversion of methanol into diesel, capturing the key energy and material flows associated with the catalytic conversion process.

These two gate-to-gate assessments provide the necessary data and process-specific insights that feed into the overall cradle-to-grave analysis. This integrated approach enables a more accurate and granular evaluation of environmental and process performance metrics across the full life cycle of methanol-to-diesel fuel production.

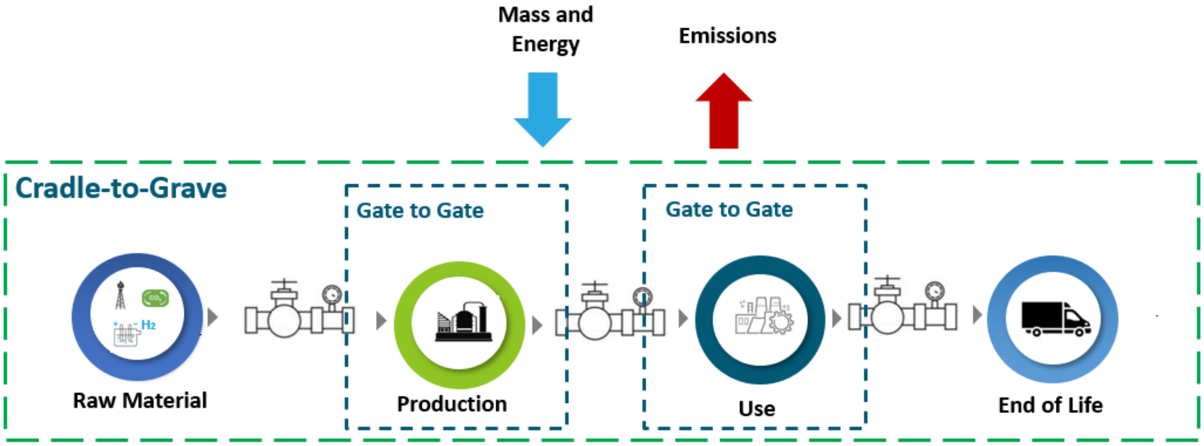

Figure 1. System boundaries of Conventional and Future Methanol and Methanol to Diesel Plant Integrated with Advanced Nuclear

For the cradle-to-grave analysis, four main stages of the process will be analyzed:

1. Raw material extraction
2. Methanol production
3. Use
4. End of life

2.1.3 Raw Material Production or Extraction

2.1.3.1 Natural Gas

Natural gas (NG) is the main raw material for SMR-based methanol production, with shale gas serving as a major source. Its extraction begins with geological surveys to locate suitable shale formations, followed by drilling and hydraulic fracturing (fracking) to release trapped natural gas. The extracted gas, primarily methane, undergoes processing to remove impurities such as CO_2, H_2S, and water vapor, ensuring it meets quality standards. Once purified, the natural gas is transported via pipelines to industrial facilities, where it is used in SMR to produce methanol [3].

2.1.3.2 Water

Steam is used to reform natural gas into syngas. In methanol production, it is the source of oxygen, later formed into a hydroxyl group. The heat recovery boilers that produce this steam require treated water.

2.1.4 Methanol production

Methanol production from SMR begins with the conversion of natural gas, primarily methane, into synthesis gas (syngas), which consists of hydrogen, carbon monoxide, and carbon dioxide. This process takes place in a reformer, where methane reacts with steam at high temperatures ranging from 700 to 1,000°C in the presence of a nickel-based catalyst. The reaction breaks down methane molecules and produces hydrogen and carbon monoxide as primary products. Additionally, a secondary reaction (the water-gas shift - WGS) occurs where carbon monoxide reacts with steam to generate more hydrogen while producing carbon dioxide [3]. To optimize the synthesis gas composition for methanol production, a separate water-gas shift reactor is used to adjust the hydrogen-to-carbon monoxide ratio. Once the synthesis gas composition is adjusted, it undergoes compression and enters a methanol synthesis reactor, where hydrogen reacts with carbon monoxide and carbon dioxide under high pressure and moderate temperature. This reaction takes place over a copper-based catalyst, facilitating the conversion of these gases into methanol. In this process, carbon monoxide reacts with hydrogen to form methanol, while carbon dioxide also participates by reacting with hydrogen to produce methanol and water as a byproduct. The crude methanol mixture is then separated and purified through distillation, removing water and other impurities to obtain high-purity methanol suitable for industrial applications.

2.1.5 Methanol use (Methanol-to-Diesel)

In the context of the LCA of methanol, diesel plays a role at the *use* stage of the life cycle when considering the potential for methanol to be converted into synthetic diesel or used as a fuel in transportation systems. However, methanol itself is not typically used directly in diesel engines. Instead, it can be converted into synthetic diesel through processes like MTD synthesis. For this study, the chemical process model for reverse water-gas shift RWGS-to-methanol-to-diesel was developed and shared by Argonne National Laboratory (ANL) [4]. In this pathway, the RWGS-based CO_2 conversion model produces methanol that is processed into liquid fuels in an integrated MTD plant. Here, methanol is dimerized and dehydrated into short-chain olefins which are then oligomerized and hydrotreated into long-chain paraffins and separated by fractionation into liquid fuel products. For the purposes of this study, Idaho National Laboratory (INL) researchers isolated the MTD model allowing for a standalone MTD plant to be used in the gate-to-gate *use* analysis as well as the cradle-to-grave analysis.

2.1.6 End of Life

At the end of the LCA of methanol, synthetic diesel derived from methanol can be used in the transportation sector, particularly in heavy-duty vehicles, shipping, and industrial machinery that rely on high-energy-density fuels. At the end of the LCA of methanol, synthetic diesel derived from methanol can be used in the transportation sector, particularly in heavy-duty vehicles, shipping, and industrial machinery that rely on high-energy-density fuels. This use of synthetic diesel made from methanol can help reduce reliance on fossil-based diesel and lower the overall carbon footprint of transportation. By integrating methanol-derived synthetic diesel into the transportation system, the life cycle of methanol closes with a product that can replace traditional diesel, benefiting from the earlier stages of methanol production, such as CO_2 recycling and clean hydrogen use. As such, the final phase of the methanol LCA contributes to reducing emissions in sectors that are otherwise difficult to electrify, enhancing the overall sustainability of the fuel.

In the context of the LCA of methanol, diesel plays a role at the end of the life cycle when considering the potential for methanol to be converted into synthetic diesel or used as a fuel in transportation systems. Methanol, when produced through sustainable processes such as nuclear-powered hydrogen production and CO_2 capture, offers a lower-carbon alternative to conventional fossil fuels. However, methanol itself is not typically used directly in diesel engines. Instead, it can be converted into synthetic diesel through processes like MTD synthesis. Table 1 summarize the assumptions in each stage considered for the cradle-to-grave analysis of individual methanol production.

Table 1: Assumptions of Each Stage of the Process for the cradle-to-grave analysis of the methanol/synthetic fuel lifecycle

Reference Plant	**Plant 1**
Raw Material	NG: Shale Gas Extraction
Transportation	NG Pipelines
Production	Steam Methane Reforming
Transportation	Methanol Pipelines
Use	Synthetic Diesel Production (Argonne Model)
Transportation	Truck
End of Life	Vehicle Operation

2.2 Life Cycle Analysis Inventory Data Collection

A Life Cycle Inventory (LCI) will be conducted to gather all necessary input and output data for the production systems based on the case studies presented in Section 2.3. This inventory will encompass resource requirements, energy inputs, and emissions data for conventional systems relying on NG, as well as advanced systems that integrate nuclear energy. For future systems, additional data on innovative technologies, such as hydrogen production via high-temperature electrolysis using nuclear heat, will be included. This phase will involve data collection from scientific literature, and process simulations to ensure the results are comprehensive and reliable.

2.3 Gate-to-Gate Methanol Production

The benchmark study for this LCA is an existing SMR-based conventional methanol synthesis plant, with a median capacity of 1 MMT/yr selected in previous work Figure 2 is a block flow diagram (BFD) that describes this plant under business-as-usual operation. It is assumed in this work and the upcoming TEA that this is an existing plant that converts NG to methanol using fully depreciated equipment. A robust waste heat recovery system uses stream cooling duties and supplemental NG to produce high-pressure steam that is let-down in backpressure turbines to produce electricity and low-pressure steam for distillation reboilers and other duties.

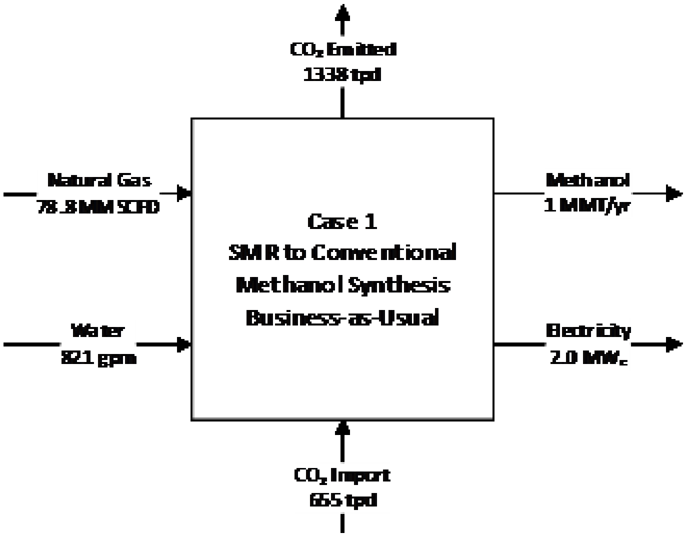

Figure 2. BFD of BAU SMR-based methanol plant.

Several possible pathways for nuclear integration are described below and illustrated in Figure 3, where dark blue blocks represent the existing plant, and the lighter colors represent new equipment required for the integration [2]. For these cases where a nuclear reactor is built on-site, low-pressure steam is also supplied to the methanol distillation columns, backing out supplemental NG fuel from the business-as-usual (BAU) waste heat recovery system; as a result, the waste heat recovery (WHR) system also produces less electricity, and the high-temperature gas reactor (HTGR) type small modular nuclear reactor (SMNR) will need to provide the plant with some electricity to power compressors, pumps, and other small duties. The material and energy balances for each of these cases are thoroughly described in previous work [1]. They are quantitatively summarized in this report by Table 2 and Figure 4:

- Case 1 – BAU operation of the existing SMR-based conventional methanol synthesis plant.
- Case 2 – Hydrogen fuel switching. Supplemental NG fuel used in BAU to drive the endothermic reformer is replaced with HTSE derived hydrogen produced by nuclear power.
- Case 3 – Furnace electrification. Supplemental NG fuel is not used. Instead, a resistive electric furnace is used to supply the reformer with high-temperature heat.
- Case 4 – Conventional CCSU. An amine-based scrubber is installed to capture CO_2 from the flue gas, and recover it for storage and later utilization for another purpose. The steam and electricity to power this CCSU system is produced by a new NG (combined heat and power (CHP), whose emissions are also captured for later utilization.
- Case 5 – Nuclear powered CCSU. Nuclear steam and electricity are used to power the CCSU system.
- Case 6 – Oxyfuel combustion with oxygen from air separation. Nitrogen is removed from the combustion air to avoid diluting the flue gas. This simplifies the CO_2 recovery.
- Case 7 – Oxyfuel combustion with oxygen from HTSE. The byproduct oxygen from HTSE is swept by CO_2 and recovered for use as combustion “air” [5]. Again, this allows the CO_2 in the flue gas to easily be recovered and utilized for another purpose.

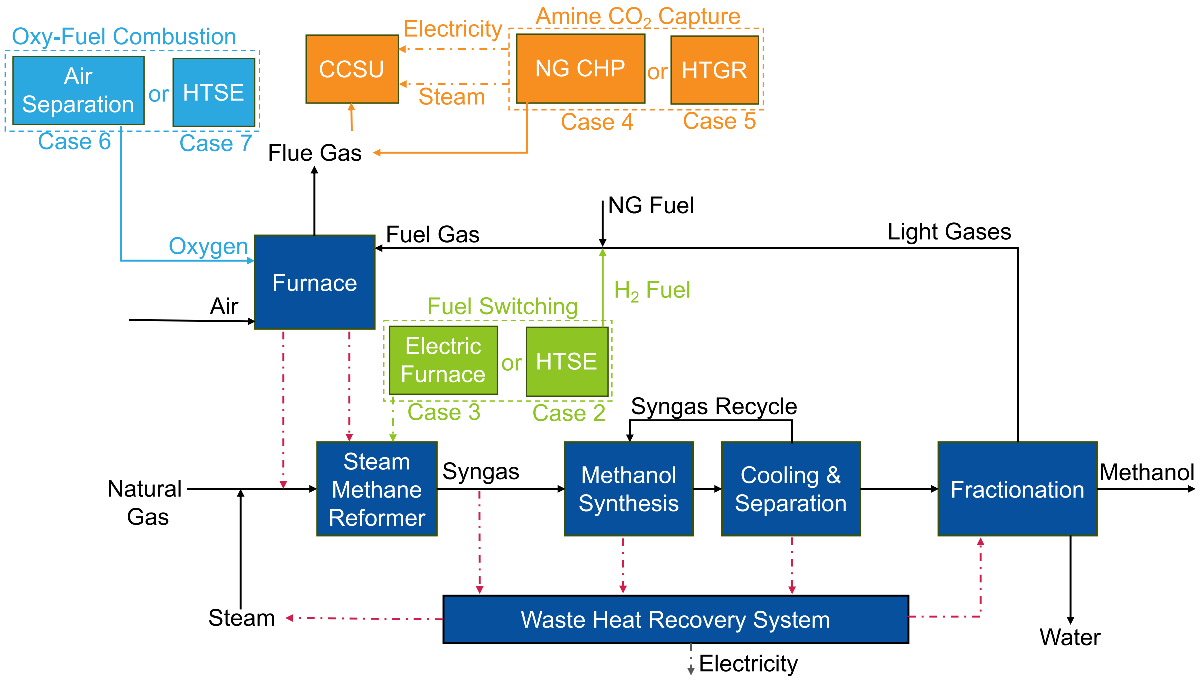

Figure 3. Schematic drawing of SMR based conventional methanol plant with potential nuclear integrations.

Table 2. HTGR-type SMNR requirements for SMR-based designs [1].

Category	BAU	Nuclear Integration		Amine-Based CCSU		Oxy-fuel Combustion	
Case Number	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7
Case Description	Business-as-Usual	H_2 Fuel Switch	Electrified Reformer	NG-CHP Powered	Nuclear Powered	O_2 from Air Separation	O_2 from Nuclear HTSE
Nuclear Thermal Power (MWth)	-	600	400	-	200	200	1200
LP Steam (MWth)	-	45.1	21.2	-	66.2	21.2	83.3
Methanol Distillation	-	*21.2*	*21.2*	-	*21.2*	*21.2*	*21.2*
CO_2 Capture	-	-	-	*67.4*	*45.0*	-	-
HTSE	-	*23.9*	-	-	-	-	*62.1*
Electricity Gen. (MWe)	-	232.6	157.3	24.5*	69.1	76.7	466.7
WHR Deficit	*-2.0*	*4.1*	*4.1*	*-2.0*	*4.1*	*4.1*	*4.1*
Electric Reformer	-	-	*154.5*	-	-	-	-
CO_2 Capture	-	-	-	*7.5*	*4.9*	*3.1*	*3.1*
HTSE	-	*167.9*	-	-	-	-	*432.2*
Air Separation	-	-	-	-	-	*25.6*	-
Export to Grid	*2.0*	*60.6*	*-1.3*	*19.0*	*60.1*	*43.9*	*27.3*

*In case 4, heat and electricity is generated by a 97.8 MW-LHV NG-CHP rather than an SMNR.

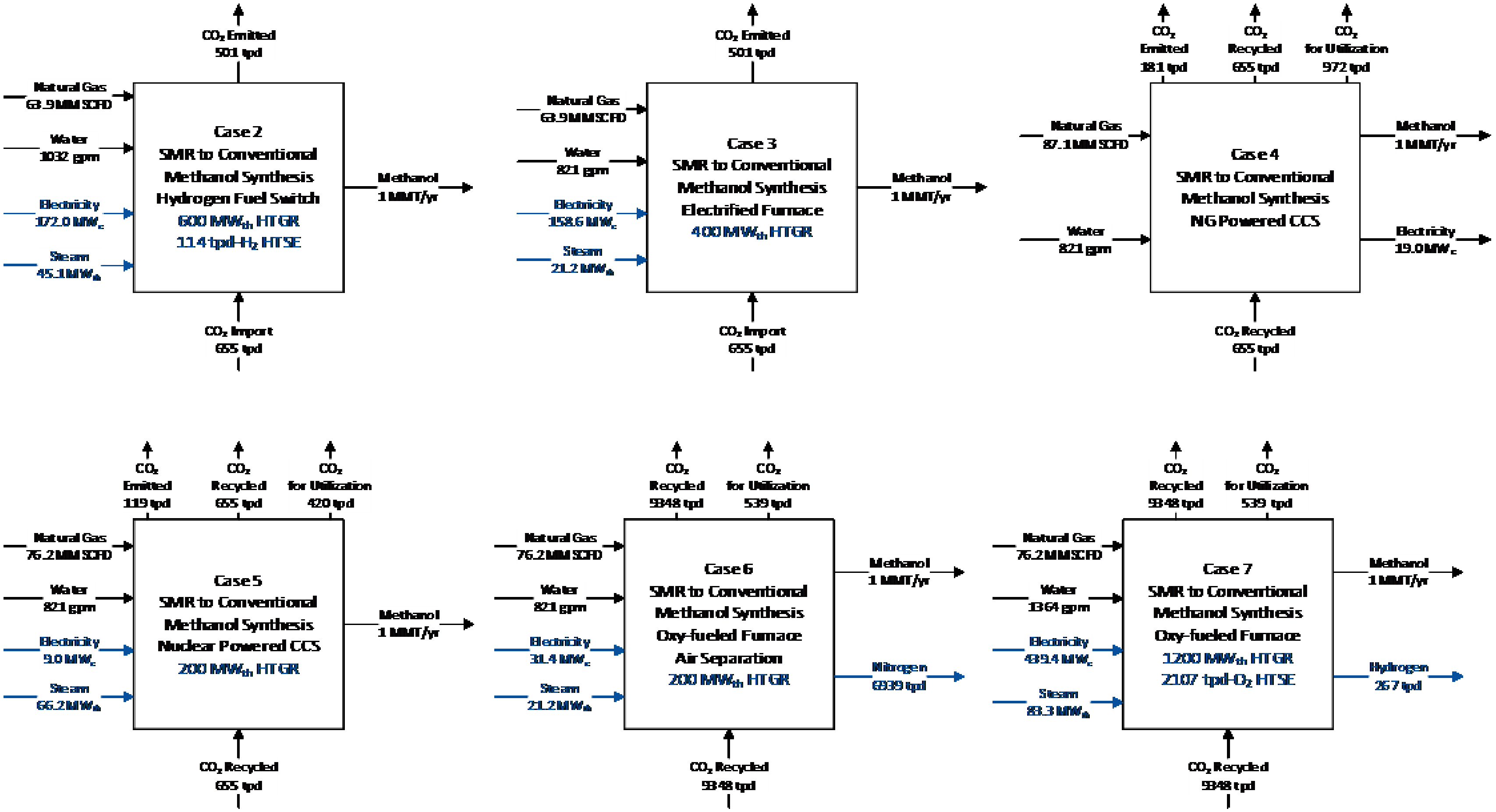

Figure 4. BFDs of SMR-based methanol plant delta cases.

2.4 Gate-to-Gate Methanol-to-Diesel Conversion

In this study, methanol is an intermediate product, with it later being converted into liquid fuels via a multi-step process. First, methanol is dimerized and dehydrated into short-chain olefins which are then oligomerized and hydrotreated into long-chain paraffins and separated by fractionation into naphtha, jet fuel, and diesel products. The residual oils and waxes are hydrocracked, and recirculated, while the gases lighter than the naphtha specifications are burned on-site. These are exothermic reactions carried out at moderate temperatures. The plant model was developed by ANL in Aspen Plus as part of an integrated RWGS-to-MTD plant model [4]; the MTD section of this plant was isolated by INL and scaled to convert 1 MMT/yr of methanol to liquid fuels. The hydrotreating and hydrocracking reactors consume hydrogen, which is assumed to be produced by HTSE. The light-gases are burned in pure oxygen, which is assumed to be produced by air separation as the burner requires more oxygen than is produced by the appropriately sized HTSE.

INL then designed a robust waste-heat recovery system that cools the exothermic reactors by making steam that can be used in the reboilers of the fractionation section and to boil HTSE feedwater. Backpressure turbines were used to make electricity and deliver reboiler steam at the appropriate temperature and pressure. A portion of this electricity was used by the compressors powering the ammonia refrigeration cycles needed for the sub-ambient condensers of some distillation columns and the n-pentane heat pump used to boost a portion of the low temperature waste heat to reboiler grade steam. With these heat pumps, the MTD plant (including HTSE) is heat neutral, meaning that only an electrical connection was required.

The WHR system for the standalone MTD plant satisfies all thermal loads of the plant, and nets 16.97 MWe after accounting for feedwater pumps and refrigeration/heat pump compressors. MTD plant house loads (pumps and compressors used to pressurize reactor feeds etc.) consume 10.49 MWe. The air separation unit (ASU) used to provide 6.19 kg/s of oxygen for oxyfiring the light gases requires 6.50 MWe, as 99 mol% O_2 requires 1.05 MJe/kg-O_2 [6]. Before powering the HTSE plant, the standalone MTD plant is essentially electricity neutral. Including rectification (95% AC-to-DC), trim heating, and product separation/compression, the HTSE plant consumes 38.8 kWh/kg-H_2. Thus, the MTD plant, including HTSE for olefin hydrotreating and wax cracking consumes 60.5 MWe. The plant is represented by the BFD shown in Figure 5.

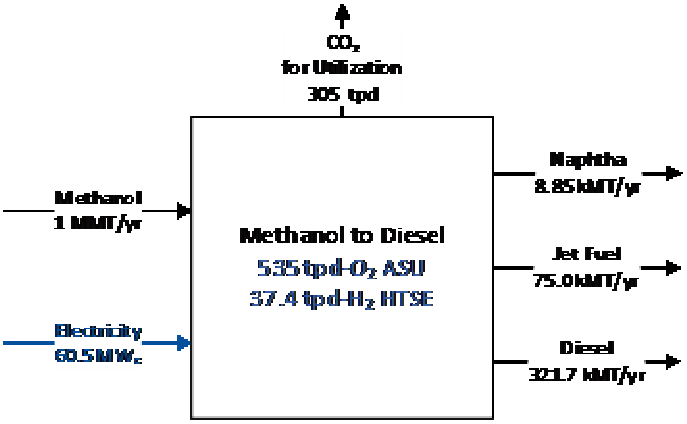

Figure 5. BFD of standalone MTD plant

Because there are no thermal interconnections between the SMR-based methanol plant and the MTD plant, the two plants do not necessarily need to be co-located. If the MTD plant is built at a different location, the plant could be powered entirely by the electrical grid. Alternatively, an 200 MWth (80 MWe) HTGR could be built on-site to produce the required 60.5 MWe and put 19.5 MWe of nuclear electricity onto the grid. When the MTD plant is co-located, there is no need to ship the methanol from the SMR-based production plant, and electricity produced at the methanol (including any SMNRs) can be transferred to the MTD plant behind the meter. Table 3 summarizes the electricity requirements of the MTD plant when associated with the 7 case studies at the conventional SMR-based methanol plant. Similarly, for each case where the MTD plant requires grid electricity after consuming the export from the methanol plant, an additional 80 MWe of SMNR capacity could be built resulting in a surplus of electricity exported to the grid.

Table 3. Grid electrical requirements for standalone MTD plant interconnected to the SMR-based methanol plant for each case

Category	BAU	Nuclear Integration		Amine-Based CCSU		Oxy-fuel Combustion	
Case Number	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7
Case Description	Business-as-Usual	H_2 Fuel Switch	Electrified Reformer	NG-CHP Powered	Nuclear Powered	O_2 from Air Separation	O_2 from Nuclear HTSE
From SMR-based methanol plant (MWe)	2.0	60.6	-	19.0	60.1	43.9	27.3
From electrical grid (MWe)	58.5	-0.1	60.5	45.5	0.4	16.6	33.2

The environmental impacts of the systems will be assessed using life cycle impact assessment (LCIA) methodologies, which convert inventory data into environmental indicators. For the life-cycle analysis (LCA) in this study, the GREET Model (Greenhouse gases, Regulated Emissions, and Energy use in Technologies) will be used to perform the calculations [7]. Particular attention will be paid to global warming potential (GWP), as the integration of advanced nuclear aims to drastically reduce carbon emissions compared to conventional fossil-fuel-based systems. GREET, developed by ANL, is a robust tool designed to evaluate the environmental impacts of energy and material systems across their life cycles. Its ability to assess greenhouse gas emissions, regulated pollutants, and energy consumption makes it ideal for analyzing the production, transportation, and utilization phases of fuels and industrial processes.

3. LIFE CYCLE ANALYSIS RESULTS AND DISCUSSION

The results from the LCA are presented in 3 different sections. First, with both the methanol production and methanol-to-diesel conversion facilities analyzed as gate-to-gate plants, then with the two facilities combined in a cradle-to-grave analysis.

3.1 Gate-to-Gate Methanol Production

Figure 6 presents the GHG emissions for different methanol production scenarios, including BAU, CCSU, and nuclear and hydrogen integration with SMR. Four key factors influence each scenario's environmental impact. Wide bars show the positive and negative lifecycle emissions from all subsystems and plant sections in the given case study, and the narrow bar displays the net lifecycle:

- Among all cases, the BAU scenario results in the highest net GHG emissions, totaling 4.3 g CO_2 eq/MJ of methanol. In contrast, integrating CCSU, hydrogen, and nuclear technologies leads to a significant reduction, with net emissions ranging from 0.2 to -89.7 g CO_2 eq/MJ of methanol.
- Comparing BAU to nuclear-integrated cases, switching to hydrogen as a fuel (Case 2) achieves a greater reduction, with net GHG emissions of -37.3 g CO_2 eq/MJ of methanol,

compared to the electrified reformer (Case 3), which results in -23.8 g CO_2 eq/MJ methanol.

- When CCSU is applied to the BAU scenario using a fossil fuel boiler (Case 4), net GHG emissions decrease from 4.3 to 0.2 g CO_2 eq/MJ of methanol.
- Further integrating hydrogen and nuclear technologies into the CCSU scenario enhances emissions reductions. The best performance is observed in Case 7, where oxy-fuel combustion (using oxygen from nuclear-powered high-temperature steam electrolysis) results in net emissions of -89.7 g CO_2 eq/MJ of methanol. This is followed by the amine-based CCSU powered by nuclear (Case 5), with net emissions of -66.1 g CO_2 eq/MJ of methanol, and oxy-fuel combustion using oxygen from an air separation unit (Case 6), which achieves -17.7 g CO_2 eq/MJ methanol.

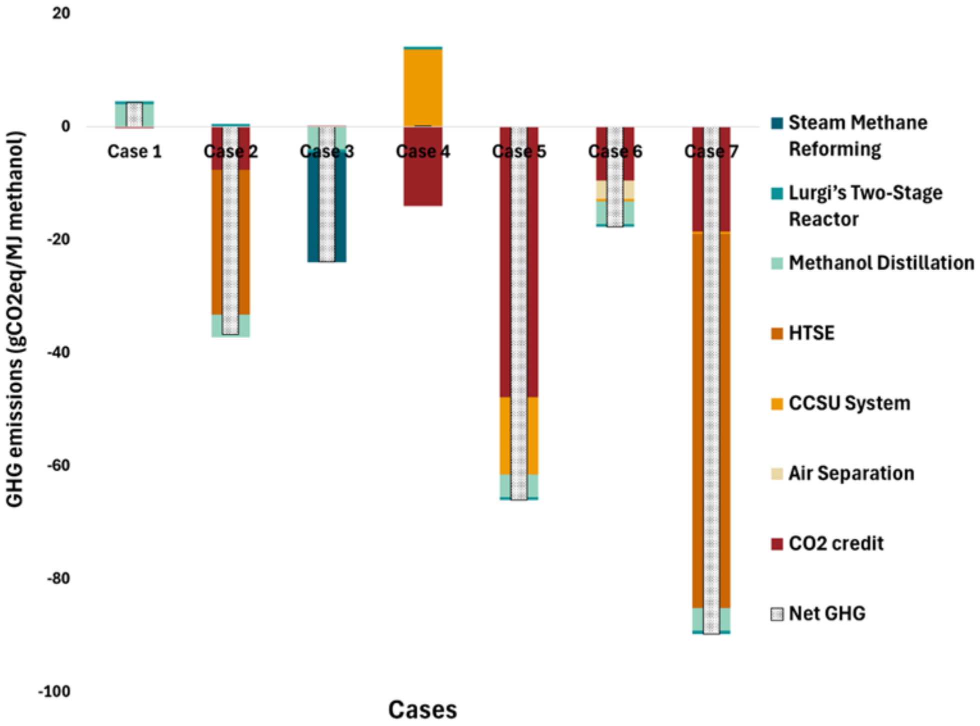

Figure *6.* GHG Emissions of Steam Methane Reforming Case Studies

The differences in net GHG emissions across the various methanol production scenarios are primarily influenced by energy requirements and the integration of CCSU, hydrogen from high-temperature steam electrolysis (HTSE), and nuclear energy. Each scenario's environmental performance depends on how these elements are incorporated into the process, either by substituting fossil-based inputs or improving carbon capture efficiency.

The business-as-usual (BAU) case exhibits the highest GHG emissions due to its reliance on fossil fuels for both hydrogen production and process heat. SMR in this scenario operates without carbon capture, allowing nearly all CO_2 generated to be released into the atmosphere. The absence of low-carbon energy sources means that both direct emissions from combustion and indirect emissions from hydrogen production contribute significantly to the overall footprint.

When nuclear energy is introduced into the system, emissions are reduced by shifting away from fossil fuel combustion. Two integration approaches are considered: replacing fossil fuels with hydrogen or electricity as a heat source. Using hydrogen from a nuclear-powered HTSE system for combustion heating leads to greater emissions reductions than the electrified reformer because it eliminates direct fossil fuel use and associated emissions.

The inclusion of CCSU in the BAU scenario significantly lowers emissions by capturing CO_2 from SMR and combustion sources. However, this approach does not fully eliminate emissions due to the energy required for capture and compression. The overall effectiveness of CCSU depends on how efficiently CO_2 can be separated and stored, as well as the energy source used to power the capture system.

Further reductions are achieved when CCSU is combined with nuclear energy and hydrogen integration. The most effective case uses an oxy-fuel combustion system where oxygen is supplied by a nuclear-powered HTSE process. This configuration enhances CO_2 capture efficiency while eliminating the need for conventional air separation, reducing energy consumption and associated emissions. Another effective approach is using nuclear energy to power an amine-based CCSU system, which improves overall process efficiency by eliminating fossil-based energy inputs. In contrast, a system that relies on an air separation unit for oxygen supply achieves a lower emissions reduction due to its additional energy demands and reliance on conventional separation technologies.

Overall, the integration of nuclear energy and hydrogen from HTSE into the methanol production process leads to substantial reductions in GHG emissions. The most effective configurations are those that maximize CO_2 capture efficiency while replacing fossil-based energy sources with nuclear power. Hydrogen substitution for fuel proves to be more effective than electrification alone and using nuclear-powered oxygen production further enhances the benefits of CCSU. These findings highlight the potential for nuclear-hydrogen integration to play a key role in decarbonizing methanol production and reducing industrial emissions.

3.2 Gate-to-Gate Methanol to Diesel Production

Figure 7 presents the GHG emissions associated with the stand-alone methanol-to-diesel conversion process. In this configuration, the system is fully integrated in terms of internal energy use. Heat and electricity required for methanol upgrading and diesel synthesis are supplied through process coupling and thermal recovery. As a result, the only significant external energy demand comes from the production of hydrogen via HTSE as it was explained in Section 2. For this analysis, two cases were evaluated: one where HTSE is powered by electricity from the grid and another where it is powered by a dedicated nuclear source.

Key findings from these two cases include:

- Grid-powered HTSE results in the highest emissions, reaching 7.6 g CO_2 eq/MJ of methanol. This reflects the mixed composition of the electricity grid, which includes a significant portion of combustion-based generation.
- Nuclear-powered HTSE provides both the high-temperature electricity required for efficient electrolysis. This configuration avoids emissions associated with fuel combustion and yields the lowest emissions in this analysis, with net emissions reaching -7.6 g CO_2 eq/MJ of methanol. The negative value reflects both the efficient integration and the potential for carbon removal through downstream capture and system coupling.

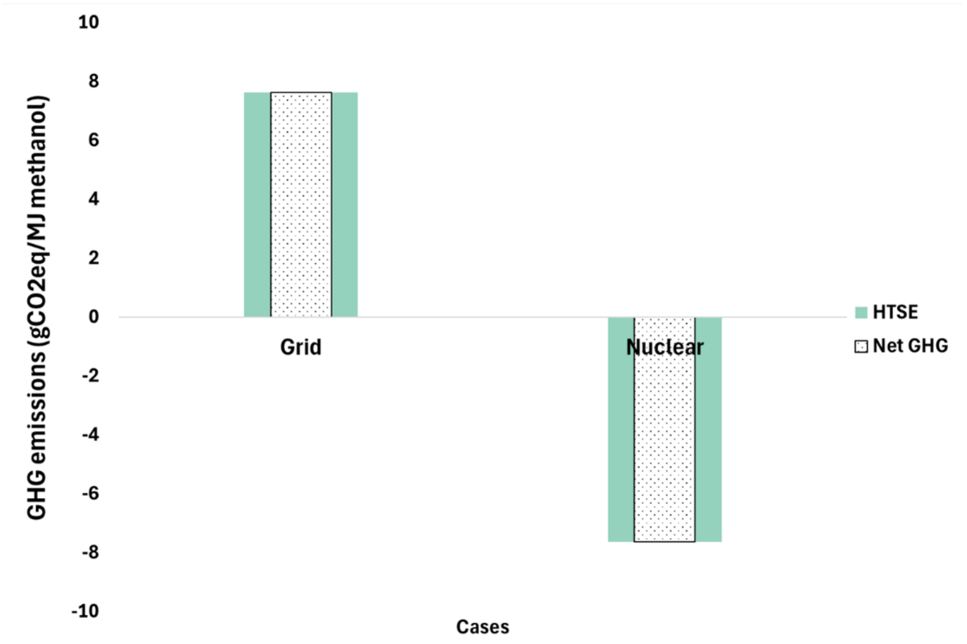

Figure 7. GHG for the stand-alone methanol to diesel process

These results highlight the importance of external energy sources in shaping the emissions profile of hydrogen-intensive fuel production pathways. While internal process integration ensures baseline efficiency, the external inputs, especially for hydrogen, can significantly alter the overall environmental performance.

3.3 Cradle-to-Grave Methanol Production

Figure 8 shows the cradle-to-grave GHG emissions associated with various methanol and methanol-to-diesel production pathways. The scenarios analyzed are based on the gate-to-gate analysis for the methanol and methanol-to-diesel processes, which include:

- A reference case representing current industrial practice (BAU) [2].
- Configurations incorporating CCSU
- Systems where hydrogen and nuclear energy are integrated with SMR
- MTD production powered by the grid and nuclear energy.

Each case is further examined under three configurations based on spatial layout and process integration:

(a) Co-located methanol and diesel plants using electricity from the grid

(b) Methanol and diesel production at separate sites, with nuclear energy used in diesel production

(c) Fully co-located and nuclear-integrated production of methanol and diesel

From this analysis, five key observations were found:

- The highest GHG emissions occur in scenarios relying on natural gas and grid electricity, particularly in the absence of nuclear integration. BAU cases (Case 1) emit 80.1 to 105.3 g CO_2 eq/MJ, while CCSU-enabled systems without alternative energy inputs (Case 4) emit 74.3 to 99.5 g CO_2 eq/MJ.

- Scenarios that combine CCSU with hydrogen and thermally driven electrolysis using nuclear heat significantly lower emissions. The most favorable configuration (Case 7c), involving co-located facilities and oxy-fuel combustion with oxygen from HTSE, achieves -17.1 g CO_2 eq/MJ of methanol.
- When CCSU is not used, hydrogen-based systems outperform electrified reforming processes. Hydrogen-powered cases (2a–2c) result in emissions between 31.1 and 57.1 g CO_2 eq/MJ, while the electrified reformer pathways (3a–3c), despite removing natural gas from the process, still yield higher emissions: 52.5 to 77.4 g CO_2 eq/MJ.
- Combining hydrogen, CCSU, and nuclear heat across the system yields the strongest GHG reductions. Case 7 (oxy-fuel with HTSE) delivers the best performance, with emissions as low as -17.1 to 8.1 g CO_2 eq/MJ, followed by Case 5 (amine-based capture powered by nuclear energy), which ranges from 2.4 to 28.3 g CO_2 eq/MJ.
- For all cases, GHG emissions associated with diesel combustion during final use are better offset when methanol and diesel plants are co-located and integrated with nuclear and hydrogen systems.

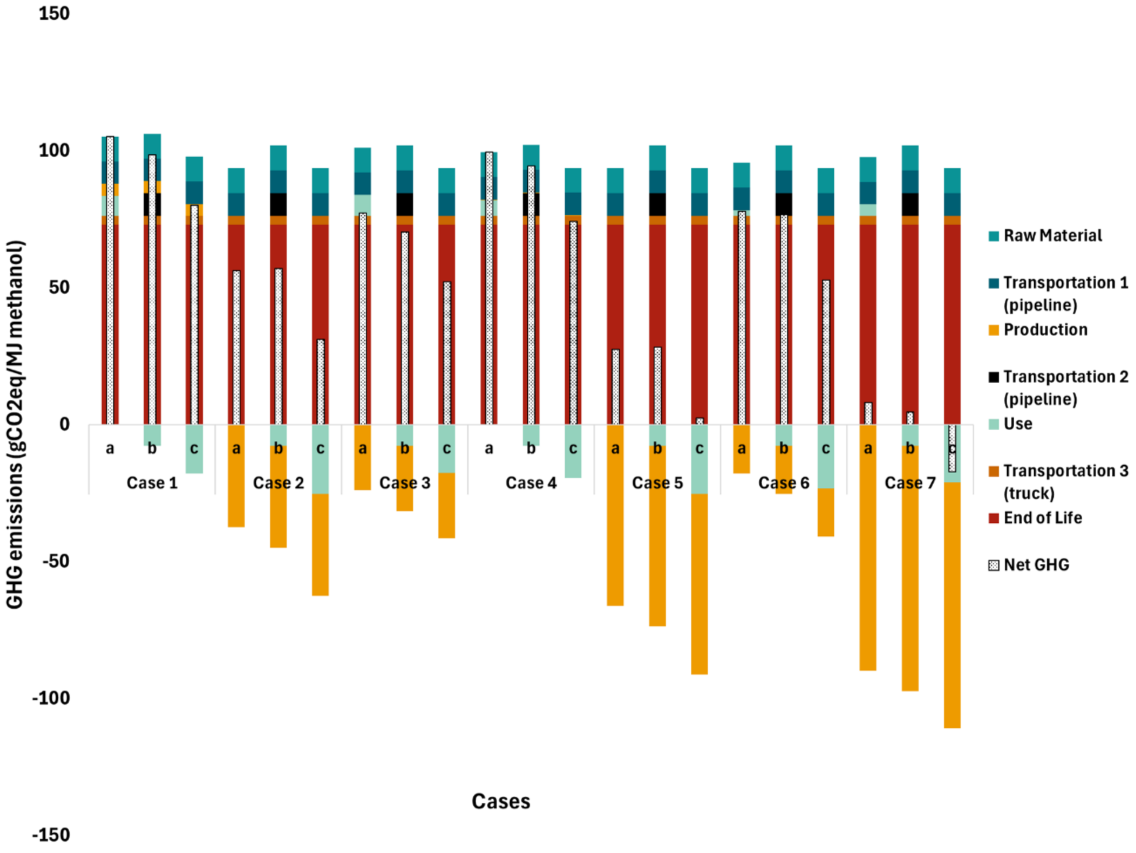

Figure 8. GHG Emissions from cradle-to-grave of Methanol Production: **a.** Co-located plants for methanol and diesel production using electricity from the grid **b.** Non-co-located plants for methanol production with nuclear integration for diesel production **c.** Co-located plants for methanol and diesel production integrated with nuclear energy

Scenarios relying on natural gas and grid electricity reflect industrial norms where combustion-based fuels and high-carbon grids dominate energy supply. These cases show the highest emissions due to both direct process emissions (e.g., from SMR) and indirect emissions from electricity generation. Even when

CCSU is applied, the capture rates are limited by energy input quality, and the emissions remain well above target ranges for performance improvement.

Substituting traditional energy carriers with hydrogen, and introducing HTSE powered by high-grade nuclear heat, enables more efficient production systems with improved capture performance. Oxy-fuel combustion, a process where fuels are burned in nearly pure oxygen, produces a more concentrated CO_2 stream that enhances capture efficiency. When both fuels are produced at a single location with shared infrastructure (as in Case 7c), the system achieves notable reductions, in some instances even producing net-negative emissions due to the combined effects of fuel substitution, process heat optimization, and near-total carbon recovery.

In configurations where carbon capture is not applied, replacing methane with hydrogen significantly improves the emissions profile. This is largely because hydrogen eliminates combustion-related CO_2 from reforming and combustion. As a result, their overall environmental performance is less favorable than hydrogen-based pathways unless the electricity supply has a very low emissions intensity.

Scenarios that align hydrogen production, carbon capture, and thermal energy supply within an integrated framework see the most substantial GHG reductions. Oxy-fuel combustion in Case 7 leverages a concentrated CO_2 stream for efficient capture, while HTSE eliminates the need for air separation units by providing high-purity oxygen using thermal input from nuclear sources. Similarly, Case 5 benefits from steady thermal and electrical input for solvent regeneration in amine systems, improving capture efficiency while minimizing parasitic energy losses. These system-level efficiencies enable emissions reductions well below those achieved by partial interventions.

Locating methanol and diesel production at the same site allows for direct energy and material integration, reducing the need for long-distance transport of intermediates and enabling real-time reuse of heat and gases. These co-located setups also reduce auxiliary emissions from pipeline networks, compression stations, and fuel transport logistics. Additionally, integrated systems can balance energy loads dynamically and optimize equipment utilization, further improving emissions performance across the product lifecycle from feedstock conversion to fuel use.

4. CONCLUSIONS

This study evaluated the GHG emissions associated with methanol and methanol-to-diesel fuel production across a range of process configurations, including conventional and advanced pathways. The analysis considered three stages: gate-to-gate methanol production, methanol-to-diesel conversion, and full cradle-to-grave fuel system performance. The primary objective was to determine how emissions vary depending on integration strategies involving carbon capture systems, hydrogen production methods, and thermal and electrical energy sources.

The results reveal that emissions intensity is highly sensitive to the energy source used for hydrogen production, the efficiency and type of carbon capture applied, and the degree of process integration between units. While conventional systems continue to rely on natural gas and grid electricity, more advanced setups benefit from strategic integration of hydrogen and high-temperature thermal energy sources, particularly when applied in co-located facilities. These system-level design choices lead to significant improvements in overall performance by minimizing both direct and indirect emissions throughout the fuel lifecycle.

Key conclusions from the analysis include:

- Conventional pathways, represented by business-as-usual (BAU) scenarios, produce the highest emissions due to their dependence on fossil-based inputs for both hydrogen production and thermal energy. Methanol production using steam methane reforming (SMR) without any form of capture or alternative energy support reached up to 4.3 g CO_2 eq/MJ, while cradle-to-grave emissions climbed to 105.3 g CO_2 eq/MJ when diesel synthesis and end use were included.

- CCSU systems reduce GHG emissions significantly. For example, applying CCSU to a fossil-fueled SMR system decreased emissions from 4.3 to 0.2 g CO_2 eq/MJ for methanol production. However, the effectiveness of CCSU is constrained by the energy required for capture and the type of system used. Oxy-fuel combustion, which produces a CO_2-rich exhaust stream, proves more effective than amine-based systems powered by conventional sources.
- Hydrogen integration, especially when produced via HTSE, delivers a notable drop in emissions compared to both fossil-derived hydrogen and electrified reformers. The best-performing configuration substituted process heat with HTSE-based hydrogen powered by a non-combustion thermal source, resulting in net emissions of -37.3 g CO_2 eq/MJ. In contrast, electrified reformers, while beneficial in eliminating direct combustion, yielded higher emissions (-23.8 g CO_2 eq/MJ) due to the continued reliance on grid electricity.
- The combination of CCSU, hydrogen from HTSE, and high-temperature energy sources led to the most favorable outcomes. Case 7c, involving oxy-fuel combustion with oxygen supplied by nuclear-powered HTSE and a fully co-located facility, achieved net-negative emissions of -17.1 g CO_2 eq/MJ of methanol on a cradle-to-grave basis. This was made possible by efficient carbon recovery, the elimination of air separation units, and minimized reliance on external fuel sources.
- Co-locating methanol and diesel production facilities improved emissions performance by enabling energy and material integration. These configurations reduce transport requirements for intermediates, optimize thermal recovery, and facilitate real-time electricity balancing between units. This integration results in both operational efficiency and lower emissions across the lifecycle.
- The methanol-to-diesel process, when isolated, relies almost exclusively on hydrogen for its external energy needs, thanks to internal heat and power integration. The source of electricity for HTSE becomes the dominant factor. Powering HTSE with grid electricity resulted in 7.6 g CO_2 eq/MJ, while nuclear-supported HTSE achieved -7.6 g CO_2 eq/MJ, reflecting the strong influence of energy input quality on hydrogen-intensive processes.

The findings confirm that GHG performance in methanol-based fuel systems is strongly dominated by the design of upstream energy and process inputs. Systems that combine high-efficiency capture, alternative thermal energy, and hydrogen production via HTSE offer substantial improvements over conventional methods. Furthermore, co-location and process integration strategies reduce auxiliary emissions and enhance the reuse of energy and materials. While not all pathways reach net-negative values, many advanced configurations approach or exceed critical performance thresholds, suggesting a clear technical direction for emissions reduction in industrial fuel production.

5. ACKNOWLEDGEMENTS

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