Berg Huettenmaenn Monatsh
https://doi.org/10.1007/s00501-025-01595-4

BHM Berg- und Hüttenmännische Monatshefte

Using Process Simulation to Support Decarbonization in the Steel Industry

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Received March 28, 2025; accepted April 4, 2025

Abstract: Being a major contributor to industrial CO_2 emissions, the iron and steel industry needs to transition towards CO_2-lean processes to achieve the carbon neutrality goal of the European Green Deal for 2050. Process simulation serves as a powerful tool for modelling and evaluating decarbonization strategies in this transition. This contribution explores a potential stepwise decarbonization pathway for the Austrian steel industry using the flowsheet simulation software gPROMS (General PROcess Modeling System). The transition from the carbon-intensive blast furnace (BF)-basic oxygen furnace (BOF) route to electric arc furnace (EAF)-based steelmaking is modelled, integrating hydrogen-based direct reduction (DR) and carbon capture and utilization (CCU) technologies. The analysis evaluates the CO_2 reduction potential and the changes in external energy demand for each scenario, including natural gas, electricity, and hydrogen. The findings of this study provide a strong basis for evaluating the European steel industry's energy demands during its transition towards sustainable steel production.

Keywords: Decarbonization, Steel industry, Process simulation, Hydrogen, Carbon capture and utilization (CCU)

Nutzung von Prozesssimulation zur Unterstützung der Dekarbonisierung in der Stahlindustrie

Zusammenfassung: Als wesentlicher Verursacher industrieller CO_2-Emissionen ist die Eisen- und Stahlindustrie aufgefordert, auf CO_2-ärmere Prozesse umzusteigen, um das Ziel der Klimaneutralität des europäischen Grünen Deals bis 2050 zu erreichen. Prozesssimulation dient als leistungsstarkes Werkzeug zur Modellierung und Bewertung von Dekarbonisierungsstrategien. In diesem Beitrag wird ein möglicher schrittweiser Dekarbonisierungspfad für die österreichische Stahlindustrie mithilfe der Prozessmodellierungssoftware gPROMS (General PROcess Modeling System) untersucht. Dabei wird der Übergang von dem kohlenstoffintensiven Hochofen-Konverter-Verfahren (BF-BOF) zu einer auf Elektrolichtbogenöfen (EAF) basierenden Stahlherstellung modelliert, ergänzt durch die Integration wasserstoffbasierter Direktreduktion (DR) und Technologien zur CO_2-Abscheidung und -Nutzung (CCU). Die Simulationsergebnisse erlauben eine detaillierte Analyse des CO_2-Reduktionspotenzials sowie der Änderungen des externen Energiebedarfs, insbesondere Erdgas, Strom und Wasserstoff. Die gewonnenen Erkenntnisse liefern eine solide Grundlage für die Bewertung des Energiebedarfs der europäischen Stahlindustrie während des Übergangs zu einer nachhaltigen Stahlproduktion.

Schlüsselwörter: Dekarbonisierung, Stahlindustrie, Prozesssimulation, Wasserstoff, CO_2-Abscheidung und -Nutzung (CCU)

1. Introduction

Despite the steel production in Europe belonging to the most CO_2 efficient worldwide, it still accounts for 5.7% of total greenhouse gas emissions in the EU-27 [1]. In 2023, 55.2% of the 126.3 million tons of crude steel in the EU-27 were produced via the coal-based BF-BOF route, while 44.8% originated from the less CO_2-emitting EAF route [2]. Fig. 1 illustrates the significant difference in CO_2 emissions of the two production routes. For every ton of crude steel produced via the traditional BF-BOF route, nearly twice as

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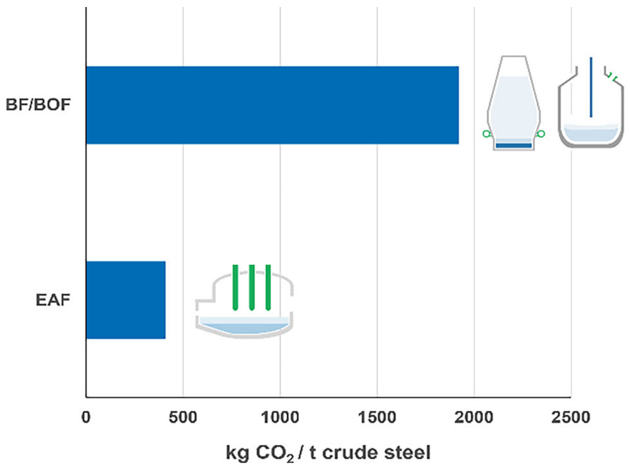


Fig. 1: CO_2 emissions ascribed to each production route

much CO_2 is emitted, whereas the scrap-based EAF-route accounts for less than 0.5 tons of CO_2 per ton of crude steel [3]. However, the scrap-based EAF-route is limited by scrap availability and steel quality, which restrict its application for high-grade steel products [4].

Eurofer [5] proposes two key strategies to reach substantial CO_2 reduction rates in the steel sector: carbon direct avoidance (CDA) and smart carbon usage (SCU). CDA relies on renewable energy and hydrogen-based steelmaking, while SCU aims to close the carbon cycle by converting captured CO_2 into valuable products, such as methane or methanol, using renewable hydrogen.

In this contribution, potential decarbonization scenarios for the Austrian steel industry are simulated with gPROMS. Initially, smaller blast furnaces are replaced by electric arc furnaces. Subsequently, direct reduction (DR) plants are integrated, operated at the beginning with a mix of natural gas and hydrogen, with the goal of transitioning to 100% hydrogen. To address residual CO_2 emissions, CCU technologies, including amine scrubber and catalytic methanation, are incorporated.

2. Potential Decarbonization Pathway for the Austrian Steel Industry

Several scenarios are defined to model the stepwise decarbonization of the Austrian steel industry between 2018 and 2050. The 2018 crude steel production level in Austria serves as the basis for the simulations, with a total of 6.9 million tons produced –90% via the BF-BOF route and 10% via the EAF route [6]. For comparative purposes, production levels are assumed to remain constant from 2018 onward. Calculations focus on the BF-BOF route, also referred to as the primary production route, as it offers the highest potential for CO_2 reductions (see Fig. 1).

Figure 2 outlines five potential decarbonization scenarios, illustrating the transition from the carbon-intensive BF-BOF route to hydrogen-based steelmaking processes:

- Scenario 2018 (Base case): All primary crude steel is produced using the BF-BOF route.
- Scenario 2030: One third of primary crude steel production is transitioned to the EAF route. The EAF input consists of 50% scrap and 50% imported hot briquetted iron (HBI), a compacted form of direct reduced iron (DRI) produced in an external DR plant. The remaining two thirds of production continues via the BF-BOF route.
- Scenario 2035: The share of crude steel produced via the EAF route increases to 53%, with the remainder pro-

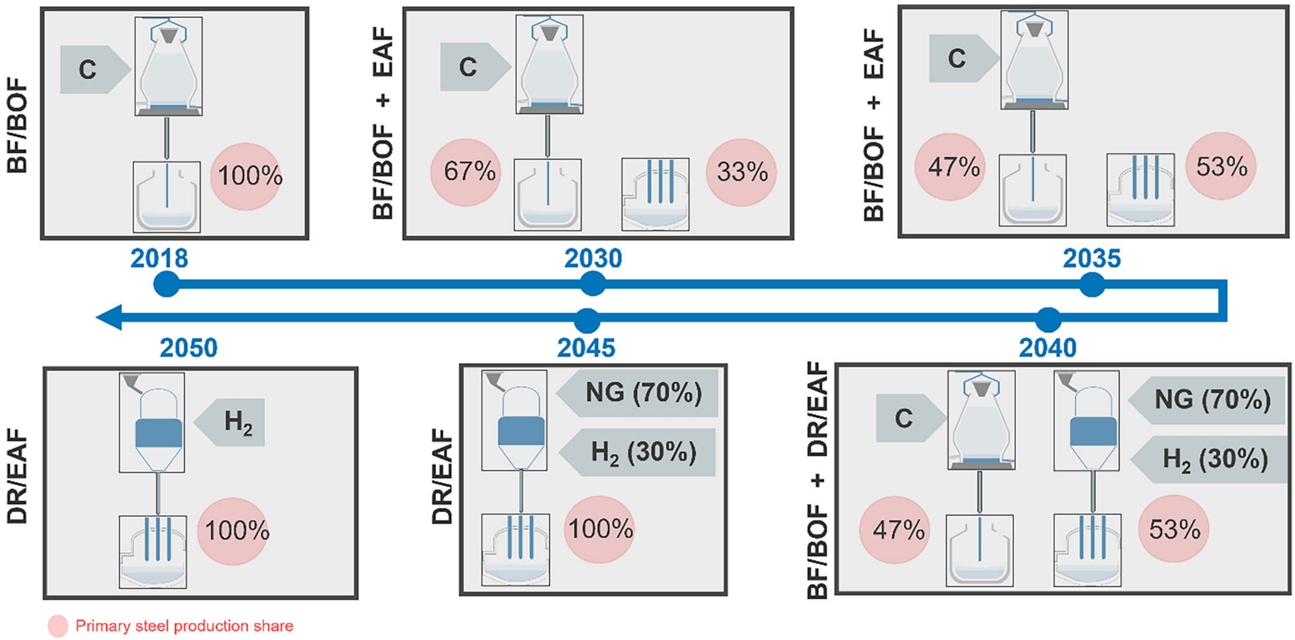
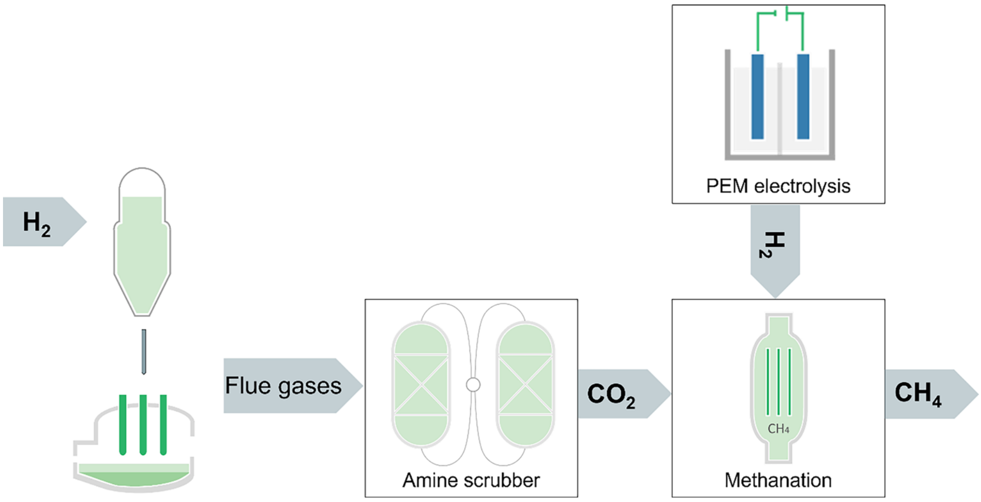


Fig. 2: Potential decarbonization scenarios for the Austrian steel industry

Fig. 3: Scenario 2050 + CCU technologies



duced through the BF-BOF route. The input mix for the EAF remains unchanged from scenario 2030.

- Scenario 2040: DR plants are introduced to supply the EAFs with DRI. These DR plants use a 70:30 volumetric flow ratio of natural gas to hydrogen. Currently, no hydrogen-based DR plants are operational at an industrial scale. However, 30% of natural gas can be substituted by hydrogen in existing DR plants without any significant modifications [7]. From this scenario onward, onsite hydrogen production via proton exchange membrane (PEM) electrolysis is also considered, with an overall efficiency of 75%, as reported in [8].
- Scenario 2045: Full transition to the DR-EAF route is achieved. Due to hydrogen availability, a mixture of 70% natural gas and 30% hydrogen is considered for the DR process.
- Scenario 2050: It is assumed that sufficient hydrogen will be available by 2050 to enable a complete transition to hydrogen-based steelmaking via the DR-EAF route. However, a small amount of natural gas is necessary to regulate the process temperature and ensure the appropriate carbon content of the DRI [7].
- Scenario 2050 + CCU: Building on scenario 2050, this scenario incorporates CCU technologies to address the remaining CO_2 emissions of the hydrogen-based DR-EAF route and is depicted in Fig. 3. The flue gases from the potential future steel mill are directed to an amine scrubber, where 90% of the CO_2 is captured using monoethanolamine (MEA) as the solvent. The captured CO_2 is subsequently converted into synthetic natural gas through catalytic methanation. This process utilizes hydrogen produced via PEM electrolysis, as described by the following reaction [9]:

$$\begin{aligned} &4H_2 + CO_2 \leftrightarrow CH_4 + 2H_2O \\ &\Delta H_R^0 = -165 kJ/mol \end{aligned} \tag{1}$$

Because of the exothermic nature of the methanation reaction, cooling is required to preserve the catalyst. The heat recovered can be utilized for steam generation, which is sufficient to cover the steam demand of the amine scrubber for CO_2 desorption.

2.1 Modelling Approach

The simulations were setup in gPROMS using literature data from the Best Available Techniques (BAT) document [10], which applies to the European steel industry. However, the results of this study are specific for Austria. gPROMS provides a unified equation-oriented simulation environment for custom modelling and process simulation. This software tool enables the modelling of complex systems through flexible steady-state and dynamic flowsheet simulation. Over recent years, the m.SIMTOP model library has been developed by Primetals Technologies, voestalpine Stahl GmbH, K1-MET and TU Wien to support the simulation of metallurgical processes [11]. The CCU technologies were modelled with Siemens libraries.

The system boundaries for the simulations encompass the key production facilities involved in the steelmaking process. In scenarios where steel is produced via the BF-BOF route, an onsite coking plant, sinter plant, and power plant for electricity and steam generation are integrated into the overall mass and energy balances. A lime plant or pelletizing unit are not part of the simulations, as they are assumed to be external. Downstream processes like hot rolling and cold rolling are not included either as their modes of operation are assumed to remain unchanged in the future scenarios analysed in this study.

The EAF model used in this study was validated with data from a plant manufacturer, as presented in [12]. Detailed models for the DR process using natural gas and hydrogen are available from [7]. The amine scrubber model was validated with experimental data obtained from a pilot plant [13] and scaled up to handle the flue gases of the potential future steel mill, which contain approximately 5 vol% CO_2. The methanation model, based on the industrially established TREMP^{TM} process (Topsøe Recycle Energy-efficient Methanation Process), was verified with measurement data from [9] and scaled up to process the captured CO_2 stream.

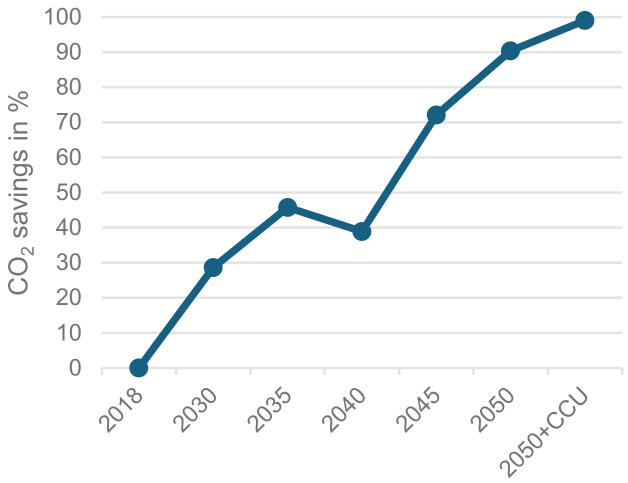


Fig. 4: Direct CO2 emissions savings

2.2 Results and Discussion

The results of the scenario simulations, focusing on direct CO$_2$ emissions savings, hydrogen and natural gas demand, as well as external electricity requirements, are presented in Figs. 4 and 5. Fig. 4 illustrates the reduction in direct CO$_2$ emissions achieved with each analysed decarbonization step. Except for scenario 2040, where DR plants are introduced on site to supply the EAFs with DRI, all scenarios show significant CO$_2$ emissions savings. In the scenarios 2030 and 2035, the import of HBI is assumed, and the associated CO$_2$ emissions from its production are not included in the direct emissions of the steel mill. Consequently, direct CO$_2$ emissions savings decrease in scenario 2040 due to the shift to onsite DR plants relying on natural gas.

Despite the transition to hydrogen-based steelmaking in scenario 2050, 10% of the direct CO$_2$ emissions from 2018 persist. These residual emissions result from the carbonaceous inputs required to achieve the specific carbon content in steel. To address these unavoidable CO$_2$ emissions, scenario 2050 + CCU was established to close the carbon cycle.

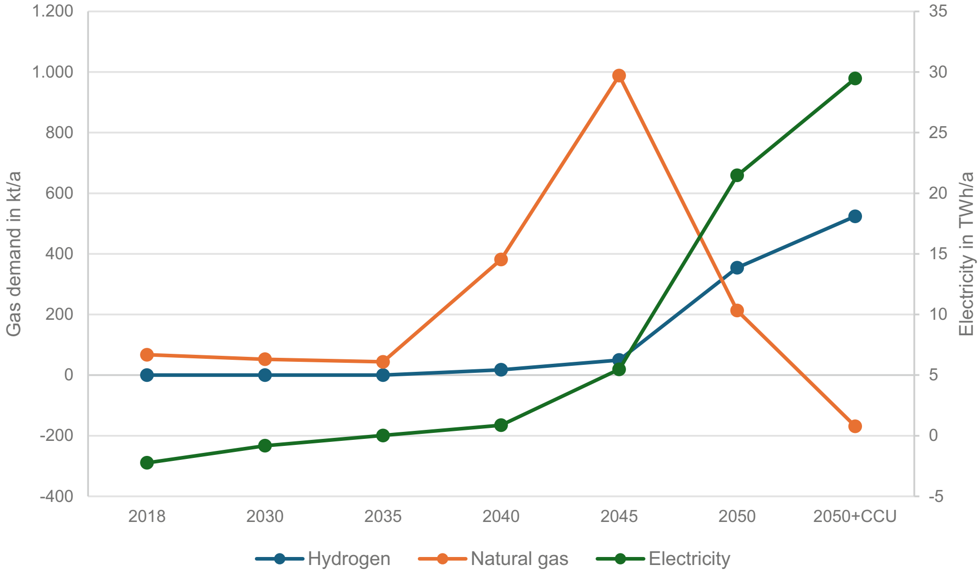
The demand for hydrogen and natural gas for each scenario is depicted in Fig. 5. Hydrogen demand begins to rise significantly in scenario 2040, driven by its extensive use in the DR process. This trend accelerates in scenario 2050 with the full transition to hydrogen-based steelmaking. In this scenario, over 350 kt/a of hydrogen are required for the DR-EAF process, with an additional 170 kt/a necessary for CCU technologies to process the residual CO$_2$ emissions.

Natural gas demand rises significantly in scenario 2040 due to the introduction of DR plants operating with a 70:30 volumetric flow ratio of natural gas to hydrogen. A peak of natural gas demand of nearly 1000 kt/a is reached in scenario 2045, driven by the full transition to the DR-EAF route with DR plants maintaining this gas ratio. To mitigate this peak in natural gas demand, an alternative pathway could involve shifting DRI production from scenario 2040 entirely to hydrogen in scenario 2045 or adding hydrogen-based DR plants to supplement the natural gas-based plants from scenario 2040. These strategies would increase hydrogen demand in scenario 2045 but offer a reduced natural gas demand.

Moreover, natural gas demand becomes negative in scenario 2050 + CCU as captured CO$_2$ is converted into methane. Catalytic methanation fully covers the natural gas demand of the potential future steel mill of approximately 200 kt/a, excluding downstream processes, where it is assumed that natural gas might be substituted with hydrogen by 2050. An additional surplus of nearly 200 kt/a can be sold externally, thereby generating revenue.

External electricity demand for each transformation scenario is illustrated in Fig. 5. The demand is negative in the earlier scenarios from 2018 to 2030. Process gases from the BF-BOF route, such as BF gas, BOF gas, and coke oven gas, are utilized to generate electricity in an internal power plant with an assumed efficiency of 37%, which is derived from the reported efficiency range of 30–40% [14]. This surplus electricity increases the energy efficiency of the integrated

Fig. 5: External gas and energy demand



steel mill by supporting processes not included in the simulations, such as the rolling mill.

However, electricity demand rises significantly from scenario 2045 onwards due to the increased use of hydrogen and its onsite production via PEM electrolysis. Scenario 2050 requires 21.5 TWh/a of external electricity to produce 'green steel' in Austria. An additional 8 TWh/a are needed in scenario 2050 + CCU for hydrogen production to support methanation and remove the remaining 10% of CO_2 emissions. Meeting these demands will require substantial investments in renewable energy infrastructure and grid capacity.

These scenarios highlight the complexity of transforming the steel industry, particularly in the later stages involving a complete revamp of steel production. Key uncertainties include the technology readiness of hydrogen-based steelmaking and CCU technologies for industrial-scale applications, the availability of green electricity and hydrogen at competitive costs, and the ability to produce steel of the required quality using low-carbon technologies. Additionally, the potential introduction of electric smelting furnaces (ESF) to process (domestic) lower-grade iron ores could further diversify decarbonization pathways, complementing DR-EAF and CCU technologies.

In addition to the amine scrubber and catalytic methanation approach modelled in this study, other CCU options could be explored to address residual CO_2 emissions. For example, CO_2 could be captured via pressure swing adsorption before being converted into methanol with hydrogen. However, methanol is not directly utilized in steel mills, and identifying external customers for methanol would be essential for implementation.

Carbon capture and storage (CCS) is also a potential alternative for managing residual CO_2 emissions. While CCS can mitigate emissions, it does not contribute to a circular economy like CCU does and does not solve the challenge of missing carbon in other industry sectors. Ultimately, the decision on which technology to implement will depend on its readiness for industrial application, economic feasibility, and overall alignment with long-term sustainability goals.

3. Conclusions and Outlook

This study demonstrates the potential for significant CO_2 emissions reductions in the steel industry through a stepwise transition to hydrogen-based DR-EAF steelmaking and the integration of CCU technologies. Using process simulation with gPROMS, this study provides detailed energy requirements for various decarbonization scenarios. For instance, the full transition to hydrogen-based steelmaking in scenario 2050 requires over 350 kt/a of hydrogen and 21.5 TWh/a of electricity, while scenario 2050 + CCU adds an additional 170 kt/a of hydrogen and 8 TWh/a of electricity to address residual emissions.

The timeline and pathways modelled in this study are based on assumptions by K1-MET and can serve as a foundation for strategic planning. It is crucial to emphasize that the CO_2 reductions presented rely on literature data and assumptions. Real-world outcomes may vary depending on technological advancements and market conditions.

Additional decarbonization strategies could include electric smelting furnaces (ESF) to process (domestic) lower-grade iron ores, which would ensure greater flexibility in adapting to resource availability. Furthermore, the substantial electricity demands identified in the scenarios 2050 and 2050 + CCU underscore the importance of expanding renewable energy infrastructure and scaling up of green hydrogen production.

Ultimately, the successful transformation of the steel industry will depend on the ability to balance technology readiness, consistent product quality, economic feasibility, and environmental sustainability to achieve net-zero emissions by 2050. During this transition, process simulation serves as a valuable tool for assessing and optimizing decarbonization strategies.

Funding. The authors gratefully acknowledge the funding support of K1-MET GmbH, metallurgical competence center. The research program of the K1-MET competence center is supported by COMET (Competence Center for Excellent Technologies), the Austrian program for competence centers. COMET is funded by the Federal Ministry for Climate Action, Environment, Energy, Mobility, Innovation and Technology, the Federal Ministry for Digital and Economic Affairs, the Federal States of Upper Austria, Tyrol, and Styria, as well as the Styrian Business Promotion Agency (SFG).

Funding. Open access funding provided by TU Wien (TUW).

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