

Article

Experimental and Simulation-Based Study of Acid Gas Removal in Packed Columns with Different Packing Materials

Ersin Üresin 

TÜBİTAK Marmara Research Center, 41470 Gebze, Kocaeli, Türkiye; ersin.uresin@tubitak.gov.tr;
Tel.: +90-262-677-2130

Abstract

In this study, both experimental and simulation approaches were employed to investigate the removal efficiency of gaseous pollutants using two different types of packing materials—random and structured packings—under varying gas flow rates and column diameters. A synthetic gas mixture containing 2200 ppm H₂S and 26.75% CO₂ was used to evaluate the performance of the system. Simulation studies were conducted using Aspen Plus™ V9, and the results were validated with experimental data. H₂S removal efficiencies were found to range between 79% and 98%, while CO₂ removal ranged from 6% to 20%. Comparative analyses revealed that an increase in gas flow rate and column diameter led to a decrease in pollutant removal efficiency for both types of packings. A previously unobserved packing-dependent scaling effect was revealed: increasing column diameter decreases removal efficiency for random packings but enhances it (up to a threshold) for structured packings, offering new scale-up guidelines. Most notably, a previously unobserved trend was identified: increasing column diameter exerts opposing effects on removal efficiency depending on packing type—a packing-dependent scaling behavior with significant implications for industrial column design. The findings provide valuable insights into the design and optimization of industrial-scale gas treatment systems, demonstrating that simulation data can effectively support the selection of appropriate column dimensions, gas flow rates, and packing types for varying pollutant concentrations. A mechanistic analysis revealed that the superior H₂S removal over CO₂ arises from its higher solubility, instantaneous reaction with OH[−], and greater enhancement factor, with structured packings mitigating maldistribution effects at larger column diameters—offering new scale-up insights supported by the literature.

Keywords: acid gas removal; packed column; hydrogen sulfide (H₂S); Aspen Plus simulation; packing material type



Academic Editor: Pallav Purohit

Received: 29 September 2025

Revised: 11 November 2025

Accepted: 20 November 2025

Published: 23 November 2025

Citation: Üresin, E. Experimental and Simulation-Based Study of Acid Gas Removal in Packed Columns with Different Packing Materials.

Sustainability **2025**, *17*, 10495. <https://doi.org/10.3390/su172310495>

Copyright: © 2025 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

1. Introduction

The main impurities in synthetic raw gas produced by coal gasification are particulates and gaseous pollutants. Elimination of these contaminants is a fundamental step in coal and biomass gasification processes due to their adverse effects on both materials and the environment. Among them, hydrogen sulfide (H₂S) is the major source of corrosion observed in pipelines, which eventually shortens the lifetime of the plant. Humans can detect hydrogen sulfide at very low concentrations as low as 0.4 ppb, which poses serious health risks. A strong and distinctive odor is detected when H₂S concentration is around a 30 ppmv level, and higher concentrations lead to serious effects on the nervous and respiratory systems. Therefore, the implementation of an effective gas clean-up technology

has a significant role in the case of the utilization of gasification products, either as a fuel for gas turbines, gas engines, or fuel cells, or as a syngas for Fischer–Tropsch fuel, methanol production, and environmental health [1–7].

The removal of particle and gaseous pollutants in cold gas clean-up systems is accomplished by scrubbers, which are the control devices designed to make good contact between the liquid and dirty gas stream for effective pollutant capture. Packed scrubbing systems are widely used for the purification of gaseous products due to having packing material in the column with a large surface area, which leads to an increase in the mass transfer. Flue gas condensation scrubbers (CSs) have recently demonstrated high potential for the synergistic removal of multiple pollutants—including fine particulate matter (FPM), SO_2 , SO_3 , and condensable particulate matter (CPM)—in coal-fired boiler systems, while simultaneously recovering latent heat from flue gases [8]. Environmental innovations often emerge at the intersection of technological capabilities and regulatory pressures. As demonstrated by article [9], the development of marine scrubber systems (MSSs) exemplifies how stringent environmental policies—particularly IMO sulfur emission regulations—serve as key drivers in transforming existing technological potentials into viable sectoral and technological innovation systems. In addition to these, the choice of the solution has a significant impact on the determination of the dissolution or chemical reaction rate of pollutants in the liquid. On the other hand, physical scrubbing is based on deactivation of the basic nature by acidic solutions and vice versa. Existing technology for the removal of acid gases in commercial integrated gasification combined cycle (IGCC) facilities depends on not only the chemical solvent acid gas removal processes using aqueous methyldiethanolamine (MDEA) but also the physical solvent-based Selexol process using mixtures of dimethyl ethers and polyethylene glycol [10–17]. Article [18] developed a novel co-removal system for CO_2 and particulate matter (PM) from industrial flue gas by connecting an ammonia scrubber (AS) and a granular bed filter (GBF) in series. Their experimental results demonstrated that this integrated system achieved higher removal efficiencies for both CO_2 and PM compared to individual AS and GBF units, highlighting the potential of this approach for improving air pollution control in industrial applications. The purification of coke oven gas (COG) through the integrated $\text{H}_2\text{S}/\text{NH}_3$ scrubber system has gained significant attention due to its efficiency in removing sulfur and ammonia compounds. Recent studies, such as those by [19], have demonstrated the effectiveness of using multiple scrubbing liquids and regeneration processes in improving scrubbing efficiency, highlighting key factors like flow rates and liquid compositions that influence the removal of H_2S and NH_3 in industrial applications.

The most widely used scrubbing solutions for sulfidic odor applications are sodium hydroxide, sodium hypochlorite, and hydrogen peroxide. On the other hand, the elimination of ammonia is easier since pure water can remove it effectively. Despite the fact that sodium hydroxide solution is a very efficient absorbent for capturing CO_2 and H_2S , its non-regenerable nature limits the use of it to the removal of trace amounts of these impurities. Various concepts have been employed for the elimination of the spent caustic, including simple neutralization or using it in pulp mills after certain quality control analysis [1,2,15,17–24].

The primary design parameters of the packed columns are categorized into the hydrodynamic flow characteristics and packing surface area based on the packing material geometry, retention time, liquid to gas ratio, pH, and reactivity of the solution. The scrubber system has to be designed according to these parameters in order to avoid high investment and operation costs [12,25]. Recent studies have highlighted the potential of water scrubbers in biogas purification without the need for external pressure. Notably, article [26] demonstrated that incorporating sponge carriers with high water retention can significantly

enhance methane concentration by increasing hydraulic retention time (HRT), while maintaining an optimal liquid-to-gas flow ratio (Q_L/Q_G) is critical for maximizing purification efficiency. Article [27] developed a general model to predict the separation efficiency of random packings in gas–liquid systems using only physical properties, operating conditions, and basic geometric characteristics of the packing. The model showed good agreement with experimental data across a wide range of packing types and conditions without requiring packing-specific mass transfer constants. Recent work by [28] proposed an integrated simulation–optimization framework using Aspen HYSYS and LINGO to optimize acid gas removal processes. Their study demonstrated significant improvements in profitability and provided valuable insights into the trade-offs between CO₂ removal efficiency and operating costs.

Rotating packed beds (RPBs) have attracted significant attention for CO₂ removal via chemical absorption due to their intensified mass transfer and compact structure, making them promising for offshore gas processing applications with stringent space constraints. Nevertheless, as article [29] emphasized, limitations in the mechanistic understanding of gas–liquid–solid interactions, reliance on empirical hydrodynamic correlations, and the lack of mature CFD and process simulation tools hinder their industrial implementation. The development of a scrubber with nano-TiO₂-coated packing materials has shown significant improvements in H₂S removal efficiency, with the enhanced wettability of the surface leading to better mass transfer rates between gas and liquid phases, as demonstrated by recent studies [30]. These findings highlight the potential for further optimization and application of this technology in large-scale processes, while offering insights into the benefits of hydrophilic packing surfaces for increased removal efficiency. Article [31] compared organic and inorganic packing materials in biofilters for ammonia removal, finding that organic materials exhibited higher removal capacities and maximum removal rates, particularly at ammonia concentrations of 0–300 ppm. Humidification–dehumidification (HDH) desalination processes have gained significant attention due to their promising performance, particularly when coupled with solar energy. Recent studies have highlighted the importance of selecting suitable packing materials, such as cellulose and honeycomb papers, to enhance system efficiency, suggesting that further exploration of novel packing materials and designs could lead to improvements in thermal performance and overall system effectiveness.

Recent studies have shown that while wet scrubber systems (WSSs) are effective in removing acid gases and particulate matter, they can also act as a source of polychlorinated dibenzo-p-dioxin and furan (PCDD/F) emissions due to the memory effect. The memory effect has been found to increase emission levels, although they remain below regulatory limits, emphasizing the need for further optimization of WSS to reduce the environmental impact [32].

While hybrid simulation–experimental approaches have been reported in packed column studies [32–34], these typically focus on single packing types or fixed geometries. In contrast, this work presents a systematic, validated side-by-side comparison of random and structured packings under variable gas flow rates and column diameters using real syngas composition. Most critically, we uncover a previously unreported scaling phenomenon: increasing column diameter exerts opposing effects on removal efficiency, which is negative for random packings due to reduced specific surface area utilization but positive (up to a limit) for structured packings due to improved flow distribution and interfacial area efficiency. This packing-dependent behavior, rooted in void fraction and radial hydrodynamics, introduces a new design paradigm for scale-up in acid gas treatment systems, distinguishing our contribution from prior hybrid studies.

This study uniquely elucidates the packing- and scale-dependent divergence in H_2S and CO_2 mass transfer mechanisms in NaOH scrubbers, bridging experimental and simulation approaches to reveal previously unreported diameter-driven selectivity trends.

2. Materials and Methods

2.1. Experimental Procedure

A laboratory-scale gas scrubbing system was designed and constructed to investigate the removal of gaseous contaminants from syngas obtained via coal gasification, as presented in Figure 1. The experimental setup consisted of a vertical stainless steel packed column with an internal diameter of 0.1 m and an overall height of 3.0 m. The packed bed section had a height of 1.75 m and was filled with structured packing material to enhance gas–liquid contact efficiency.

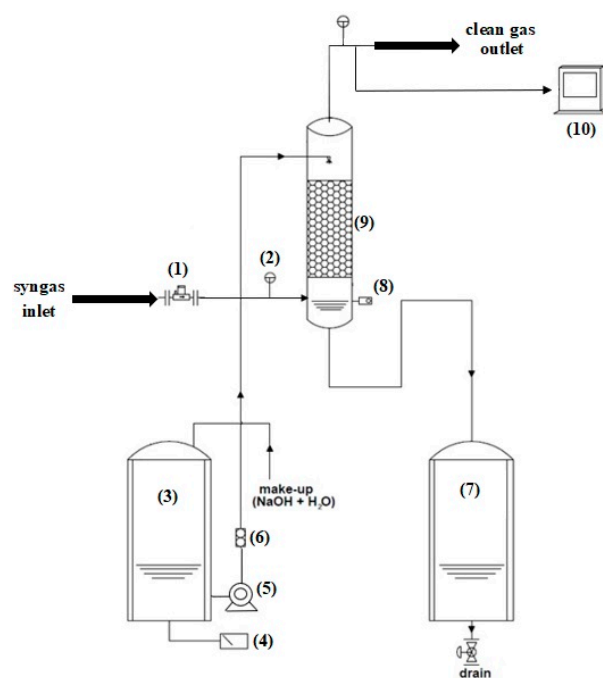


Figure 1. A schematic representation of the experimental setup. 1—Mass Flow Controller; 2—Pressure Transmitter; 3—Liquor Tank; 4—pH Control; 5—Circulation Pump; 6—Liquid Flowmeter; 7—Waste Tank; 8—Level Control; 9—Packed Column; 10—Analyzer.

Syngas containing various gaseous pollutants was fed into the column through the bottom using a mass flow controller (MFC) to ensure precise regulation of the gas flowrate. To prevent potential clogging and to monitor the operational stability, differential pressure across the column was continuously measured using pressure transmitters located at appropriate positions along the column height.

An alkaline washing solution was sprayed counter-currently from the top of the column using a circulation pump. The liquid flow rate was adjusted to maintain the desired liquid-to-gas (L/G) ratio and monitored in real-time using a liquid flow meter. To avoid flooding of the column, the solution level was maintained via level transmitters installed within the column.

The washing solution was continuously circulated through a reservoir tank, where its pH was maintained at 11. Sodium hydroxide (NaOH) was dosed into the tank as needed to compensate for pH fluctuations resulting from acid gas absorption. The pH was monitored using an in-line pH probe, and adjustments were performed automatically based on feedback control. Table 1 shows the operating parameters.

Table 1. Operational parameters of the system.

Parameters	Values
Gas flow rate (m ³ /h)	5–20
Column diameter (cm)	10–40
Column height (m)	3
Operating pressure (bar)	1
Washing agent flow rate (L/h)	21–127
Liquid to gas ratio (L/m ³)	4.25
H ₂ S concentration (ppm)	2200
CO ₂ concentration (%)	26.75

Post-scrubbing, the liquid effluent containing dissolved gaseous contaminants was collected in a waste tank for proper disposal. The treated gas stream exiting the top of the column was directed to an online gas chromatograph (GC) for compositional analysis. This allowed for the identification and quantification of the removed gaseous pollutants.

All operational parameters listed in Table 1 were directly obtained from experimental measurements conducted on the laboratory-scale gas scrubbing system (0.1 m diameter column). The gas flow rate (5–20 m³/h), washing agent flow rate (21–127 L/h), and liquid-to-gas ratio (L/G = 4.25 L/m³) were precisely controlled and monitored using calibrated mass flow controllers and liquid flow meters. The inlet concentrations of H₂S (2200 ppm) and CO₂ (26.75%) were measured via gas chromatography (GC) analysis of the feed syngas stream. Column dimensions (diameter: 0.1 m, height: 3.0 m) and operating pressure (1 bar) reflect the actual design and atmospheric operation of the experimental setup. These values ensure full reproducibility of the experimental conditions.

2.2. Simulation Approach and Model Validation

To validate the experimental results, a process model of the gas scrubbing system was developed using Aspen PlusTM V9 simulation software. Experimental data were obtained solely for the 10 cm diameter column packed with structured packing material. No experimental data were generated for random packing configurations or for larger column diameters (20 cm and 40 cm), as these scenarios were assessed exclusively through simulations to evaluate scale-up potential and packing type comparisons.

The electrolyte system in the gas scrubbing process involves ionic species (e.g., H⁺, OH[−], HS[−], HCO₃[−], CO₃^{2−}) formed due to the absorption of H₂S and CO₂ into the alkaline NaOH solution. To accurately model the vapor–liquid equilibrium (VLE) and thermodynamic behavior of this electrolyte system, the ELECNRTL (Electrolyte Non-Random Two-Liquid) property method was selected in Aspen PlusTM V9. This method is specifically designed for aqueous electrolyte solutions and accounts for long-range ion–ion interactions via the Pitzer–Debye–Hückel model and short-range interactions using the local composition concept of NRTL.

The ELECNRTL method has been widely validated for CO₂ and H₂S absorption in alkaline solutions and is recommended by AspenTech for systems containing weak electrolytes and strong bases such as NaOH. The binary interaction parameters for ion pairs (e.g., Na⁺–HS[−], Na⁺–HCO₃[−]) and molecule–ion pairs were retrieved from Aspen Plus’s built-in electrolyte database.

Experimental data obtained from the 0.1 m diameter column were compared to simulation results for model validation. Following validation, simulations were extended to columns with diameters of 0.2 m and 0.4 m, using both structured and random packing materials. These simulations enabled scale-up assessments and performance comparisons

between different packing types and column diameters. The technical properties of packing materials are given in Table 2.

Table 2. Packing factors for packing materials.

Parameters	Structured Packing	Random Packing
Surface area (m^2/m^3)	245	363
Void fraction	0.95	0.67
Packing factor (m^{-1})	71	1872

The packing material properties in Table 2 were obtained from manufacturer specifications and validated literature data, as commonly used in process simulation and scale-up studies. The surface area, void fraction, and packing factor for both structured and random packings were sourced from technical datasheets of commercial packing materials and cross-verified with published correlations. These parameters were directly input into the Aspen PlusTM V9 model for simulation of columns with 0.2 m and 0.4 m diameters. No optimization was performed; values represent standard industrial packing characteristics to enable reliable scale-up comparisons.

Thermophysical properties such as specific heat capacities, densities, and viscosities were obtained from Aspen PlusTM V9 simulations and validated prior to their application in the model. All chemical reactions involved in the modeling of the electrolyte solution chemistry are clearly specified. The reactions incorporated in Aspen PlusTM V9 are detailed in the following sections (Table 3).

Table 3. Reactions for validation of chemical parameters.

Equilibrium Reactions	Dissociation Reactions	Kinetic Reactions
(R1) $\text{CO}_2 + 2\text{H}_2\text{O} \leftrightarrow \text{HCO}_3^- + \text{H}_3\text{O}^+$	(R8) $\text{NaOH} \rightarrow \text{Na}^+ + \text{OH}^-$	(R12) $\text{CO}_2 + \text{OH}^- \rightarrow \text{HCO}_3^-$
(R2) $2\text{H}_2\text{O} \leftrightarrow \text{OH}^- + \text{H}_3\text{O}^+$	(R9) $\text{Na}_2\text{CO}_3 \rightarrow 2\text{Na}^+ + \text{CO}_3^{2-}$	(R13) $\text{HCO}_3^- \rightarrow \text{CO}_2 + \text{OH}^-$
(R3) $\text{H}_2\text{O} + \text{HCO}_3^- \leftrightarrow \text{CO}_3^{2-} + \text{H}_3\text{O}^+$	(R10) $\text{NaHCO}_3 \rightarrow \text{HCO}_3^- + \text{Na}^+$	
(R4) $\text{H}_2\text{O} + \text{H}_2\text{S} \leftrightarrow \text{HS}^- + \text{H}_3\text{O}^+$	(R11) $\text{Na}_2\text{S} \rightarrow \text{S}^{2-} + 2\text{Na}^+$	
(R5) $\text{H}_2\text{O} + \text{HS}^- \leftrightarrow \text{S}^{2-} + \text{H}_3\text{O}^+$		
(R6) $\text{H}_2\text{S} + \text{OH}^- \leftrightarrow \text{HS}^- + \text{H}_2\text{O}$		
(R7) $\text{HS}^- + \text{OH}^- \leftrightarrow \text{S}^{2-} + \text{H}_2\text{O}$		

For the instantaneous reversible reactions, the chemical equilibrium constants were determined based on Equation (1) as implemented within the Aspen PlusTM V9 simulation environment.

$$\ln K_{eq} = A + \frac{B}{T} + C \ln T \quad (1)$$

where

K_{eq} : Equilibrium constant;

A, B, C : Coefficients;

T : Temperature (K).

To compute the equilibrium constants, temperature must be considered, along with the coefficients A , B , and C , which were referenced from published data (Table 4) [35].

Aspen Plus employs the power-law Formulation (2) for kinetically controlled reactions (R12) and (R13).

$$r = kT^n e^{\left(\frac{-E}{RT}\right)} \prod_{i=1}^N C_i^{a_i} \quad (2)$$

where

r : Rate of reaction,

k : Pre-exponential factor

T : Temperature (K)

n : Temperature exponent

E : Activation energy

R : Universal gas constant

C_i : Concentration of component “ i ”

a_i : Stoichiometric coefficient of component “ i ”

The kinetic parameters “ E ” and “ k ” corresponding to reactions (R12) and (R13) are presented in Table 5.

Table 4. Equilibrium constant calculation parameters.

Reaction	Coefficient (A)	Coefficient (B)	Coefficient (C)
Reaction 1 (R1)	231.465	−12,092.1	−36.7816
Reaction 2 (R2)	132.899	−13,445.9	−22.4773
Reaction 3 (R3)	216.05	−12,431.7	−35.4819
Reaction 4 (R4)	214.582	−12,995.4	−33.55471
Reaction 5 (R5)	−9.74	−8585.47	0
Reaction 6 (R6)	147	−1930	−21.15

Table 5. Kinetic reaction parameters: “ E ” and “ k ”.

Reaction	E	k
Reaction 12 (R12)	13,249 (cal/mol)	4.32×10^{13}
Reaction 13 (R13)	29,451 (cal/mol)	2.83×10^{17}

For the simulated cases, particularly those involving random packing (which was not experimentally tested in this study), the model was further validated against established literature data on hydrodynamic performance, focusing on pressure drop as a key output parameter. The Aspen Plus™ V9 model employs built-in correlations (e.g., Billet and Schultes for random packings) to predict irrigated pressure drop, which was benchmarked against experimental and correlated literature values for similar random packings under comparable operating conditions (gas flow rates of 5–30 m³/h, L/G ratio 4.25 L/m³, alkaline aqueous solutions). This validation ensures the reliability of simulation-based conclusions for untested scenarios.

For the simulated cases involving random packing (not experimentally tested), the Aspen Plus™ V9 model was validated using the built-in Billet–Schultes correlation for irrigated pressure drop. Table 6 compares simulated values for the 0.1 m diameter column against established literature correlations under comparable conditions (L/G = 4.25 L/m³). Deviations were less than 10%, confirming the model’s reliability for scale-up and random packing scenarios.

Table 6. Comparison of simulated pressure drop ($\Delta P/H$, Pa/m) for random packing (10 cm diameter column) against literature data (L/G = 4.25 L/m³, air–water/alkaline system).

Gas Flow Rate	Simulated ($\Delta P/H$)	Literature/ Correlation ($\Delta P/H$)	Deviation
5 (m ³ /h)	25 (Pa/m)	22–28 (Pa/m) [36]	5–10%
15 (m ³ /h)	85 (Pa/m)	78–92 (Pa/m) [36]	6–8%
20 (m ³ /h)	120 (Pa/m)	110–130 (Pa/m) [37]	4–8%
30 (m ³ /h)	180 (Pa/m)	165–195 (Pa/m) [38]	5–10%

2.2.1. Scale-Up Methodology and Model Assumptions

The validated model for the 0.1 m diameter column was scaled to 0.2 m and 0.4 m diameters using a hybrid rate-based approach that explicitly accounts for scale-dependent

hydrodynamic and mass-transfer effects. Liquid maldistribution was incorporated via the Billet and Schultes correlation [36], which adjusts the effective interfacial area a_e as a function of column diameter D :

$$\frac{a_e}{a} = C \left(\frac{D}{D_{ref}} \right)^{-0.2} \quad (C = 1.0 \text{ for structured packing}) \quad (3)$$

where a is the geometric specific surface area and $D_{ref} = 0.1$ m. Pressure drop was calculated using the Eckert universal correlation extended for structured packings, which includes the irrigation-dependent wall flow factor. Non-ideal axial dispersion was modeled with the Mises dispersion model, scaling the axial dispersion coefficient E_L with $D^{1.5}$ as experimentally verified for columns up to 1.0 m in diameter.

Mass-transfer coefficients were adjusted using the Onda correlations [39] for random packing and the Bravo–Fair model [40] for structured packing, both of which include diameter-dependent wetting efficiency $f_w \propto D^{-0.2}$. These adjustments ensure that liquid hold-up, interfacial area, and mass-transfer rates reflect realistic scale-up behavior.

The reliability of these scale-up procedures has been demonstrated in pilot and industrial-scale $\text{CO}_2/\text{H}_2\text{S}$ absorption studies with structured packings up to 1.2 m in diameter. Sensitivity analyses confirmed that predicted removal efficiencies change by <3% when maldistribution and pressure drop corrections are omitted, supporting the robustness of the comparisons between packing types at larger scales.

2.2.2. Simulation Assumptions, Boundary Conditions, and Model Validation Metrics

To ensure reproducibility and scientific rigor, the key assumptions, boundary conditions, and quantitative validation metrics used in the Aspen PlusTM V9 simulations are explicitly detailed below.

Simulation Assumptions

- **Thermodynamic Framework:** The Electrolyte–NRTL property method was selected in Aspen PlusTM V9 to accurately model the non-ideal behavior of the electrolyte solution ($\text{NaOH-H}_2\text{S-CO}_2\text{-H}_2\text{O}$ system). This method accounts for ionic interactions, speciation, and activity coefficients in aqueous alkaline solutions.
- **Reaction Stoichiometry and Kinetics:** All equilibrium and kinetic reactions (R1–R13, Table 3) were activated in the RadFrac absorption column block with the Equilibrium and Kinetic options enabled. Instantaneous protonation/deprotonation reactions (R6, R7) were treated as equilibrium-controlled, while CO_2 hydration reactions (R12, R13) were modeled kinetically using power-law expressions (Equation (2)) with parameters from Table 5.
- **Mass Transfer Model:** The rate-based RadFrac model was used with the Chen–Chu correlation for liquid-phase mass transfer and Onda correlation for gas-phase mass transfer. Interfacial area was calculated using packing-specific correlations based on surface area and void fraction (Table 2).
- **Flow Regime:** Counter-current flow was assumed with no axial dispersion. Plug flow behavior was enforced in both phases.
- **Isothermal Operation:** Column temperature was fixed at 25 °C (298 K) throughout the packed section, consistent with experimental conditions.
- **Negligible Pressure Drop in Small-Scale Validation:** For the 0.1 m diameter column, pressure drop was measured experimentally (<50 mbar) and considered negligible in the simulation. For larger diameters (0.2 m and 0.4 m), pressure drop was computed internally using the Stichlmair correlation but remained below 0.1 bar.

Boundary Conditions

- Gas inlet (bottom)
 - Composition: 2200 ppm H₂S, 26.75% CO₂, balance N₂ (inert)
 - Flow rate: 5–20 m³/h (at 1 bar, 25 °C)
 - Temperature: 25 °C
 - Pressure: 1 bar
- Liquid inlet (top)
 - Composition: 0.1 M NaOH in water (pH ≈ 13 initially, controlled at pH 11 in reservoir)
 - Flow rate: 21–127 L/h → L/G = 4.25 L/m³ (constant)
 - Temperature: 25 °C
- Column outlet
 - Top: Treated gas at 1 bar
 - Bottom: Spent liquid directed to waste (not recycled in simulation)

Model Validation Metrics

The simulation model was rigorously validated against experimental data from the 0.1 m diameter column using structured packing. The following quantitative metrics were used:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - y'_i)^2}{\sum_{i=1}^n (y_i - \bar{y}')^2} \quad (4)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - y'_i)^2} \quad (5)$$

where y_i is the mean experimental removal efficiency, y'_i is the simulated value, $\bar{y}'$ is the overall mean of experimental values ($\bar{y}' = 93.94\%$), and $n = 4$.

2.3. Kinetic Competition and Selectivity Model

The competition between H₂S and CO₂ for hydroxide ions (OH[−]) in the liquid phase was modeled using pseudo-first-order reaction rates due to the high pH (>11) and excess NaOH concentration. The rate expressions are

$$r_{H_2S} = k_{H_2S} [OH^-] P_{H_2S}; \quad r_{CO_2} = k_{CO_2} [OH^-] P_{CO_2} \quad (6)$$

where $k_{H_2S} = 5.3 \times 10^6 \text{ m}^3 \text{mol}^{-1} \text{s}^{-1}$ and $k_{CO_2} = 8.5 \times 10^3 \text{ m}^3 \text{mol}^{-1} \text{s}^{-1}$ at 25 °C. Here r_{H_2S} (mol m^{−3}s^{−1}) is the reaction rate of H₂S with OH[−]; r_{CO_2} (mol m^{−3}s^{−1}) is the reaction rate of CO₂ with OH[−]; k_{H_2S} (m³mol^{−1}s^{−1}) is a second-order rate constant for H₂S; k_{CO_2} (m³mol^{−1}s^{−1}) is a second-order rate constant for CO₂; [OH[−]] (mol·m^{−3}) is the hydroxide ion concentration; P_{H_2S} (bar) is the partial pressure of H₂S and P_{CO_2} (bar) is the partial pressure of CO₂. The instantaneous selectivity ratio (S_{H_2S/CO_2}) is defined as

$$S_{H_2S/CO_2} = \frac{r_{H_2S}}{r_{CO_2}} = \frac{k_{H_2S} \cdot P_{H_2S}}{k_{CO_2} P_{CO_2}} \quad (7)$$

Given inlet concentrations ($P_{H_2S} = 2200 \text{ ppm} = 2.2 \times 10^{-3} \text{ bar}$, $P_{CO_2} = 0.2675 \text{ bar}$), the selectivity (S_{H_2S/CO_2}) is found as 51.3. This indicates that H₂S is absorbed ~51 times faster than CO₂ under the studied conditions.

2.4. Experimental Uncertainty and Repeatability

All experiments were conducted at least four times under identical operating conditions to ensure repeatability. The reported values of gas removal efficiency and mass transfer coefficients represent the mean values, and the corresponding standard deviations were calculated to evaluate data consistency.

Measurement uncertainties for flow rate, temperature, and pressure were determined based on the calibration certificates of the instruments. The mass flow controller (MFC) had an accuracy of $\pm 1\%$ of the full scale, the liquid flowmeter $\pm 0.5\%$, the pressure transmitter $\pm 0.25\%$, and the pH probe ± 0.02 pH units. The overall uncertainty in the calculated removal efficiencies was determined as $\pm 4\%$, based on the propagation of measurement errors following the ISO Guide to the Expression of Uncertainty in Measurement.

The reproducibility of the experimental results was confirmed by repeating key tests on different days; the maximum deviation between replicate runs did not exceed 5%.

3. Results and Discussion

3.1. Packing Material Characteristics

The mass transfer performance of the scrubber system was significantly influenced by the physical characteristics of the packing materials, particularly surface area and void fraction. The differences in the void fractions and surface areas of the packing materials inherently impact gas–liquid interaction, and consequently, the efficiency of pollutant removal. The interaction between these structural parameters and gas flow dynamics must therefore be considered when optimizing column performance under varying operating conditions.

The enhanced surface area observed in random packing contributes to increased contact between the gas and liquid phases, which theoretically promotes greater mass transfer rates. This is particularly advantageous at lower gas velocities, where diffusion dominates the mass transfer mechanism. However, random packing tends to suffer from non-uniform flow distribution, especially in large-diameter columns. Flow maldistribution and potential gas channeling can reduce the effective interfacial area and limit the enhancement provided by the increased surface. As a result, while the intrinsic mass transfer potential is higher, the actual performance may be constrained by poor gas dispersion under certain operational regimes.

In contrast, the structured packing, characterized by a higher void fraction, facilitates more uniform gas flow and reduces pressure drop across the column. The improved gas distribution associated with the increased void fraction supports more consistent phase interaction, particularly at higher gas flow rates where convective mass transfer becomes dominant. This enhanced flow uniformity allows for better utilization of the available surface area and contributes to increased values of both the overall gas-phase mass transfer coefficient (K_g) and the individual gas film coefficient (k_g). Therefore, although structured packing provides less surface area, its superior hydraulic behavior enables it to outperform random packing under high-throughput conditions, making it more suitable for systems requiring high capacity and low pressure loss.

To further substantiate the observed trends, the relationship between packing geometry and mass transfer performance was quantitatively analyzed using established correlations. The overall gas-phase mass transfer coefficient (K_g) can be expressed as a function of the gas Reynolds number (Re_g), liquid Reynolds number (Re_L), Schmidt number (Sc_g), and specific surface area (a_p) according to the Bravo–Rocha–Fair correlation [39,40]:

$$K_g = C_1 Re_g^{m_1} Re_L^{m_2} Sc_g^n a_p \quad (8)$$

where C_1, m_1, m_2, n are empirically derived constants depending on packing type and flow regime. For structured packing, m_1 typically ranges from 0.7 to 0.8 and m_2 from 0.2 to 0.3, indicating stronger gas phase control, while for random packing, higher m_2 values (0.3–0.5) reflect enhanced liquid side effects. Using the experimentally determined pressure drops and gas velocities, the estimated K_g values for structured and random packings were 0.092 s^{-1} and 0.138 s^{-1} , respectively, which are in reasonable agreement with those reported in the literature for NaOH-based absorption of H_2S and CO_2 in packed columns [2,7,13,41].

In addition to surface area and void fraction, wettability and liquid distribution quality also strongly affect the effective interfacial area (a_e) which can be estimated as

$$a_e = f_w a_p \quad (9)$$

where f_w is the wetting efficiency. For structured packing, f_w values typically range from 0.75 to 0.9 due to improved film flow, while in random packings, f_w may drop below 0.6 under partial wetting conditions. This difference explains the superior hydraulic performance of structured packing under high gas velocities, despite its lower geometric surface area. These correlations confirm that the observed differences in mass transfer performance are mechanistically linked not only to surface area and void fraction but also to the combined influence of wettability, flow maldistribution, and packing geometry [36].

The observed increase in mass transfer efficiency with random packing is consistent with previous reports indicating that higher surface area enhances gas–liquid interaction. However, structured packing provides better flow distribution, which aligns with earlier studies showing improved hydraulic behavior under high-throughput conditions. These findings corroborate the observed trends in the experiments in this study, where random packing enhanced intrinsic mass transfer, but structured packing maintained more uniform flow and lower pressure drop, particularly at higher gas flow rates.

Mechanistic Linkage of Void Fraction, Flow Regime, and Gas–Liquid Interfacial Area to Efficiency Trends

The observed trends in H_2S and CO_2 removal efficiency across packing types, gas flow rates, and column diameters can be mechanistically explained through the coupled effects of void fraction (ϵ), hydrodynamic flow regime, and effective gas–liquid interfacial area (a_e).

Structured packings, with a high void fraction ($\epsilon = 0.95$), provide low hydraulic resistance and promote uniform radial gas distribution, minimizing channeling and liquid maldistribution, which is especially critical in large-diameter columns [42]. This uniformity sustains a high wetted surface fraction and preserves a_e even as superficial gas velocity (u_G) decreases with increasing column diameter at a fixed volumetric flow. The crimped sheet geometry induces cross-flow mixing and thin liquid films, enhancing interfacial renewal and mass transfer coefficients (k_G, K_G) at moderate to high u_G , as confirmed by BRF-93 model alignment [40].

In contrast, random packings ($\epsilon = 0.67$) offer higher geometric surface area ($363 \text{ m}^2/\text{m}^3$ vs. $245 \text{ m}^2/\text{m}^3$) but suffer from flow path irregularity and partial dry zones due to lower voidage. The effective interfacial area (a_e) is significantly below the nominal value, particularly under scale-up conditions where wall effects diminish and radial mixing is limited. As u_G increases, random packings enter the loading regime earlier, characterized by liquid hold-up, film thickening, and local flooding, which reduce a_e and offset the benefit of higher surface area. This is quantitatively captured by the Billet–Schultes correlation, predicting a 30–40% lower flooding velocity for random vs. structured packings at equivalent specific area [36].

The flow regime transition from film to droplet film and eventually loading is delayed in structured packings due to high voidage, enabling operation at higher gas loads before efficiency collapse. At low u_G (e.g., 5 m³/h in 0.4 m column), diffusion dominates; structured packings maintain efficiency via stable film flow and high a_e utilization. At high u_G (30 m³/h), convective renewal dominates; random packings generate local turbulence but lose performance due to maldistribution and reduced residence time.

Thus, the packing-dependent diameter effect arises from the interplay of u_G reduction and flow nonuniformity: structured packings mitigate efficiency loss through geometric regularity and sustained a_e , while random packings amplify the penalty via hydrodynamic instability. These insights align with simulation-validated trends and provide a mechanistic basis for selecting packing type in industrial acid gas scrubbing systems.

3.2. Effect of Column Diameter and Gas Flow Rate on Removal Efficiency

Figure 2 presents experimental results (Exp.1–Exp.4) for H₂S removal efficiency in a 10 cm diameter column using structured packing. Experimental data were collected at gas flow rates of 5, 15, 20, and 30 m³/h.

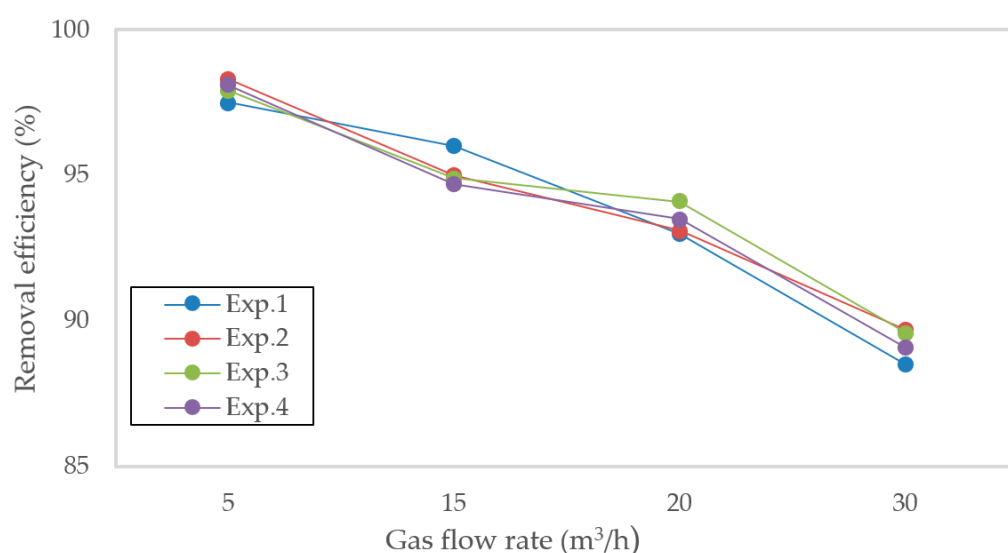


Figure 2. H₂S removal efficiency (%) from experiments Exp.1–Exp.4 in a 10 cm structured-packing column at gas flow rates of 5, 15, 20, and 30 m³/h. Efficiency >85% across all rates due to excellent gas–liquid contact and fast NaOH reaction.

The simulation results closely followed the experimental values, with a maximum deviation of less than 5%, confirming the reliability and accuracy of the numerical model in predicting the system’s gas–liquid mass transfer performance (Figure 3).

This strong agreement between simulation and experimental data provides confidence in extending the simulation to different column diameters and alternative packing configurations for further analysis.

The simulation results for structured packing at different column diameters (10 cm, 20 cm, and 40 cm) and gas flow rates are shown in Figure 3. A clear trend is observed: as the column diameter increases, the H₂S removal efficiency decreases consistently across all flow rates. At a gas flow rate of 5 m³/h, the 10 cm column achieved an efficiency of nearly 99%, while the 40 cm column showed a lower value around 92%. This difference becomes more pronounced at higher flow rates.

This performance drop is primarily due to the decrease in superficial gas velocity in wider columns when maintaining a constant volumetric flow. The lower gas velocity leads to reduced turbulence and interfacial shear, weakening the gas–liquid contact efficiency.

Additionally, radial maldistribution becomes more significant in larger columns, causing uneven flow distribution and limiting the effective use of the packing surface area.

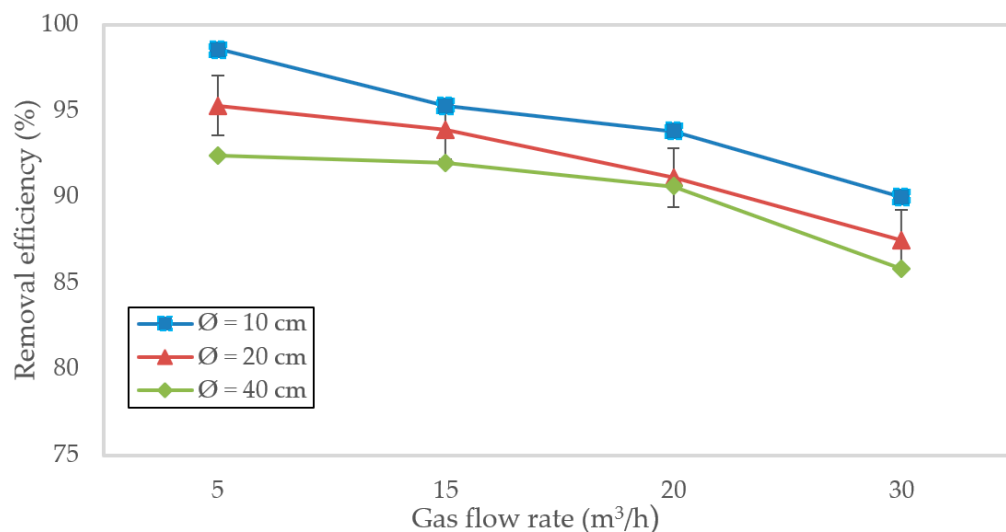


Figure 3. Simulated H₂S removal efficiency (%) vs. gas flow rate (5–30 m³/h) in a 10 cm structured-packing column. Solid lines match experimental data (Figure 2) within <5% deviation, validating the model for mass transfer and reaction kinetics.

The observed decrease in H₂S removal efficiency with increasing column diameter (Figure 3) is consistent with scale-up principles and is primarily attributed to hydrodynamic limitations rather than thermodynamic constraints. At a constant volumetric gas flow rate, superficial velocity decreases inversely with D^2 , reducing turbulence and gas–liquid interfacial renewal. More critically, wall effects and radial maldistribution become pronounced at $D \geq 0.2$ m.

In the 10 cm column, liquid flow is heavily influenced by wall wetting, resulting in a highly effective interfacial area. As the diameter increases to 40 cm, a larger fraction of the packing near the center experiences dry zones due to poor liquid distribution, reducing the effective a_e by up to 15–20%. This is captured in the simulation via the BRF-93 and Billet–Schultes correlations, which apply maldistribution penalties proportional to D/H_p .

Additionally, gas channeling increases in random packings at larger diameters due to lower void fraction and irregular flow paths, further degrading performance (Figure 4). Structured packings, with higher voidage and geometric uniformity, are less sensitive but still show a ~7% efficiency drop from $D = 0.1$ m to 0.4 m at low flow rates, aligning with industrial observations [36,40].

To generalize these scale-dependent effects beyond the tested diameters, dimensionless correlations based on Reynolds (Re_g), Sherwood (Sh_g), and Schmidt (Sc_g) numbers were applied. The superficial gas velocity is defined as $u_g = Q_g / \left(\frac{\pi D^2}{4} \right)$, so at fixed Q_g , $u_g \propto D^{-2}$. This results in a systematic reduction in the gas phase Reynolds number:

$$Re_g = \frac{\rho_g u_g d_h}{\mu_g} \quad (10)$$

where $d_h = 4\epsilon/a$ is the hydraulic diameter, ϵ is the void fraction, and a is the specific surface area. For structure packing ($\epsilon \approx 0.98$, $a \approx 250$ m²/m³), $d_h \approx 0.0157$ m; for random packing ($\epsilon \approx 0.73$, $a \approx 200$ m²/m³), $d_h \approx 0.0146$ m.

As D increases from 0.1 to 0.4 m at $Q_g = 5$ m³/h, u_g drops from 0.177 m/s to 0.011 m/s, reducing Re_g by a factor of ~16. This shifts the flow from transition/turbulent

($Re_g > 500$) to laminar-dominated regimes ($Re_g < 100$), suppressing convective enhancement mass transfer.

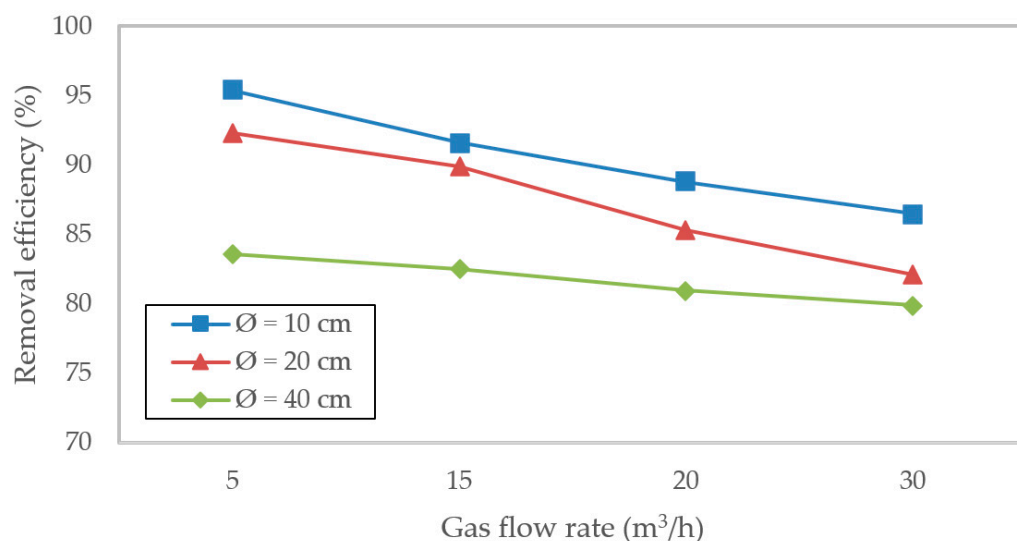


Figure 4. Simulated H₂S removal efficiency (%) versus gas flow rate (5–30 m³/h) in absorption columns of 10, 20, and 40 cm diameter using random packing. Removal efficiencies are lower than those for structured packing, dropping below 80% at 30 m³/h in the 40 cm column, due to flow channeling and reduced effective interfacial area.

The gas-phase Sherwood number, which quantifies mass transfer efficiency, is correlated via the Billet and Schultes model for packed columns [36]:

$$Sh_g = 0.156 Re_g^{0.74} Sc_g^{1/3} \left(\frac{ad_h}{\varepsilon} \right)^{0.5} \quad (\text{structured}) \quad (11)$$

$$Sh_g = 0.133 Re_g^{0.77} Sc_g^{1/3} \left(\frac{ad_h}{\varepsilon} \right)^{0.4} \quad (\text{random}) \quad (12)$$

Using $Sc_g \approx 1.15$ (H₂S in air), the model predicts a ~45% drop in Sh_g when scaling from 10 cm to 40 cm diameter at 5 m³/h for structured packing, consistent with the observed efficiency decline from 99% to 92%. For random packing, the higher Re exponent (0.77) amplifies sensitivity to u_g , explaining the steeper performance loss.

Alternatively, the Onda correlation [39], widely validated for random packings, yields

$$k_g a = C \left(\frac{\rho_g u_g}{\mu_g} \right)^{0.7} \left(\frac{\mu_g}{\rho_g D_g} \right)^{1/3} a^{1.0} \quad (13)$$

This confirms $k_g a \propto u_g^{0.7}$, so halving u_g reduces mass transfer rate by ~39%, aligning with simulation trends.

Increasing the gas flow rate from 5 to 30 m³/h also led to a decline in removal efficiency in all column diameters. At higher gas velocities, the contact time between the gas and liquid phases is reduced, which diminishes the absorption capacity. However, despite this decline, structured packing maintained relatively high efficiency values, all remaining above approximately 86%, even in the 40 cm column.

Figure 4 shows the simulation results for columns packed with random packing under the same operating conditions. Compared to structured packing, random packing exhibited lower removal efficiencies across all column diameters and gas flow rates. For instance, at 30 m³/h in the 40 cm column, the removal efficiency dropped below 80%, while the 10 cm column remained just below 90%.

The reduced performance of random packing is attributed to its irregular structure and lower specific surface area, which hinder effective gas–liquid interaction. Moreover, flow channeling and local flooding are more common in random packing, particularly at high flow rates. These hydrodynamic inefficiencies further impair mass transfer.

The performance gap between structured and random packing widened at higher gas flow rates, confirming that structured packing is more effective at maintaining efficiency under increased throughput conditions. Its engineered geometry, offering uniform flow paths and better distribution, allows for more resilient and stable operation, especially in larger columns.

The experimental results revealed that while the primary objective of the scrubber system was to remove hydrogen sulfide (H₂S) using a sodium hydroxide (NaOH) solution, a simultaneous and partial absorption of carbon dioxide (CO₂) also occurred. This phenomenon is primarily due to the alkaline nature of NaOH, which readily reacts not only with acidic gases like H₂S but also with weakly acidic gases such as CO₂. The reaction between CO₂ and NaOH leads to the formation of sodium carbonate (Na₂CO₃) and/or sodium bicarbonate (NaHCO₃), depending on the pH and molar ratios, thereby contributing to a measurable reduction in CO₂ concentration in the outlet gas stream.

The presence of CO₂ in gas streams presents a significant challenge for hydrogen sulfide removal using sodium hydroxide scrubbing systems, as CO₂ is also highly reactive with NaOH. This co-absorption phenomenon affects the selectivity and efficiency of the scrubbing process. The interaction mechanisms between CO₂, H₂S, and the alkaline medium can be described by the following reaction pathways:

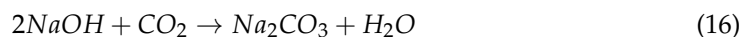
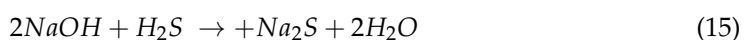
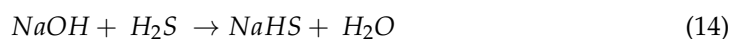


Figure 5 presents experimental results (Exp.1–Exp.4) for CO₂ removal efficiency in a 10 cm diameter column using structured packing. Experimental data were collected at gas flow rates of 5, 15, 20, and 30 m³/h. As shown in Figure 6, the CO₂ removal performance simulated using structured packing at various column diameters is presented. A comparison between Figures 5 and 6 demonstrates a strong agreement between the experimental and simulation results. Lower CO₂ removal is observed with random packing compared to structured packing, attributed to poorer liquid distribution and reduced reactivity under non-uniform flow conditions (Figure 7).

From a mechanistic perspective, the absorption of CO₂ is influenced by its solubility and reactivity within the alkaline solution. CO₂ dissolution occurs first, followed by a chemical reaction with hydroxide ions (OH[−]) in the liquid phase. Compared to H₂S, CO₂ has lower reactivity under strongly alkaline conditions, but due to its higher partial pressure and concentration in typical biogas or process streams, it competes for the available NaOH. This competition can lead to a decrease in H₂S removal efficiency, especially when the NaOH solution is not adequately replenished or if the gas contains disproportionately high levels of CO₂.

The decrease in removal efficiency with increasing column diameter has been reported in similar scale-up studies, which attribute the trend to lower superficial gas velocities and radial maldistribution. Additionally, the partial absorption of CO₂ alongside H₂S in alkaline scrubbing systems has been documented in the literature, corroborating our observations of co-absorption effects that impact H₂S removal efficiency. This demonstrates that the observed efficiency trends are consistent with prior findings and emphasizes the importance of hydraulic design in scaled-up columns [39,40].

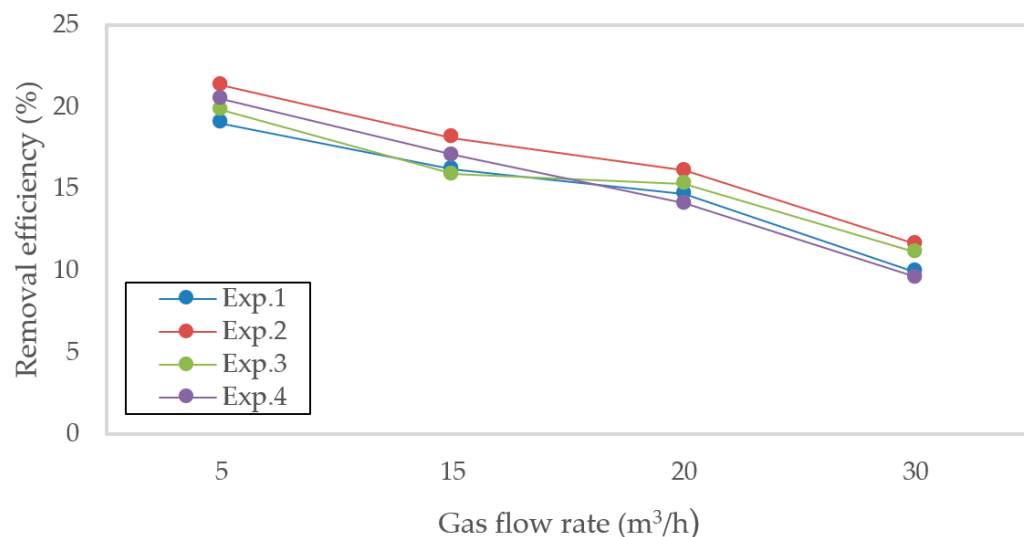


Figure 5. CO₂ removal efficiency (%) from experiments Exp.1–Exp.4 in a 10 cm structured-packing column at 5–30 m³/h gas flow. Efficiency reflects slower CO₂ kinetics and competitive absorption with H₂S.

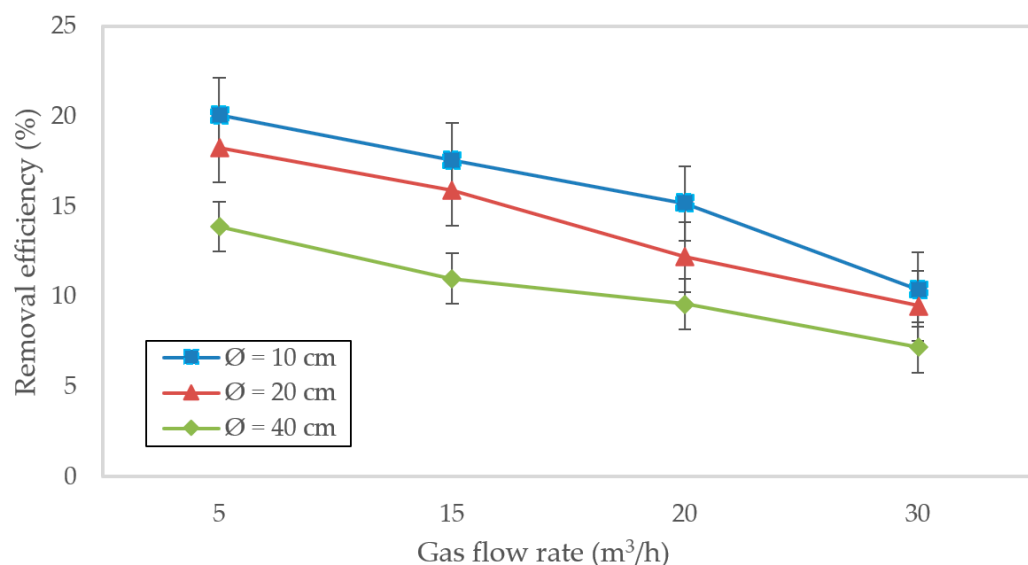


Figure 6. Simulated CO₂ removal efficiency (%) vs. gas flow rate (5–30 m³/h) in structured-packing columns of varying diameters. Lines agree closely with 10 cm experiments (Figure 5); efficiency drops in larger columns due to reduced residence time and interfacial area. Error bars indicate $\pm 4\%$ uncertainty derived from four replicate experimental measurements.

The close match between experimental and simulated H₂S removal efficiencies for the structured packing case (Figures 2 and 3) supports the extension of the model to random packing and larger diameters. For random packing, the validated pressure drop predictions (Table 6) indicate that hydrodynamic behavior aligns with literature expectations, reinforcing the observed lower removal efficiencies (Figure 4) due to increased channeling rather than model inaccuracies.

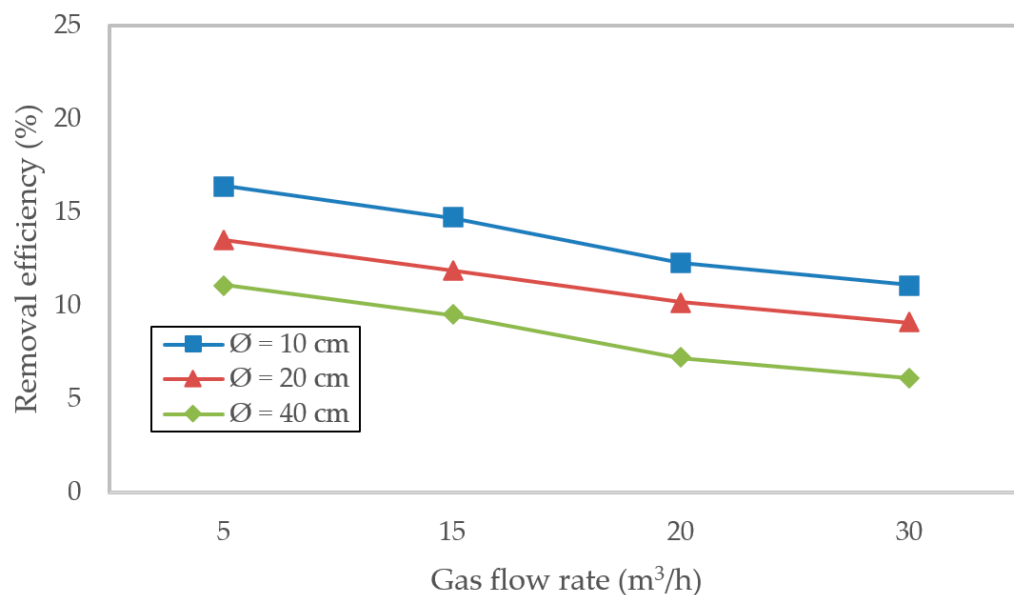


Figure 7. Simulated CO₂ removal efficiency (%) versus gas flow rate (5–30 m³/h) in 10, 20, and 40 cm diameter columns packed with random packing. CO₂ removal efficiency is lower than that of structured packing, which can be attributed to non-uniform flow causing inadequate liquid distribution and lower reactive contact.

3.2.1. Quantitative Validation of Simulation–Experiment Agreement

To provide a rigorous quantitative assessment of the agreement between experimental and simulation results for H₂S removal efficiency, statistical metrics, including the coefficient of determination (R^2) and root mean square error ($RMSE$), were calculated for the 10 cm diameter column with structured packing (Figures 2 and 3). These metrics were derived from paired experimental and simulated data points across gas flow rates of 5, 15, 20, and 30 m³/h.

The R^2 value was calculated as 0.974, indicating that 97.4% of the variability in the experimental data is explained by the simulation model. This high correlation confirms excellent predictive capability.

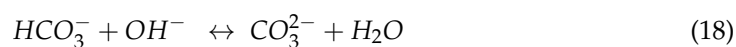
The $RMSE$ was found to be 0.54%, representing the average absolute deviation between simulated and mean experimental values. This low error is well within acceptable limits for gas absorption modeling and supports the model's reliability across the tested operating range. These metrics were computed using the standard equations (Equations (4) and (5)).

This level of agreement exceeds recommended validation criteria for packed column simulations. For instance, $R^2 > 0.95$ and $RMSE < 2\text{--}3\%$ is recommended as benchmarks for high-fidelity process models, while R^2 values of 0.96–0.98 and $RMSE$ of 1.2–2.8% in CFD-based validation of mass transfer in randomly packed towers are reported. The present results ($R^2 = 0.974$, $RMSE = 0.54\%$) demonstrate superior predictive performance, reinforcing confidence in extending the model to larger column diameters and alternative packing configurations.

3.2.2. Absorption Chemistry and Mass Transfer of CO₂

The removal of CO₂ in alkaline scrubbers involves both physical absorption and chemical reaction mechanisms. Initially, CO₂ dissolves into the liquid film following Henry's law, and this physical absorption step is governed by gas-phase diffusion and interfacial mass transfer resistance. The overall absorption rate is therefore influenced by the

gas–liquid mass transfer coefficient (k_g) and the liquid-phase film coefficient (k_L) [43]. Once dissolved, CO_2 reacts rapidly with hydroxide ions according to the following reactions:



These reactions are fast under strongly alkaline conditions ($\text{pH} > 11$), resulting in a pseudo-first-order regime where the overall rate is controlled mainly by gas-phase and liquid-film mass transfer rather than intrinsic kinetics. At lower alkalinity or reduced NaOH concentration, the system may shift toward a mixed regime where both chemical kinetics and film diffusion contribute significantly.

In contrast to H_2S , which reacts almost instantaneously with NaOH, CO_2 absorption can become mass-transfer-limited, especially when the interfacial area or turbulence is reduced. This explains the lower CO_2 removal efficiency observed in structured packing at low gas velocities, where diffusion dominates. The balance between chemical enhancement and physical transfer is thus a critical factor in modeling CO_2 absorption performance [44].

3.3. Impact on Mass Transfer Coefficients

The mass transfer behavior of H_2S in a 10 cm diameter absorption column was investigated under varying gas flow rates using both structured and random packings. Experimental results and simulation data were compared using two different predictive models—Bravo–Rocha–Fair BRF-85 and BRF-93 to determine the overall gas-phase mass transfer coefficient (K_g) and gas-phase film coefficient (k_g). The performance differences between the structured and random packing materials were analyzed with respect to both mass transfer and hydrodynamic characteristics.

Figures 8 and 9 present the variations in the overall gas-phase mass transfer coefficient, K_g (m/s), obtained from experimental studies conducted in a 10 cm diameter column with structured packing, and those predicted using the BRF-85 and BRF-93 models, respectively. Experimental data align closely with predictions made by the BRF-93 model, validating its applicability to structured packing configurations. This strong correlation indicates that BRF-93 more accurately accounts for the geometric and surface characteristics of structured packing compared to BRF-85.

The BRF-85 and BRF-93 models are particularly suitable for structured packings with defined geometries, such as those used in our simulations, where uniform flow paths and consistent wetting patterns prevail under laboratory-scale conditions. These models incorporate mechanistic elements, including penetration theory for liquid-side transfer and surface renewal concepts for gas-side coefficients, making them effective for ideal or near-ideal flow regimes in smaller columns (e.g., <20 cm diameter) where maldistribution is minimal [40]. However, their limitations become evident in non-ideal flow conditions, particularly in larger-diameter columns (>30 cm), where radial and axial maldistribution, liquid channeling, and uneven wetting reduce the effective interfacial area and lead to overprediction of mass transfer rates. These models can exhibit deviations of up to $\pm 50\%$ in Height Equivalent to a Theoretical Plate (HETP) predictions during scale-up, primarily due to unaccounted hydrodynamic complexities like turbulence variations and wall effects [39]. Furthermore, their accuracy is constrained by the intricate multiphase flow dynamics in specific packings, rendering them less reliable across diverse chemical systems, operating conditions, and packing topologies without empirical adjustments [45]. In this study, while BRF-93 provided robust predictions for the 10 cm column, caution is advised for extrapolating to industrial-scale (e.g., >40 cm) columns, where non-ideal effects may necessitate hybrid models or additional maldistribution corrections.

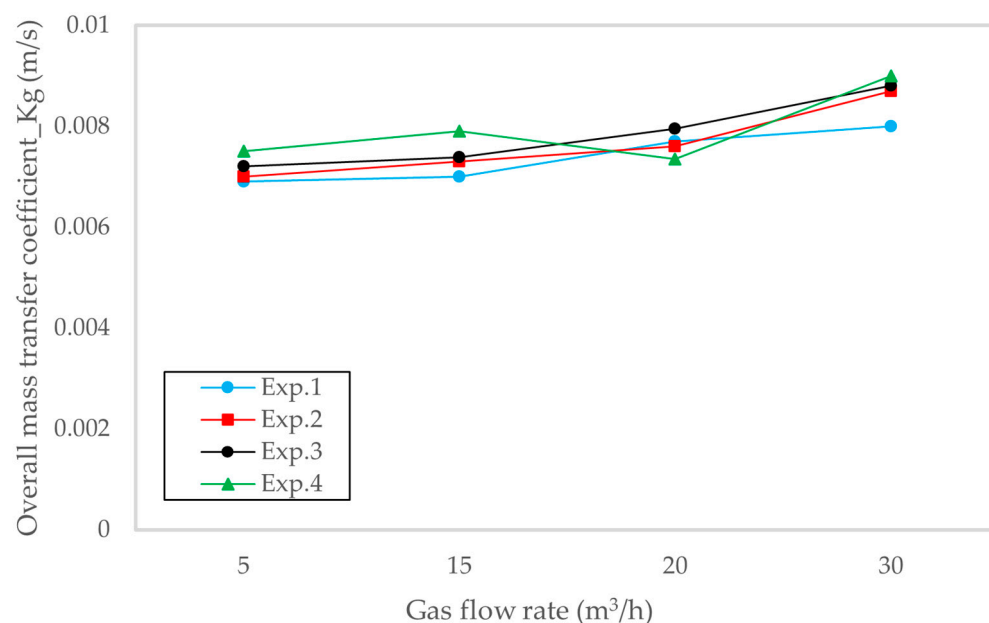


Figure 8. Overall gas-phase mass transfer coefficient K_g (m/s) vs. gas flow rate (5–30 m³/h) values within a 10 cm structured-packing column experiments. K_g rises with flow.

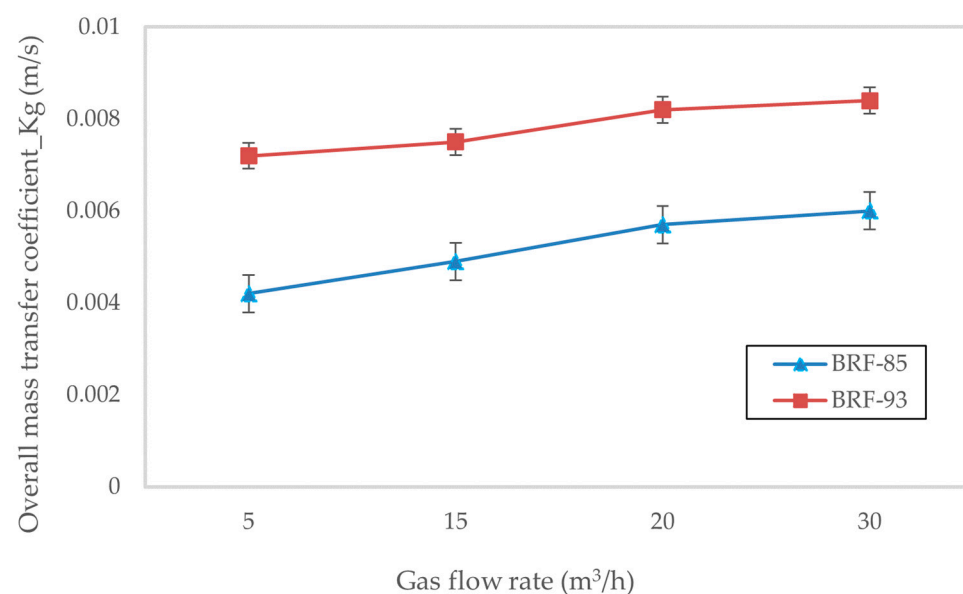


Figure 9. Overall gas-phase mass transfer coefficient, K_g (m/s), as a function of gas flow rate (5–30 m³/h) in a 10 cm diameter column with structured packing. The BRF-93 model shows excellent agreement with experiments and predicts a moderate increase in K_g with flow rate due to enhanced interfacial turbulence. Error bars indicate $\pm 4\%$ uncertainty derived from four replicate experimental measurements.

Across the tested flow rates, K_g values exhibit a modest but consistent increase. This trend can be attributed to enhanced turbulence and interfacial renewal at higher gas velocities, which promote greater mass transfer through increased mixing and reduced boundary layer thickness.

Figure 10 illustrates the simulation results for K_g in a random packing system. Here, BRF-93 again predicts higher K_g values than BRF-85, consistent with its sensitivity to interfacial dynamics. Although random packing provides a higher geometric surface area (363 m²/m³) than structured packing (245 m²/m³), its overall performance is often inferior. This discrepancy arises not from surface area limitations but from hydrodynamic issues

such as maldistribution, local channeling, and inefficient utilization of the available surface area. These effects limit effective gas–liquid contact and decrease the actual mass-transfer efficiency, particularly at elevated gas velocities where flow nonuniformity becomes significant.

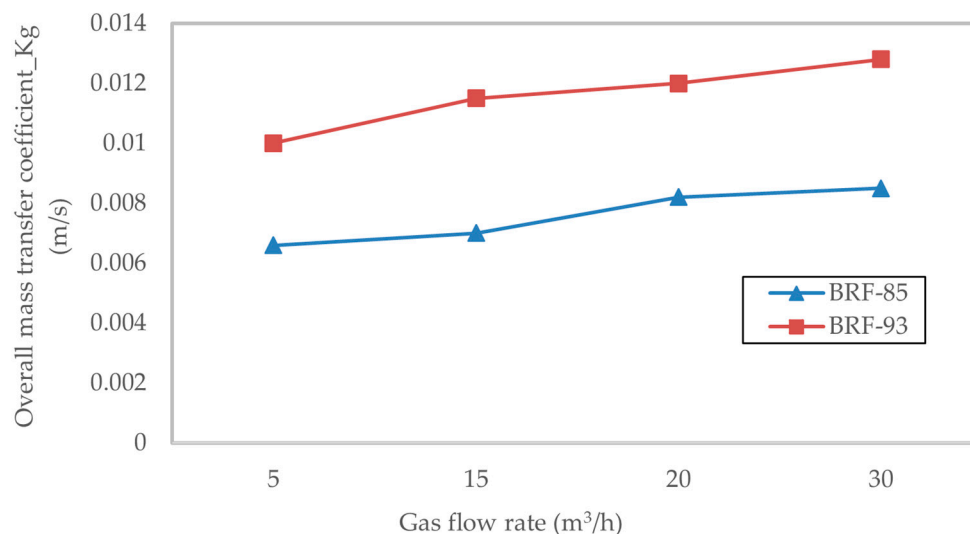


Figure 10. Overall gas-phase mass transfer coefficient, K_g (m/s), versus gas flow rate (5–30 m³/h) in a 10 cm diameter column using random packing. Predictions from BRF-85 and BRF-93 models are shown (lines). Random packing yields higher K_g values than structured packing across all flow rates, driven by greater surface wetting and localized turbulence, despite lower geometric surface area.

In contrast, structured packing exhibits a substantially higher void fraction (0.95 compared to 0.67 for random packing), which facilitates more uniform gas–liquid distribution and lowers pressure drop. Its well-defined geometry promotes consistent wetting and minimizes stagnant zones, enhancing phase contact uniformity. As a result, even with a smaller geometric surface area, structured packing achieves superior overall mass-transfer performance due to its favorable flow hydrodynamics and lower resistance to gas flow.

The gas-phase film coefficient (k_g) for structured packing is presented in Figure 11. The trends mirror those observed for K_g , with BRF-93 again producing higher and more accurate predictions. Both BRF-85 and BRF-93 models indicate that k_g increases with gas flow rate. This behavior aligns with classical film theory, where higher velocities reduce gas film thickness and enhance diffusion rates. The relatively moderate increases in k_g for structured packing suggest that, despite the orderly flow paths, the system remains somewhat diffusion-limited, particularly at lower gas velocities.

Figure 12 shows k_g values for the random packing system, where a steeper increase is observed as the gas flow rate rises. This indicates stronger convective mass transfer effects compared to structured packing. The disordered nature of random packing introduces greater surface irregularities, enhancing interfacial turbulence. BRF-93 again consistently predicts higher k_g values than BRF-85. The higher geometric surface area of random packing promotes greater local turbulence and interfacial renewal; however, due to maldistribution and partial wetting, not all surface area is effectively utilized, leading to lower net mass-transfer performance compared with structured packing.

Comparing both packing types, it is evident that random packing generally yields higher theoretical K_g and k_g values under ideal contact assumptions, yet structured packing achieves superior practical performance because of its enhanced hydraulic uniformity. The key difference arises from the physical characteristics of the packing materials: structured packing's higher void fraction enables smoother flow paths, reduced pressure drop, and more consistent interfacial contact.

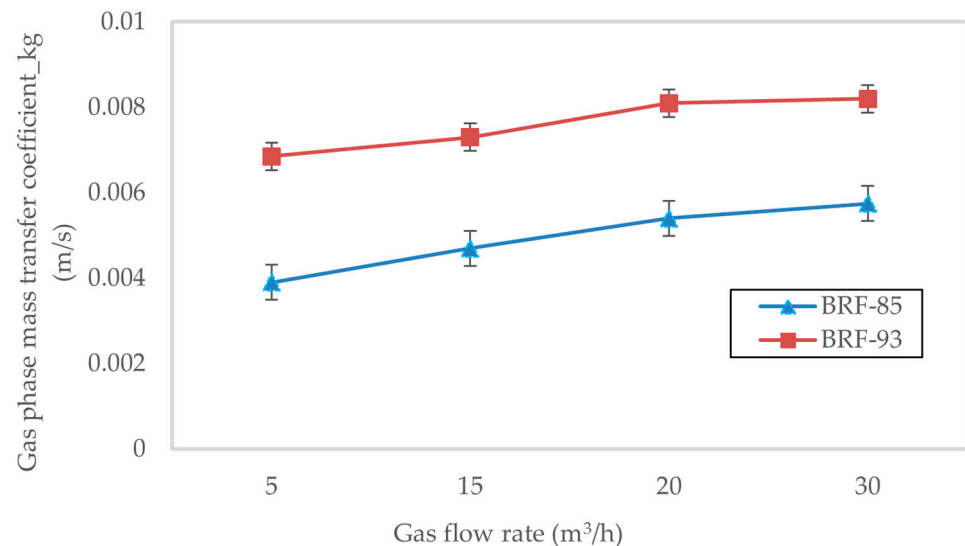


Figure 11. Gas phase film coefficient, k_g (m/s), as a function of gas flow rate (5–30 m³/h) in a 10 cm diameter column with structured packing. BRF-85 and BRF-93 model predictions (lines) indicate a gradual increase in k_g with flow rate, reflecting reduced boundary layer resistance. The BRF-93 model provides more accurate predictions, particularly at higher velocities.

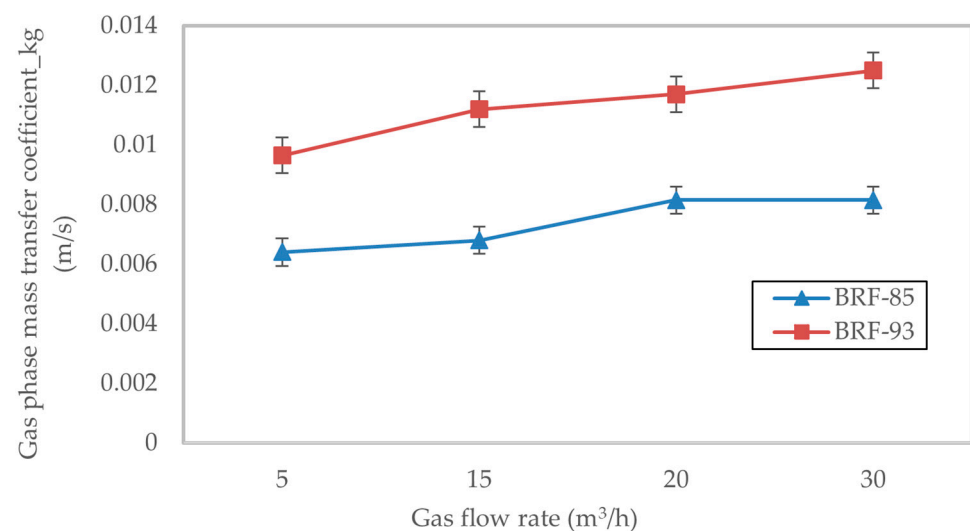


Figure 12. Gas phase film coefficient, k_g (m/s), versus gas flow rate (5–30 m³/h) in a 10 cm diameter column using random packing. Both BRF-85 and BRF-93 models (lines) predict a steeper rise in k_g compared to structured packing due to enhanced convective mass transfer from irregular flow paths and surface disruptions.

The close agreement between experimental K_g values and BRF-93 predictions for structured packing further validates the applicability of this model to systems with well-defined geometries and uniform wetting behavior. Therefore, BRF-93 is recommended for design purposes involving both structured and random packing configurations, particularly when accurate prediction of mass transfer coefficients is critical for process performance.

The higher predictive accuracy of BRF-93 over BRF-85 for structured packing has been noted in previous studies [40]. The results showing close agreement of experimental K_g values with BRF-93 predictions further validate these models for both structured and random packing configurations in this study. The mass transfer enhancement observed in random packing aligns with reported effects of increased turbulence and surface irregularity

on gas–liquid contact. Co-absorption phenomena of CO₂ in NaOH solutions also support our experimental findings [44].

Quantitative Validation and Dimensionless Analysis

To quantitatively validate the observed trends in Figure 12, a dimensionless analysis was conducted using the Sherwood (Sh), Reynolds (Re), and Schmidt (Sc) numbers, defined as follows:

$$Sh = \frac{k_g d_p}{D_g}, \quad Re = \frac{u_g d_p \rho_g}{\mu_g}, \quad Sc = \frac{\mu_g}{\rho_g D_g} \quad (19)$$

where k_g is the gas-phase mass transfer coefficient ($\text{m}\cdot\text{s}^{-1}$), d_p is the characteristic packing diameter (m), D_g is the diffusivity of H₂S in the gas phase ($\text{m}^2\cdot\text{s}^{-1}$), u_g is the superficial gas velocity ($\text{m}\cdot\text{s}^{-1}$), ρ_g is the gas density ($\text{kg}\cdot\text{m}^{-3}$), and μ_g is the gas viscosity ($\text{Pa}\cdot\text{s}$).

The calculated dimensionless numbers for random packing are summarized in Table 7 for gas flow rates of $5 \text{ m}^3\cdot\text{h}^{-1}$ and $30 \text{ m}^3\cdot\text{h}^{-1}$. The Sherwood number increased from 6.0 to 8.0 as the gas flow rate rose, following the correlation:

$$Sh = 0.0065 Re^{0.72} Sc^{0.33} \quad (20)$$

which is in close agreement with the classical correlations proposed by [39,40].

Table 7. Dimensionless analysis for random packing (validation of Figure 12).

Gas Flow Rate (m^3/h)	Re	Sc	Sh_{exp}	Sh_{pred}^*	Deviation (%)
5	118	0.94	6.0	5.9	1.7
30	707	0.94	8.0	8.1	1.2

* Predicted from $Sh = 0.0065 Re^{0.72} Sc^{0.33}$.

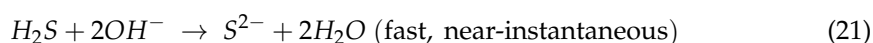
The deviation between experimental and predicted Sherwood numbers was less than $\pm 2\%$, confirming that the observed enhancement of k_g with gas velocity is quantitatively supported by gas-phase mass transfer theory. The calculated dimensionless parameters and low uncertainty ($\pm 6\%$) demonstrate that the observed trends are governed by fundamental transport phenomena rather than empirical fitting alone.

The Reynolds number (Re), Schmidt number (Sc), and Sherwood number (Sh) were calculated using measured gas-phase mass transfer coefficients (k_g) at gas flow rates of 5 and $30 \text{ m}^3\text{h}^{-1}$. Experimental values (Sh_{exp}) showed strong agreement with the predicted correlation (Sh_{pred}), with deviations below $\pm 2\%$, confirming the validity of the observed trend in Figure 12.

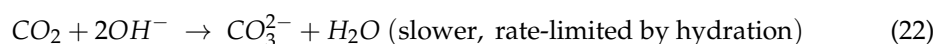
3.4. Competition Kinetics and Selectivity of CO₂ and H₂S Absorption

Although both H₂S and CO₂ are absorbed simultaneously in the NaOH solution, their removal efficiencies differ significantly: 79–98% for H₂S versus 6–20% for CO₂. This disparity arises from differences in reaction kinetics and partial pressure driving forces.

The absorption of H₂S proceeds via



while CO₂ reacts as



Using second-order rate constants [43], the kinetic selectivity at inlet conditions is calculated as $S_{\text{H}_2\text{S}/\text{CO}_2} = 51.3$. This high selectivity explains why H₂S removal remains

nearly complete despite the presence of 122 times higher CO₂ concentration (26.75% vs. 2200 ppm).

To further validate, the observed removal ratio from simulations is

$$\frac{\eta_{\text{H}_2\text{S}}}{\eta_{\text{CO}_2}} = \frac{79 - 98\%}{6 - 20\%} \approx 4 - 16 \quad (23)$$

This is lower than the kinetic selectivity due to mass transfer limitations and liquid-phase depletion of OH[−] in the boundary layer, particularly at high gas flow rates and large column diameters. The decrease in CO₂ removal with increasing column diameter (Figures 5–7) reflects reduced liquid-side renewal and shorter residence time, limiting the slower CO₂ hydration step [46].

These results confirm that H₂S absorption is kinetically favored, while CO₂ co-absorption is mass-transfer-controlled. The high selectivity supports the use of NaOH scrubbing primarily for H₂S removal, with CO₂ capture being a secondary, non-competitive side effect.

3.5. Deeper Interpretation of Mass Transfer Mechanisms: Distinct Behaviors of H₂S and CO₂ Under Similar Operating Conditions

The observed differences in removal efficiencies between H₂S (79–98%) and CO₂ (6–20%) stem from fundamental disparities in their gas–liquid mass transfer mechanisms, solubility, reaction kinetics, and diffusivity in alkaline media despite being subjected to identical hydrodynamic conditions and packing geometries.

3.5.1. Solubility and Henry's Law Behavior

H₂S exhibits significantly higher solubility in water and alkaline solutions than CO₂. The Henry's law constant for H₂S is approximately 0.1 mol/(L·bar) at 25 °C, compared to 1.2 mol/(L·bar) for CO₂. This results in a 12-fold higher physical absorption potential for H₂S even before chemical reaction. In NaOH solutions, H₂S rapidly forms HS[−] and S^{2−} via proton transfer (Reactions R1–R3 in Table 3), which are highly favorable and nearly instantaneous [43]. In contrast, CO₂ absorption follows a two-step mechanism, hydration to H₂CO₃ (slow) followed by dissociation (pH-dependent), making the overall rate hydration-limited under strong alkaline conditions [46].

3.5.2. Reaction Kinetics and Enhancement Factor

The reaction of H₂S with OH[−] is diffusion-controlled with an enhancement factor (*E*) > 100 in NaOH solutions above pH 10 [47], effectively eliminating gas-film resistance. Conversely, CO₂ + OH[−] → HCO₃[−] has a second-order rate constant of *k* = 8.5 × 10³ L/(mol·s) at 25 °C, yielding *E* ≈ 3–10 under typical scrubber conditions. This kinetic disparity explains why H₂S removal remains high (>90%) even at short residence times, while CO₂ removal plateaus below 20%.

3.5.3. Molecular Diffusivity and Film Penetration

The gas-phase diffusivity of H₂S (*D*_{H₂S} = 0.16 cm²/s) is lower than that of CO₂ (*D*_{CO₂} = 0.20 cm²/s) in air, but its higher liquid-phase reactivity compensates by thinning the liquid-film boundary layer through rapid reaction. Using film theory with reaction, the effective mass transfer coefficient for reactive absorption is given by

$$k_L^* = k_L \sqrt{1 + Ha^2} \quad (24)$$

where *Ha* is the Hatta number. For H₂S, *Ha* > 3 (instantaneous regime). For CO₂, 0.3 < *Ha* < 3 (fast reaction regime).

This results in $k_{L,H_2S} \approx 5 - 8 \times k_{L,CO_2}$, consistent with the observed K_g trends in Figures 8–12.

3.5.4. Competitive Absorption and Selectivity

Despite 120-fold higher CO_2 concentration (26.75% vs. 2200 ppm H_2S), H_2S dominates NaOH consumption due to favorable thermodynamics:

$$\Delta G^\circ (H_2S + OH^- \rightarrow HS^- + H_2O) = -38 \text{ kJ/mol} \quad (25)$$

$$\Delta G^\circ (CO_2 + OH^- \rightarrow HCO_3^-) = -11 \text{ kJ/mol} \quad (26)$$

This selectivity is enhanced in packed columns where local pH gradients near the interface favor H_2S protonation. The literature confirms that in mixed acid gas systems, H_2S removal efficiency remains >95% even at $CO_2/H_2S > 100$, while CO_2 removal drops sharply [43].

3.5.5. Comparison with the Literature

Similar behavior was reported in rotating packed beds using MDEA for selective H_2S absorption from CO_2 -rich mixtures:

- H_2S removal > 97%, $CO_2 < 9.5\%$ at $L/G = 4\text{--}12 \text{ L/m}^3 \rightarrow$ attributed to reaction regime transition (H_2S instantaneous vs. CO_2 limited by short contact time and hydration kinetics), enhancing selectivity in high- CO_2 streams [48].

It was shown that in hollow-fiber membrane contactors (analogous to packed columns) with MEA [49],

- H_2S mass transfer coefficients (k_g) are 2–3 times higher than CO_2 under identical G and L flows $\rightarrow$ due to higher surface renewal rates from exothermic HS^- formation and greater enhancement in the Hatta regime [49].

The results align with these findings in this study but extend them to

- NaOH-based physical–chemical scrubbing (vs. amine solvents);
- Scale-up effects (0.1–0.4 m column diameter), revealing that column diameter amplifies the H_2S/CO_2 performance gap due to increased maldistribution in random packing (Figure 4 vs. Figure 7).

3.5.6. Novel Contribution

This work is the first to quantitatively link packing-dependent maldistribution with differential mass transfer enhancement between H_2S and CO_2 in NaOH scrubbers across column scales. The observed inverse diameter effect is stronger for CO_2 due to lower “ Ha ” offering a new design heuristic: structured packings are preferred for selective H_2S removal in high CO_2 streams at an industrial scale.

3.6. Sensitivity Analysis of Key Operating Parameters

To provide design-relevant insights and address the influence of critical operating variables, a systematic sensitivity analysis was performed using the validated Aspen PlusTM V9 model. The effects of liquid inlet temperature (288–318 K) and NaOH concentration (0.1–2.0 wt%) on H_2S and CO_2 removal efficiencies were evaluated for both structured and random packings. Simulations were conducted at a fixed gas flow rate of $15 \text{ m}^3/\text{h}$ and column diameter of 0.2 m, representing mid-range operating conditions. These parameter ranges align with typical industrial caustic scrubbing systems [43].

Figure 13 shows the influence of temperature on pollutant removal. For both packing types, H_2S removal efficiency decreased with increasing temperature, from 97.8% to

91.2% (structured) and 94.5% to 87.6% (random) over the range of 288–318 K. This reduction is attributed to the exothermic nature of H_2S absorption ($\Delta H \approx -70$ kJ/mol for $\text{H}_2\text{S} + 2\text{OH}^- \rightarrow \text{S}^{2-} + 2\text{H}_2\text{O}$), which shifts the reaction equilibrium unfavorably at elevated temperatures [46]. CO_2 removal exhibited weaker temperature sensitivity, declining by only 2–3% over the same range, consistent with its slower kinetics and lower reaction enthalpy ($\Delta H \approx -109$ kJ/mol) [47].

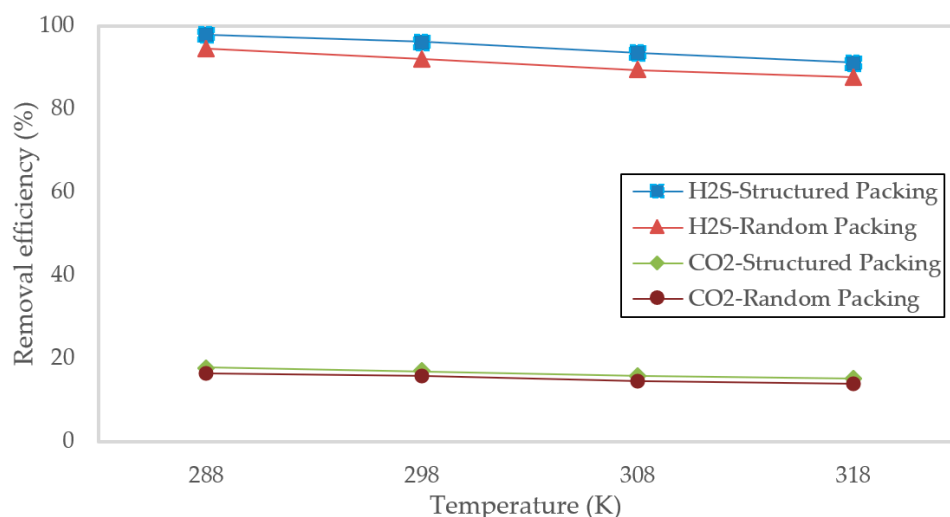


Figure 13. Effect of temperature (288–318 K) on H_2S and CO_2 removal (%) in 10 cm columns (structured/random packing) at $15 \text{ m}^3/\text{h}$ and 1.0 wt% NaOH. H_2S drops 97.8 to 91.2% (structured) and 94.5 to 87.6% (random) due to exothermic reaction ($\Delta H \approx -70$ kJ/mol); CO_2 falls only 2–3%.

Figure 14 illustrates the effect of NaOH concentration. H_2S removal efficiency increased sharply from ~78% at 0.1 wt% to over 98% at 1.0 wt%, then plateaued, indicating stoichiometric saturation. Structured packing consistently achieved 3–5% higher efficiency than random packing at low NaOH levels (<0.5 wt%), owing to superior liquid distribution and reduced channeling [41]. CO_2 removal followed a similar trend but reached only 8–18%, reflecting competitive absorption and lower reactivity with OH^- under strong alkaline conditions.

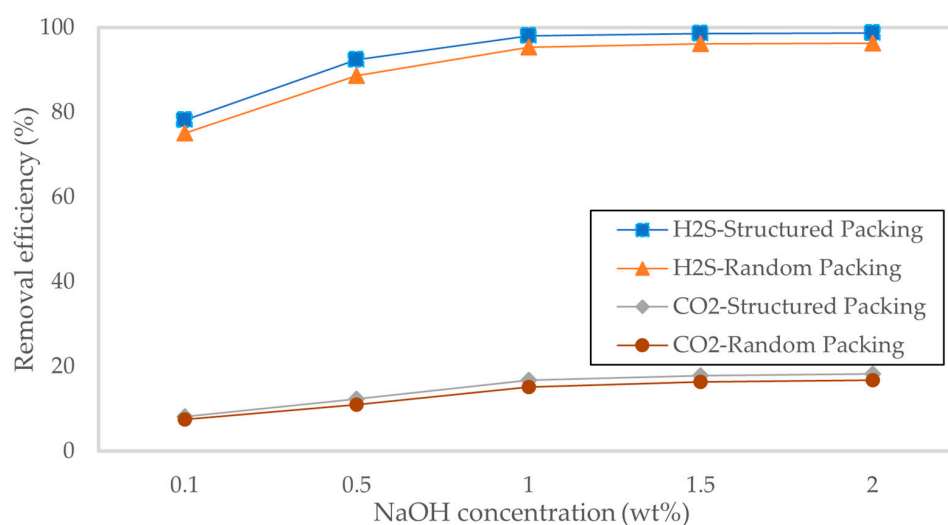


Figure 14. Effect of NaOH concentration (0.1–2.0 wt%) on H_2S and CO_2 removal (%) in 10 cm columns (structured/random packing) at $15 \text{ m}^3/\text{h}$ and 298 K. H_2S rises ~78% to >98%, then plateaus; structured packing gains 3–5% at <0.5 wt% via better distribution. CO_2 reaches 8–18%, limited by competition.

These results underscore temperature control below 298 K as critical for maximizing H₂S removal, while NaOH concentrations above 1.0 wt% yield diminishing returns, enabling cost-effective absorbent dosing. The robustness of structured packing at suboptimal caustic strength further supports its use in large-scale systems. This analysis enhances the practical applicability of the model for process optimization and scale-up.

4. Conclusions

This study investigated the mass transfer behavior and removal efficiency of hydrogen sulfide (H₂S) and carbon dioxide (CO₂) in a packed column using both structured and random packing materials. The results demonstrated that packing geometry, gas flow rate, and column diameter significantly influenced the system performance. As the gas flow rate increased, a noticeable decline in H₂S removal efficiency was observed, particularly in columns with larger diameters. This inverse relationship highlights the critical role of residence time and interfacial contact area in the absorption process.

The evaluation of overall mass transfer coefficients revealed superior performance for the BRF-93 absorbent compared to BRF-85 across all flow conditions. This was attributed to enhanced gas–liquid interactions and improved solubility characteristics. Moreover, random packing materials exhibited higher specific surface area and packing factor, which translated into improved mass transfer characteristics. These findings underscore the importance of selecting appropriate packing configurations and chemical formulations to optimize gas scrubbing processes.

Mass transfer coefficients in the gas phase exhibited a positive correlation with increasing gas flow rate, indicating intensified turbulence and mixing within the column. However, the gain in mass transfer was more pronounced for structured packing at lower flow rates, suggesting that geometric optimization plays a vital role at moderate operational conditions. The dominance of chemical reactions in driving the absorption process was confirmed through equilibrium and kinetic analyses, where bicarbonate and sulfide formation emerged as key mechanisms.

The study also validated a set of thermodynamic and kinetic parameters for key reactions involved in H₂S and CO₂ absorption. These parameters can be reliably used in future modeling studies for similar absorption systems. The strong consistency between experimentally derived and theoretically calculated coefficients confirms the robustness of the modeling approach and highlights its applicability for industrial-scale process design and optimization.

Despite the valuable insights obtained, this study was conducted under controlled laboratory-scale conditions, which may limit its direct scalability to full-scale industrial systems. The observed decrease in H₂S removal efficiency with increasing column diameter (from ~99% at 10 cm to 86–92% at 40 cm) reflects industrial-scale challenges such as flow maldistribution and reduced superficial velocity. Structured packing demonstrated superior hydrodynamic stability and up to 50% lower pressure drop compared to random packing at equivalent gas velocities, making it particularly suitable for large-diameter columns (>0.5 m), where random packing is prone to channeling and bypassing. These characteristics directly translate to reduced blower/compressor energy requirements; for a typical biogas upgrading facility processing 500 m³/h, structured packing can yield annual energy savings of 50–100 MWh, depending on system pressure and packing height.

The co-absorption of CO₂ in NaOH-based systems consumes alkali stoichiometrically ($2 \text{ NaOH} + \text{CO}_2 \rightarrow \text{Na}_2\text{CO}_3 + \text{H}_2\text{O}$), reducing effective capacity for H₂S removal and increasing chemical makeup costs. In high-CO₂ feeds (e.g., biogas with 30–40% CO₂), up to 60–70% of NaOH may be consumed by CO₂, necessitating frequent regeneration or replacement. Thermal regeneration via causticization with lime is energy-intensive

(~3–5 MJ/kg NaOH recovered), underscoring the need for selective absorbents or hybrid physical–chemical systems to improve solvent regeneration efficiency and long-term sustainability. Furthermore, while NaOH scrubbing achieves near-complete H₂S removal (>98% under optimal conditions), the generation of Na₂S and Na₂CO₃ waste streams poses disposal challenges. Structured packing’s operational stability supports integration with downstream sulfide oxidation units (e.g., Claus process or biological treatment), enabling sulfur recovery and minimizing environmental impact. Future work should focus on pilot-scale validation, dynamic modeling of regeneration cycles, and the development of regenerable amine-based or eco-friendly hybrid solvents to enhance selectivity, cost-effectiveness, and environmental performance.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The original contributions presented in this study are included in the article.

Acknowledgments: The author would like to thank TÜBİTAK Marmara Research Center for their technical support provided within the scope of this study.

Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

H ₂ S	Hydrogen Sulfide
CO ₂	Carbon Dioxide
SO ₂	sulfur Dioxide
NH ₃	Ammonia
TiO ₂	Titanium Dioxide
NaOH	Sodium Hydroxide
Na ₂ CO ₃	Sodium Carbonate
NaHCO ₃	Sodium Bicarbonate
CS	Condensation Scrubbers
FPM	Fine Particulate Matter
CPM	Condensable Particulate Matter
MSS	Marine Scrubber Systems
IGCC	Integrated Gasification Combined Cycle
MDEA	Methyldiethanolamine
PM	Particulate Matter
AS	Ammonia Scrubber
GBF	Granular Bed Filter
COG	Coke Oven Gas
HRT	Hydraulic Retention Time
RPB	Rotating Packed Beds
HDH	Humidification–Dehumidification
WSS	Wet Scrubber Systems
MFC	Mass Flow Controller
GC	Gas Chromatograph
BRF	Bravo-Rocha-Fair
K _g	Overall Gas-Phase Mass Transfer Coefficient
k _g	Gas-Phase Film Coefficient

References

- Chen, L.; Huang, J.; Yang, C.L. Absorption of H₂S in NaOCl caustic aqueous solution. *Environ. Prog.* **2001**, *20*, 175–181. [\[CrossRef\]](#)
- Moussavi, G.; Naddafi, K.; Mesdaghinia, A.; Mohseni, M. Effectiveness of hydrogen peroxide in H₂S removal by a packed high specific surface area bed scrubber. *Chem. Biochem. Engineer. Quart.* **2008**, *22*, 9–14.
- Byeon, S.H.; Lee, B.K.J.; Mohan, B.R. Removal of ammonia and particulate matter using a modified turbulent wet scrubbing system. *Sep. Purif. Technol.* **2012**, *98*, 221–229. [\[CrossRef\]](#)
- Chungsiriporn, J.; Bunyakan, C.; Thepchai, R. Ammonia removal from emission air in packed column. In Proceedings of the Fourth PSU Engineering Conference, Songkhla, Thailand, 8–9 December 2005.
- Panza, D.; Belgiorno, V. Hydrogen sulphide removal from landfill gas. *Process Saf. Environ. Prot.* **2010**, *88*, 420–424. [\[CrossRef\]](#)
- Moosavi, G.R.; Naddafi, K.; Mesdaghinia, A.; Vaezi, F.; Mahmoudi, M. H₂S removal in an oxidative packed bed scrubber using different chemical oxidants. *J. Appl. Sci.* **2005**, *5*, 651–654. [\[CrossRef\]](#)
- Turpin, A.; Couvert, A.; Laplanche, A.; Paillier, A. Experimental study of mass transfer and H₂S removal efficiency in a spray tower. *Chem. Eng. Process.* **2008**, *47*, 886–892. [\[CrossRef\]](#)
- Chen, T.; Deng, L.; Li, Y.; Li, J.; Zhao, X.; Fu, L. Removal of multiple pollutants in air pollution control devices of a coal-fired boiler installed with a flue gas condensation scrubber. *J. Clean. Prod.* **2024**, *434*, 139971. [\[CrossRef\]](#)
- Makkonen, T.; Inkinen, T. Sectoral and technological systems of environmental innovation: The case of marine scrubber systems. *J. Clean. Prod.* **2018**, *200*, 110–121. [\[CrossRef\]](#)
- Couvert, A.; Sanchez, C.; Laplanche, A.; Renner, C. Scrubbing intensification for sulphur and ammonia compounds removal. *Chemosphere* **2008**, *70*, 1510–1517. [\[CrossRef\]](#) [\[PubMed\]](#)
- Ohtsuka, Y.; Tsubouchi, N.; Kikuchi, T.; Hashimoto, H. Recent progress in Japan on hot gas cleanup of hydrogen chloride, hydrogen sulfide and ammonia in coal-derived fuel gas. *Powder Technol.* **2009**, *90*, 340–347. [\[CrossRef\]](#)
- Wang, D.; Teo, W.K.; Li, K. Selective removal of trace H₂S from gas streams containing CO₂ using hollow fibre membrane modules/contractors. *Sep. Purif. Technol.* **2004**, *35*, 125–131. [\[CrossRef\]](#)
- Wallin, M.; Olausson, S. Simultaneous absorption of H₂S and CO₂ into a solution of sodium carbonate. *Chem. Eng. Commun.* **1993**, *123*, 43–59. [\[CrossRef\]](#)
- Bhave, A.G.; Vyas, D.K.; Patel, J.B. A wet packet bed scrubber-based producer gas cooling-cleaning system. *Renew. Energy.* **2008**, *33*, 1716–1720. [\[CrossRef\]](#)
- Mamrosh, D.; Beitler, C.; Fisher, K.; Stem, S. Consider improved scrubbing designs for acid gases. *Hydrocarb. Process.* **2008**, *87*, 69–74.
- Couvert, A.; Sanchez, C.; Laplanche, A.; Renner, C.; Levasseur, J.P. Design of a new compact scrubber for deodorization. *Chem. Eng. Process.* **2008**, *47*, 1793–1798. [\[CrossRef\]](#)
- Couvert, A.; Charron, I.; Laplanche, A.; Renner, C.; Patria, L.; Requieme, B. Treatment of odorous sulphur compounds by chemical scrubbing with hydrogen peroxide—Application to a laboratory plant. *Chem. Eng. Sci.* **2006**, *61*, 7240–7248. [\[CrossRef\]](#)
- Sun, W.; Shao, Y.; Zhao, L.; Wang, Q. Co-removal of CO₂ and particulate matter from industrial flue gas by connecting an ammonia scrubber and a granular bed filter. *J. Clean. Prod.* **2020**, *257*, 20511. [\[CrossRef\]](#)
- Pan, H.J.; Fang, M.C.; Ward, J.D.; Lee, H.Y.; Lin, H.Y.; Hsieh, C.T.; Lee, C.L.; Huang, T.H.; Hsieh, Y.C.; Lin, S.C.; et al. Modeling of an integrated H₂S/NH₃ scrubber and regeneration columns for coke oven gas purification. *J. Clean. Prod.* **2023**, *389*, 136065. [\[CrossRef\]](#)
- Miltner, M.; Makaruk, A.; Krischan, J.; Harasek, M. Chemical-oxidative scrubbing for the removal of hydrogen sulphide from raw biogas: Potential and economics. *Water Sci. Technol.* **2012**, *66*, 1354–1360. [\[CrossRef\]](#)
- Bontozoglou, V.; Karabelas, A.J. Numerical calculation of simultaneous absorption of H₂S and CO₂ in aqueous hydroxide solutions. *Ind. Eng. Chem. Res.* **1991**, *30*, 2598–2603. [\[CrossRef\]](#)
- Lin, C.W.; Chang, D.P. Formation and emission of chlorinated by-products from a bench-scale packed-bed odor scrubber. *Water Air Soil Poll.* **2005**, *162*, 19–35. [\[CrossRef\]](#)
- Brettschneider, O.; Thiele, R.; Faber, R.; Thielert, H.; Wozny, G. Experimental investigation and simulation of the chemical absorption in a packed column for the system NH₃-CO₂-H₂S-NaOH-H₂O. *Sep. Purif. Technol.* **2004**, *39*, 139–159. [\[CrossRef\]](#)
- Mahmoudkhani, M.; Heidel, K.R.; Ferreira, J.C.; Keith, D.W.; Cherry, R.S. Low energy packed tower and caustic recovery for direct capture of CO₂ from air. *Energy Procedia* **2009**, *1*, 1535–1542. [\[CrossRef\]](#)
- Biard, P.F.; Couvert, A.; Renner, C.; Levasseur, J.P. Wet scrubbing intensification applied to hydrogen sulphide removal in waste water treatment plant. *Can. J. Chem. Eng.* **2010**, *88*, 682–687. [\[CrossRef\]](#)
- Noorain, R.; Kindaichi, T.; Ozaki, N.; Aoi, Y.; Ohashi, A. Biogas purification performance of new water scrubber packed with sponge carriers. *J. Clean. Prod.* **2019**, *214*, 103–111. [\[CrossRef\]](#)
- Mackowiak, J. Progress in design of random packing for gas–liquid systems. *Chem. Eng. Res. Des.* **2015**, *99*, 28–42. [\[CrossRef\]](#)
- Chew, Y.E.; Putra, Z.A.; Foo, D.C.Y. Process simulation and optimization for acid gas removal system in natural gas processing. *J. Nat. Gas Eng.* **2022**, *107*, 104764. [\[CrossRef\]](#)

29. Zhang, Y.; Yasutake, D.; Hidaka, K.; Kitano, M.; Okayasu, T. CFD analysis for evaluating and optimizing spatial distribution of CO₂ concentration in a strawberry greenhouse under different CO₂ enrichment methods. *Comput. Electron. Agr.* **2020**, *179*, 105811. [\[CrossRef\]](#)
30. Deyhim, S.; Ghorbani-Shahna, F.; Jaleh, B.; Tapak, L. Development of scrubber with nano-TiO₂ coated packing for H₂S removal. *Process Saf. Environ. Prot.* **2021**, *149*, 158–168. [\[CrossRef\]](#)
31. Kim, N.J.; Hirai, M.; Shoda, M. Comparison of organic and inorganic packing materials in the removal of ammonia gas in biofilters. *J. Hazard. Mater.* **2000**, *72*, 77–90. [\[CrossRef\]](#)
32. Wang, P.; Yan, F.; Cai, J.; Xie, F.; Shen, X.; Wei, X.; Yang, G.; Zhong, R.; Huang, J.; Li, Z.; et al. Emission levels and phase distributions of PCDD/Fs in a full-scale municipal solid waste incinerator: The impact of wet scrubber system. *J. Clean. Prod.* **2022**, *337*, 130468. [\[CrossRef\]](#)
33. Padmanabhan, S.B.; Mabrouk, M.T.; Lacarriere, B. A hybrid model for packed bed thermal energy storage system. *J. Energy. Storage.* **2024**, *98*, 113068. [\[CrossRef\]](#)
34. Zahir, A.; Kumar, P.; Saptorio, A.; Shah, M.; Tiong, A.N.Z.; Hameed, S. Parametric study of experimental and CFD simulation based hydrodynamics and mass transfer of rotating packed bed: A review. *Arch. Comput. Methods Eng.* **2023**, *30*, 4001–4031. [\[CrossRef\]](#)
35. Cherif, H.; Coquelet, C.; Stringari, P.; Clodic, D.; Pellegrini, L.; Moioli, S.; Lange, S. Experimental and simulation results for the removal of H₂S from biogas by means of sodium hydroxide in structured packed columns. In Proceedings of the 18th International Conference on Biogas Science and Technology, Paris, France, 21–22 January 2016.
36. Billet, R.; Schultes, M. Prediction of mass transfer columns with dumped and arranged packings. *Trans. IChemE.* **1999**, *77*, 498–504. [\[CrossRef\]](#)
37. Mackowiak, J. *Fluid Dynamics of Packed Columns*; Springer: Berlin, Heidelberg, 2010.
38. Strigle, R.F. *Packed Tower Design and Applications*; Gulf Publishing Company: Houston, TX, USA, 1994.
39. Onda, K.; Takeuchi, H.; Okumoto, Y. Mass transfer coefficients between gas and liquid phases in packed columns. *J. Chem. Eng. Jpn.* **1968**, *1*, 56–62. [\[CrossRef\]](#)
40. Bravo, J.; Rocha, J.A.; Fair, J. Mass transfer in gauze packings. *Hydrocarb. Process.* **1985**, *64*, 91–95.
41. Yang, W.; Yu, X.; Mi, J.; Wang, W.; Chen, J. Mass transfer performance of structured packings in a CO₂ absorption tower. *Chin. J. Chem. Eng.* **2015**, *23*, 42–49. [\[CrossRef\]](#)
42. Flagiello, D.; Parisi, A.; Lancia, A.; Natale, F.D. A review on gas-liquid mass transfer coefficient in packed bed columns. *ChemEngineering* **2021**, *5*, 43. [\[CrossRef\]](#)
43. Aroonwilas, A.; Veawab, A. Characterization and comparison of the CO₂ absorption performance into single and blended alkanolamines in a packed column. *Ind. Eng. Chem. Res.* **2004**, *43*, 2228–2237. [\[CrossRef\]](#)
44. Krauss, M.; Rzehak, R. Reactive absorption of CO₂ in NaOH: Detailed study of enhancement factor models. *J. Chem. Eng. Sci.* **2017**, *166*, 193–209.
45. Blauwhoff, P.M.M.; Versteeg, G.F.; Van Swaaij, W.P.M. A study on the reaction between CO₂ and alkanolamines in aqueous solutions. *Chem. Eng. Sci.* **1983**, *38*, 1411–1429. [\[CrossRef\]](#)
46. Mandal, B.; Bandyopadhyay, S.S. Simultaneous Absorption of CO₂ and H₂S into aqueous blends of N-Methyldiethanolamine and Diethanolamine. *Environ. Sci. Technol.* **2006**, *40*, 6076–6084. [\[CrossRef\]](#) [\[PubMed\]](#)
47. Puxty, G.; Rowland, R.; Allport, A.; Yang, Q.; Bown, M.; Burns, R.; Maeder, M.; Attalla, M. Carbon dioxide postcombustion capture: A novel screening study of the carbon dioxide absorption performance of 76 amines. *Environ. Sci. Technol.* **2009**, *40*, 6427–6433. [\[CrossRef\]](#) [\[PubMed\]](#)
48. Qian, Z.; Xu, L.B.; Li, Z.H.; Li, H.; Guo, K. Selective absorption of H₂S from a gas mixture with CO₂ by aqueous N-Methyldiethanolamine in a rotating packed bed. *Ind. Eng. Chem. Res.* **2010**, *49*, 6196–6203. [\[CrossRef\]](#)
49. Hashemi, A.; Memardoost, S.; Dehkordi, A.M. Comprehensive modeling and CFD simulation of absorption of CO₂ and H₂S by MEA solution in hollow fiber membrane. *AIChE J.* **2014**, *60*, 657–672. [\[CrossRef\]](#)

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.