



# Digital twin-based modeling of heat transfer processes in soda ash production

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## Abstract

The production of soda by the Solvay process is based on complex phenomena of mass and heat transfer in multiphase systems, involving gas–liquid and liquid–solid reactions. The foundation of such analyses lies in understanding and optimizing the nonlinearity and dynamics of the processes involved. This paper presents a digital design, optimization, and comparison of process data obtained through simulation of the post-filtration liquor heating together with ammoniacal recirculating condensates cooling using plate heat exchangers, aimed at replicating realistic operational conditions of the process. The obtained results demonstrate the potential of modeling technologies in predicting process parameters, optimizing operations, and identifying operational deviations. As a result of the simulations conducted in the digital environment, 99.04% agreement was achieved between the process parameters obtained from the model and those measured in production. The simulation data served as the input basis for production tests, which resulted in an increase of 25 K in the temperature of the post-filtration liquor directed to the distillation unit, which enables further research towards the potential reduction of heat consumption in the form of steam within the ammonia recovery installation.

## Keywords

Industry 5.0, digital twin, soda ash production, chemical process simulation, plate heat exchangers

## 1. INTRODUCTION

The use of digital twins in chemical processes aligns with the concept of Industry 5.0. Human intelligence and modern machines work together in Industry 5.0, a manufacturing and industrial revolution. Unlike Industry 4.0, Industry 5.0 prioritizes human–machine collaboration over automation and cyber-physical systems. In this era, human creativity and problem-solving skills, combined with the precision of robotics and artificial intelligence, contribute to a more productive and harmonious industrial environment (Khan et al., 2025)

The concept of the Digital Twin (DT) was first introduced in 2002 by Michael Grieves at the University of Michigan (Grieves and Vickers, 2017). Since then, the term has appeared in numerous frameworks, including an early version of NASA's technology roadmap in 2010 (Shafto et al., 2010).

In an era marked by continuous technological advancement and industrial innovation, the concept of Digital Twins (DT) has emerged as a powerful driver of transformation, revolutionizing conventional approaches within the pervasive chemical industry. The integration of cutting-edge technologies such as artificial intelligence, the Internet of Things (IoT), and big data analytics is redefining long-established industrial processes (Mane et al., 2024). It is expected that Digital Twin frameworks will increasingly support the design and development of intelligent control systems, based on five-dimensional models. These models create a virtual representation of a real

system or process, consisting of two key components: a mathematical or descriptive model and a tangible visual representation (Kherbache et al., 2021; Tepljakov 2023; Vaclavova et al., 2022; Werbińska-Wojciechowska and Winiarska, 2023). Digital Twins (DT) represent an emerging technology that has recently gained significant popularity in case studies related to lifecycle management and predictive analytics across various industries and domains (Botín-Sanabria et al., 2022). The application of digital twins offers a range of benefits, including more accurate determination of product lifecycle stages, reduction of costs associated with the construction of prototype installations (or multiple prototype systems), which can also be time-consuming, and the ability to simulate experiments that cannot be conducted on a laboratory or industrial scale due to safety or practical constraints. Furthermore, digital twins enable real-time monitoring, analysis, and prediction of potential issues, thereby supporting critical decision-making in emergency situations and helping to reduce the risk of failures and losses. They also facilitate the optimization of complex systems within industrial plants including process parameters and raw material consumption indicators across the entire scale of the process, which may consist of multiple interconnected units (Szczepblewski et al., 2025).

In the production of soda by the Solvay process, a number of multiphase flows occur due to the chemical reactions taking place in systems where different phases (gas–liquid–solid) come into contact. Within the gas–liquid absorption process,



the following key stages can be distinguished: ammonia ( $\text{NH}_3$ ) absorption, carbon dioxide ( $\text{CO}_2$ ) absorption, and ammonia regeneration. The filtration stage of the suspension occurs in a liquid–solid system, utilizing the differences in solubility between sodium bicarbonate and ammonium chloride, while the crucial carbonation process involves a gas–liquid–solid system. In such complex systems and numerous inter process connections, modeling tools are increasingly being employed to holistically optimize production systems.

In this study, the gPROMS Process 2024.1.0 digital twin modeling software was used to develop equation-oriented models simulating the process of post-filtration liquor heating and ammoniacal recirculating condensates cooling. This approach enabled the determination of equipment and process parameters that can be implemented in an industrial soda production facility operating according to the Solvay process. In the analyzed process system, the heating of the post-filtration liquor together with ammoniacal recirculating condensates cooling is carried out in plate heat exchangers (PHE). PHEs are among the most commonly used heat exchanger designs in the chemical industry, energy sector, and many other fields. The construction of a PHE is based on a stack of thin metal plates (typically made of stainless steel, titanium, or nickel) arranged in parallel. These plates have specially embossed patterns that induce flow turbulence and increase the heat transfer coefficient. The plates are separated by gaskets, which both seal and direct the flow of the two media through alternating channels (Zhang et al., 2019).

The literature provides several examples of the application of digital twins in the chemical industry, including methanol production (Ferranti et al., 2021; Moretta et al., 2022), bioethanol distillation plants (Botín-Sanabria et al., 2022; Xu et al., 2023), as well as instances of their use in soda production processes (Golubev et al., 2023; Szczeblewski et al., 2025). However, a review of the available literature revealed no publications addressing the application of digital twin-based heat exchange process modeling in post-filtration liquor heating and ammoniacal recirculating condensates cooling systems within the soda production industry.

## 2. RAW MATERIALS AND MODELING APPROACH

### 2.1. Post-filtration liquor

The inlet substrate heated in the plate heat exchangers is the post-filtration liquor, in which ammonia is present both as “free” ammonia—ammonium carbonate and bicarbonate ( $(\text{NH}_4)_2\text{CO}_3$ ,  $\text{NH}_4\text{HCO}_3$ ,  $\text{NH}_4\text{OH}$ ) at concentrations of 18.7–22.1 g/dm<sup>3</sup> – and as “bound” ammonia in the form of ammonium chloride ( $\text{NH}_4\text{Cl}$ ) and, in small amounts, ammonium sulfate ( $(\text{NH}_4)_2\text{SO}_4$ ) at 55.25–62.9 g/dm<sup>3</sup>. The remaining components of the post-filtration liquor are NaCl

and  $\text{H}_2\text{O}$ . The medium has a temperature of 293.15 K, a density of 1145.01 kg/m<sup>3</sup>, and a specific heat capacity of 3.18 kJ/(kg · K) (Bukowski, 1958; Bukowski, 1978).

### 2.2. Ammoniacal condensates

The stream of recirculating condensates in the plate heat exchanger system and the KDS-type shell tube cooler has a temperature of 331.15 K, a density of 975.66 kg/m<sup>3</sup>, and a specific heat capacity of 3.88 kJ/(kg · K).

### 2.3. Cooling water

The cooling water used for the cooling of circulating ammonia condensate at a temperature of 293.15 K, with a density of 998.2 kg/m<sup>3</sup> and a specific heat capacity of 4.182 kJ/(kg · K).

### 2.4. Modeling approach

An analysis of the software available for heat exchanger modeling reveals the presence of several types of tools on the market. Professional industrial tools for the design and simulation of heat exchangers, including plate heat exchangers, such as HTRI – Xchanger Suite / Xphe, provide an environment that integrates numerical modeling with experimental data (Maina et al., 2018). AspenTech modules allow for the design and performance evaluation of plate heat exchangers (gasketed, welded, brazed), commonly used in conjunction with Aspen HYSYS/Aspen Plus for the design and operational optimization of heat exchangers, including in full-scale production (Janaun et al., 2016). General CFD (Computational Fluid Dynamics) tools are used in numerical studies of plate heat exchangers, particularly when detailed analysis of flow behavior, temperature distribution, and pressure drop is required (Pianko-Oprych and Jaworski, 2017). The authors of the publication focused on the gProms environment due to the software’s extended capabilities, which align well with the realistic modeling of the soda production process via the Solvay method. Siemens’ gProms software enables the simulation of heat and mass transfer processes throughout the entire production process, taking into account the ionic concentrations of individual raw material and product components. This is particularly important for the soda industry, as it allows for the analysis of sodium ion migration and  $\text{CO}_3^{2-}$  groups. Such a model facilitates a comprehensive analysis of the entire production process.

The digital models used for the simulations were developed using gPROMS Process 2024.1.0. This process simulation software supports key design and operational decisions based on equation-oriented models, allowing the construction of process block diagrams through drag-and-drop of both basic and advanced unit operations from the model library, as well as the creation of custom models using the gPROMS modeling language. The resulting block diagram can then

be simulated or used for optimization and validation studies. To conduct detailed investigations in the digital environment, a model replicating the real industrial production process was created. Figure 1 illustrates the model of the post-distillation gas cooling system in a KDS-type shell tube cooler, including the heating of the post-filtration liquor in the plate heat exchanger PHE<sub>1</sub> and the recirculating condensates cooling system in the plate heat exchanger PHE<sub>2</sub>. This publication focuses on the studies conducted in the digital environment using the plate heat exchangers: PHE<sub>1</sub> and PHE<sub>2</sub>.

### 3. SYSTEM MODELING AND VALIDATION OF PROCESS PARAMETERS

In order to accurately represent the process, models of the plate heat exchangers PHE<sub>1</sub> and PHE<sub>2</sub> were developed as separate units and in the next steps they were implemented to full installation model. Figure 2 shows the plate heat exchanger no 1 (PHE<sub>1</sub>). Figure 3 shows the plate heat exchanger no 2 (PHE<sub>2</sub>).

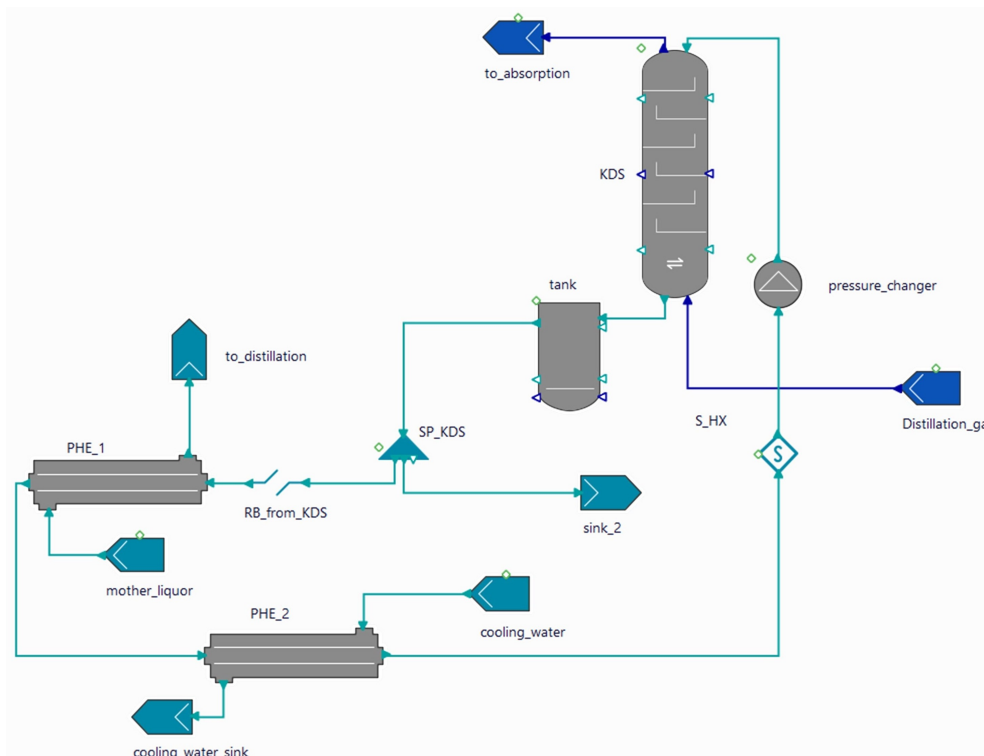


Figure 1. Model of the post-distillation gas cooling system, including the post-filtration liquor preheater and the circulating condensate cooler developed in gPROMS Process 2024.1.0.

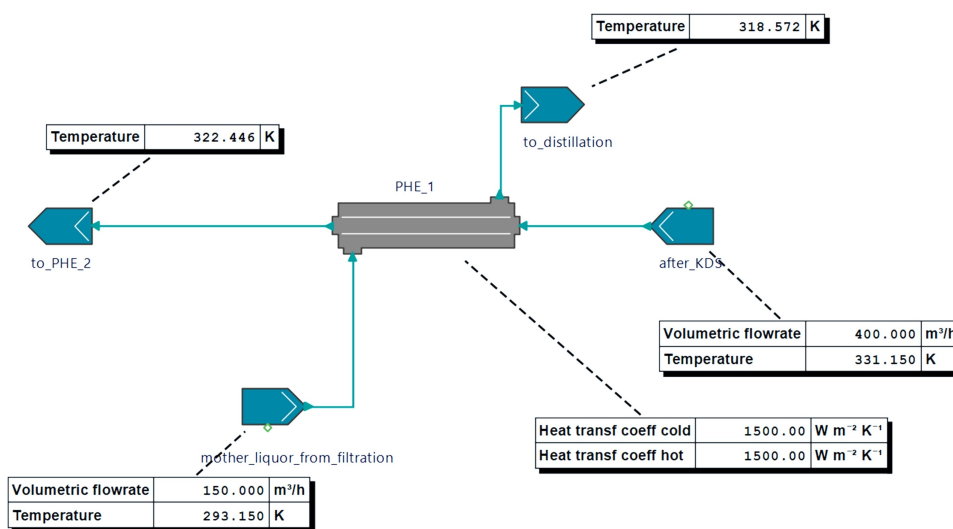
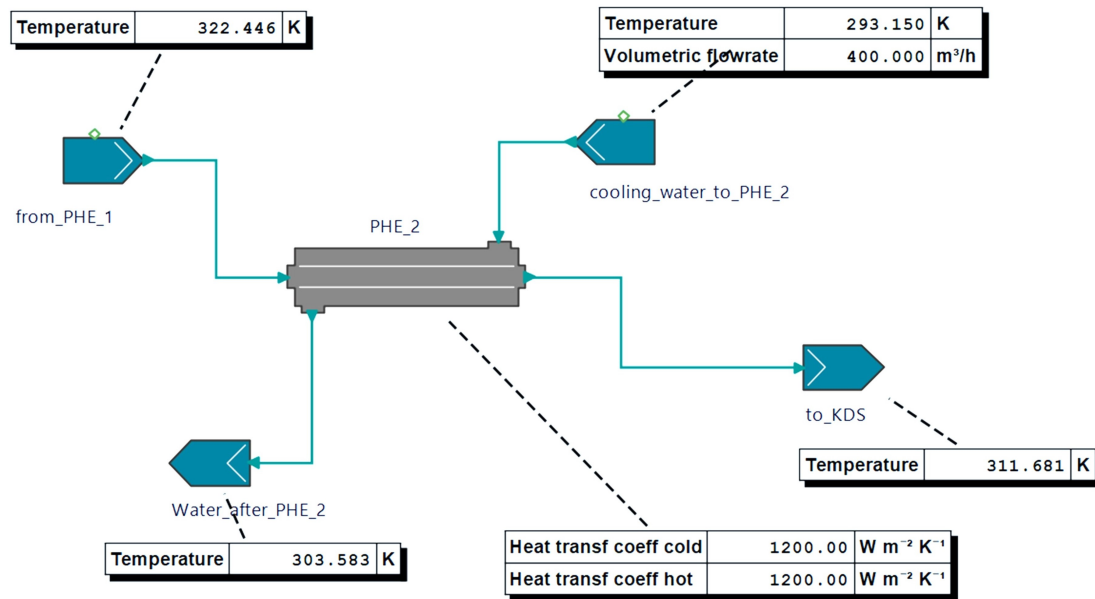


Figure 2. Plate heat exchanger (PHE<sub>1</sub>) model developed in gPROMS Process 2024.1.0.

Figure 3. Plate heat exchanger (PHE<sub>2</sub>) model developed in gPROMS Process 2024.1.0.

In the initial stage, the volumetric flow rate, temperature, and composition of the inlet media streams to the plate heat exchangers were determined based on experimental data. In the subsequent stage, the parameters of the plate heat exchangers were defined, beginning with the constructional dimensions  $1.4 \text{ m} \times 0.9 \text{ m} \times 2.1 \text{ m}$  ( $H \times W \times L$ ), followed by the determination of the pressure drop on the hot (0.594 bar) and cold (0.12 bar) sides, evaluation of the surface enlargement factor, calculation of the heat transfer coefficient ( $1500 \text{ W}/(\text{m}^2 \cdot \text{K})$  for PHE<sub>1</sub> and  $1200 \text{ W}/(\text{m}^2 \cdot \text{K})$  for PHE<sub>2</sub>), and estimation of the required number of plates for each exchanger (130 plates). The equation-based models employed in this study constituted the theoretical heat balance of the heat exchangers. In subsequent stages of the research, the simulation results obtained from the digital environment were compared with real operational data acquired from the production process.

### 3.1. Surface enlargement factor

#### 3.1.1. Geometrical definition of the corrugation factor

$$\Phi = \frac{A_{\text{dev}}}{A_{\text{proj}}} \quad (1)$$

where  $A_{\text{dev}}$  is the developed area or true surface area and  $A_{\text{proj}}$  is the projected area. Typical values  $\Phi = 1.10\text{--}1.30$  for most industrial chevron plates with angles of  $30\text{--}65^\circ$ .

#### 3.1.2. Sinusoidal model (for a sinusoidal profile)

For a simplified corrugation shape, assumed as a sinusoidal wave with amplitude  $a$ ,  $L_{\text{dev}}$  developed length,  $L_{\text{proj}}$  projected length and wavelength  $\lambda$ :

$$\Phi = \frac{L_{\text{dev}}}{L_{\text{proj}}} = \frac{1}{\lambda} \int_0^\lambda \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx \quad (2)$$

Assuming  $y = a \sin\left(\frac{2\pi x}{\lambda}\right)$ :

$$\Phi = \frac{1}{\lambda} \int_0^\lambda \sqrt{1 + \left(\frac{2\pi a}{\lambda}\right)^2 \cos^2\left(\frac{2\pi x}{\lambda}\right)} dx \quad (3)$$

After integration (or approximation for small slopes)  $a/\lambda \ll 1$ :

$$\Phi \approx 1 + \frac{1}{4} \left(\frac{2\pi a}{\lambda}\right)^2 = 1 + \pi^2 \left(\frac{a}{\lambda}\right)^2 \quad (4)$$

#### 3.1.3. Chevron plate model (with angled embossments)

For plates with a “chevron” geometry (diagonal corrugations at an angle  $\beta$ ), a simplified formula is used (Sodagar-Abardeh et al., 2020):

$$\Phi = \frac{1}{\cos \beta} \quad (5)$$

or, when the effect of corrugation depth is also considered:

$$\Phi = \frac{1}{\cos \beta} \left(1 + \frac{2a}{\lambda}\right) \quad (6)$$

where  $\beta$  is an inclination angle of the corrugations (chevron angle,  $30\text{--}65^\circ$ ),  $a$  is the half of the fold height (corrugation amplitude),  $\lambda$  is the wavelength (distance between corrugation peaks). In practice,  $1/\cos \beta$  typically gives the following coefficients: for  $\beta = 30^\circ$   $\Phi \approx 1.15$ , for  $\beta = 45^\circ$   $\Phi \approx 1.41$  and for  $\beta = 60^\circ$   $\Phi = 2.00$  (theoretically, but lower in practice due to flow limitations).

In plate heat exchanger models (PHE<sub>1</sub> and PHE<sub>2</sub>) created in gProms Process 2024.1.0, the surface corrugation factor is introduced as an effective (corrected) parameter, rather than as an exact geometric description of the plate. In actual heat exchangers, surface corrugation factors typically range from 1.1 to 1.3, reflecting the real developed surface area resulting from the plate's corrugations (chevrons). In one-dimensional (1D) models, such as those used in the present study, this value is often increased above the typical range of 1.3–1.6 to better match the model behavior to experimental or real process data.

gProms Process utilizes the Logarithmic Mean Temperature Difference method (LMTD) for plate heat exchangers calculations. The Logarithmic Mean Temperature Difference (LMTD) method is commonly used to analyze heat exchangers, including condensers, as it effectively calculates heat transfer rates by accounting for the varying temperature differences between hot and cold fluids throughout the heat exchanger (Cartaxo and Fernandes, 2011; Claesson, 2005; Swardhamana et al., 2024; Xia et al., 2009).

### 3.2. Calculation methodology used during the simulation

The heat transfer area was expressed as the global design equation:

$$Q = UA \Delta T_{lm} \quad (7)$$

where  $U$  is the overall heat transfer coefficient [ $W/(m^2 \cdot K)$ ],  $A$  is the total area of heat transfer [ $m^2$ ] and  $\Delta T_{lm}$  is log mean temperature difference [ $K$ ], which is a function of the inlet and outlet liquid temperature.  $\Delta T_{lm}$  is log mean temperature difference [ $K$ ] method also used to compare process data with process simulation data.

$$\Delta T_{lm} = \frac{\Delta T_2 - \Delta T_1}{\ln \left( \frac{\Delta T_2}{\Delta T_1} \right)} \quad (8)$$

### 3.3. Methods for comparing real and simulated values

Log mean temperature difference [ $K$ ] from LMTD method was also used to compare process real data with process simulation data. The real temperature  $T_{lm,real}$  and simulated temperature  $T_{lm,sim}$  were compared together with mass flowrates  $\dot{V}_{real}$ ,  $\dot{V}_{sim}$

by determining the relative error:

$$\text{Relative error} = \frac{|T_{lm,real} - T_{lm,sim}|}{T_{lm,real}} \times 100\% \quad (9)$$

$$\text{Relative error} = \frac{|V_{lm,real} - V_{lm,sim}|}{V_{lm,real}} \times 100\% \quad (10)$$

In order to compare the data obtained from plate heat exchanger simulations with data collected from online measurements in the production environment, the Mean Squared Error (MSE) and the Root Mean Squared Error (RMSE) were employed.

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (11)$$

where  $n$  is the number of observations,  $y_i$  is the real production value and  $\hat{y}_i$  is the predicted value from the model.

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (12)$$

A total of 50 simulations of the process were performed in a digital environment ( $n = 50$ ).

### 3.4. Parameters and calculations

Table 1 presents the data obtained from PHE<sub>1</sub> simulations in a digital environment, along with process data acquired from online measurements during production process. The specific heat values ( $C_{p,h} = 3.88 \text{ kJ}/(\text{kg} \cdot \text{K})$ , ( $C_{p,c} = 3.18 \text{ kJ}/(\text{kg} \cdot \text{K})$ ), density ( $\rho_h = 975.6 \text{ kg}/\text{m}^3$ ,  $\rho_c = 1145.0 \text{ kg}/\text{m}^3$ ) and the heat transfer coefficient  $U$  ( $1500 \text{ W}/(\text{m}^2 \cdot \text{K})$ ) were assumed to be constant. The calculated heat transfer area  $A$  was  $127 \text{ m}^2$ . During the research, a total of 50 process simulations were performed using digital twins ( $n = 50$ ). The simulation results were compared with actual production data, which were averaged from monthly measurements obtained from the industrial plant.

The data used to develop the digital twin models were introduced progressively in stages, taking into account that the models employ machine learning processes to perform successive simulations. Results from the initial simulations were stored in SVS (Saved Variable Set) files, which then served as the basis for subsequent heat transfer process analyses. In this way, the prepared virtual laboratory relies on multiple variables that are continuously utilized throughout the simulations, thereby avoiding restriction to a narrow data range.

Table 1. Comparison of data obtained from simulations with process data for PHE<sub>1</sub>.

	$T_{h,in}$ [K]	$T_{h,out}$ [K]	$\dot{V}_{h,in}$ [kg/s]	$\dot{V}_{h,out}$ [kg/s]	$T_{c,in}$ [K]	$T_{c,out}$ [K]	$\dot{V}_{c,in}$ [kg/s]	$\dot{V}_{c,out}$ [kg/s]
PHE <sub>1</sub> gProms simulation	331.1	322.4	108.4	106.9	293.1	318.5	47.7	47.4
PHE <sub>1</sub> process data	332.1	323.7	107.7	106.2	294.4	319.8	46.8	46.5

Table 2 presents the data obtained from PHE<sub>2</sub> simulations in a digital environment, along with process data acquired from online measurements during production process. The specific heat values ( $C_{p,h} = 3.88 \text{ kJ}/(\text{kg} \cdot \text{K})$ ,  $C_{p,c} = 4.182 \text{ kJ}/(\text{kg} \cdot \text{K})$ ), density ( $\rho_h = 975.6 \text{ kg}/\text{m}^3$ ,  $\rho_c = 998.2 \text{ kg}/\text{m}^3$ ) and the heat transfer coefficient  $U$  ( $1200 \text{ W}/(\text{m}^2 \cdot \text{K})$ ) were assumed to be constant. The calculated heat transfer area  $\lambda$  was  $206 \text{ m}^2$ . During the research, a total of 50 process simulations were performed using digital twins ( $n = 50$ ). The simulation results were compared with actual production data, which were averaged from monthly measurements obtained from the industrial plant.

In Tables 3 and 4, the temperature differences and mass flow rates obtained from the PHE<sub>1</sub> and PHE<sub>2</sub> digital models were calculated with industrial process data for  $n = 50$  observations.

The following Figure 4 presents the temperature profile in the plate heat exchanger PHE<sub>1</sub> for the cold and hot inlet streams. The plot correlates the temperature across the entire cross-section of the heat exchanger. The values on the X-axis represent the length of the exchanger, with 0.00 corresponding to the inlet of the cold stream and the outlet of the hot stream, and 1.0 corresponding to the outlet of the cold stream and the inlet of the hot stream. Analysis of the profile clearly shows an increase in the post-filtration liquor temperature from  $293.15 \text{ K}$  to  $318.57 \text{ K}$  ( $\Delta T = 25.42 \text{ K}$ ). An increase in the post-filtration liquor temperature leads to a reduction in process steam consumption in the distillation columns used in the ammonia recovery process. The post-filtration liquor fed to the columns requires less heating to reach the desired temperature, which consequently reduces energy demand.

Lower steam consumption decreases operational costs while simultaneously improving the overall energy efficiency of the process. An additional benefit of increasing the post-filtration liquor temperature is the stabilization of the plant operation. In practical terms, such energy savings have a significant economic impact, particularly in large-scale industrial process installations.

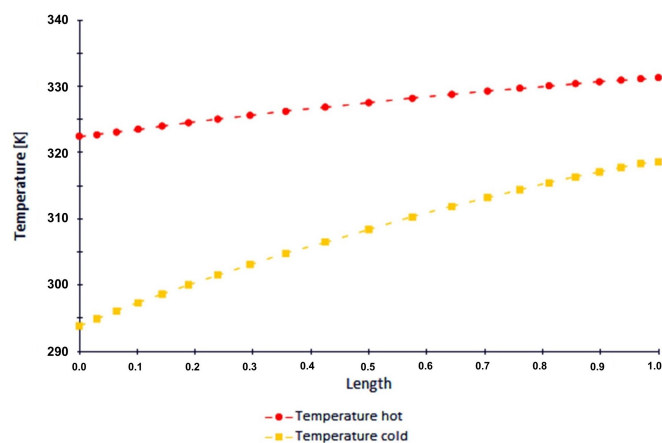


Figure 4. Temperature profile of PHE<sub>1</sub> generated in gPROMS Process 2024.1.0. (value 0 on X-axis corresponds to the beginning of the heat exchanger, and 1.0 corresponds to its full length).

The following Figure 5 presents the temperature profile in the plate heat exchanger PHE<sub>2</sub> for the cold and hot inlet streams. The plot correlates the temperature across the entire cross-section of the heat exchanger. The values on the X-axis represent the length of the exchanger, with 0.00 correspond-

Table 2. Comparison of data obtained from simulations with process data for PHE<sub>2</sub>.

	$T_{h,in}$ [K]	$T_{h,out}$ [K]	$\dot{V}_{h,in}$ [kg/s]	$\dot{V}_{h,out}$ [kg/s]	$T_{c,in}$ [K]	$T_{c,out}$ [K]	$\dot{V}_{c,in}$ [kg/s]	$\dot{V}_{c,out}$ [kg/s]
PHE <sub>2</sub> gProms simulation	322.4	311.6	106.9	105.4	293.1	303.5	111.9	111.2
PHE <sub>2</sub> process data	323.7	313.0	104.9	104.9	294.3	305.6	110.8	110.9

Table 3. Comparison of temperature differences and mass flow rates obtained from simulations and real data for PHE<sub>1</sub>.

	$T_{h,in}$ [K]	$T_{h,out}$ [K]	$\dot{V}_{h,in}$ [kg/s]	$\dot{V}_{h,out}$ [kg/s]	$T_{c,in}$ [K]	$T_{c,out}$ [K]	$\dot{V}_{c,in}$ [kg/s]	$\dot{V}_{c,out}$ [kg/s]
RMSE	0.95	1.32	0.7	0.7	1.26	1.29	0.9	0.9
Relative error [%]	0.28	0.408	0.65	0.659	0.42	0.403	1.92	1.94

Table 4. Comparison of temperature differences and mass flow rates obtained from simulations and real data for PHE<sub>2</sub>.

	$T_{h,in}$ [K]	$T_{h,out}$ [K]	$\dot{V}_{h,in}$ [kg/s]	$\dot{V}_{h,out}$ [kg/s]	$T_{c,in}$ [K]	$T_{c,out}$ [K]	$\dot{V}_{c,in}$ [kg/s]	$\dot{V}_{c,out}$ [kg/s]
RMSE	1.27	1.39	2	0.5	1.2	2.1	1.1	0.31
Relative error [%]	0.39	0.44	1.91	0.47	0.41	0.687	0.99	0.28

ing to the inlet of the cold stream and the outlet of the hot stream, and 1.0 corresponding to the outlet of the cold stream and the inlet of the hot stream. Analysis of the profile clearly shows an decrease in the ammoniacal recirculating condensate temperature from 322.44 K to 311.68 K ( $\Delta T = 10.76$  K). The use of lower temperature ammonia circulating condensates directed to a KDS-type cooler reduces the temperature of the gas fed to the absorption system and may improve the concentration of the ammonia solution in brine. Precise control of the post-distillation gas temperature helps minimize the risk of thermal stress or corrosion in process equipment and additionally optimizes the overall operation of the plant.

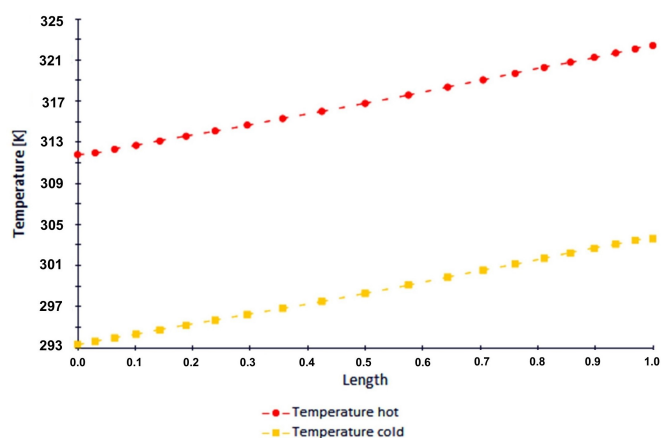


Figure 5. Temperature profile of PHE<sub>2</sub> generated in gPROMS Process 2024.1.0. (value 0 on X-axis corresponds to the beginning of the heat exchanger, and 1.0 corresponds to its full length).

## 4. RESULTS AND SUMMARY

The software used for creating digital twins in this study was gPROMS Process 2024.1.0, a next-generation process modeling environment that supports the entire design of lifecycle from conceptual design to operation. By leveraging advanced analytical and optimization technologies based on high-fidelity models, gPROMS process digital twins accelerate process design, risk quantification and management, and identify optimal process configurations that generate value throughout the plant's operational lifetime (Astesauin et al., 2001; Näf et al., 1994; Tanvir and Mujtaba, 2008). gPROMS Process 2024.1.0 provides an intuitive and flexible platform for graphically constructing process flow diagrams along with the corresponding master model, which automatically integrates the equations of individual unit models during simulation and optimization (Said et al., 2010).

Analysis of process data from the actual production facility and the digital model reveals a close correlation between the datasets. During the analysis of the obtained data (using the average conformity method by dividing the sum of conformity values by the number of analyses), a 99.04% agreement

was achieved between the data obtained from the digital twin simulation and the process measurements. The lowest relative errors were observed when comparing the inlet and outlet temperatures of the media based on production data and simulation results (relative error ranging from 0.28% to 0.687% and RMSE in the range of 0.95–2.1). For mass flow rates, the relative error was higher (0.28% to 1.94% and RMSE in range of 0.31–2) but still within acceptable deviations. Given that the simulation data obtained from the digital twin environment closely matched real measurements, they could be used as input for subsequent production tests.

The digital simulations provided insights into the assumptions for production tests, reduced the risk associated with on-site testing, shortened the preparation time for pilot installations, and minimized the risk of production downtime. During the simulations, the desired temperature of the post-filtration liquor directed to the distillation unit was successfully achieved. Increasing the temperature of the post-filtration liquid directed to the RH-DS distillation unit (where the RH section serves as the distiller heater and the DS section is the actual distiller) may result in reduced consumption of steam supplied to the unit. Due to the need for a continuous energy supply to the distillation process in the form of steam, a subsequent study will be conducted to analyze potential energy cost reductions in the ammonia recovery section.

The achieved agreement of the digital twin model with real operational data at a level of 99.04% enabled research to be conducted within the digital environment and allowed the integration of simulation results into actual production. This approach not only reduced the time required for traditional heat exchanger design but also facilitated holistic analysis, i.e., studying the impact of obtained parameters on the entire ammonia recovery installation using large-scale optimization. In a traditional approach, such tests would involve risks of deteriorating process parameters due to incorrect assumptions, reduced production efficiency, and, in extreme cases, shutdowns of production lines. Designing heat exchangers in-house clearly demonstrates the benefits of reducing costs associated with employing external design companies. Most importantly, the data used in the model, which constitutes the industrial plant's know-how, remains confidential. The number of articles describing real-world implementations and the associated benefits is limited due to the innovative nature of utilizing digital twins in the chemical industry, particularly in soda production (Szczepkowski and Gębicki, 2025).

While the modeling of heat exchange processes using gPROMS software has been reported in the scientific literature (Chang et al., 2021; Garma et al., 2024), to the best of the authors' knowledge, heat exchange modeling in the soda production process has not yet been performed. This study highlights a substantial knowledge gap concerning the application and practical implementation of Digital Twins in soda ash production.

## SYMBOLS

$C_p$	heat capacity, J/(kg · K)
$\rho$	density, kg/m <sup>3</sup>
$\Phi$	geometrical correction factor
$\alpha$	wave amplitude
$\lambda$	wavelength, mm
$\beta$	angle, °
$\dot{V}$	mass flowrate, kg/s

### Subscripts

in	inlet
out	outlet

### Abbreviations

CFD	Computational Fluid Dynamics
PHE	plate heat exchanger

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