Numerical study of sodium bicarbonate production in industrial bubble columns

Abstract

Aims of this study is to explore the physico-chemical factors that affect sodium bicarbonate synthesis in industrial bubble columns employing CFD simulations The model represents gasliquid-solid systems, and introduces turbulent phenomena into the model and chemical reactions, as well. Parameter optimizations are undertaken to analyze the operational parameters such as gas flow rate, liquid phase characteristics, column geometry, and reaction kinetics. The study permits one to understand the optimal reaction conditions for maximum NaHCO₃ yielding, fast enough kinetic reaction and less un-desired byproducts formation. The work has a role in shaping more productive and environmentally friendly approaches to the synthesis of chemical products. The width of column leads the turbulent mass diffusivity and viscosity increases but the turbulent diffusivity and viscosity decreases. Column pH gradient decreases as column width increases due to the increased liquid amount. 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 (the height of 200 mm). Supersaturation increases with column height. For the 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.

1. Introduction

The existing CFD simulations are used to investigate the production of sodium bicarbonate in industrial bubble columns. The process known as Solvay that goes back to the 19th century 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 gasliquid interfacial area and remarkable mass transfer efficiency. The study 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 the field of chemical production.

(Taborda and Sommerfeld, 2021) [1] Bubble columns are more complicated than conventional reactors leading to enhanced mass and chemical transfer efficiencies. CFD (computational fluid dynamics) is used to learn about these systems and make processes better. Numerical implementations of reactive bubble columns adopt the LES-Euler/Lagrange approach, with the oscillation of bubbles being simulated using a model that is random 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 taken into account. Large-Scale Simulation (LSES) is employed in computation of fluid flows. (Bonfim-Rocha et al., 2020) [2] several

production processes for the synthesis of sodium bicarbonate and the chemical reactions involved in the crystallization reactor. It contrasts soda ash generaion procedures from trona, the Solvay and the sodium ammonium sulfate route. The primary raw material is sodium chloride that is due to its general availability in seawater and food applications considered to be economically feasible. Solvay process suggests the technology having the best performance and economic benefits. The application of sodium sulfate is promising, however may not be idealized since it is characterized by a limitation in its product separation and purification. The review focuses on the absence of research studies related to sodium bicarbonate crystallization and purification. (Abdel-Rahman and Abdullah, 2019) [3] The mathematical model was constructed for designing and simulating highly diluted CO_2 (2-18%)into the flue gases for the production of sodium bicarbonate in a bubble column reactor. This model employs mass balance equations and Danckwerts concept to consider mass transfer and crystallization. The model came up with CO_2 conversion varying from 34% to 71% and the size range of the particles as 0 to 400 µm.

(Lee et al., 2019) [4] evaluated the techno-economic vicinity of a CO₂ mineralization process in sodium carbamate production. The process involves the flue gas of a coal-fired power plant to create the sodium carbonate solution containing CO₂. Reduction potential was found to be CO₂ of 0.33 ton of sodium bicarbonate produced and isolate exclusion value of 0.10 ton of CO₂ emissions were considered. The economic analysis of a plant operating at the capacity of 30,000 tonnes of sodium bicarbonate production with give a positive result, with benefit-cost ratio and an internal rate of return of 1.45 and 80,5%, respectively. (Adnan Abdel-Rahman, 2018) [5] sodium bicarbonate production model based on bubble column with high particle retention to minimize filtration and drying processes was implemented. A three-variable (CO₂ gas content, temperature, and time) batch bubble column of a lab-scale is employed to study the impact of elevated CO₂ on aquatic organisms. The outcome of the experiments was getting the reaction time and temperature as the highest performance in terms of yield and crystal size respectively. Kinetic study is consistent to zero order with respect to either carbonate sodium concentration or CO₂ concentration. Sorption/desorption process is governed by parameters - sodium carbonate and CO₂ concentrations.(Zhang et al., 2018) [6] the dimensional analysis of mass transfer turbulent model for computational evaluation of the CO₂ chemisorption in the bubble column reactor. The theory is a correlation between the turbulent mass diffusivity and the metrics of concentration variance and dissipation rate, which eventually gives out the easy prediction of the diffusion pattern of the species concentration. By contrast with the constancy 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., 2017) [7] catalytically presented to provide a new sodium bicarbonate production approach using an industrial bubble column reactor. Of all the components of this model, a portion of the outlet CO_2 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 produces 314 mol/m2.s of the CO2 emission reduction, 50% increase in the power of the particles made, and great decrease in the amount of pollutants. (Shim et al., 2016) [8] CO₂ capture and conversion with NaOH in coal-fired power stations. CO₂ gas reacts with sodium hydroxide to produce sodium bicarbonate (NaHCO₃). Bench-scale reactor system was one of the things which was designed, capturing 2 kg of carbon dioxide each day. This experiment verified the feasibility of carbon capture technologies for coal-based power plants which operate on the basis of sodium hydroxide with useful data for construction and operation of the full scale plants. (Goharrizi and Abolpour, 2015) [9] investigated the effects of diverse situations on the nucleation and boom rate of sodium bicarbonate crystals. It uses Danckwerts principle for mass switch between gasoline and liquid levels and a population stability to derive a nucleation and growth formula. The outcomes show that production of sodium bicarbonate crystals decreases under unique running situations.

(Jain et al., 2015) [10] a unit operation that is based on the micro-structured bubble column (microsieves) type and is safer than the safety risks of 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 the proximity of high interfacial contact and dynamic interface behavior. The paper numerically analyzes MSBC and the usage of hybrid-volume of fluid (VOF)-discrete bubble model (DBM) and a variant which handles mass switch with chemical reaction. Study indicates that installing a greater number of the mesh stacking in the columns leads to a significant enhancement of mass transfer. (Goharrizi and Abolpour, 2014) [11] studied gas-liquid mass transfer accompanied by chemical reactions, gas-liquid-solids mass transfer, and the crystallization in bubble column reactor. The reactor will cause emission of sodium bicarbonate that includes carbonate and bicarbante and carbon dioxide. A bubble column flow and a reactor column additive investigated with mole balances, while a cell population stability examines the nucleation and addition of cubic phase. The principle of Danckwerts is used for gasoil-gasoline mass levitation. In the current example, the model predicts the behavior of a number of parameters in terms of the production quantity of sodium bicarbonate crystals and also for the conversion process of carbon dioxide. Simulation outcomes is compared with the observations to validate the model. Different parameters effects on manufacturing processes and morphology of. Sodium bicarbonate crystals are considered and absorbent of CO₂ is investigated. (Saberi et al., 2009) [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 decide crystal length distribution. The 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., 2004) [13] specializes in developing 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 is constructed, along side a gasoline-liquid mass switch model. (Wylock et al., 2011) [14] constructed following a multi-scale approach, as illustrated on 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. Results of the examine at the scale of the bubble have already been supplied in preceding papers. In this paper, focus might be given on the results of the studies at the size of the lab and at the dimensions of the economic column. (Abolpour and Goharrizi, 2003) [15] Sodium bicarbonate is produced throughout soda ash manufacturing, in which carbon dioxide fuel is injected right into a bubble column reactor. This observe examines gas-liquid mass switch, chemical reactions, and liquid-strong mass transfer. A mathematical modeling version predicts the size distribution of sodium bicarbonate crystals. The version changed into tested the use of 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, recent synthesized activated carbon-based adsorbents show better adsorption capacities and effectiveness as compared to the traditional activated carbon due to the providence of 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 operational conditions, including the width of the column, to get the highest possible output and the least quantity of unwanted products. Besides, it looks at 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 and specific optimization [18]. It verifies the results obtained from the simulation and makes the results accurate as well as reliable, which set 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 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 parameters analysis with validation with experimental data make this work different from some of the existing literature which may be losely simulated, less-parameterized or in some cases without experimental validation.

2. Methodology

In this paragraph, all the governing equations will be discussed in using the ANSYS and MATLAB programs to complete the full simulation regarding the 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 the MATLAB program.

2.1 Geometry design

Validated were the results obtained with a three-dimensional cylindrical bubble column that was used in their experimental study, a one and a half meter liquid level was established, 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.

2.2 Boundary condition

The jacket attached on the bubble column and become heated to 25 'C.' The column initially contained aqueous sodium hydroxide solution with pH=13.3 and CO2 was sparged with a liquid upflow rate of .035m/s. Probes for pH price dimension were installed in specific reactor width : 107mm, 150mm and 200mm just above the feeder pipe. The exact substances samples had been taken both at the same heights and carbonate concentrations had been determined. [6] performed the precipitation test by adding barium chloride and doing hydrochloric acid titration. These processes were conducted to detect the carbonated nature of the liquid but the outcomes could be affected by the presence of hydrogen carbonate in the liquid.

In order to determine the range of the best width of the column for sodium bicarbonate production in the large scale industrial bubble columns, a comparison should be made with the novel wider ranges of the column width, for example, 250, 300 and 350 mm using the CFD models. Carry out a thorough comprehensive numerical and experimental parametric analysis and sensitivity analysis to assess the effects on; the mass transfer, the turbulence and the reaction kinetics. Better conditions for yield can be discovered using optimization such as Response Surface Methodology. The final step on Simulation is to compare the simulation results with experimental results and conduct a Cost Benefit Analysis of the Simulation. In this approach efficiency, yield and environmental sustainability of the process is planned and desired.

2.3 Mesh

Grid with a number of 495664 meshes became selected in this paintings after thinking about the computational accuracy and the time required as compared with a grid of 659305 meshes. Figure 1 indicates the computational domain and the grid used on this simulation. A time step of

zero.001s modified into used inside the calculation for the solution of the equations for a time spent of 300s' chemisorption procedure.



An accurate mesh must be created in order to solve the equations because the simulation process depends on complicated algorithms to work on the matrices present in the domain. After that, 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 more than one mesh dependability due to the variety of models that have been simulated. The value of the element was 659305 when the turbulent mass diffusivity $m^2/s 0.0349$ as in Table 1

Table (1): Mesh independency	
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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

2.3 Governing equations

With the pinnacle of 22 m. The temperature of activity is accepted to be consistent inside the length of segment as a result of low intensity of response and utilizing of a water coat round 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 to the section from its posterior. The accompanying balance responses can be mounted inside the segment:

$$CO_{2}(g) \leftrightarrow CO_{2}(l)$$
(1)

$$CO_{2}(l) + OH \leftrightarrow HCO_{3}$$
(2)

$$HCO_{3}^{-} + OH^{-} \leftrightarrow CO_{3}^{2-} + H_{2}O$$
(3)

$$Na^{+} + HCO_{3}^{-} \rightarrow NaHCO_{3}.$$
(4)

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 inside the presence of Na2 CO3 is given inside the Ref. [11] as underneath:

$$\log(x^*) = 6.71535 - \frac{843.0681}{T} - 2.24336 \times \log(T).$$
(4)

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

$$\frac{\mathrm{d}G}{\mathrm{d}z} = -N_{\mathrm{CO}} \times \alpha_8 \tag{5}$$

that:

$$\alpha_{\rm g} = \frac{6 \times \varepsilon_{\rm g}}{d_{\rm B}} \tag{6}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}z} \left(G \times y_{\mathrm{CO}_2} \right) - \frac{\varepsilon_{\mathrm{g}} \cdot D_{\mathrm{g}}}{U_{\mathrm{g}}} \times \frac{\mathrm{d}^2}{\mathrm{d}z^2} \left(G \times y_{\mathrm{CO}_2} \right) = -N_{\mathrm{CO}_2} \times \alpha_{\mathrm{g}} \tag{7}$$

that gas velocity is given by:

$$U_g = \frac{4 \times G_{FR}}{\pi \cdot d_R^2 + \varepsilon_g} \tag{8}$$

The delivered sodium bicarbonate will stable area. In the event that gulf answer has an immersion or supersaturation consideration of sodium bicarbonate, the essential zone can be killed and the subsequent one zone covers the total section ($I_0=0$). The reaction of sodium bicarbonate producing is a quick response in over the top temperatures. Consequently, it is accepted that the charge of carbon dioxide utilization response be equivalent with its retentiveness expense. Consequently, the molar speed of fluid section and added substances is determined the utilization of carbon dioxide absorbance and response stoichiometry. Mole soundness inside the primary locale (which has no steady) can be composed inside the accompanying shape [11]:

$$\frac{\mathrm{d}L}{\mathrm{d}z} = 0 \tag{9}$$

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

$$\frac{\varepsilon_1 \cdot D_1}{U_1} \times L \times \frac{\mathrm{d}^2}{\mathrm{d}z^2} \left(x_{\mathrm{Na}_2 \mathrm{CO}_3} \right) + L \times \frac{\mathrm{d}}{\mathrm{d}z} \left(x_{\mathrm{Na}_2} \mathrm{CO}_3 \right) = N_{\mathrm{CO}_2} \times \alpha_8 \tag{10}$$

$$\frac{\varepsilon_1 \cdot D_1}{U_1} \times L \times \frac{d^2}{dz^2} (x_{\text{NaHCO}_3}) + L \times \frac{d}{dz} (x_{\text{NaHCO}_3})$$

$$= -2 \times N_{\text{CO}_2} \times \alpha_g$$
(11)

$$\frac{\varepsilon_1 \cdot D_1}{U_1} \times L \times \frac{d^2}{dz^2} (x_{H_2 0}) + L \times \frac{d}{dz} (x_{H_2 0}) = N_{CO_2} \times \alpha_g$$
(12)

Mole balance inside the 2d quarter (that created sodium bicarbonate is embedded to stable stage) might be composed as the accompanying differential condition [11]:

$$\frac{\mathrm{d}L}{\mathrm{d}z} = N_{\mathrm{NaHCO}} \times \alpha_s \tag{13}$$

and for each component:

$$\frac{b_1 \cdot D_1}{U_1} \times \frac{\mathrm{d}^2}{\mathrm{d}z^2} \left(L \times x_{\mathrm{Na}_2\mathrm{CO}_3} \right) + \frac{\mathrm{d}}{\mathrm{d}z} \left(L \times x_{\mathrm{Na}_2\mathrm{CO}} \right) = N_{\mathrm{CO}_2} \times \alpha_{\mathrm{g}}$$
(14)

$$\frac{E_1 \cdot D_1}{U_1} \times \frac{d^2}{dz^2} (L \times x \text{NaHCO}_3) + \frac{d}{dz} (L \times \text{NaHCO}_3)$$
$$= N_{\text{NaHCO}_3} \times \alpha_{\text{s}} - 2 \times N_{\text{CO}_2} \times \alpha_g$$
(15)

$$\frac{E_1 \cdot D_1}{U_1} \times \frac{\mathrm{d}^2}{\mathrm{d}z^2} \left(L \times x_{\mathrm{H}_2 \mathrm{O}} \right) + \frac{\mathrm{d}}{\mathrm{d}z} \left(L \times x \mathrm{H}_2 \mathrm{O} \right) = N \mathrm{CO}_2 \times \alpha_{\mathrm{B}}.$$
(16)

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

$$U_1 = \frac{4 \times L_{FR}}{\pi \cdot d_R^2 \cdot \varepsilon_1 \cdot \rho_1}.$$
(17)

3. Results and discussion

3.1 The effect of column width on turbine mass diffusivity

The effect of column width on turbulent diffusion mass transfers of bubbling columns in the integrated Solvay process is important to develop an optimum process flow. Industrial bubble columns are employed by the chemical companies owing to their great mass transfer properties. In spite of reduced cross-section the more effective mass transfer may be achieved but higher pressure drops and flooding risks can occur. 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 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 Figure 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 during the width of 107 mm, as in the previous research [6], and increased to 0.0189 m2/s in Width 150 mm. This increase also increased to 0.0349 m2/s in width 200 mm.





Figure 2: Contour of turbulent mass diffusivity (m²/s) of OH- at 90s. (a) 107 mm , (b) 150mm, (c) 200 mm.

Through Figure 3, which shows the turbulent viscosity, it is noted that the increase in the width of the column reduces the amount of turbulent viscosity, as during the width of 107 mm, as in the previous research [6], it reached 0.98 kg/(m·s) within 90 seconds and decreased to 0.92 kg/ (m s) in width 150 mm. This reduction also increased to 0.88 kg/(m s) in width 200 mm.





Figure 3: Contour of turbulent viscosity $(kg/(m \cdot s))$ of the liquid phase at 90s. (a) 107 mm, (b) 150mm, (c) 200 mm.

3.2 The effect of column width on Species concentration

The influence of column underwork on species concentration during generation of sodium bicarbonate in the industrial bubble columns is one of the main issues discussed in the process optimization. The bubbling coulumn industrial 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. The broader columns can have lower velocities and lower mixing rate, resulting to 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. As for 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 Figure 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.





As for Figure 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 reach 82 mmol/L at a width of 200 mm.



Figure 5: CO $_{2-}$ ³ concentration with time of different column width.

3.3 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 where a solution becomes saturated above equilibrium solubility of sodium bicarbonate 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 can have larger gas-liquid interfacial areas with higher mass transfer rates, reaches higher levels of supersaturation and thus faster crystal growth kinetics. The knowledge of how column width affects operations and design specifications is indispensable for the optimum functioning of a specific cell. In Figure 6, which shows the amount of Supersaturation with column height, it is noted that the amount of Supersaturation increases with increasing column width, reaching 0.015 Kg NAHCO3/Kg liquid. At a width of 200 mm at the beginning of the column, it reaches more than 0.015 Kg NAHCO3/Kg liquid at the end of the column.



Figure 6: Supersaturation in the length of column of different column width.

3.4 Effect of column width on Magma density

Column width has an essential role on 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 and denser magma, as well as larger sediments. Column width optimization aids in clarifying the supernatant, improves the homogenization, and enhances the conversion rates and product yield. In Figure 7, which shows the amount of 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.



Figure 7: Magma density in the length of column of different column width.

3.5 The effect of column width on Molar fraction of carbon dioxide

The concentration of CO2 mol (in liquid phase) is of vital importance for the bubble column in the industrial production of NaHCO3. 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, thus, the CO2 capacity is limited. Column width's impact can be assessed by studying fluid dynamics, mass transfer as well as chemical reaction rate. The optimization of column width can enhance the efficient way of carbonation for sodium bicarbonate production. In Figure 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.



Figure 8: Molar fraction of carbon dioxide in gas in the length of column of different column width.

The study explores the impact of column width on various aspects of sodium bicarbonate production. It reveals that wider columns improve mass transfer rates, enhancing mixing and faster reaction rates. This is crucial for industrial applications, as column geometry plays a vital role in reactor performance. The 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 CO₂ 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.

4. Conclusions

The results will be summarized as follows:

1. The paper reported that the higher a column width was, the bigger the turbulence mass diffusivity became. The peak value of 0.01 m2/s was reached at 107 mm width, and 0.0189 m2/s with 150 mm width. Nevertheless, this layer reduces eddy viscosity and, in

90 seconds, at the 107 mm width, reaches the value of 0.98 kg/($m\cdot s$). In this case the value of 200 mm width decreases to 0.88 kg/($m\cdot s$). Analytical experiments that used MATLAB showed that the column widths affects pH value as they tend to contain more fluid than other sizes of columns.

- 2. The concentration of the solution increased to 95 mmol/L when the width was 107 mm and then 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 Kg NAHCO3/Kg liquid at 4 cm to 0.01 Kg/Kg at 22 cm. At 200 mm width it was as high as 0.015 Kg NAHCO₃/Kg liquid at the outlet of the buffer.
- 3. With the widening of the column, the Density of the Magma rises upto 0.58 at 200mm width and 0 towards the end. CO_2 moles 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 the fact that the 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 as well as reaction conditions. Consequently, an ideal width of the column improves on the rate of CO_2 absorption and the density magma to increase 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 inform the development of better and/or new processes for sodium bicarbonate production that enjoy higher densities of returns.

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