



Numerical Study of Sodium Bicarbonate Production in Industrial Bubble Columns

Jasim Humadi¹ * , Ekehwanh Rasheed²

1. Baghdad, Iraq. E-mail: jasim_alhashimi_ppe@tu.edu.iq
2. Department of Chemical Engineering, Tikrit University, Tikrit, Iraq. E-mail: ekehwanh.a.almajeed@tu.edu.iq

| ARTICLE INFO | ABSTRACT |
|--|---|
| <p>Article History: Received: 21 July 2024 Revised: 04 August 2024 Accepted: 12 August 2024</p> <p>Article type: Research</p> <p>Keywords: Bubble Column, CFD, NaHCO₃, Simulation, Supersaturation</p> | <p>The purpose of this study is to explore the physio-chemical factors that affect sodium bicarbonate synthesis in industrial bubble columns employing CFD simulations. The model represents gas-liquid-solid systems and introduces turbulent phenomena and chemical reactions into the model. Parameter optimizations are performed to analyze the operational parameters such as gas flow rate, liquid phase characteristics, column geometry, and reaction kinetics. This study demonstrates a better understanding of the optimal reaction conditions for maximum NaHCO₃ yielding, fast enough kinetic reaction, and less undesired byproduct formation, as well as introducing productive and environmentally friendly approaches to synthesizing chemical products. The broader width of the column increases turbulent mass diffusivity, but decreases turbulent viscosity. With a broader column width, column pH gradient decreases, due to the increased liquid amount. The concentration of the solutions falls, as the width of the column decreases. For the height of 107 mm, the concentration is 95 mmol/L; this value is 82 mmol/L for the height of 200 mm. Supersaturation increases with column height. For a height of 200 mm, the supersaturation is equal to 0.015. The molar proportion of carbon dioxide in gas is a function of column height, thus 35% at 200 mm and 20% at the air end.</p> |

Introduction

The existing CFD simulations are used to investigate the production of sodium bicarbonate in industrial bubble columns. The process known as Solvay goes back to the 19th century and involves the reaction between sodium chloride and ammonia, carbon dioxide, and water. The industrial foam column boilers are the key elements due to their high capacity of bubble gas-liquid interfacial area and remarkable mass transfer efficiency. The study's purpose is to discover the maximum operating conditions, design criteria, and feature increase strategies that are needed for efficiency and sustainability enhancement. The study provides opportunities for progress in process efficiency, lowering of environmental impact, and advances in chemical production.

Taborda and Sommerfeld [1] showed that bubble columns are more complicated than conventional reactors, enhancing mass and chemical transfer efficiencies. CFD (computational fluid dynamics) is used to learn about these systems and improve processes. Numerical

* Corresponding Author: J. Humadi (E-mail address: jasim_alhashimi_ppe@tu.edu.iq)





implementations of reactive bubble columns adopt the LES-Euler/Lagrange approach, with the oscillation of bubbles being simulated using a random model in the eccentricity and the inclination angle of motion. The behavior of the bubbles is examined in surface forces, and the impact of the chemicals on the reactants is also considered. Large-scale simulation (LSS) is employed in the computation of fluid flows. Bonfim-Rocha et al. proposed several production processes for synthesizing sodium bicarbonate and the chemical reactions involved in the crystallization reactor [2]. It contrasts soda ash generation procedures from trona, the Solvay, and the sodium ammonium sulfate route. The primary raw material is sodium chloride, which due to its general availability in seawater and food applications, is considered economically feasible. The Solvay process suggests the technology has the best performance and economic benefits. The application of sodium sulfate is promising, however may not be ideal, since there are limitations in its product separation and purification, as well as the absence of research studies related to this matter. Abdel-Rahman and Abdullah constructed a mathematical model for designing and simulating highly diluted CO₂ (2-18%) into the flue gases, for the production of sodium bicarbonate in a bubble column reactor [3]. This model employs mass balance equations and Danckwerts concept to consider mass transfer and crystallization. The model came up with CO₂ conversion varying from 34% to 71% and the particle size ranges between 0 to 400 μm.

Lee et al. evaluated the techno-economic vicinity of a CO₂ mineralization process in sodium carbamate production [4]. The process involves the flue gas of a coal-fired power plant to create a sodium carbonate solution containing CO₂. Reduction potential was found to be CO₂ of 0.33 tons of sodium bicarbonate produced and an isolate exclusion value of 0.10 tons of CO₂ emissions was considered. The economic analysis of a plant operating at the capacity of 30,000 tons of sodium bicarbonate production gave a positive result, with a benefit-cost ratio and an internal rate of return of 1.45 and 80,5%, respectively. Adnan Abdel-Rahman implemented a sodium bicarbonate production model based on a bubble column, with high particle retention to minimize filtration and drying processes [5]. A three-variable (CO₂ gas content, temperature, and time) batch bubble column of a lab-scale was employed to study the impact of elevated CO₂ on aquatic organisms. The outcome of the experiments was getting the highest performance in terms of yield and crystal size respectively. The kinetic study is consistent with zero concerning carbonate sodium concentration or CO₂ concentration. The sorption/desorption process is governed by parameters - sodium carbonate and CO₂ concentrations. Zhang et al. proposed a dimensional analysis of the mass transfer turbulent model for computational evaluation of the CO₂ chemisorption in the bubble column reactor [6]. The theory is a correlation between the turbulent mass diffusivity, the metrics of concentration variance, and the dissipation rate, which eventually gives out the easy prediction of the diffusion pattern of the species concentration. By contrast, with the constancy of Schmidt number in traditional SPC simulations, this model avoids this assumption. The simulation is in agreement with the experimental data, and the model can be applied even in the cases when the empirical turbulent mass diffusivity is not available.

Maharloo et al. [7] presented a new sodium bicarbonate production approach, using an industrial bubble column reactor. Of all the components of this model, a portion of the outlet CO₂ stream is given back for recycling, which greatly cuts down on greenhouse gases and the production of mineral acid. In this model, the concept of translational and rotational behavior of a liquid, CO₂ conversion, and its pressure-gas profile are considered. The model predicts a 314 mol/m².s reduction in CO₂ emission, a 50% increase in the power of the particles made, and a great decrease in the amount of pollutants. Shim et al. [8] performed CO₂ capture and conversion with NaOH in coal-fired power stations. CO₂ gas reacts with sodium hydroxide to produce sodium bicarbonate (NaHCO₃). This experiment verified the feasibility of carbon

capture technologies for coal-based power plants, which operate based on sodium hydroxide with useful data for the construction and operation of the full-scale plants. Goharrizi and Abolpour [9] investigated the effects of diverse situations on the nucleation and boom rate of sodium bicarbonate crystals. It uses Danckwert's principle for mass switch between gasoline and liquid levels, growth formula, and population stability to derive nucleation. The outcomes showed that the production of sodium bicarbonate crystals decreases under unique running situations.

Jain et al. [10] designed a unit operation based on the micro-structured bubble column type (microsieves), which proved to be safer than the slurry bubble column (SBC) and trickle mattress (TB) types in chemical, petrochemical, and pharmaceutical industries. The static mesh of thin wires coated with the catalyst serves to further micro-shape the catalyst service area and prevent bubbles from occurring in the interface, consequently leading to high interfacial contact and dynamic interface behavior. The paper numerically analyzes MSBC and the usage of a hybrid-volume of fluid (VOF)-discrete bubble model (DBM) and a variant, which handles mass switch with chemical reaction. Studies indicate that installing a greater number of mesh stacking in the columns leads to a significant enhancement of mass transfer. Goharrizi and Abolpour [11] studied gas-liquid mass transfer, accompanied by chemical reactions, gas-liquid-solids mass transfer, and crystallization in bubble column reactors. The reactor will cause the emission of sodium bicarbonate, which includes carbonate, bicarbonate, and carbon dioxide. A bubble column flow and a reactor column additive were investigated with mole balances, while cell population stability analyzes the nucleation and addition of cubic phase. The principle of Danckwerts is used for gasoil-gasoline mass levitation. In the current work, the model predicts the behavior of several parameters, in terms of the production quantity of sodium bicarbonate crystals and also the conversion process of carbon dioxide. Simulation outcomes are compared with observations to validate the model. The effects of different parameters on manufacturing processes and morphology of Sodium bicarbonate crystals are considered and absorption of CO₂ is investigated. Saberi et al. [12] investigated the formation and boom of sodium bicarbonate in the middle ranges of soda ash manufacturing. It uses titration, magma density monitoring, and sieving to determine crystal length distribution. These effects display correlations between nucleation and growth costs, which can be used to simulate the crystallization of sodium bicarbonate flowers in industrial reactor situations.

Haut et al. [13] developed a mathematical version for a particular commercial column for refined sodium bicarbonate production. Using measurements and experimental data, an ID model with two bubble populations was constructed, alongside a gasoline-liquid mass switch model. Wylock et al. [14] followed a multi-scale approach, as illustrated in the picture beneath. Three essential steps are concerned in its creation: research at the scale of the bubble, studies at the size of the lab, and research at the dimensions of the industrial columns. The necessary data for the scale of the bubble have already been supplied in preceding papers. In this paper, we focus on the results of the studies at the size of the lab and the dimensions of the economic column. Abolpour and Goharrizi [15] produced sodium bicarbonate throughout soda ash manufacturing, in which carbon dioxide fuel is injected right into a bubble column reactor. This observation analyses gas-liquid mass switch, chemical reactions, and liquid-strong mass transfer. A mathematical modeling version predicts the size distribution of sodium bicarbonate crystals. This version used the experimental results from Shiraz Petrochemical Complex's bubble column reactor.

Specific types of carbon-based adsorbents, like the ones for phenolic compounds removal, exhibit high efficiency, because of the highly developed surface area and potential adsorption sites. In the case of the removal of sulfur from heavy gas oil, recently synthesized activated carbon-based adsorbents show better adsorption capacities and effectiveness, compared to the traditional activated carbon, due to porosity and surface defects [16, 17]. Although these materials emphasize several absorptive uses of bubble columns, the production of sodium bicarbonate using bubble columns depends on versatile CFD Modeling. This approach strives

to adjust the operational conditions, including the width of the column, to get the highest possible output and the least quantity of byproducts. Besides, it considers the environmental aspect, particularly in the course of employing the CO₂ recycling mechanism and techno-economic analysis, which makes it different from other methods that might not have such specific optimization [18]. It verifies the obtained results from the simulation, making them more accurate and reliable results, which sets this work apart from other works in the literature [19].

To the best of the author's knowledge, this study is the first to couple comprehensive CFD simulations with LES-Euler/Lagrange models to predict sodium bicarbonate production in the industrial bubble columns, with satisfactory prediction of gas-liquid-solid interactions. It describes the impact of column width in the distribution of turbulent mass diffusivity, viscosity of species, concentration of the particular species, supersaturation, and magma density, with a suggested range on how column width should be designed. The latter is a global parameter optimization with the yield on the top and byproducts on the bottom, where environmental sustainability comes into play, with concepts like CO₂ recycling and the techno-economic assessment. Extensive parameter analysis and validation with experimental data, make this work different from some of the existing literature, which may be loosely simulated, less-parameterized, or in some cases, without experimental validation.

Methodology

In this section, all the governing equations will be discussed using ANSYS and MATLAB, to complete the full simulation and details of the flow through the column, which will be done by CFD. The values of the variables in the results will also be extracted through the equations in MATLAB.

Geometry Design

The obtained results were validated with a three-dimensional cylindrical bubble column. The liquid level was maintained at 1.5 meters, and the diameter of the column was set to zero, regardless of the height. A sintered metal frit covering the entire length of a sparger was used to evenly distribute fuel in the modeling domain. Therefore, in our simulation, we can treat the uniform distribution of inlet bubbles as the best assumption.

Boundary Condition

The jacket attached to the bubble column is heated, so the temperature reaches 25 °C. The column initially contained an aqueous sodium hydroxide solution with pH = 13.3 and CO₂ was sparged with a liquid flow rate of .035 m/s. pH probes were installed in specific reactor widths: 107 mm, 150 mm, and 200 mm just above the feeder pipe. The exact substance samples were taken at the same heights and carbonate concentrations were determined [6]. Precipitation test was conducted by adding barium chloride and performing hydrochloric acid titration. These processes were undertaken to detect the carbonated nature of the liquid, but the outcomes could be affected by the presence of hydrogen carbonate.

To determine the best width of the column for sodium bicarbonate production in industrial bubble columns, a comparison should be made with the wider ranges of the column width, for example, 250, 300, and 350 mm, using the CFD models. A thorough comprehensive numerical and experimental parametric analysis and sensitivity analysis needs to be carried out to assess the effects on mass transfer, turbulence, and reaction kinetics. Better yield conditions can be discovered using optimizations, such as Response Surface Methodology. The final step in

Simulation is to compare the simulation results with experimental results and conduct the cost-benefit analysis of the Simulation. In this approach, factors such as efficiency, yield, and environmental sustainability of the process are planned and desired.

Mesh

A grid with a number of 495664 meshes was selected in these paintings, after thinking about the computational accuracy and the time required, as compared with a grid of 659305 meshes. Fig. 1 indicates the computational domain and the grid used in this simulation. A time step of 0.001 s is modified in the calculation. For the solution of the equations, we use a time spent of 300s' chemisorption procedure.

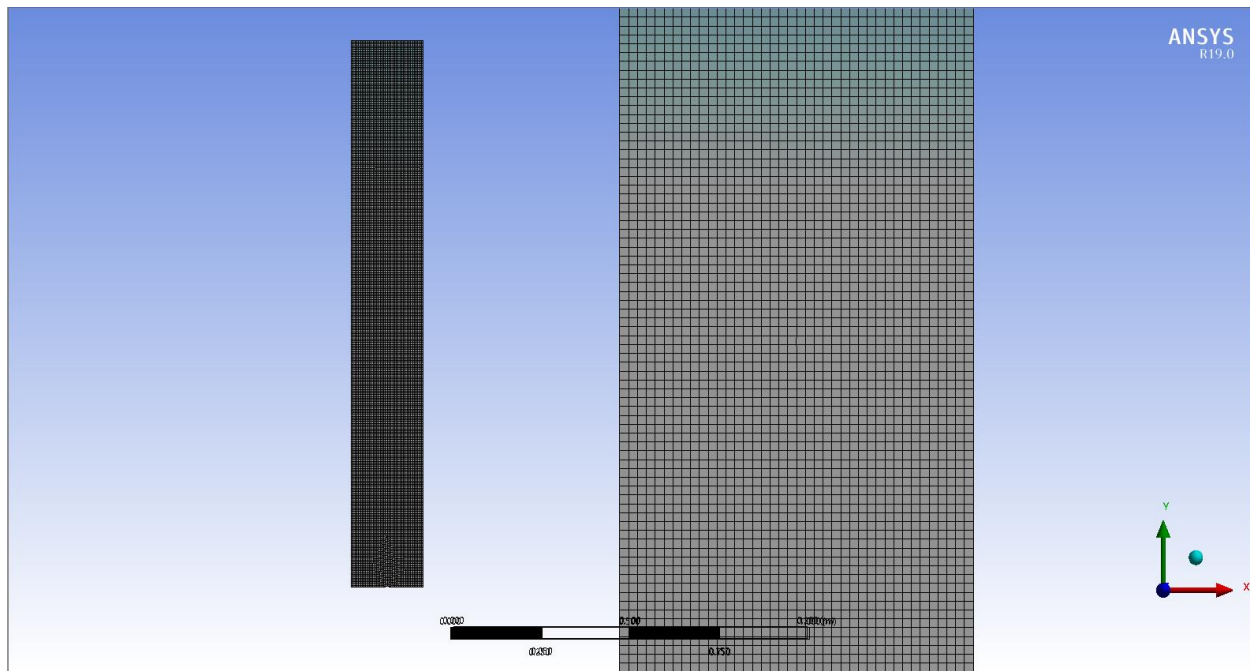


Fig. 1. Mesh generated

An accurate mesh must be created to solve the equations because the simulation process depends on complicated algorithms to work on the matrices present in the domain. After that, we use the mesh's dependability to find a remedy and bring the outcomes to a stable condition. It is important to create more than one mesh and mesh dependability, due to the variety of simulated models. The value of the element was 659305, with the turbulent mass diffusivity m^2/s 0.0349, as presented in Table 1.

Table 1. Mesh independency

| Case | Element | Node | turbulent mass diffusivity m ² /s |
|------|---------|--------|--|
| 1 | 495664 | 274388 | 0.0421 |
| 2 | 563457 | 307675 | 0.0359 |
| 3 | 604365 | 321576 | 0.0351 |
| 4 | 659305 | 334358 | 0.0349 |

Governing Equations

With the pinnacle of 22 m, the temperature of activity is accepted to be consistent inside the length of the segment, as a result of the low intensity of response and utilization of a water coat around it. The response incorporates water, sodium carbonate, and sodium bicarbonate. This arrangement enters the segment from its top feature and a vaporous mix of carbon dioxide and air is continually infused into the section from its posterior. The accompanying balance responses can be mounted inside the segment:



At the point when the consciousness of created sodium bicarbonate arrives at its dissolvability limitation inside the response (answer diverts into immersed from sodium bicarbonate), response 4 happens and the precious stones start to shape inside the segment [11]. The dissolvability of NaHCO₃ in the presence of Na₂CO₃ is given inside the Ref. [11] as underneath:

$$\log(x^*) = 6.71535 - \frac{843.0681}{T} - 2.24336 \times \log(T) \quad (5)$$

a mole balance for the gas stage around the detail yields the ensuing differential overseeing condition:

$$\frac{dG}{dz} = -N_{\text{CO}} \times \alpha_g \quad (6)$$

in which α_g is defined as:

$$\alpha_g = \frac{6 \times \epsilon_g}{d_B} \quad (7)$$

Also, mole strength for carbon dioxide results inside the accompanying differential condition:

$$\frac{d}{dz} (G \times y_{CO_2}) - \frac{\varepsilon_g \cdot D_g}{U_g} \times \frac{d^2}{dz^2} (G \times y_{CO_2}) = -N_{CO_2} \times \alpha_g \quad (8)$$

where gas velocity is given by:

$$U_g = \frac{4 \times G_{FR}}{\pi \cdot d_R^2 + \varepsilon_g} \quad (9)$$

The delivered sodium bicarbonate will stabilize the area. The gulf answer has an immersion or supersaturation consideration of sodium bicarbonate, the essential zone can be destroyed and the subsequent zone covers the total section ($I_0 = 0$). The production of sodium bicarbonate is a quick response in extreme temperatures. Consequently, it is accepted that the charge of carbon dioxide utilization response is equivalent to its retentiveness expense. Consequently, the molar speed of the fluid section and added substances is determined by the utilization of carbon dioxide absorbance and response stoichiometry. Mole soundness inside the primary locale can be composed inside the accompanying shape [11]:

$$\frac{dL}{dz} = 0 \quad (10)$$

Mole solidness for sodium carbonate, sodium bicarbonate, and water in this zone might be composed inside the accompanying structures [11]:

$$\frac{\varepsilon_1 \cdot D_1}{U_1} \times L \times \frac{d^2}{dz^2} (x_{Na_2CO_3}) + L \times \frac{d}{dz} (x_{Na_2CO_3}) = N_{CO_2} \times \alpha_B \quad (11)$$

$$\frac{\varepsilon_1 \cdot D_1}{U_1} \times L \times \frac{d^2}{dz^2} (x_{NaHCO_3}) + L \times \frac{d}{dz} (x_{NaHCO_3}) = -2 \times N_{CO_2} \times \alpha_g \quad (12)$$

$$\frac{\varepsilon_1 \cdot D_1}{U_1} \times L \times \frac{d^2}{dz^2} (x_{H_2O}) + L \times \frac{d}{dz} (x_{H_2O}) = N_{CO_2} \times \alpha_g \quad (13)$$

Mole balance inside the 2d quarter might be composed as the accompanying differential condition [11]:

$$\frac{dL}{dz} = N_{NaHCO_3} \times \alpha_s \quad (14)$$

and for each component:

$$\frac{b_1 \cdot D_1}{U_1} \times \frac{d^2}{dz^2} (L \times x_{Na_2CO_3}) + \frac{d}{dz} (L \times x_{Na_2CO_3}) = N_{CO_2} \times \alpha_g \quad (15)$$

$$\begin{aligned} \frac{E_1 \cdot D_1}{U_1} \times \frac{d^2}{dz^2} (L \times x_{\text{NaHCO}_3}) + \frac{d}{dz} (L \times \text{NaHCO}_3) &= \\ = N_{\text{NaHCO}_3} \times \alpha_s - 2 \times N_{\text{CO}_2} \times \alpha_g & \end{aligned} \quad (16)$$

$$\frac{E_1 \cdot D_1}{U_1} \times \frac{d^2}{dz^2} (L \times x_{\text{H}_2\text{O}}) + \frac{d}{dz} (L \times x_{\text{H}_2\text{O}}) = N_{\text{CO}_2} \times \alpha_B \quad (17)$$

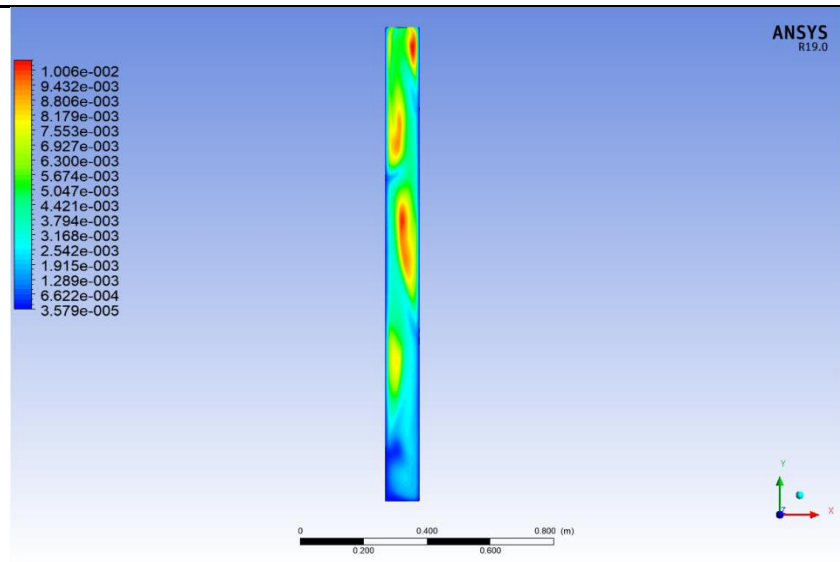
the first and 2d terms of late conditions are obtained from the outspread scattering in the fluid segment (that is raised from the development of water by bubbles movement) and liquid mass development, separately. The speed of the fluid is given with the resulting condition [11]:

$$U_1 = \frac{4 \times L_{FR}}{\pi \cdot d_R^2 \cdot \varepsilon_1 \cdot \rho_1} \quad (18)$$

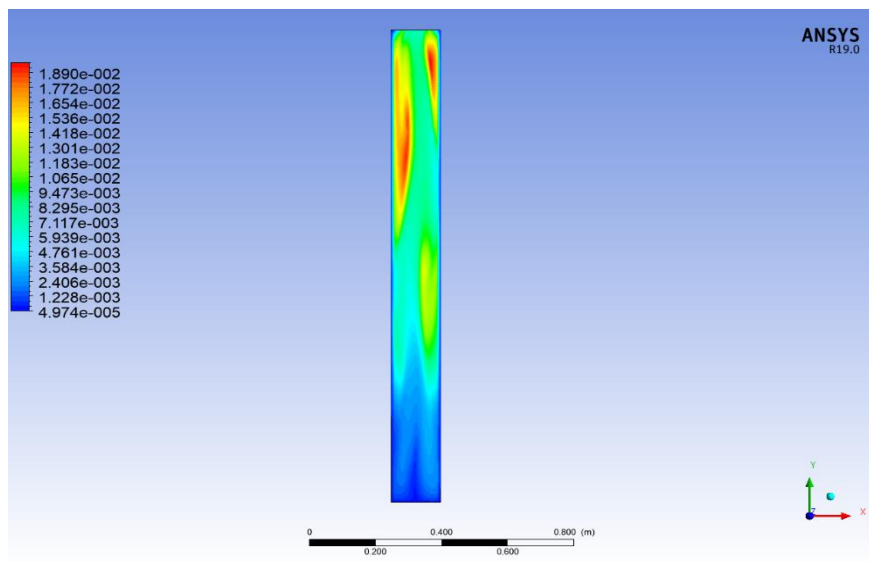
Results and Discussion

The Effect of Column Width on Turbine Mass Diffusivity

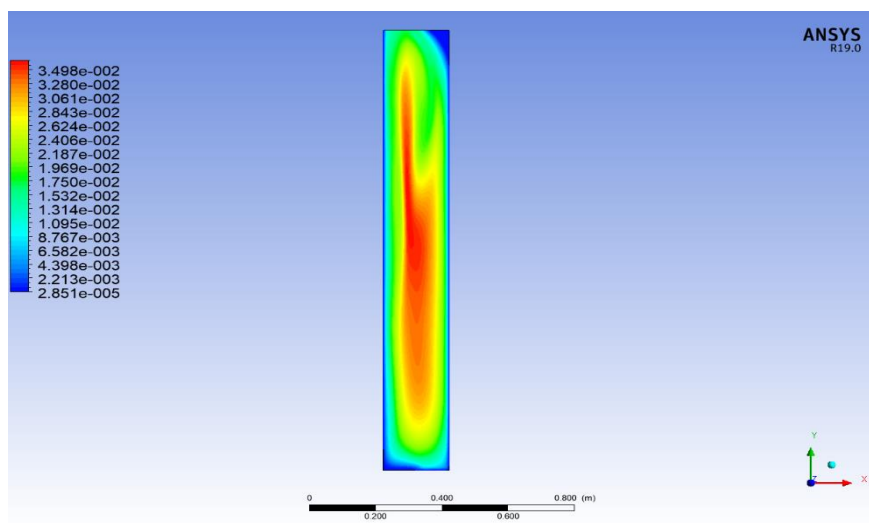
The effect of column width on turbulent diffusion mass transfer of bubbling columns, in the integrated Solvay process, is important to develop an optimum process flow. Industrial bubble columns are employed by chemical companies, owing to their great mass transfer properties. Despite a reduced cross-section, a more effective mass transfer may be achieved, but higher pressure drops and flooding risks are increased. The mass diffusivity of the reactants and products is strongly influenced by such properties as column width, intensity of gas-liquid agitation, gas-liquid properties, and operating conditions. Adjusting the number of columns and turbine design types strikes the optimum balance between these competing factors. Computational simulation methodologies play a key role in enhancing the understanding of processes by providing valuable information. Through Fig. 2, which shows the turbulent mass diffusivity, it is noted that the increase in the width of the column increases the amount of turbulent mass diffusivity, as it reached 0.01 m²/s in the width of 107 mm, as in the previous research [6]. This factor is increased to 0.0189 m²/s and 0.0349 m²/s, in width of 150 mm and 200 mm, respectively.



a



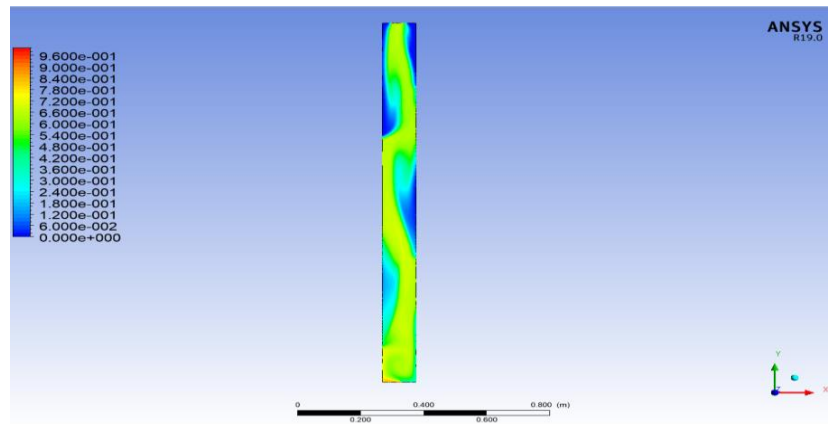
b



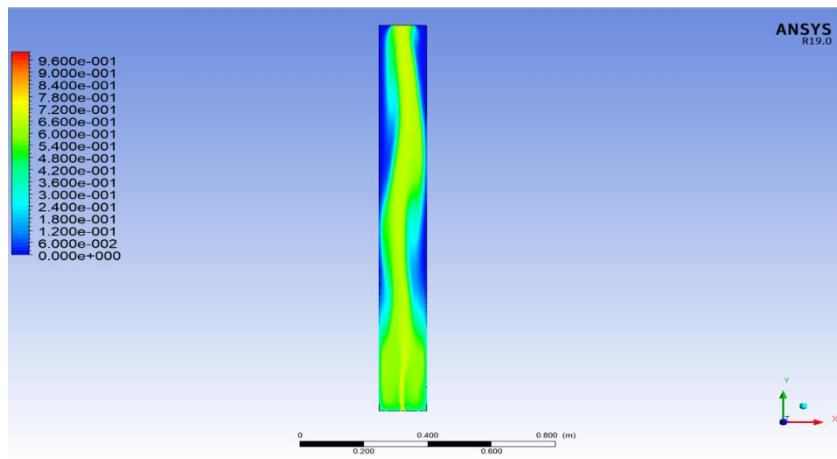
c

Fig. 2. Contour of turbulent mass diffusivity (m^2/s) of OH^- at 90s. (a) 107 mm, (b) 150 mm, (c) 200 mm

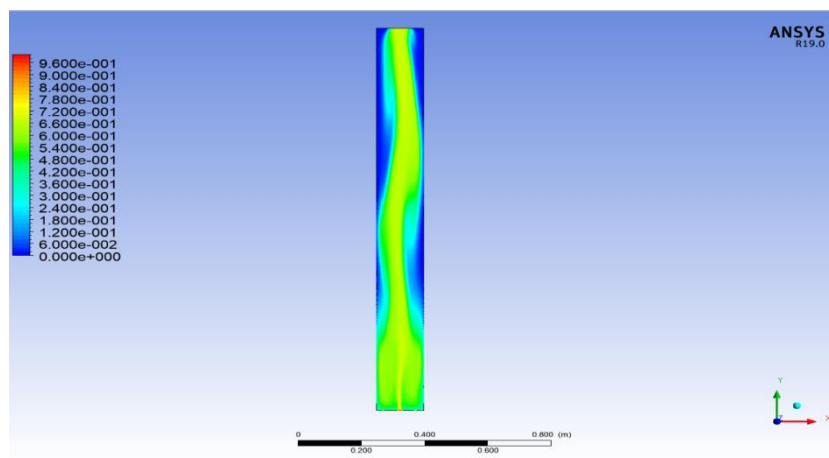
Through Fig. 3, which shows the turbulent viscosity, it is noted that the increase in the width of the column reduces the amount of turbulent viscosity. It reached 0.98 kg/(m.s) within 90 seconds at the width of 107 mm, 0.92 kg/ (m.s) at the width of 150 mm, and 0.88 kg/(m s) at the of width 200 mm.



a



b



c

Fig. 3. Contour of turbulent viscosity (kg/(m·s)) of the liquid phase at 90s. (a) 107 mm, (b) 150 mm, (c) 200 mm

The Effect of Column Width on Species Concentration

The influence of column width on species concentration, during the generation of sodium bicarbonate in the industrial bubble columns, is one of the main issues discussed in the process optimization. The industrial bubbling column reactors are an efficient way of producing a good gas-liquid-solid interaction, in the Solvay process, for changing common table salt into baking soda. Column dimensions and hydrodynamics influence the concentration of species by affecting fluid flow, mass transfer rates, and residence time. Shallower columns have higher velocities and more efficient mixing, which ensures an improved dispersion and uniform distribution of species. Broader columns can have lower velocities and lower mixing rates, resulting in the concentration gradient and non-uniform distribution of the stream. The exploration and comprehension of this relationship is, therefore, crucial for the improvement of the column width and bringing about the best process effectiveness and efficiency. In another study, through analytical experiments using the MATLAB program [11], where the column width is manipulated to obtain better results, through a pH chart as in Fig. 4, it is observed that an increase in the column width reduces the pH value, due to the large amount of fluid in the column.

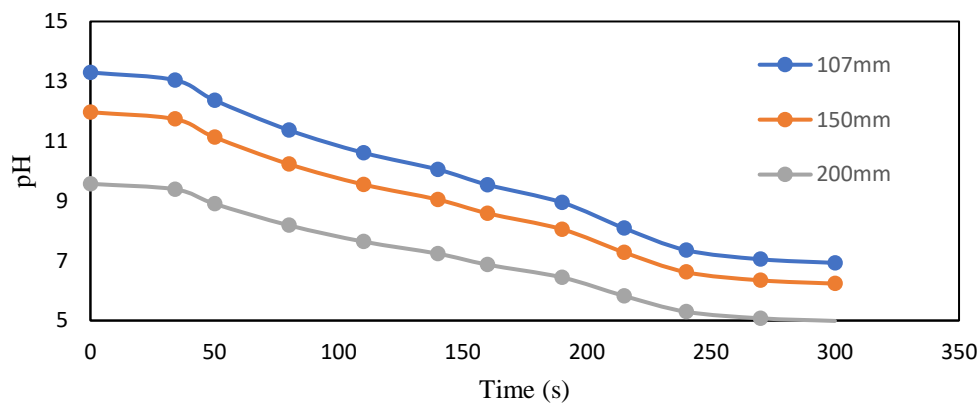


Fig. 4. pH with a time of different column width

As for Fig. 5, which represents the concentration of solutions, it is noted that the value of the solution reached 95 mmol/L at a width of 107 mm [11], and it decreased as the width increased to 82 mmol/L at a width of 200 mm.

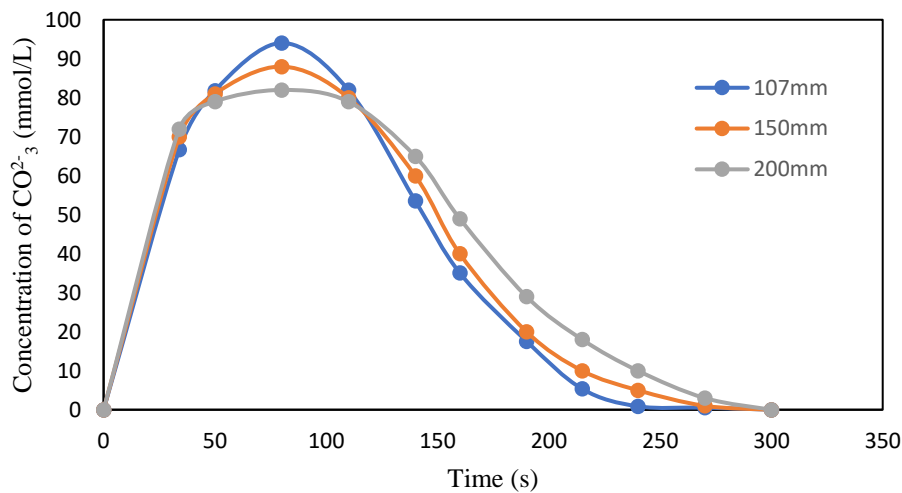


Fig. 5. CO_3^{2-} concentration with time of different column width

The Effect of Column Width on Supersaturation

column width in the industrial bubble columns plays a crucial role in the saturation of supersaturation in the production of sodium bicarbonate and crystallization kinetics, as well as the quality. Supersaturation is critical to the nucleation and growth of the crystals in the Solvay process. Columns with more reduced diameters have higher gas-liquid interfacial areas and mass transfer rates, with more saturation and supersaturation levels. Narrower columns with larger gas-liquid interfacial areas and higher mass transfer rates reach higher levels of supersaturation and faster crystal growth kinetics. The understanding of how column width affects operation and design specifications is essential for the optimum functioning of a specific cell. In Fig. 6, which shows the changes of Supersaturation with column height, it is noted that the amount of Supersaturation increases with increasing column width, reaching 0.015 Kg NAHCO_3/Kg liquid, at a width of 200 mm and the beginning of the column. It reaches more than 0.015 Kg NAHCO_3/Kg liquid at the end of the column.

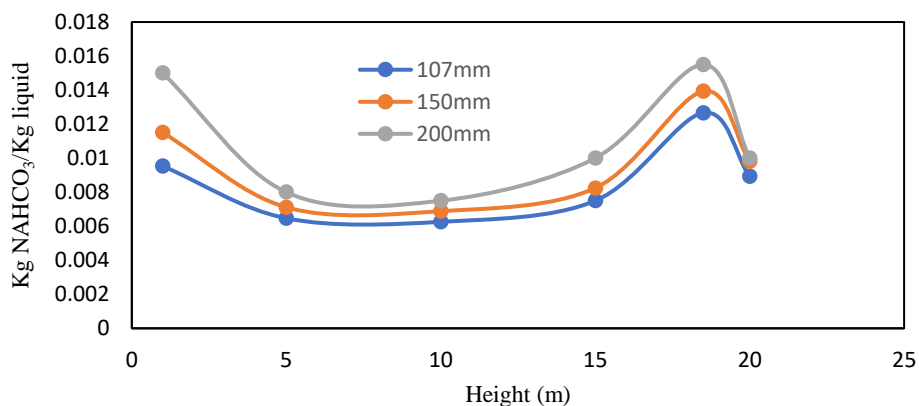


Fig. 6. Supersaturation in the length at different column width

Effect of Column Width on Magma Density

Column width has an essential role in magma density in industrial sodium bicarbonate production when bubbles form in industrial bubble columns and thus, process parameters as well as equipment design are optimized. The density of magma, the density of the slurry or the mixture, is regulated over mass transfer rates, hydrodynamics, and the final working performance. More confined columns have higher gas-liquid interfaces and better mixing that result in higher magma density. Thicker columns may have lower gas-liquid interfacial areas, lower mixing efficiency, denser magma, and larger sediments. Column width optimization aids in clarifying the supernatant, improves the homogenization and enhances the conversion rates and product yield. In Fig. 7, which shows the Magma density with the height of the column, it is noted that the amount of Magma density increases with increasing column width, reaching 0.58 at a width of 200 mm at the beginning of the column, and reaching 0 at the end of the column.

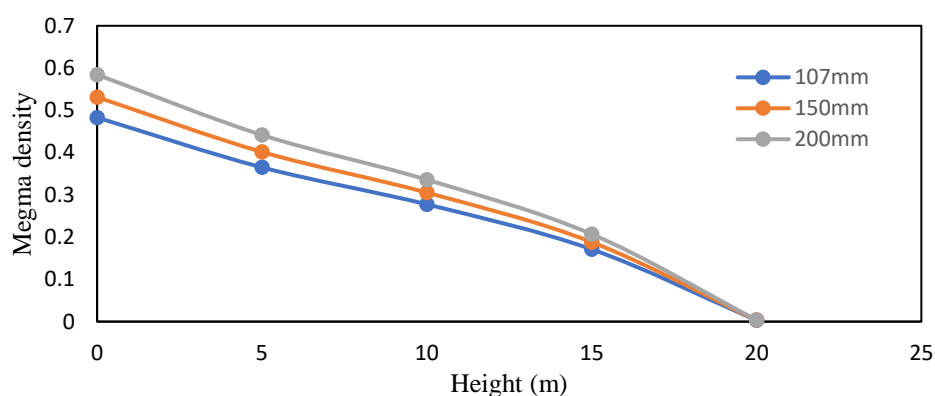


Fig. 7. Magma density in the length of columns of different column width

The Effect of Column Width on Molar Fraction of Carbon Dioxide

The concentration of CO_2 mol (in the liquid phase) is of vital importance for the bubble column in the industrial production of NaHCO_3 . Column width impacts all of these by affecting liquid flow properties, mass transfer properties, and reaction kinetics. More wide columns dissolve more carbon dioxide, causing higher molar ratios and further formation of bicarbonate ions. However, pills with a wider diameter might have a low molar fraction and thus, the CO_2 capacity is limited. Column width's impact can be assessed by studying fluid dynamics, mass transfer, and chemical reaction rate. The optimization of column width can enhance the efficient way of carbonation for sodium bicarbonate production. In Fig. 8, which shows the amount of Molar fraction of carbon dioxide in gas with the height of the column, it is noted that the amount of molar fraction of carbon dioxide in gas decreases as the width of the column increases, reaching 35% at the width of 200 mm at the beginning of the column, and reaching 20% at the end of the column.

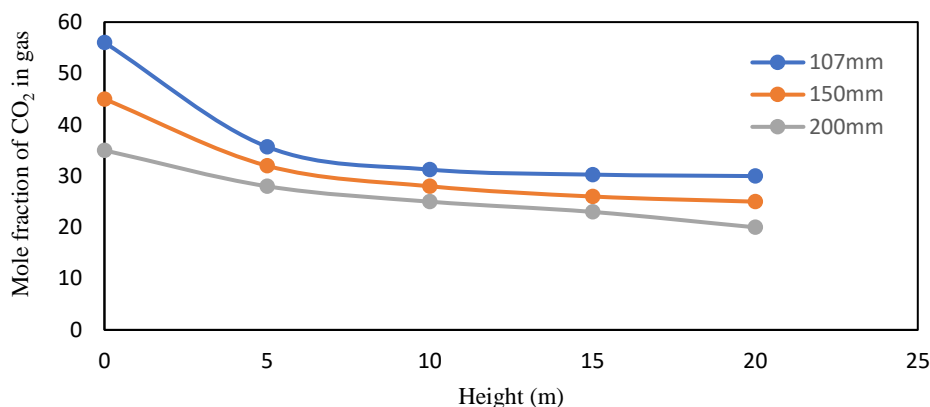


Fig. 8. Molar fraction of carbon dioxide in gas in the length at different column width

This study explores the impact of column width on various aspects of sodium bicarbonate production. It reveals that wider columns improve mass transfer rates, enhance mixing, and lead to faster reaction rates. This is crucial for industrial applications, as column geometry plays a vital role in reactor performance. This study also shows that wider columns result in lower turbulent viscosity, indicating better fluid dynamics and improved mixing efficiency. This can enhance reaction kinetics and reduce energy consumption, making the process more cost-effective. Wider columns tend to decrease species concentration, which can affect reaction rates and yield. The balance between column width and species concentration is crucial for achieving high efficiency. The study also highlights the importance of optimizing column width for crystal formation, with higher supersaturation levels promoting faster nucleation and growth of sodium bicarbonate crystals. Magma density increases with column width, indicating improved mixing and crystallization conditions. This is crucial for high-quality product formation and efficient crystal growth. The study suggests that optimizing column width can enhance production efficiency. Lastly, the study shows a decrease in the molar fraction of CO_2 in the gas phase, suggesting enhanced CO_2 absorption. This is beneficial for the carbonation process, maximizing sodium bicarbonate yield and minimizing environmental impact. The findings suggest that wider columns can improve the overall sustainability of the production process.

Conclusion

This paper reported that with higher a column width, the turbulence mass diffusivity became higher. The peak value of $0.01 \text{ m}^2/\text{s}$ was reached at 107 mm width and $0.0189 \text{ m}^2/\text{s}$ at 150 mm width. Nevertheless, this layer reduces eddy viscosity and in 90 seconds, at the 107 mm width, reaches the value of $0.98 \text{ kg}/(\text{m}\cdot\text{s})$ and at the 200 mm width, decreases to $0.88 \text{ kg}/(\text{m}\cdot\text{s})$. Analytical experiments that used MATLAB, showed that the column widths affect pH value, as they tend to contain more fluid than other sizes of columns.

The concentration of the solution increased to 95 mmol/L when the width was 107 mm. It started to decrease to 82 mmol/L when the width became 200 mm. Supersaturation curves were also a function of column width, with values ranging from $0.015 \text{ Kg NAHCO}_3/\text{Kg liquid}$ at 4 cm, to 0.01 Kg/Kg at 22 cm. At 200 mm width, it was as high as $0.015 \text{ Kg NAHCO}_3/\text{Kg liquid}$ at the outlet of the buffer.

With the widening of the column, the density of the magma rises to 0.58 at 200 mm width and 0 towards the end. CO₂ mole fraction matches that of 35% at 200 mm wide column and 20% at the end. The Carbon dioxide in the gas phase is dependent on both the length and width of the column.

The investigation proves that a broader width of the column enhances the turbulent mass diffusivity and also, increases the supersaturation, which is quite crucial for the fabrication of sodium bicarbonate. The use of wider columns also decreases turbulent viscosity and species concentration, implying improved mixing and reaction conditions. Consequently, an ideal width of the column improves the rate of CO₂ absorption and magma density, which leads to an increase in the yield and quality of the product. The results reveal that it is possible to have improved production parameters by increasing the width of columns. More comprehensive studies with even larger widths and superior methods of optimization should be conducted to determine the appropriate running conditions for the application in industries. These outcomes can help to develop better and/or new processes for sodium bicarbonate production that enjoy higher densities of return.

References

- [1] Taborda MA, Sommerfeld M. Reactive LES-Euler/Lagrange modelling of bubble columns considering effects of bubble dynamics. *Chemical Engineering Journal*. 2021 Mar 1;407:127222. <https://doi.org/10.1016/j.cej.2020.127222>
- [2] Bonfim-Rocha L, Silva AB, de Faria SH, Vieira MF, de Souza M. Production of sodium bicarbonate from CO₂ reuse processes: A brief review. *International Journal of Chemical Reactor Engineering*. 2020 Jan 28;18(1):20180318. <https://doi.org/10.1515/ijcre-2018-0318>
- [3] Z.A. Abdel-Rahman, Z.A. Abdullah, Utilization of CO₂ in Flue Gas for Sodium Bicarbonate Production in a Bubble Column, *Tikrit J. Eng. Sci.* 26 (2019) 28–38. <https://doi.org/10.25130/tjes.26.2.05>. <https://doi.org/10.25130/tjes.26.2.05>
- [4] Lee JH, Lee DW, Kwak C, Kang K, Lee JH. Technoeconomic and environmental evaluation of sodium bicarbonate production using CO₂ from flue gas of a coal-fired power plant. *Industrial & Engineering Chemistry Research*. 2019 Aug 4;58(34):15533-41. <https://doi.org/10.1021/acs.iecr.9b02253>
- [5] Abdel-Rahman ZA, Hamed HH, Khalaf FK. Optimization of Sodium Bicarbonate Production Using Response Surface Methodology (RSM). <https://doi.org/10.24237/djes.2018.11304>
- [6] Zhang C, Yuan X, Luo Y, Yu G. Prediction of species concentration distribution using a rigorous turbulent mass diffusivity model for bubble column reactor simulation part I: Application to chemisorption process of CO₂ into NaOH solution. *Chemical Engineering Science*. 2018 Jul 20;184:161-71. <https://doi.org/10.1016/j.ces.2018.03.031>
- [7] Maharloo DG, Darvishi A, Davand R, Saidi M, Rahimpour MR. Process intensification and environmental consideration of sodium bicarbonate production in an industrial soda ash bubble column reactor by CO₂ recycling. *Journal of CO₂ Utilization*. 2017 Jul 1;20:318-27. <https://doi.org/10.1016/j.jcou.2017.06.005>
- [8] J.G. Shim, D.W. Lee, J.H. Lee, N.S. Kwak, Experimental study on capture of carbon dioxide and production of sodium bicarbonate from sodium hydroxide, *Environ. Eng. Res.* 21 (2016) 297–303. <https://doi.org/10.4491/eer.2016.042>
- [9] Goharrizi RS, Abolpour B. Estimation of nucleation and growth rate of sodium bicarbonate crystals in a steady-state bubble column reactor. *Research on Chemical Intermediates*. 2015 Mar;41:1459-71. <https://doi.org/10.1007/s11164-013-1285-y>
- [10] Jain D, Kuipers JA, Deen NG. Numerical modeling of carbon dioxide chemisorption in sodium hydroxide solution in a micro-structured bubble column. *Chemical Engineering Science*. 2015 Dec 1;137:685-96. <https://doi.org/10.1016/j.ces.2015.07.025>
- [11] Goharrizi AS, Abolpour B. Modeling an industrial sodium bicarbonate bubble column reactor. *Applied Petrochemical Research*. 2014 Jun;4:235-45. <https://doi.org/10.1007/s13203-014-0064-z>



- [12] Saberi A, Goharrizi AS, Ghader S. Precipitation kinetics of sodium bicarbonate in an industrial bubble column crystallizer. *Crystal Research and Technology: Journal of Experimental and Industrial Crystallography*. 2009 Feb;44(2):159-66. <https://doi.org/10.1002/crat.200800429>
- [13] Haut B, Halloin V, Cartage T, Cockx A. Production of sodium bicarbonate in industrial bubble columns. *Chemical engineering science*. 2004 Nov 1;59(22-23):5687-94. <https://doi.org/10.1016/j.ces.2004.07.110>
- [14] Wylock C, Larcy A, Cartage T, Haut B. Optimization of the Sodium Bicarbonate Production Process, using High Performance Computing. In *Proceedings of the 18th International Congress of Chemical and Process Engineering 2008 Aug 27*.
- [15] Abolpour B, SOLTANI GA. Estimation of Sodium Bicarbonate Crystals Size Distribution in Bubble Column Reactor.
- [16] Humadi J, Nawaf AT, Khamees LA, Abd-Alhussain YA, Muhsin HF, Ahmed MA, Ahmed MM. Development of new effective activated carbon supported alkaline adsorbent used for removal phenolic compounds. *Communications in Science and Technology*. 2023 Dec 31;8(2):164-70. <https://doi.org/10.21924/cst.8.2.2023.1244>
- [17] Nawaf AT, Jarullah AT, Hameed SA, Mujtaba IM. Design of new activated carbon based adsorbents for improved desulfurization of heavy gas oil: experiments and kinetic modeling. *Chemical Product and Process Modeling*. 2021 Sep 16;16(3):229-49. <https://doi.org/10.1515/cppm-2020-0107>
- [18] Nawaf AT, Jarullah AT, Hameed SA, Mujtaba IM. Design of new activated carbon based adsorbents for improved desulfurization of heavy gas oil: experiments and kinetic modeling. *Chemical Product and Process Modeling*. 2021 Sep 16;16(3):229-49. <https://doi.org/10.1515/cppm-2020-0107>
- [19] Shihab MA, Nawaf AT, Mohamedali SA, Alsalmoney MN. Improving porosity of activated carbon nanotubes via alkali agents for the enhancement of adsorptive desulfurization process. In *Materials Science Forum 2020 Aug 14 (Vol. 1002, pp. 423-434)*. Trans Tech Publications Ltd. <https://doi.org/10.4028/www.scientific.net/MSF.1002.423>

How to cite: Humadi J, Rasheed E. Numerical Study of Sodium Bicarbonate Production in Industrial Bubble Columns. *Journal of Chemical and Petroleum Engineering* 2024; 58(2): 391-406.