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Optimizing Steam flux for Energy efficiency in Ammonia Recovery during Sodium carbonate production

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ABSTRACT

Industrial decarbonization is crucial to reducing global emissions. Efficient processes lower energy use and reduce the environmental impacts, such as material use and waste, decreasing the overall industrial footprint. In this context, the present study explores the impact of reducing steam consumption (thermal energy) during the ammonia regeneration process in the production of sodium carbonate. A key feature of the Solvay process is ammonia recycling, which significantly reduces raw material consumption and ensures both economic and environmental sustainability. However, this stage is highly energy-intensive. To enhance energy efficiency in soda ash production, a study was conducted to analyze variation in temperature, pressure, and steam flow introduced into the ammonia regeneration system. The objective is to understand its impact on both ammonia recovery and the process's energy consumption. Variations in steam pressure do not impact on energy consumption of the process. By reducing the temperature and steam flow introduced into the system, in order to reduce the energy consumption, it was found that there is no decrease in ammonia recovery. The reduction in both the total injected steam flow and operating temperature led to lower heat exchange requirements and a decreased the cooling energy demand, highlighting the potential for optimizing steam flow as an effective strategy to improve process efficiency. Instead, it underscores a potential for energy optimization, promoting a more sustainable and cost-effective operation.

Keywords: Energy Efficiency, Modelling and Simulations, Aspen Plus, Energy, Optimization

INTRODUCTION

Sodium carbonate is a key industrial chemical with widespread applications across several sectors, including glass manufacturing, paper production, detergents, and the chemical industry. Its strategic importance is reflected in the steady growth of the global sodium carbonate market, primarily driven by the expansion of the glass and detergent industries [1]). This trend is further reinforced by increasing urbanization and industrialization, particularly in emerging economies. According to market projections, the global sodium carbonate market is expected to reach USD 14.42 billion in 2025 and expand to approximately USD 25.74 billion by 2035 [1].

The Ammonia Process or Solvay Process, a widely used and efficient method to produce sodium carbonate also known as soda ash. The production of sodium carbonate through the Solvay process is divided into four stages. The first stage is limestone calcination, in which calcium carbonate ($CaCO_3$) is thermally decomposed to produce carbon dioxide (CO_2) and calcium oxide (CaO). The carbon dioxide generated in this step is subsequently utilized in the following stage. In the second stage, carbonation, the carbon dioxide is bubbled through a brine solution containing sodium chloride (NaCl), ammonia (NH_3), and water. Within this medium, carbon dioxide reacts with ammonia and sodium ions, leading to the formation of sodium bicarbonate ($NaHCO_3$), which precipitates due to its low solubility. Sodium bicarbonate constitutes the desired intermediate product, whereas ammonium chloride (NH_4Cl) is simultaneously formed as a by-product. The third stage involves the thermal decomposition of sodium bicarbonate. The solid obtained from carbonation is separated by filtration and subsequently subjected to calcination. Upon heating, sodium bicarbonate decomposes into sodium carbonate

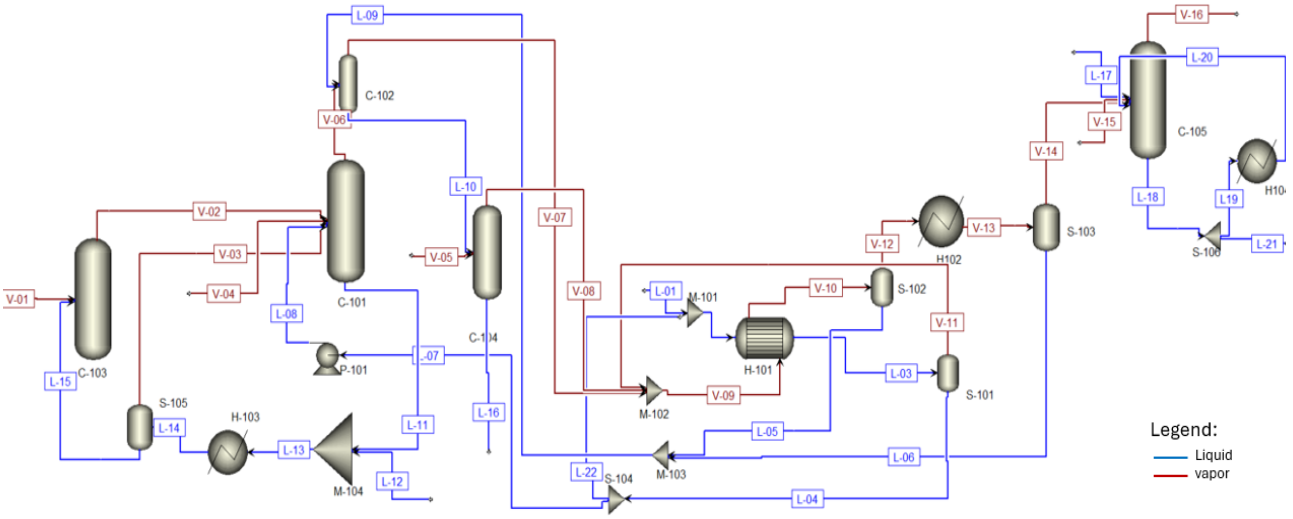

Figure 1: Ammonia regeneration process flow diagram in sodium carbonate production.

(Na_2CO_3), water, and carbon dioxide. The regenerated carbon dioxide is recycled within the process, contributing to its overall sustainability. Finally, the fourth stage is ammonia regeneration. In this step, ammonium chloride reacts with hydrated calcium oxide ($Ca(OH)_2$), yielding free ammonia and calcium chloride ($CaCl_2$). The recovered ammonia is recycled into the process through absorption in brine, thus closing the operational cycle and ensuring the economic and environmental viability of the Solvay process [2].

The production of sodium carbonate is both energy-intensive and CO2-intensive [3], in part because the ammonia recovery step requires a substantial amount of steam. Despite this significant energy requirement, ammonia recovery is the operation that ensures the economic viability of the Solvay process when compared with alternative sodium carbonate production routes (Book: Manufacture of Soda). Nevertheless, even though it plays an important role in process efficiency and overall performance, the ammonia recovery step remains insufficiently addressed in the scientific literature. Most existing studies focus on eliminating the ammonia recovery stage [4, 5], replacing ammonia as the process intermediate [6, 7] or integrating carbon capture strategies into the Solvay process [8]. However, although such strategies can reduce environmental impacts, they require major modifications to existing industrial plants, which in turn demand substantial capital investment. For this reason, these modified methods have generally not been favored by manufacturers due to economic considerations[9].

The ammonia regeneration process investigated in this study presents significant advantages with respect to process efficiency, operational costs, and environmental performance. The effective recovery of ammonia and carbon dioxide reduces waste streams and decreases the requirement for fresh ammonia make-up, thereby lowering operating expenses. To further improve the energy performance of soda ash production, this study focuses on assessing the impact of steam flow rate variations in the ammonia regeneration stage. The analysis evaluates the relationship between steam input, ammonia recovery efficiency, and overall energy consumption, providing a technical basis for the optimization of industrial-scale sodium carbonate production systems.

METHODOLOGY

Thermodynamic model

In this study, process modeling is performed in Aspen Plus® V14.0. The Electrolyte Wizard is used to identify possible reactions, components, and intermediates, and to calculate equilibrium constants and properties. For systems with inorganic electrolytes, such as sodium bicarbonate, ionic species and reactions are also considered. The thermodynamic model ELECNRTL-RK is applied, combining the NRTL electrolyte model for the aqueous phase with the Redlich-Kwong equation of state for the vapor phase. This thermodynamic model has been validated in previous studies, such as the methodology used by Yoshi et al. (2022) [10], specifically in the simulation of the Solvay process.

Process simulation

The simulated system (Figure 1) is based on ammonia regeneration, focusing on the processing of cold

mother liquor (L-01), which is predominantly composed of water and ammonium chloride (NH_4Cl), also known as fixed ammonia, as well as dissolved carbon dioxide (CO_2) and free ammonia (NH_3). Initially, L-01 is directed to the heat exchanger (H-101), where it absorbs heat for pre-heating, causing part of the dissolved gasses to gas phase. After this stage, the heated fluid proceeds to a gas separator (S-101), where the liquid and vapor phases are separated. The liquid phase is then sent to the column C-101.

Column C-101, designed as a stripping unit, functions to remove carbon dioxide (CO_2) and free ammonia present in the mother liquor. The liquid effluent from this stage is sent to the mixer (M-104), where calcium hydroxide ($Ca(OH)_2$) is added. The chemical reaction occurring here can be detailed as follows: $Ca(OH)_2 + 2NH_4Cl \rightarrow 2NH_3 + CaCl_2 + 2H_2O$. The chemical reaction between calcium hydroxide and ammonium chloride results in the formation of free ammonia and calcium chloride ($CaCl_2$). Subsequently, the mixture is transferred to a foam separator, whose primary function is to remove the gases formed, mainly composed of ammonia. The vapor extracted in this separator is redirected to column C-101, while the liquid phase proceeds to column C-103.

Column C-103, also configured as a stripping unit, is responsible for removing the free ammonia generated in the previous stage (M-104). The liquid effluent from this column is now characterized as de-ammoniated mother liquor. The vapors generated in C-103 are sent back to column C-101, along with the vapor from the foam separator and an additional flow of steam introduced into the system.

The vapor from the top of column C-101 is directed to column C-102, another stripping unit. C-102 receives condensed water from the heat exchangers in the ammonia regeneration system (H-101 and H-102). At this stage, ammonia and carbon dioxide present in the condensates are recovered and reincorporated into the vapor flow. The liquid collected at the bottom of C-102 is sent to a second stripping column (C-104), where residual NH_3 and CO_2 in the condensate are transferred to the vapor phase.

The ammonia recovered in systems C-102, C-104, and S-101 is routed to the heat exchangers (H-101 and H-102) for cooling before being introduced into the absorber. In this equipment, the gas is absorbed by the NaCl brine, allowing its reintegration into the sodium carbonate production process.

The formation of ammonia brine is accompanied by the release of a significant amount of heat, characterizing it as an exothermic process. To control the temperature and optimize NH_3 absorption, a pre-cooled ammonia brine (H-104) is recycled in the system, ensuring ideal conditions for the continuity of the process.

Test optimization

The process has three steam inputs: the V-01 stream, which is added to the stripping column C-103 and represents the main steam flow of the system, with a flow rate of 38, 700 kg/h; the V-04 stream, a supplemental steam flow with a flow rate of 3, 000 kg/h, directed to column C-101; and the V-05 stream, with a flow rate of 5, 573 kg/h, introduced into column C-104.This study analyzed the variation in temperature, pressure, and mass flow rate of steam introduced into the fixed ammonia regeneration process, with the aim of understanding the impact of these variables on ammonia recovery efficiency. The temperature, pressure, and mass flow conditions of these three steam streams were modified as presented in Table 1, one variable at a time. The proposed variations are based on values practiced by the soda ash production industry.

Table 1: Variation in the temperature, pressure, and mass flow rate of the process's steam inputs.

Stream	Temperature	Pressure	Mass Flow
V-01	116-145 °C	1.68-1.80 bar	10% reduction
V-04	116-145 °C	1.30-1.50 bar	10% reduction
V-05	116-145 °C	1.30-1.50 bar	10% reduction

RESULTS AND DISCUSSION

The effects of temperature, pressure, and mass flow rate variations on the vapor flow rate the main equipment of the ammonia regeneration process are analyzed, and the effect of mass flow variation is presented in Figure 2. The mass flow rate results of the system's vapor streams were normalized with respect to the mass flow rate obtained when the analyzed variable was at its maximum value. In addition, the results highlight the effect of reducing the analyzed variable on system behavior; therefore, in Figures 2, the *x*-axis is presented from the highest to the lowest value of the variable.

The variation in temperature and pressure has a minimum impact on ammonia recovery Similarly to the influence on the process steam flow, some variations are so small that they can be attributed to changes caused by model convergence. The most significant change observed was a 2% reduction in the steam flow exiting the C-105 column, which does not impact ammonia recovery or the stream entering the absorption column.

The low influence of temperature and pressure variations on ammonia recovery and steam mass flow rate in the system indicates that, despite the reduction in thermal energy transported by the steam stream fed into the system columns, the energy supplied is sufficient to achieve ammonia recovery. Under these conditions, the steam acts predominantly as an entraining agent, and

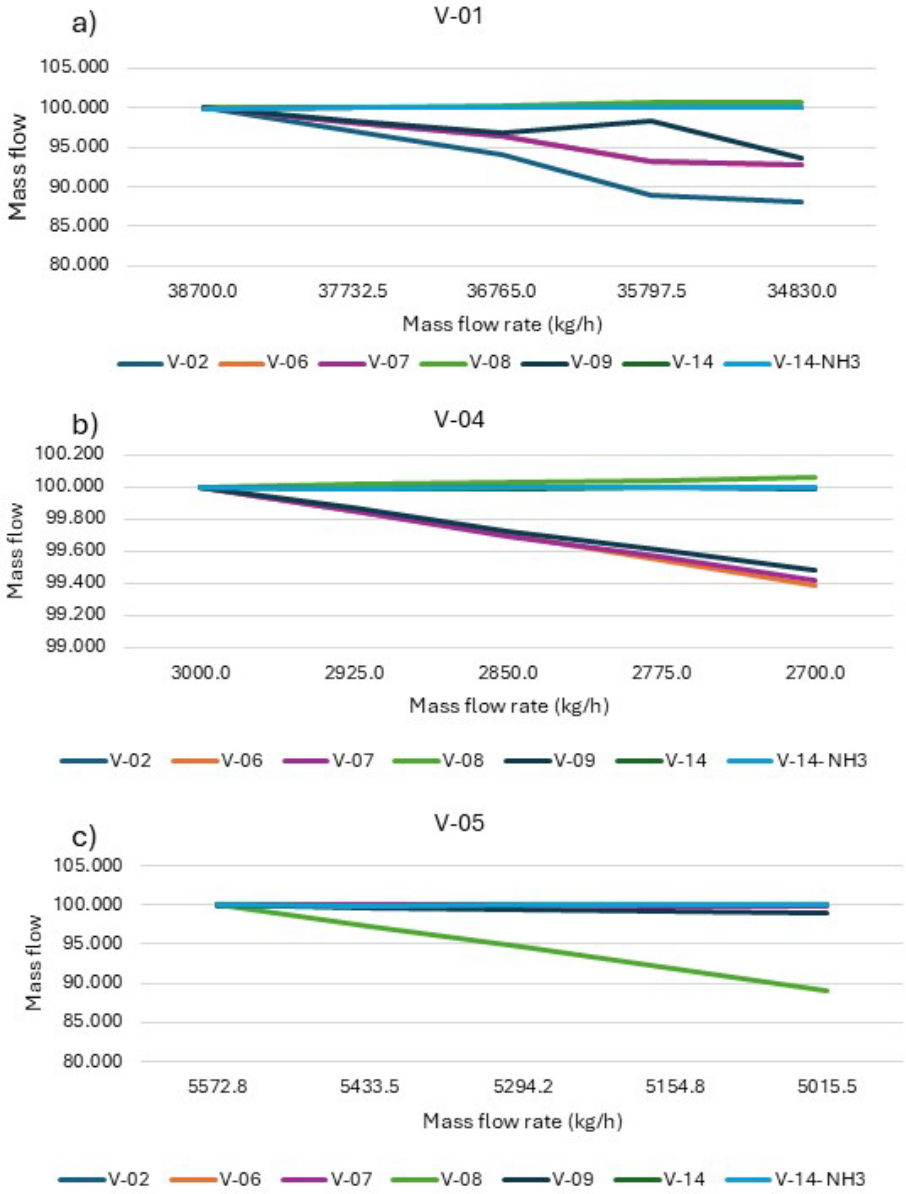

Figure 2. Influence of vapor mass flow rate input on the vapor mass flow rate for different vapor outputs of equipment: a) vapor input V-01, b) vapor input V-04, and c) vapor input V-05.

small variations in its temperature or pressure do not result in significant changes in the thermodynamic gradient required for ammonia vaporization. Despite the reduction in thermal energy introduced into the system, it continues to operate without major alterations. More details about the influence of temperature and pressure variations on ammonia recovery and steam mass flow rate in the system in the supplementary material.

The reduction in steam flow introduced into the system (Figure 2) implies changes in the dynamics of the vapor streams, although with variable impacts depending on the stream analyzed. In the case of stream V-04, the reduction in steam flow is minimal, less than 1% in streams V-06, V-07, and V-09, demonstrating little sensitivity to this change. On the other hand, stream V-05 shows a significant reduction of approximately 11% in the V-08 flow, which originates from column C-104, a column where the V-05 vapor stream is added, directly impacting the amount of vapor exiting this column. For the other system streams, including the absorption column's inlet stream, no significant impact is observed, with the NH_3 percentage remaining constant. The low influence of the reduction in the flow of V-04 and V-05 is due to the small change in the total energy supplied to the system. The

flow of V-04 represents only 6% of the steam introduced into the system, and a 10% reduction in this value results in a decrease of less than 1% in the total heat supplied to the system.

In the case of stream V-01, which is the main source of steam for the system, its reduction has a considerable impact on several vapor streams. This occurs because the steam introduced into column C-103 flows through multiple units within the system and accounts for approximately 82% of the total steam supplied to the process. This reduction, however, does not compromise ammonia recovery, which remains constant, as does the performance of the vapor stream feeding the absorption column (line v-14 and V-14NH3, which corresponds to the mass flow rate of ammonia entering the absorption column).

The observed behavior can be attributed to the thermodynamic properties of the involved compounds. Due to the high volatility of ammonia, even with the reduction in steam flow in the stripping columns, ammonia continues to efficiently migrate to the vapor phase. On the other hand, a larger amount of water remains in the liquid phase, as water requires more energy to transition to the vapor phase.

Table 2: Energy balance exchanged by the equipment streams in different equipment for various pressure of steam stream introduced into the system.

Pressure	V-01	C101	C102	C103	C104	H101	H102
	bar	Gcal/h	Gcal/h	Gcal/h	Gcal/h	Gcal/h	Gcal/h
V-01	1.80	38.86	12.44	23.33	3.73	-11.27	-8.77
	1.68	38.86	12.45	23.33	3.73	-11.27	-8.77
V-04	1.50	38.86	12.45	23.33	3.73	-11.28	-8.78
	1.30	38.85	12.45	23.33	3.73	-11.28	-8.77
V-05	1.50	38.85	12.46	23.33	3.74	-11.28	-8.78
	1.30	38.85	12.45	23.33	3.73	-11.28	-8.78

In the system's heat exchangers, the reduction in steam mass flow rate impacts the performance of heat transfer. In heat exchanger H-101, it is observed that the effluent steam exhibits a lower temperature compared to the scenario where the system operates with a higher steam flow rate, and a smaller amount of steam is condensed during the heat exchange process. More details regarding the temperature variation in the steam streams are available in the supplementary material. In the subsequent heat exchanger, H-102, designed to ensure that the steam reaches a temperature of 64 °C, required for entry into the absorption column, the reduction in steam mass flow rate does not alter the final steam flow rate coming from the ammonia regeneration system or the ammonia concentration present. The only modification occurs in the fraction of steam that is condensed at this stage of the process.

To better understand the heat exchange occurring within the process equipment, Tables 2, 3, and 4 present the energy transfer in the liquid phase between process streams at the maximum and minimum values of the following variables: pressure, temperature, and mass flow rate, respectively. The analysis of energy variation in a stripping column is highly complex, since the enthalpy of the liquid stream is a function of temperature, pressure, and chemical composition. The latter changes along the column as a result of mass transfer phenomena between the liquid and vapor phases. Consequently, an increase in the energy associated with the outlet stream may be attributed, among other factors, to the transfer of vapor to the liquid phase, which supplies latent heat to the system. In order to simplify the overall energy analysis, the parameter adopted to quantify the reduction of the system's thermal energy is the heat duty removed in the heat exchangers responsible for vapor cooling. These units are located at the end of the process and are designed to remove heat from the vapor stream, thus constituting the primary mechanism for energy removal from the system.

Table 3: Energy balance exchanged by the equipment streams in different equipment for various temperature of steam stream introduced into the system.

Temperature	V-01	C101	C102	C103	C104	H101	H102
	°C	Gcal/h	Gcal/h	Gcal/h	Gcal/h	Gcal/h	Gcal/h
V-01	145	38.94	13.31	19.75	3.75	-11.27	-9.25
	116	38.86	12.43	23.33	3.73	-11.27	-8.77
V-04	145	38.86	12.43	23.33	3.73	-11.27	-8.77
	116	39.13	12.42	23.34	3.73	-11.27	-8.74
V-05	145	38.85	12.46	23.33	3.73	-11.28	-8.78
	116	38.86	12.40	23.33	4.16	-11.27	-8.72

In the heat exchangers, the thermal behavior shows specific variations. Heat exchanger H-101 maintains its thermal exchange capacity almost unchanged in the three tables, as the equipment operates within its design range, allowing energy exchange between the hot and cold fluid streams to occur small variations. On the other hand, in heat exchanger H-102, designed to cool the vapor before its entry into the absorption column, the reduction in mass flow rate and vapor temperature results in a lower amount of heat exchanged. This reduction represents the most significant thermal alteration observed in the system, indicating a direct adaptation to the decrease in vapor flow introduced.

In Table 2, it is observed that the heat exchanged in the H-102 exchanger does not present significant variation, except for a reduction of 0.01 Gcal/h in stream V-04, indicating that pressure changes do not result in relevant

alterations in the system's thermal exchange. Changes in the temperature and mass flow rate of the vapor stream show, as presented in Tables 3 and 4, a reduction in energy consumption in the H-102 exchanger, with the most significant impact observed when modifying stream V-01, as it is the most important vapor stream in the process. Although both strategies promote a reduction in energy consumption, the reduction in vapor flow led to more pronounced decreases compared to temperature variation, considering the range of variation proposed in this study.

Table 4: Energy balance exchanged by the equipment streams in Different Equipment for Various Mass Flow Rates of V-01 Introduced into the System.

Mass flow	V-01	C101	C102	C103	C104	H101	H102
	Kg/h	Gcal/h	Gcal/h	Gcal/h	Gcal/h	Gcal/h	Gcal/h
V-01	38700	38.86	12.43	23.33	3.73	-11.27	-8.77
	34830	38.48	10.40	23.39	3.66	-11.27	-6.88
V-04	3000	38.85	12.90	23.33	3.73	-11.28	-8.79
	2700	38.88	12.67	23.33	3.73	-11.28	-8.66
V-05	5573	38.86	12.48	23.33	3.73	-11.27	-8.78
	5015	38.86	12.06	23.33	3.73	-11.27	-8.54

Additionally, the decrease in energy required to cool the vapor in the absorption column reflects the impact of the reduced amount of vapor generated in the system. This change not only reduces the overall energy consumption of the process but also improves the thermal efficiency of the system by operating with lower energy demands without compromising operational stability.

This scenario reinforces the robustness of the system in response to adjustments in vapor flow, demonstrating that the reduction in the mass flow rate of vapor V-01 does not compromise critical operations, such as ammonia removal or the efficiency of the heat exchangers. On the contrary, it highlights an opportunity for energy optimization, enabling sustainable and economically advantageous operation.

However, it is important to emphasize that the present work is strictly theoretical in nature and is therefore subject to the inherent limitations of mathematical models and the simplifying assumptions adopted. While the findings indicate potential operational benefits, the analyzed system exhibits high complexity, as it involves an electrolytic system where the formation of solid species (salts) may occur depending on the operational conditions of composition, temperature, and pressure. The precipitation of these species can lead to the formation of deposits on the system's surfaces, resulting in a loss of operational efficiency, changes in mass and energy transfer coefficients, as well as potential hydrodynamic impacts. Although the model calculates the formation of solids, such phenomena were not incorporated into the model used, which may limit the applicability of the results to real systems.

CONCLUSION

Process optimization plays a fundamental role in industrial decarbonization, establishing itself as a viable strategy for reducing energy consumption and inputs in industrial processes. The results of this study demonstrate that variations in temperature and pressure do not significantly impact the system's operational performance (flow rate, temperature, composition), allowing adjustments in these variables without compromising overall operation. However, only the reduction in temperature resulted in a 5% decrease in energy consumption. Among the evaluated strategies, reducing the flow of steam injected into the process proved to be the most effective, promoting considerable reductions in steam flows, temperatures, and heat exchange, without compromising the efficiency of ammonia recovery, a crucial factor for process sustainability. These results suggest that there is significant potential for operational adjustments in the steam used in the system, even within the limits already practiced in the industry. However, to achieve even more significant advances in the process's energy efficiency, more detailed investigations involving other operational parameters are necessary. Future studies may focus on the interaction between different process variables, the impact of extreme conditions, and the application of emerging technologies, aiming to identify additional opportunities for optimization and emission reduction, thereby strengthening the commitment to industrial sustainability.

DIGITAL SUPPLEMENTARY MATERIAL

Further details on the effects of variations in steam pressure and temperature on the system temperature and mass flow rate are provided in the digital supplementary material (LAPS.2026.0023)

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