Received: 1 August 2022 | Revised: 8 October 2022 | Accepted: 25 October 2022

DOI: 10.1002/cae.22583

RESEARCH ARTICLE

WILEY

Virtual mimic of lab experiment using the computer-based Aspen Plus® Sensitivity Analysis Tool to boost the attainment of experiment's learning outcomes and mitigate potential pandemic confinements

Ahmed M. Elkhatat | **Shaheen A. Al-Muhtaseb**

Department of Chemical Engineering, Qatar University, Doha, Qatar

Correspondence
Ahmed M. Elkhatat, Department of Chemical Engineering, Qatar University, P.O. Box 2713, Doha, Qatar.
Email: ahmed.elkhatat@qu.edu.qa

Abstract

The computer-based Aspen Plus® Sensitivity Analysis Tool (APSAT) was used as a virtual environment to mimic a gas absorption lab experiment in the Unit Operations Lab within the curriculum for the Bachelor of Science in Chemical Engineering at Qatar University. A pool of 35 students enrolled in three lab sections was utilized. The approach was applied in three stages to foster the attainment of the learning outcomes of the experiment by testing and evaluating some parameters that cannot be examined using the physical lab equipment. Results show that the approach helped the students gain a profound understanding and address conceptual mistakes while discussing the results of the APSAT outputs. Students who were engaged in the APSAT activity demonstrated a strong interest in this approach. This approach can be implemented to facilitate the teaching of lab courses. Furthermore, it is a practical choice to optimize the resources and a good substitute for lab experiments in case of any pandemic, confinement or interest in testing the effects of hazardous conditions to ensure sustaining the learning outcomes from corresponding experiments.

KEYWORDS

Aspen Plus® Sensitivity Analysis, computer-aided learning, engineering laboratory course, virtual lab experiment

1 | INTRODUCTION

The rising needs for environmental and industrial solutions, along with the latest trends in technologies, push chemical engineering education programs to update their curricula and education paradigms to provide students with the required skills and knowledge to master designing, operating, maintaining, and developing chemical processes in various environmental and industrial fields [2, 22, 44].

According to Bloom's taxonomy, Lab education promotes high-level learning outcomes through

Abbreviations: ABET, Accreditation Board for Engineering and Technology; APSAT, Aspen Plus Sensitivity Analysis Tool; CLO, course learning outcomes; EAC, Engineering Accreditation Commission; SO, student outcome.

applying, analyzing, synthesizing, and evaluating the experimental results [4, 15, 19]. Accordingly, it enhances mastery of science by developing practical and reasoning skills that enhance a grasp of practical work's complexness and ambiguity [33]. Moreover, laboratory courses also equip students with a sense of physical systems and assist them in developing an understanding of engineering operations [16, 18, 26, 30, 32]. In this sense, the Engineering Accreditation Commission (EAC) of the Accreditation Board for Engineering and Technology (ABET) defined a specific Student Outcome (SO6) that involves "an ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions [1]," which ensures achieving all Bloom's taxonomy levels.

Although laboratory courses are beneficial to students through well-designed experiment schemes, physical lab equipment is commonly designed with limited options, leading to some challenges for development and synthesis activities. Therefore, computer-based simulations can provide students with a promised land for designing and testing experiments. Computer-based simulations offer many benefits, including, but not limited to, saving lab space and operation costs. Besides, they can be considered a safer substitute for those operations that might include hazards and a more versatile substitute for lab experiments with limited specifications [24, 25]. Computer-based simulations can hone the students' creative and critical thinking by investigating and testing a virtual environment that enhances an understanding of empirical work's potential complexity and ambiguity [17, 23]. The need for computer-based simulations has been spotlighted in the COVID-19 pandemic to promote learning opportunities by ensuring inclusive and equitable quality education [16, 27].

One of the trusted market-leading chemical process simulators is *Aspen Plus®* [6], an extensive simulator with capabilities for rigorous modeling of various chemical processes flexibly and powerfully. One of the powerful built-in capabilities of Aspen plus is the Sensitivity Analysis tool. This advanced built-in tool iterates its calculation sequence through a range of values provided for an independent variable to inspect its effect on the corresponding result for a dependent variable. Hence, it can be used as a virtual environment to mimic a Lab experiment to foster its learning outcomes by testing and evaluating some parameters that cannot be examined using the lab equipment.

This work presents the use of the *Aspen Plus* Sensitivity Analysis Tool (APSAT) as a virtual mimic of the Gas Absorption Experiment. The examined pool of students involved 35 enrolled in three Unit Operations Laboratory course sections. The Unit Operations Laboratory course is a part of the undergraduate curriculum in the Chemical Engineering program at Qatar University. This lab course includes hands-on and computerized experiments in mass transfer phenomena and separation processes. This paper aims to investigate how this approach can help improve the attainment of course learning outcomes (CLOs). The APSAT was introduced and demonstrated to the students through a dedicated tutorial session. The attainment of CLOs was evaluated for each student via a multiple-choice questions test at the beginning of the session, and the same test was repeated after the session. The students' opinions were surveyed at the end of the second quiz.

2 | THEORY

Carbon dioxide (CO_2) is a primary greenhouse gas contributing to global warming. About 50% of the CO_2 emissions are from stationary sources such as power plants. Therefore, carbon capture and storage (CCS) research aims to develop technologies, methods, and units to increase the efficiency of CO_2 capture [12].

CO_2 is a typical acid gas that reacts with aqueous NaOH to form sodium carbonate and sodium bicarbonate. The wet scrubbing of CO_2 from atmospheric air using alkaline solutions such as Sodium hydroxide (NaOH) has been examined for a half-century [41], where CO_2 is absorbed into a lean aqueous NaOH solution, leaving behind a rich aqueous solution of NaOH and sodium carbonate (Na_2CO_3). Two reactions are possible, as outlined below:

$$\begin{aligned} CO_2(g) + 2NaOH(aq) &\rightarrow Na_2CO_3(aq) \\ &+ H_2O(\Delta H^o = -169.8\,\text{kJ/mol}, \\ &\Delta S^o = -0.137\,\text{kJ/mol K}, \\ &\Delta G^o = -128.97\,\text{kJ/mol}), \end{aligned} \tag{1}$$

$$\begin{aligned} CO_2(g) + Na_2CO_3(aq) + H_2O &\rightarrow 2NaHCO_3 \\ &(aq)(\Delta H^o = -129.1\,\text{kJ/mol}, \\ &\Delta S^o = -0.1334\,\text{kJ/mol}, \\ &\Delta G^o = -29.65\,\text{kJ/mol}). \end{aligned} \tag{2}$$

Although these two reactions are exothermic and spontaneous, reaction (2) has a much smaller Gibbs free energy than that of reaction (1), and thus reaction (2) can be ignored compared relative to reaction (1).

CO_2 also dissolves in water to form carbonic acid (H_2CO_3), dissociating into bicarbonate ions (HCO_3^-) and donating a proton (H^+) to a water molecule to form hydronium ions (H_3O^+). Bicarbonate ions can further

FIGURE 1 Sample pre-lab test

In a packed absorption column to capture **carbon dioxide** from the **air** by **NaOH**.

The Gas stream was introduced into the packed column counter-currently with a Liquid stream.

The experiment is designed to study the effect of

(1) Packing height, (2) Column Diameter, (3) Inlet gas pressure, and (4) Inlet liquid temperature) on the absorbed CO_2 from the gas stream.

Check your expectation for the results:

Q1: When the packing height increases, does the absorbed CO_2 from the inlet gas stream increase?

a) True b) False c) I am not sure

Q2: When the column diameter increases, does the absorbed CO_2 from the inlet gas stream increase?

a) True b) False c) I am not sure

Q3: When the inlet gas pressure increases, does the absorbed CO_2 from the inlet gas stream increase?

a) True b) False c) I am not sure

Q4: When the inlet liquid temperature increases, does the absorbed CO_2 from the inlet gas stream increase?

a) True b) False c) I am not sure

donate a proton to a water molecule and thus form carbonate ions (CO_3^{2-}). In addition, sodium hydroxide, sodium carbonate, and sodium bicarbonate undergo dissociation reactions to form sodium (Na^+), hydroxyl (OH^-), carbonate (CO_3^{2-}), and bicarbonate (HCO_3^-) ions as follows:

$$CO_2(g) + 2H_2O \xleftrightarrow{\text{equilibrium}} HCO_3^-(aq) + H_3O^+(aq), \tag{3}$$

$$HCO_3^-(aq) + H_2O \xleftrightarrow{\text{equilibrium}} CO_3^{2-}(aq) + H_3O^+(aq), \tag{4}$$

$$2H_2O \xleftrightarrow{\text{equilibrium}} OH^-(aq) + H_3O^+(aq), \tag{5}$$

$$NaOH(aq) \xleftrightarrow{\text{dissociation}} OH^-(aq) + Na^+(aq), \tag{6}$$

$$Na_2CO_3(aq) \xleftrightarrow{\text{dissociation}} CO_3^{2-}(aq) + 2Na^+(aq), \tag{7}$$

$$NaHCO_3(aq) \xleftrightarrow{\text{dissociation}} HCO_3^-(aq) + Na^+(aq). \tag{8}$$

Packed columns using NaOH are the most frequently suggested designs for a 50% capture rate of CO_2 from the air with concentrations up to 500 ppm [5, 7, 45]. Moreover, NaOH-packed columns have been used to capture higher amounts of up to 75,000 tonnes/year of CO_2 from a flue gas

TABLE 1 Components used in the simulation

Components	Formula	Aspen Plus ID	Type
Water	H_2O	H2O	Conventional
Carbon dioxide	CO_2	CO2	Conventional
Sodium carbonate	Na_2CO_3	NA2CO3	Conventional
Hydronium ion	H_3O^+	H3O+	Conventional
Hydroxyl ion	OH^-	OH-	Conventional
Bicarbonate ion	HCO_3^-	HCO3-	Conventional
Carbonate ion	CO_3^{2-}	CO3-2	Conventional
Sodium-ion	Na^+	NA+	Conventional
Sodium hydroxide	NaOH	NAOH	Conventional
Sodium bicarbonate	$NaHCO_3$	NAHCO3	Conventional
Nitrogen gas	N_2	N2	Conventional
Oxygen gas	O_2	O2	Conventional

TABLE 2 Property method options

Description	Method name
Base method	ELECNRTL
Henry components	GLOBAL
Electrolyte calculation method	CAUSTIC

TABLE 3 CAUSTIC chemistry model

	Reactants		Products			
Reaction	**Component**	**Coefficient**	**Component**	**Coefficient**	**Type**	**Equilibrium constants**[a]
(3)	CO_2	−1	HCO_3^-	1	Equilibrium	A: 231.465
	H_2O	−2	H_3O^+	1		B: −12092.1
						C: −36.7816
(4)	HCO_3^-	−1	H_3O^+	1	Equilibrium	A: 216.05
						B: −12431.7
	H_2O	−1	CO_3^{2-}	1		C: −35.4819
(5)	H_2O	−2	OH^-	1	Equilibrium	A: 132.899
			H_3O^+	1		B: −13445.9
						C: −22.4773
(6)	NAOH	N/A	NA+	1	Dissociation	N/A
			OH^-	1		
(7)	NA_2CO_3	N/A	NA+	1	Dissociation	N/A
			CO_3^{2-}	1		
(8)	$NAHCO_3$	N/A	NA+	1	Dissociation	N/A
			HCO_3^-	1		

[a] $\ln(K_{eq}) = A + \frac{B}{T} + C \times \ln(T) + D \times T\,[T \text{ in Kelvin}]$.

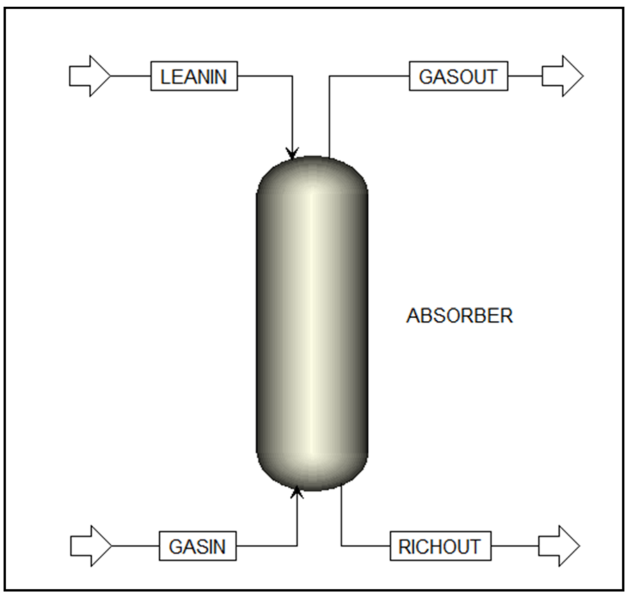


FIGURE 2 Absorber block and streams modeling flowsheet

stream in large-scale CO_2 capture processes [29, 34, 38]. Designing packed columns depends on the information available from experiments, empirical formulas, models, and codification in Unit Operation design [20]. For basic academic/educational purposes, the design criteria for a lab-scale packed column can be obtained from classical handbooks on Unit Operations that provide enough data to support the initial design of absorbers. Nevertheless, the accuracy of this approach is often limited by the stream properties and column internals (e.g., packing hydrodynamics and multiphase flow) [14, 31, 39].

For industrial, research, and advanced academic purposes, chemical process simulators (e.g., Aspen Plus®, Aspen Hysys®, Aveva Pro II®, ChemCAD®) provide many correlations and rigorous models of many chemical processes and operations. Examples of rigorous models applied for random and structured packing in packed column design are Onda et al. (random backing: Rasching rings, Berl Saddles, and Spheres) [36], Billet and Schultes (random backing: Pall rings, Hiflow rings, Ralu Pak, Impulse packing, Montzpak, and Euroform.) [8], Hanley and Chen (random backing: Pall rings) [28], Bravo et al. (structured packing: gauze Sulzer BX) [10, 9], Brunazzi and Paglianti (Mellapak 250.Y and BX) [11], Oluji'c et al. (corrugated structured packings) [35]. The equations and formulas of these models are presented elsewhere [20]. It's noteworthy that Flagiello and his colleagues [21] developed an Excel tool for calculating liquid-gas mass transfer coefficients in packed towers for educational purposes.

Many factors affect the mass transfer process for the scrubbing process of CO_2 from the air by alkaline solutions, including packing height and type, column diameter, feed stream concentration, streams' properties such as temperature, pressure, viscosity, surface tension, and others. However, to improve the quality of acquired

TABLE 4 Design and specifications of the streams and absorber block

Stream/unit	Specifications and parameters
GASIN	• Temperature:20°C • Pressure: 103.15 kPa • Total flowrate: 0.138 mol/s • Composition (mole fraction): N_2: 0.65, O_2: 0.165, CO_2: 0.155, H_2O: 0.03
LEANIN	• Temperature: 20°C • Pressure: 103.15 kPa • Total flowrate: 0.106 m^3/s • Composition (mole concentration): NaOH: 1.9 kmol m^{-3}, Solvent: H_2O
Absorber (RadFrac type)	Configuration: • Calculation type: Rate based • Number of stages: 18 • Condenser: None • Reboiler: None • Valid phases: Vapor-liquid Streams: LEANIN: stage 1 (on stage), GASIN: stage 18 (on stage), GASOUT: stage 1 (vapor phase), RICHOUT: stage 18 (liquid phase) Pressure: Stage 1 pressure: 101.15 kPa
Column internals	Mode: Rating, Stages: 1–18, Internal type: Packed, Packing type: Berl, Vendor: Generitic, Material: Ceramic, Dimension: 13 mm, Packed height: 5 m, Column Diameter: 0.1 m
Rate-based modeling	Global setup: • Reaction condition factor: 0.9, Film discretization ratio: 5 Sections: • Flow model: Mixed. • Interfacial area factor: 2 • Liquid phase: Film resistance: Discrxn film, discretization points: 5 • Vapor phase: Film resistance: Consider film. • Correlation methods: Mass transfer coefficient method: Onda et al. [36], Heat transfer coefficient method: Chilton and Colburn, Interfacial area method: Onda et al. [36]. Holdups: • Correlation: Stichlmair et al. [42]
Reactions	The reaction model was created in the simulation environment with ID CAUSTIC-R, and includes two types of reaction **1)** Equilibrium reactions Include reactions (3) and (4). **2)** Kinetic reactions $CO_2 + OH^- \xrightarrow{K=4.3e+13,\ E=13{,}249\,cal/mol} HCO_3^-$ (9) $HCO_3^- \xrightarrow{K=2.8e+17,\ E=29{,}451\,cal/mol} CO_2 + OH^-$ (10)

TABLE 5 Streams summary of components mole flow, and mole fraction

	GASIN		GASOUT		LEANIN		RICHOUT	
	Mole flows (kmol/s)	Mole fraction	Mole flows (kmol/s)	Mole fraction	Mole flows (kmol/s)	Mole fraction	Mole flows (kmol/s)	Mole fraction
Total	0.000138	1	0.000117	1	0.001752	1	0.001753	1
H_2O	4.14E−06	3.00E−02	2.61E−06	2.24E−02	0.00164	9.36E−01	0.001661	9.47E−01
CO_2	2.14E−05	1.55E−01	1.54E−06	1.32E−02	0	0	1.59E−12	9.04E−10
H_3O^+	0	0	0	0	0	0	0	0
OH^-	0	0	0	0	5.59E−05	2.31E−16	1.62E−05	3.58E−15
HCO_3^-	0	0	0	0	0	0	5.41E−09	9.27E−03
CO_3^{2-}	0	0	0	0	0	0	1.98E−05	3.09E−06
NA+	0	0	0	0	0	0	5.59E−05	1.13E−02
NAOH	0	0	0	0	0	0	0	0
NA_2CO_3	0	0	0	0	0	0	0	0
N_2	8.97E−05	6.50E−01	8.97E−05	7.69E−01	0	0	6.85E−09	3.91E−06
O_2	2.28E−05	1.65E−01	2.28E−05	1.95E−01	0	0	3.33E−09	1.90E−06

learning outcomes and avoid distractions, this work focused on the effects of four parameters: (1) packing height, (2) column diameter, (3) liquid stream temperature, and (4) gas stream pressure. The conventional (physical) lab experiment cannot examine these parameters due to equipment limitations (i.e., fixed packing height and column diameter) and safety considerations (in case of high stream pressure and temperature). Hence, the APSAT approach was implemented in this work as a virtual mimic of the gas absorption experiment to investigate the effect of these parameters on CO_2 absorption while avoiding the limitations of the physical experiment.

3 | METHODOLOGY

The APSAT approach was applied in the gas diffusion experiment in the Spring 2022 semester. Three sections of the Unit Operations Laboratory course (a part of the undergraduate curriculum in the Chemical Engineering program at Qatar University), involving 35 students, were considered the platform for this study. The approach was applied through three stages: (1) Pre-lab test, (2) Aspen Plus Analysis Tool (APSAT), and (3) Quiz and questionnaire.

3.1 | Stage-I: Pre-lab test

In stage-I, students were given a pre-lab test of multiple-choice questions on the effect of investigated parameters on CO_2 absorption. Students were informed that this test is not graded, so they can only answer if they know the correct answers or otherwise select the answer option of "I am not sure." Students have not received any feedback on their answers. An example of the pre-lab test is shown in Figure 1.

3.2 | Stage II: Applying the APSAT

This stage involves three steps (1) building the simulation environment, (2) running the simulation environment and checking its outputs, and (3) applying the APSAT. These steps are outlined below.

3.2.1 | Step 1: Building the simulation environment

Gas absorption process simulation was created as a rate-based model of the CO_2 absorption process from the air (a gas mixture of N_2, O_2, and H_2O) by using NaOH. The model consists of a rate-based *RadFrac* absorber, which is the most rigorous column type in *Aspen Plus*. To apply the APSAT, the module was first built based on the unit design and operation data provided by a pilot plant [43]. The reaction kinetics was set based on Pinsent [37]. The physical properties, including thermo-physical and transport models, were validated using data from the literature. The details of these design criteria are presented elsewhere [5]. The components, property method, chemistry model, and

TABLE 6 Specifications and parameters of Aspen Plus® Sensitivity Analysis Tool (APSAT)

APSAT-ID	HEIGHT	DIAMETER	L-T	G-P
Description	**Effect of Packing Height**	**Effect of Column Diameter**	**Effect of Liquid Stream Temperature**	**Effect of Gas Stream Pressure**
Specifications and parameters	Manipulated variable [Vary]	Manipulated variable [Vary]	Manipulated variable [Vary]	Manipulated variable [Vary]
	• Type: Block-Var	• Type: Block-Var	• Type: Stream-Var	• Type: Stream-Var
	• Block: ABSORBER	• Block: ABSORBER	• Stream: LEANIN	• Stream: GASIN
	• Variable: CA-PACK-HT	• Variable: CA-DIAM	• Substream: Mixed	• Substream: Mixed
	• Units: meter	• Units: meter	• Variable: TEMP	• Variable: PRES
	• Start point: 2 m	• Start point: 0.09 m	• Units: C	• Units: kPa
	• Endpoint: 10 m	• Endpoint: 0.5 m	• Start point: 10°C	• Start point: 101.15 kPa
	• Increment: 0.1 m	• Increment: 0.01 m	• Endpoint: 50°C	• Endpoint: 200 kPa
	Measure variable [Define]	Measure variable [Define]	• Increment: 1°C	• Increment: 5 kPa
	• Variable ID: CO2	• Variable ID: CO_2	Measure variable [Define]	Measure variable [Define]
	• Category: Streams	• Category: Streams	• Variable ID: CO_2	• Variable ID: CO_2
	• Ref.-Type: Mole-Frac	• Ref.-Type: Mole-Frac	• Category: Streams	• Category: Streams
	• Ref.-Stream: GASOUT	• Ref.-Stream: GASOUT	• Ref.-Type: Mole-Frac	• Ref.-Type: Mole-Frac
	• Substream: Mixed	• Substream: Mixed	• Ref.-Stream: GASOUT	• Ref.-Stream: GASOUT
	• Component: CO2	• Component: CO_2	• Substream: Mixed	• Substream: Mixed
	Display results [Tabulate]	Display results [Tabulate]	• Component: CO_2	• Component: CO_2
	• Column No.: 1	• Column No.: 1	Display results [Tabulate]	Display results [Tabulate]
	• Tabulated variable expression: CO_2	• Tabulated variable expression: CO_2	• Column No.: 1	• Column No.: 1
			• Tabulated variable expression: CO_2	Tabulated variable expression: CO_2

unit operation blocks and streams utilized in this study are outlined below.

Components used in the simulation

The components' list includes gas stream components (N_2, O_2, H_2O, CO_2), liquid stream components (NaOH, H_2O), and all chemical reaction compounds and ions, as indicated in Table 1.

Property method used in the simulation

The absorption of carbon dioxide into aqueous sodium hydroxide is a system that involves an electrolyte of chemical species that can dissociate partially or totally into ions. Hence, the appropriate property method in Aspen Plus is electrolyte nonrandom two-liquid (ELECNRTL). Henry components' option was set as GLOBAL, where Henry's constants are retrieved from the Aspen Plus database. The property method options utilized in this study are summarized in Table 2.

Chemistry model

The chemistry model was created with the CAUSTIC ID and was embedded in the electrolyte calculation method. In this model, reactions (3)–(5) were identified as equilibrium reactions, while reactions (6)-(8) were identified as dissociation reactions, as detailed in Table 3.

Building unit operation blocks and streams

After running the property model and ensuring no errors or warning messages were reported, the absorber block and

TABLE 7 Five-point Likert scale anonymous survey statements and choices

Statements	
1	Simulation of Gas Absorption Lab experiments using the Aspen Plus Sensitivity Analysis Tool helped me understand the theoretical concepts of mass transfer in a packed column.
2	Simulation of Gas Absorption Lab experiments using the Aspen Plus Sensitivity Analysis Tool helped me learn practical concepts of Aspen Plus simulation.
3	Simulation of Gas Absorption Lab experiments using the Aspen Plus Sensitivity Analysis Tool is helpful to examine parameters that cannot be examined using the lab equipment.
4	I would like to simulate other Lab experiments using the Aspen Plus Sensitivity Analysis Tool in future Lab courses.
Five-point Likert scale choices	
1	Strongly disagree
2	Disagree
3	Neutral (neither agree nor disagree)
4	Agree
5	Strongly agree

streams are modeled in the simulation flowsheet, as shown in Figure 2. The detailed design and specifications of the absorber block and streams are presented in Table 4.

3.2.2 | Step 2: Running the simulation environment and checking its outputs

The summary of various streams shown in Figure 2 is presented in Table 5. This simulation aims to check the mole flow/fraction of CO_2 in both *GASIN* and *GASOUT* streams to evaluate the efficiency of the current simulation in removing CO_2 from atmospheric air. Results indicated that the CO_2 mole fraction has depleted from 0.15 in the GASIN stream to 0.013 in the GASOUT stream, indicating a 91.49% removal of CO_2 from atmospheric air using the alkaline NaOH solution.

3.2.3 | Step 3: Applying the APSAT

The APSAT was performed as a virtual mimic of the Gas Absorption Experiment to study the effects of packing height, column diameter, liquid stream temperature, and gas stream pressure on scrubbing CO_2 from the air using an alkaline NaOH solution. A sensitivity analysis scenario was created for each investigated parameter to iterate the calculation sequence through a range of provided values to investigate each parameter's effect on the mole fraction of carbon dioxide in the exit gas stream.

In this step, students were trained on how to create the APSAT, and each student created, executed, and investigated the APSAT individually. After that, students were allowed to discuss the results with their classmates. They also were allowed to use the online literature to discuss the results with the instructor. The details of each APSAT model are given in Table 6.

3.3 | Stage III: Quiz and questionnaire

In stage III, students were given multiple-choice questions on the effect of investigated parameters on CO_2 absorption, similar to stage I. In addition, they were also requested to submit an individual short report on the resulting plots of the effects of the four investigated parameters with reflections and discussions. The students' opinions were collected at the end of stage III through a five-point Likert scale anonymous survey. The choices ranged from "Strongly Agree" to "Strongly Disagree." The anonymous survey questions and choices are presented in Table 7.

4 | RESULTS AND DISCUSSION

4.1 | Evaluation of the APSAT outputs

The results of each APSAT scenario were plotted to study the effects of packing height, column diameter, liquid stream temperature, and gas stream pressure on removing CO_2 from air using an alkaline NaOH solution.

4.1.1 | Effect of packing height on scrubbing CO_2 from the air using an alkaline NaOH solution

The packing height is the multiplication product of the height of the transfer unit (HTU) and the number of transfer units (NTU), and is determined according to the following equation [31, 40]:

$$z = \underbrace{\frac{G}{A_c K_{oG} a_e}}_{HTU} \underbrace{\int_{y_A}^{y_B} \frac{(1-y)_{LM}}{(1-y)(y-y^*)}}_{NTU}, \tag{9}$$

where G is the molar flux of the gas stream (kmol/s), A_c is the cross-sectional column area (m^2), respectively,

$K_{oG}a_e$ is the gas phase overall volumetric mass transfer coefficient (kmol/m^3/s), y_A and y_B are the mole fractions of CO_2 in the gas streams at the top and bottom of the packed column, respectively. The subscript LM refers to the logarithmic mean.

NTU indicates the difficulty of the mass transfer process, and it depends on the solute concentration; HTU indicates the system's effectiveness in the mass transfer process and depends on the operation conditions and packing properties. Packing with a larger wet surface area (a_e) promotes the mass transfer process.

When the APSAT was used to inspect the effect of packing height on the scrubbing of CO_2 from the air using an alkaline NaOH solution by iterating the calculation sequence through a range of packing height (from 2 to 10 m with an increment of 0.1 m) for of its effect on the mole fraction of carbon dioxide in the exit gas stream. Other parameters were fixed, as listed in Table 4. Results showed that the absorption of CO_2 increases proportionally with packing height. The percentage of CO_2 uptake increased significantly from 65% to 87% when increasing the packing height from 2 to 4 m, respectively. The scrubbing rate increased slowly to 95% at 6.5 m; after that, the effect of packing height can be considered negligible. Figure 3 shows the resulting curves plotted based on APSAT outputs and their derivatives.

4.1.2 | Effect of column diameter on scrubbing CO_2 from the air using an alkaline NaOH solution

The diameter of the packed column diameter is designed to suit the maximum anticipated counter-current gas and liquid flow rates. The diameter is generally sized based on flow and flooding parameters, where flooding parameters can be determined empirically or experimentally [13]. Although practically, column diameter is not taken into consideration for

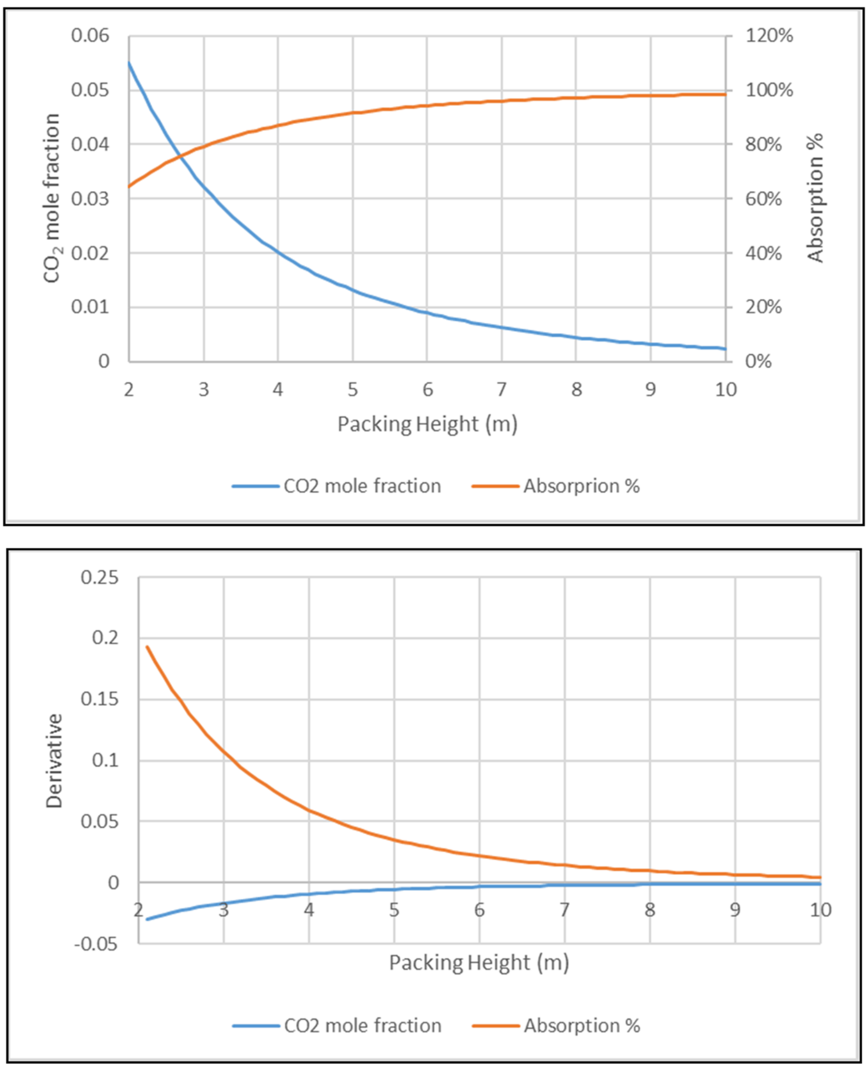


FIGURE 3 Effect of packing height on scrubbing CO_2 from air using an alkaline NaOH solution

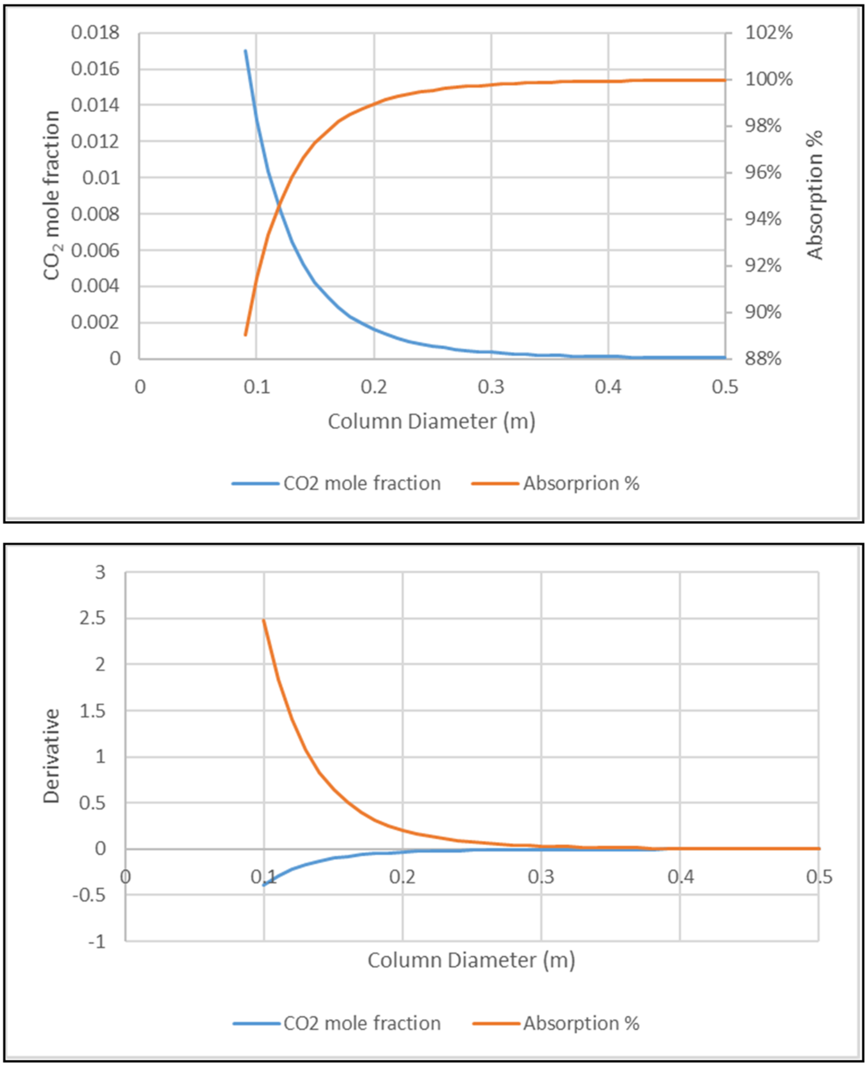


FIGURE 4 Effect of column diameter on scrubbing CO_2 from air using an alkaline NaOH solution

enhancing the absorption in a packed column, it plays an indirect role, where increasing the column diameter increases the packing volume, which leads to increasing the wet surface area.

When the APSAT was used to inspect the effect of column diameter on scrubbing CO_2 from air using an alkaline NaOH solution by iterating the calculation sequence through a range of column diameter (from 0.09 to 0.5 m with an increment of 0.01 m) for its effect on the mole fraction of carbon dioxide in the exit gas stream, other parameters were fixed as listed in Table 4. Results show that the absorption of CO_2 increases proportionally with the column diameter. The percentage of CO_2 uptake increased significantly from 89% to 99% when increasing the column diameter from 0.09 to 0.19 m, respectively, at a column height of 5 m. After that, the effect of the column diameter on the absorption of CO_2 can be considered negligible. Figure 4 shows the resulting curves plotted based on APSAT outputs and their derivatives.

4.1.3 | Effect of the liquid stream temperature on the removal of CO_2 from the air using an alkaline NaOH solution

There are two factors of opposite effects that impact the scrubbing of CO_2 from the gas phase. The first factor is solubility, where the gas solubility decreases as the liquid stream temperature increases. In contrast, when the temperature increases, the kinetic energy of the involved chemical reactions increases, increasing the chances of successful collisions and the rate of reaction. The combined effect of these two factors on the liquid stream temperature will be evaluated.

The APSAT was used to inspect the effect of liquid stream temperature on the scrubbing of CO_2 from the air using an alkaline NaOH solution by iterating the calculation sequence through a range of liquid stream temperature (from 10°C to 50°C with an increment of 1°C) for investigating its effect on the mole fraction of carbon dioxide in the exit gas stream. Other parameters

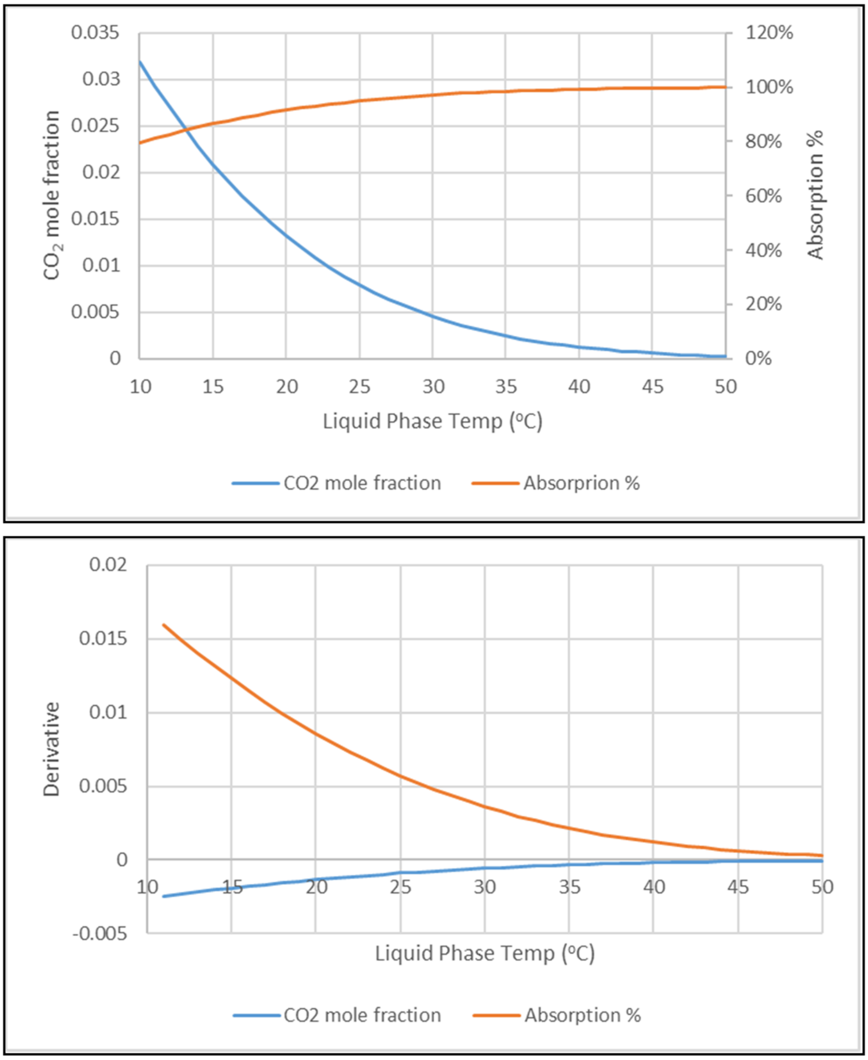


FIGURE 5 The effect of liquid stream temperature on scrubbing CO_2 from air using an alkaline NaOH solution

were fixed, as listed in Table 4. Results show that the absorption of CO_2 increases proportionally with liquid stream temperature. The percentage of CO_2 uptake increased significantly from 79% (at 10°C) to 97% (at 30°C). After that, the effect of temperature can be considered negligible. Figure 5 shows the resulting curves plotted based on APSAT outputs and their derivatives.

4.1.4 | Effect of gas stream pressure on scrubbing CO_2 from the air using an alkaline NaOH solution

Similarly, the gas stream pressure has two opposite effects on scrubbing CO_2 from the gas phase. Although the solubility of a gas in the liquid phase increases as its pressure increases, the high gas pressure decreases the gas-liquid interfacial area, which in turn reduces the mass transfer rate [3].

The APSAT was used to inspect the effect of gas stream pressure on the scrubbing CO_2 from air using an alkaline NaOH solution by iterating the calculation sequence through a range of gas phase pressure (from 101.15 to 200 kPa with an increment of 2 kPa) for investigating its effect on the mole fraction of carbon dioxide in the exit gas stream. Other parameters were fixed, as listed in Table 4. Results show that the absorption of CO_2 decreases negligibly when the gas stream pressure increases. The percentage of CO_2 uptake decreased negligibly from 91.49% (at 101.15 kPa) to 91.46% (at 200 kPa). Figure 6 shows the resulting curves plotted based on APSAT outputs and their derivatives.

4.2 | Evaluation of the learning outcomes of APSAT

The learning outcome of the APSA approach was evaluated based on the difference between the correct

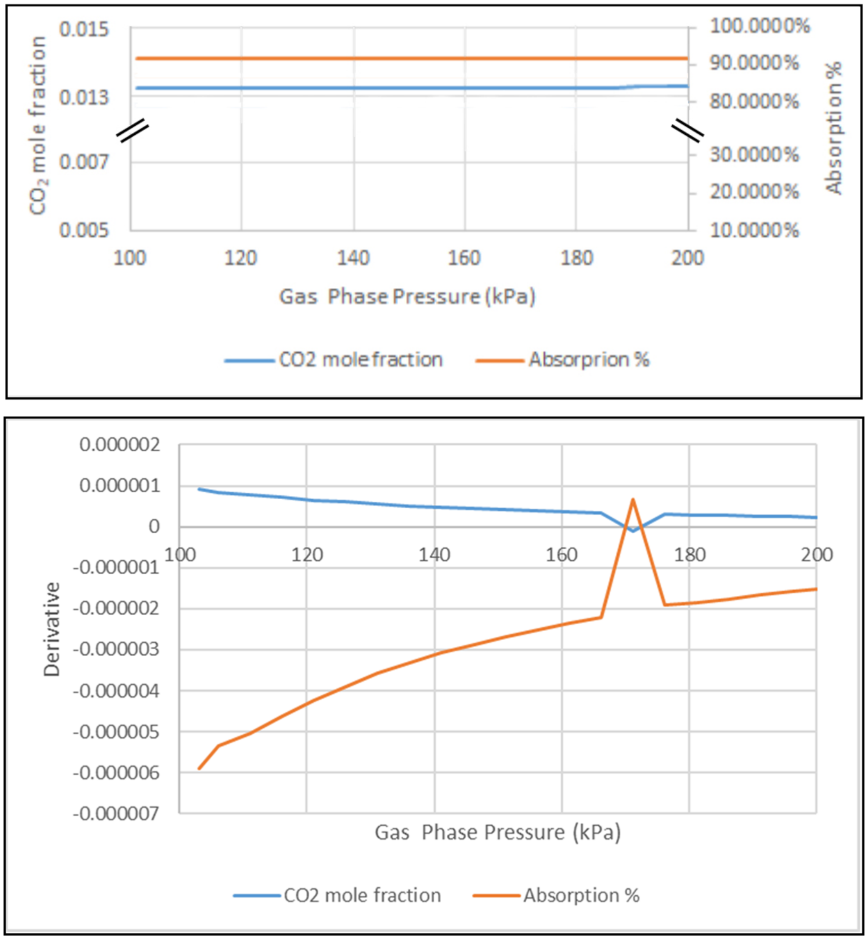


FIGURE 6 The effect of gas stream pressure on scrubbing CO_2 from air using an alkaline NaOH solution

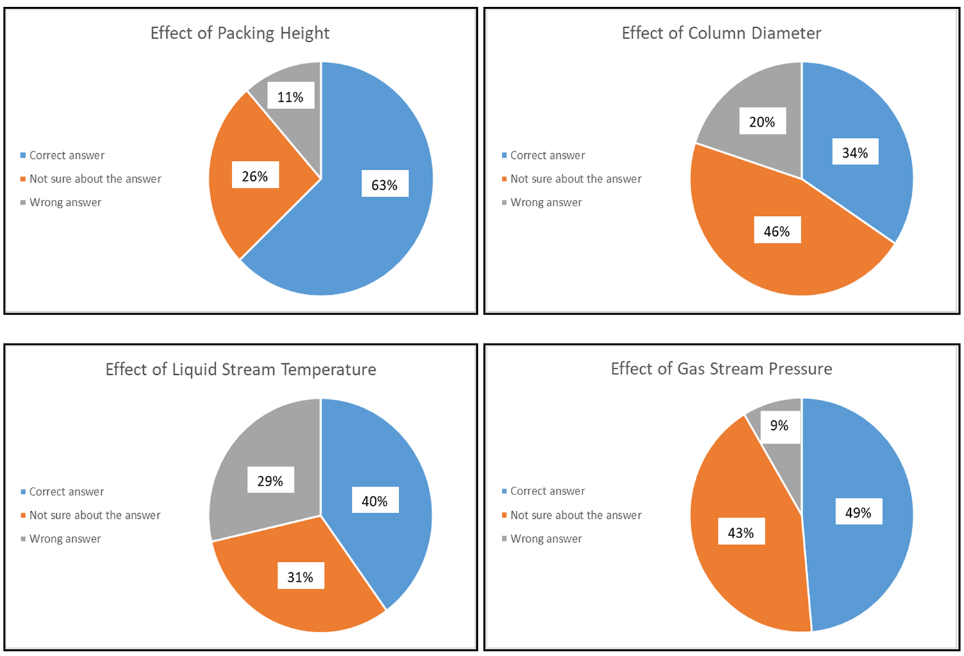


FIGURE 7 Evaluation of Students' judgment on the effects of studied parameters before the Aspen Plus® Sensitivity Analysis Tool

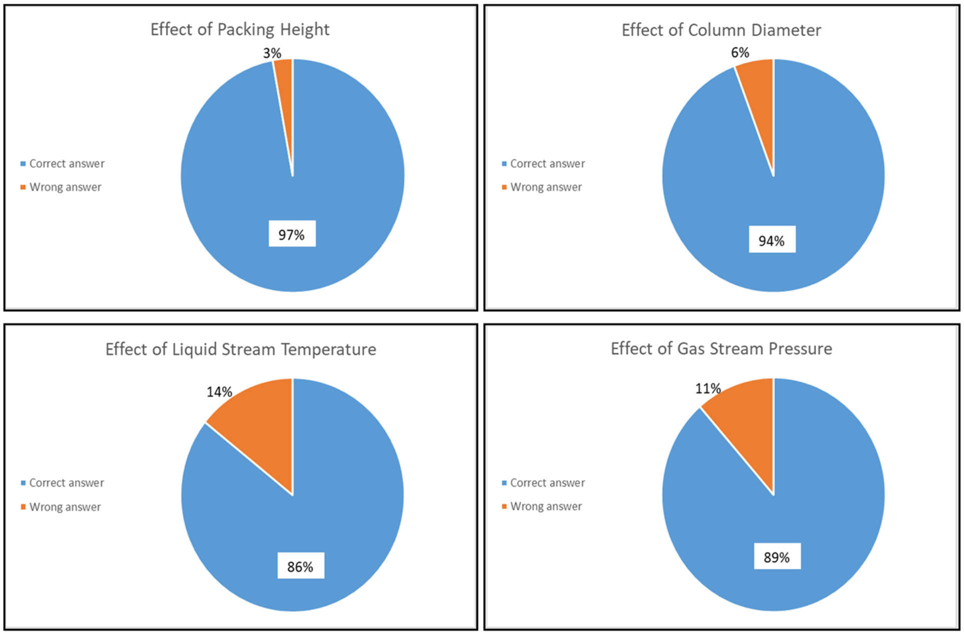


FIGURE 8 Evaluation of Students' judgment on the effects of studied parameters after the Aspen Plus® Sensitivity Analysis Tool

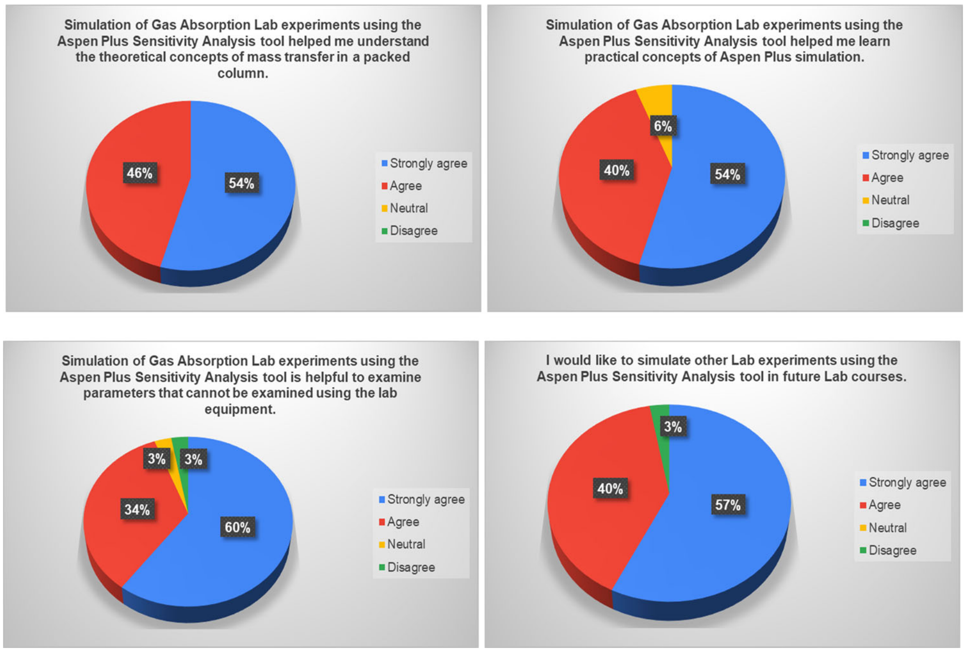


FIGURE 9 Evaluation of students' feedback on Aspen Plus® Sensitivity Analysis Tool

answers in the quiz given in stage I and that given in stage III (as shown in Figures 7 and 8, respectively).

Students' responses in stage I revealed a high percentage of uncertainty, where students were not sure about the correct answer. The highest degrees of uncertainty was in the "effect of column diameter" (at 46%) and in the "effect of gas stream pressure" (at 43%). On the contrary, the "effect of the packing height" shows the lowest percentage of uncertainty (at 26%). Moreover, the misconceptions were analyzed from the wrong answers, where the height extent of misconceptions was faced in the "effect of liquid stream temperature" (at 29%) followed by the "effect of column diameter" (at 20%).

Hence, except for the "effect of the packing height," other investigated parameters show high percentages of uncertainties and misconceptions. This can be attributed to the fact that, while the "effect of the packing height" is a straightforward concept studied in other mass transfer courses, the other parameters are a bit complex and need further critical thinking and analysis.

As mentioned earlier, the students did not receive any feedback on their performance in stage I, and they were engaged in stage II, where students used their critical thinking and online resources to gain a profound understanding while discussing the APSAT results. This was reflected in their performance in stage III, which significantly improved the students' learning outcomes. The correct answers jumped from 63% to 97%, 34% to 94%, 40% to 86%, and 49% to 89% for the effects of height, diameter, temperature, and pressure, respectively.

4.3 | Evaluation of students' feedback on APSAT

Students who were engaged in the APSAT activity demonstrated a strong interest in this approach as a virtual environment to mimic a Lab experiment, which fosters their learning outcomes by testing and evaluating some parameters that cannot be examined using the physical lab equipment. A summary of their perceptions of the APSAT is shown in Figure 9. An analysis of the results shown in Figure 9 is presented below:

- All 35 students agreed that the APSAT approach helped them understand the theoretical concepts of mass transfer in a packed column (19 students [54%] strongly agreed, and 16 students [46%] agreed).
- Most of the students (33 out 35 students [94%]) agreed that the APSAT approach helped them learn practical concepts of Aspen Plus simulation (19 students [54%] strongly agreed, and 14 students [40%] agreed).
- Most of the students (33 out 35 students [94%]) agreed that the APSAT approach helped them examine parameters that cannot be examined using the physical lab equipment (21 students [60%] strongly agreed, and 12 students [34%] agreed). However, one student (3%) disagreed!
- The majority (34 out of 35 students [97%]) would like to simulate future Lab experiments using the APSAT in future Lab courses (20 students [57%] strongly agreed, and 14 students [40%] agreed). However, one student [3%] did not wish to apply the APSAT approach in future lab experiments!

5 | CONCLUSIONS

The computer-based APSAT is a promising approach for mimicking lab experiments to avoid possible hazards or test and evaluate some parameters that cannot be examined using the lab equipment due to possible limitations. The APSAT approach enabled the students to iterate the calculation sequence of independent parameters through a range of values to investigate their effect on certain dependent variables, which honed their creativity and critical thinking skills.

Results showed that this approach helped the students gain a profound understanding of addressing conceptual mistakes while discussing the results of the APSAT outputs. In addition, students demonstrated a strong interest in this approach as a supporting tool to understand the theoretical concepts of mass transfer in a packed column, learn practical concepts of Aspen Plus simulation, and examine parameters that cannot be examined using the lab equipment. Moreover, they recommended using the APSAT in future Lab experiments.

Hence, this approach can be implemented to facilitate the teaching of lab courses. Furthermore, it is a practical choice to optimize the resources and a good substitute for lab experiments in case of any pandemic, confinement, or interest in testing the effects of hazardous conditions to ensure sustaining the learning outcomes from corresponding experiments.

AUTHOR CONTRIBUTIONS

Ahmed M. Elkhatat conceived, designed, analyzed, interpreted the data, and wrote the paper. Shaheen A. Al-Muhtaseb contributed to data analysis and interpretation, paper proofreading, and improvement. All authors read and approved the final manuscript.

ACKNOWLEDGMENTS

The Qatar National Library and Qatar University funded the publication of this article. Funding Open access funding is provided by the Qatar National Library.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

The data sets used and/or analyzed during the current study are available from the corresponding author on reasonable request.

ORCID

Ahmed M. Elkhatat http://orcid.org/0000-0003-0383-939X

Shaheen A. Al-Muhtaseb http://orcid.org/0000-0002-9240-930X

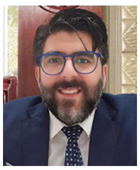
REFERENCES

1. ABET. Criteria for Accrediting Engineering Programs, 2021–2022. https://www.abet.org/accreditation/accreditation-criteria/criteria-for-accrediting-engineering-programs-2021-2022/, 2021.

2. Y. Alice, Y. Kolb, and D. A. Kolb, *Learning styles and learning spaces: Enhancing experiential learning in higher education*, Acad. Manag. Learn. Educ. **4** (2005), no. 2, 193–212.
3. A. Almoslh, F. Alobaid, C. Heinze, and B. Epple, *Influence of pressure on gas/liquid interfacial area in a Tray column*, Applied Sciences **10** (2020), no. 13, 4617.
4. P. Armstrong. *Bloom's taxonomy*. https://cft.vanderbilt.edu/guides-sub-pages/blooms-taxonomy/
5. Aspen.Plus, *Rate-based model of the CO_2 capture process by NaOH using Aspen Plus*, Aspen Technology Inc., Cambridge, MA, 2008.
6. Aspen.Plus. https://www.aspentech.com/en/products/engineering/aspen-plus
7. R. Baciocchi, G. Storti, and M. Mazzotti, *Process design and energy requirements for the capture of carbon dioxide from air*, Chem. Eng. Process. Process Intensif. **45** (2006), no. 12, 1047–1058.
8. R. Billet and M. Schultes, *Predicting mass transfer in packed columns*, Chem. Eng. Technol. **16** (1993), no. 1, 1–9.
9. J. Bravo, J. Rocha, and J. Fair, A comprehensive model for the performance of columns containing structured packings, Hemsphere Publishing Corporation, New York, USA, 1992.
10. J. L. Bravo, J. A. Rocha, and J. R. Fair, *Mass-transfer in Gauze packings*, Hydrocarbon Process. **64** (1985), no. 1, 91–95.
11. E. Brunazzi and A. Paglianti, *Liquid-film mass-transfer coefficient in a column equipped with structured packings*, Ind. Eng. Chem. Res. **36** (1997), no. 9, 3792–3799.
12. J. G. Canadell, C. Le Quéré, M. R. Raupach, C. B. Field, E. T. Buitenhuis, P. Ciais, T. J. Conway, N. P. Gillett, R. A. Houghton, and G. Marland, *Contributions to accelerating atmospheric CO_2 growth from economic activity, carbon intensity, and efficiency of natural sinks*, Proc. Natl. Acad. Sci. U. S. A. **104** (2007), no. 47, 18866–18870.
13. A. K. Coker, *Chapter 14—Packed towers*, Ludwig's applied process design for chemical and petrochemical plants (A. K. Coker, ed.), 4th ed., Gulf Professional Publishing, Boston, 2010, pp. 483–678.
14. J. R. Couper, W. R. Penney, J. R. Fair, and S. M. Walas, Chemical process equipment: Selection and design, Gulf professional Publishing, Houston, Texas, USA, 2005.
15. A. N. Darwazeh, *A new revision of the [Revised] Bloom's taxonomy*. Distance Learning, 14 (2017)no. **3**, 13–28.
16. A. M. Elkhatat and S. A. Al-Muhtaseb, *Hybrid online-flipped learning pedagogy for teaching laboratory courses to mitigate the pandemic COVID-19 confinement and enable effective sustainable delivery: Investigation of attaining course learning outcome*, SN Soc. Sci. **1** (2021), no. 5, 113.
17. A. M. Elkhatat and S. A. Al-Muhtaseb, *Fostering engineering laboratory course teaching by embedding inquiry-guided learning approach using computer-aided learning packages*, Chem. Eng. Educ. **56** (2022), no. 3, 190–198.
18. L. D. Feisel and A. J. Rosa, *The role of the laboratory in undergraduate engineering education*, Learn. Educ. **94** (2013), no. 1, 121–130.
19. R. M. Felder, R. Brent, and M. J. Prince, *Engineering instructional development: programs, best practices, and recommendations*, J. Eng. Educ. **100** (2011), no. 1, 89–122.
20. D. Flagiello, A. Parisi, A. Lancia, and F. Di. Natale, *A review on gas-liquid mass transfer coefficients in packed-bed columns*. ChemEngineering **5** (2021), no. 3, 43.
21. D. Flagiello, A. Parisi, A. Lancia, and F. Di Natale, *A tool for mass transfer evaluation in packed-bed columns for chemical engineering students*, Educ. Chem. Eng. **37** (2021), 29–39.
22. S. Freeman, S. L. Eddy, M. McDonough, M. K. Smith, N. Okoroafor, H. Jordt, and M. P. Wenderoth, *Active learning increases student performance in science, engineering, and mathematics*, Proc. Natl. Acad. Sci. U. S. A. **111** (2014), no. 23, 8410–8415.
23. J. Glassey, K. Novakovic, and M. Parr, *Enquiry based learning in chemical engineering curriculum supported by computer aided delivery*, Educ. Chem. Eng. **8** (2013), no. 3, e87–e93.
24. L. Gomes and S. Bogosyan, *Current trends in remote laboratories*, IEEE Trans. Ind. Electron. **56** (2009), no. 12, 4744–4756.
25. C. Gravier et al., *State of the art about remote laboratories paradigms—Foundations of ongoing mutations*, Int. J. Online Eng. **4** (2008), no. 1, 9–25.
26. L. P. Grayson, The making of an engineer, John Wiley and Sons, New York, 1993.
27. F. Hadjeris, *Revisiting sustainable development Goal 4 in the context of COVID-19 pandemic: A case study of online teaching in Algerian higher education institutions*, Human Behav. Emerg. Technol. **3** (2021), no. 1, 160–168.
28. B. Hanley and C-C Chen, *New mass-transfer correlations for packed towers*, AIChE J. **58** (2012), no. 1, 132–152.
29. J. Joe, C. Barton, M. Clayton, A. Yablonsky, and D. Legere, *SkyMine Carbon Mineralization Pilot Project*. Technical Report: OSTI.GOV. 2010. https://doi.org/10.2172/1027801
30. A. Leva, *A Hands-On experimental laboratory for undergraduate courses in automatic control*, IEEE Trans. Educ. **46** (2003), no. 2, 263–272.
31. W. L. McCabe, J. C. Smith, and P. Harriott, Unit operations of chemical engineering, vol. **5**. McGraw-Hill, New York, 1993.
32. D. J. Moore and D. R. Voltmer, *Curriculum for an engineering renaissance*, IEEE Trans. Educ. **46** (2003), no. 4, 452–455.
33. National Academies of Sciences, Engineering, and Medicine, *Laboratory experiences and student learning*, America's lab report: Investigations in high school science (S. R. Singer, M. L. Hilton, and H. A. Schweingruber, eds.), The National Academies Press, Washington, DC, 2006, p. 75.
34. A. G. Olabi, T. Wilberforce, K. Elsaid, E. T. Sayed, H. M. Maghrabie, and M. A. Abdelkareem, *Large scale application of carbon capture to process industries—A review*, J. Clean. Prod. **362** (2022), 132300.
35. Z. Olujic, M. Behrens, L. Colli, and A. Paglianti, *Predicting the efficiency of corrugated sheet structured packings with large specific surface area*, Chem. Biochem, Eng. Quater. **18** (2004), 2, 89–96.
36. K. Onda, H. Takeuchi, and Y. Okumoto, *Mass transfer coefficients between gas and liquid phases in packed columns*, J. Chem. Eng. Jpn. **1** (1968), no. 1, 56–62.
37. B. Pinsent, L. Pearson, and F. J. W. Roughton, *The kinetics of combination of carbon dioxide with hydroxide ions*. Trans. Faraday Soc. **52** (1956), 1512–1520.

38. M. G. Plaza, S. Martínez, and F. Rubiera, *CO_2 capture, use, and storage in the cement industry: State of the art and expectations*, Energies **13** (2020), no. 21, 5692.
39. A. Sinha and P. De, Mass transfer: Principles and operations, PHI Learning Pvt. Ltd, New Delhi, India, 2012.
40. R. K. Sinnott, Chemical engineering design, vol. **6**., 4th ed., Elsevier, Oxford, UK, 2005.
41. N. A. Spector and B. F. J. Dodge, *Removal of carbon dioxide from atmospheric air*. Am. Inst. Chem. Eng. **42** (1946), nos. 5–6, 827–848.
42. J. Stichlmair, J. L. Bravo, and J. R. Fair, *General model for prediction of pressure drop and capacity of countercurrent gas/liquid packed columns*. Gas Sep. & Purif. 3 (1989), no. **1**, 19–28.
43. R. Thiele, R. Faber, J. U. Repke, H. Thielert, and G. Wozny, *Design of industrial reactive absorption processes in sour gas treatment using rigorous modelling and accurate experimentation*. Chem. Eng. Res. Des. **85** (2007), no. 1, 74–87.
44. M. M. Waldrop, *Why we are teaching science wrong, and how to make it right*, Nature **523** (2015), 272–274.
45. F. Zeman, *Energy and material balance of CO_2 capture from ambient air*, Environ. Sci. Technol. **41** (2007), no. 21, 7558–7563.

AUTHOR BIOGRAPHIES



Ahmed M. Elkhatat is PhD qualified and experienced in the entire spectrum of activities associated with chemical engineering's academic position, with a track record of patents and peer-reviewed publications in pedagogy and chemical engineering. He is active in teaching, lab safety, and infrastructure management to accommodate multiple needs and the Department's broader functioning. Extramural interests include judging and helping schools with science competitions, innovation to produce patentable ideas, and promoting science in the mass media.

Shaheen A. Al-Muhtaseb earned his PhD degree in chemical engineering from the University of South Carolina in 2001. He also earned his MSc and BSc degrees in chemical engineering from the Jordan University of Science and Technology. He is currently a professor of chemical engineering at Qatar University. His main research interests are the various fields of advanced materials, with special attention to adsorption equilibria, membranes for gas separation, and energy storage materials.

How to cite this article: A. M. Elkhatat and S. A. Al-Muhtaseb, *Virtual mimic of lab experiment using the computer-based Aspen Plus® Sensitivity Analysis Tool to boost the attainment of experiment's learning outcomes and mitigate potential pandemic confinements*, Comput. Appl. Eng. Educ. (2022), 1–16. https://doi.org/10.1002/cae.22583