INTRODUCTION

The increase in anthropogenic CO₂ emissions mainly from natural gas-fired and coal power plants has stimulated intense interest in CO₂ capture and storage (CCS) or CO₂ application in oil recovery.¹ The most exceptional near-term solution for reducing CO₂ emissions is through postcombustion CO₂ capture technologies because these technologies can be retrofitted to existing electricity generation units.² Among various technologies, CO₂ capture using solid sorbents is being recognized as an up-and-coming technology and has attracted intense attention from both academic and industrial fields in

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Abstract
A comprehensive computational fluid dynamic (CFD) model of CEES-developed polyethylenimine impregnated protonated titanate nanotubes (PEI-PTNTs) was developed using the Multiphase Flow with Interphase eXchanges (MiX) package to evaluate the performance of the PEI-PTNTs in a 1-MW pilot-scale carbon capture reactor developed by the National Energy Technology Laboratory (NETL). In this CFD model, the momentum, continuity, and energy transport equations were integrated with the first-order chemistry model for chemical kinetics of heterogeneous reactions to predict the adsorption of CO₂ onto amine-based sorbent particles and the reactor temperature. Based on the amount of the CO₂ adsorption obtained in the small-scale experiment, the coefficients for the chemical reaction equations of PEI-PTNTs are adjusted. The adjusted PEI-PTNTs model is applied to the simplified numerical model of 1-MW pilot-scale carbon capture system, which is calibrated through the comparison between our simulation results and the results provided by NETL. This calibrated CFD model is used for selecting the optimized flow rate of the gas phase. Our study shows that the optimized gas flow rate to absorb 100% CO₂ without loss is 1.5 kg/s, but if higher absorption rate is preferable despite some loss of CO₂ absorption in the reactor, a higher flow rate than 1.5 kg/s can be selected.

KEYWORDS
computational fluid dynamic simulation, chemical reactions, MiX, solid amine-based carbon capture, titanate nanotubes
the last decade. Reliable sorbent-based CO₂ capture offers some advantages such as the potential to reduce energy consumption, improve regeneration, enable higher capacity, and offer good selectivity, as well as ease in handling.

There are various solid substrates used to fabricate solid amine adsorbents, but titanate nanotubes are known as the most effective materials because they can easily be synthesized through a simple hydrothermal treatment method. Regarding the hydrothermal treatment methods to functionalize the titanate nanotubes to attain the titanate nanotube-based adsorbents, some studies were carried out changing the loading ratios of PEI used to impregnate PTNTs. Based on the results, they found that the optimized loading was 50 wt% of PEI to reach the highest CO₂ capture capacity. Additionally, in an earlier study, Kommalapati, et al investigated the effect of hydrothermal treatment conditions of PTNTs, for example, temperature and hydrothermal treatment time. In the study, PTNTs were synthesized at 130 and 140°C within 1, 3, and 5 days, PEI-functionalized PTNTs were obtained by impregnating PTNTs with PEI, and the effects of some PTNTs synthesis conditions on the capture capacity were evaluated. CO₂ capture with PEI-PTNTs was conducted at 75°C from mixed CO₂ and N₂ gas, and CO₂ desorption was done at 110°C by purging the adsorbent with pure nitrogen gas (N₂), and the 130°C and 3-day hydrothermal treatment of anatase TiO₂ is suggested for effectively capturing CO₂.

Application of computational fluid dynamic (CFD) to the solid sorbent-based CO₂ capture system has gotten attention in the recent past. CFD modeling is a valuable tool to predict the performance of CO₂ capture including the chemical reactions because CFD analysis has resulted in rapid progress in the applications of CFD in performance analysis, design, and optimization of various equipment and systems. However, CFD modeling of the CO₂ absorption process is challenging because of the complex hydrodynamics of gas-solid flow within the reactor, as well as the different types of chemical reactions taking place simultaneously. Recently, various efforts are underway to increase the fidelity of the CFD model including complex physical and chemical processes of sorbent-based carbon capture and gain more insights on-flow field and reaction behavior in reactors.

Wang, et al performed device-scale CFD simulations to study hydrodynamics and CO₂ absorption behavior in a conceptual fluidized bed reactor using the micro-encapsulated carbon dioxide sorbent, which is considered as a promising material because of high capture rate, low fabrication cost, and efficient energy consumption. Chen developed CFD simulation models for the solid sorbent CO₂ capture in the applications of the long-term integrated gasification combined cycle by using ANSYS FLUENT. The CFD models were validated by experimental data and applied to commercial size fixed-bed reactor design and simulations. Barelli, et al presented a new reactor solution based on rotating fixed beds for CO₂ capture with solid sorbents. For the design of the innovative system, they developed a suitable CFD model considering the kinetic capture process. The model was validated with experimental results, showing a potential reduction of energy penalties with current technologies. Breault, et al simulated the adsorber performance of a lower temperature CO₂ absorption reactor operating in the core-annular flow regime using multiphase computational fluid dynamics with chemistry and heat transfer. The three-dimensional geometry is based on the lower mixing section of a riser from a recently operated CO₂ capture test unit. An eight-point test matrix was used to evaluate the performance of the riser adsorber concerning solids circulation rate, gas flow rate, and heat removal. Also, Ryan et al performed the CFD simulation of the solid sorbent carbon capture system. They focused on comparing between Eulerian-Eulerian and Eulerian-Lagrangian simulation approaches. Through this comparison, they investigated the accuracy of modeling the system using current state-of-the-art CFD modeling tools and explored the benefits and weaknesses of using different multiphase modeling methods for simulating solid sorbent carbon capture systems. Abbasi et al and Chalermsinsuwan et al developed the CFD model for the CO₂ capture process in the riser part of a circulating fluidized bed using a potassium-based solid sorbent and validated the model through comparison with the experimental data.

In this paper, a comprehensive CFD model of CEES-developed PEI-PTNTs was developed using the MFIX package to evaluate the performance of the PEI-PTNTs in a 1-MW pilot-scale carbon capture reactor developed by the National Energy Technology Laboratory (NETL). In this CFD model, the momentum, continuity, and energy transport equations were integrated with the first-order chemistry model for chemical kinetics of heterogeneous reactions to predict the adsorption of CO₂ onto amine-based sorbent particles and the reactor temperature. The CFD model is verified through the comparison of the amount of the CO₂ adsorption between the simulation and the experiment on a small scale, and the coefficients for the chemical reaction equation of PEI-PTNTs are adjusted. The adjusted PEI-PTNTs model is applied to the simplified numerical model of 1-MW pilot-scale carbon capture reactor system developed by NETL. NETL has independently verified the pilot-scale CFD model for various simple and small-scale multiphase reactive flow problems by using a two-fluid model (TFM). For the calibration of the CEES-developed simulation model, the same reactor model developed by NETL was built using MFIX, and the results are compared to those provided by NETL. Because of some limits in our CFD simulation for the large-scale model including heat transfer and chemical reaction like 1-MW NETL reactor, the heating and cooling effects on the CO₂ absorption are considered entering the uniform and higher temperature distribution for the entire reactor and the
gas flow than initial temperature of the gas. The best temperature to make CO₂ capture ratio the same as the NETL result is identified, and the temperature is applied to the simulation model for the NETL reactor. This calibrated simulation model is employed to examine the performance of the solid sorbents and find the optimized flow rate in the reactor model developed by NETL.

2 | CHEMISTRY OF CARBON CAPTURE IN THE ABSORBER

A first-order chemistry model for chemical kinetics is used to model the adsorption and desorption of CO₂ and water vapor onto amine-based sorbent particles. The chemical reactions considered in the current kinetics model include the following:

1. Reaction of CO₂ with the impregnated amine to form carbamate,
2. Reaction of CO₂, physisorbed H₂O, and amine to form bicarbonate,
3. Physical absorption of H₂O to the sorbent, that is, water physisorption. Equations for the three respective reactions are written as follows:

\[ 2R₂NH + CO₂(g) \rightarrow R₂NCO₂⁻ + R₂NH₂⁺ \]  \hspace{1cm} (1)
\[ R₂NH + H₂O(phys) + CO₂(g) \rightarrow HCO₃⁻ + R₂NH₂⁺ \]  \hspace{1cm} (2)
\[ H₂O(phys) \rightarrow H₂O(phys) \]  \hspace{1cm} (3)

The following reaction rates for all three chemical equations can be derived by assuming most species react ideally:

\[ \frac{\partial x}{\partial t} = k_c \left( s^2 p_c - \frac{x_w}{k_c} \right) \]  \hspace{1cm} (4)
\[ \frac{\partial b}{\partial t} = k_b \left( sa p_c - \frac{b_w}{k_b} \right) \]  \hspace{1cm} (5)
\[ \frac{\partial a}{\partial t} = k_h \left( p_h - \frac{a}{k_h} \right) \]  \hspace{1cm} (6)

where \( x, s, \) and \( w \) are the fraction of amine sites occupied by carbamate ions, the fraction of unreacted amine sites, and the fraction of protonated amine sites; \( b \) and \( a \) are concentration of bicarbonate and concentration of water molecules (mol/m³); and \( p_c \) and \( p_h \) are partial pressures of CO₂ and water in the gas. Reaction rate equations and the equilibrium constants above are entered in the MFiX as the user-defined code. The equilibrium and kinetic parameters are adjusted based on the comparison of CO₂ capture capacity between experiment and simulation, and their values are tabulated in Table 1.

3 | EXPERIMENT

In this section, the previous experimental work of PVAMU-CEES is briefly explained. Anatase TiO₂ nanopowder of 2 g was mixed with 75 mL of 10 mol/L NaOH solution. The mixture was poured into a Teflon-lined stainless steel autoclave and hydrothermally treated at preselected temperature (130 or 140°C) for either 1, 3, or 5 days, respectively. The 50 wt% PEI loading functionalized PTNTs was obtained in our experiments by dissolving 1 g PEI in 25 mL methanol, dispersing 1 g PTNTs in 60 mL with sonication, and then mixing them, where PTNTs were PTNTs-130°C-1 day, PTNTs-140°C-1 day, PTNTs-130°C-3 days, PTNTs-140°C-3 days, or PTNTs-130°C-5 days. PEI with molecular weight 10 000 was used in the experiment. The adsorbent-filled tube was placed to the oven under 13.5 vol% CO₂/N₂ for 60-90 minutes at 75°C for CO₂ adsorption. The CO₂ absorbed by the adsorbent was released by heating at 110°C under pure N₂ for 60 minutes. One complete adsorption-desorption cycle consisted of CO₂ adsorption at 75°C followed by CO₂ desorption at 110°C. The process was repeated to obtain 7-10 cycles for each adsorbent. The higher adsorption capacities are observed for PEI-PTNTs-130°C-3 days. The average capture capacity of the adsorbent PEI-PTNTs-130°C-3 days is 78.1 mg/g in Trial 1 and 79.2 mg/g in Trial 2. The adsorbents took about 90 minutes to reach the maximum adsorption. More detailed information of the experiment is given in Kommalapati, et al. Additional details about the multiphase flow theory and the numerical techniques employed in MFiX are provided in the MFiX documentation. The gas phase is comprised of four chemical species, which are N₂, O₂, CO₂, and H₂O(g), and the solids phase (sorbent) comprises six chemical species, which are R₂NH,
KIM et al. R2NCO−, R2NH+, HCO−, absorbed H2O, and H2Ti3O7. A total of 20 transport equations are solved at each time step: two continuity, six momentum, two energy, and 10 species equations. The simulation case included in Xu, et al24 is selected for the evaluation of our CFD model.

To achieve steady-state operation, the simulations for the NETL reactor and for the PVAMU-CEES reactor are run to 100 and 900 seconds, respectively. It takes about thirty days to finish the 100-second simulation and about twenty days to finish the 900-second simulation, respectively. Each case uses four processors for the parallel simulation with work stations belonging to PVAMU-CEES. The computational cost significantly increases because of the chemical reaction complexity.

4.2 | Numerical modeling design

4.2.1 | Reactor used in PVAMU-CEES experiment

This section includes a detailed description of the MFiX model for the absorber reactor column. A two-dimensional (2D) MFiX model is built for the 0.6 × 1.0 cm absorber column. The entire domain is discretized into 6 × 10 grids. As shown in Figure 1, the solid inlet is modeled as a mass flow inlet at the bottom of the absorber column. The corresponding gas outlet on the top side is designed as a constant pressure outflow. The flue gas is entered at the bottom of the absorber column as a mass inflow boundary condition. The inlet mass flow rate for flue gas is 20 mL/s. To avoid escaping of sorbents either from the bottom inlet or top outlet, a semipermeable membrane is used to allow only the gas phase to pass through. In the experiment, both ends of adsorption tubes were filled with high-temperature resistant fibers, but in the simulation, they are replaced with the semipermeable membranes, R1 and R2. They are modeled for preventing the solid sorbents from passing through, and their dimensions do not affect the results in the bed. No-slip boundary condition was used for both sidewalls. The summation of initial and boundary conditions is listed in Tables 2 and 3. Figure 1 shows the solid and gas inlets and outlets from the conceptual design. Sorbent particles enter through the bottom of the fluidized bed region where most chemical reactions occur. The solid sorbent particles have a density of 381.6 kg/m³ with an average size of 118 μm, and the density and the average diameter are directly measured by using scale and microscope in the laboratory.

4.2.2 | NETL reactor

A sorbent-based 1-MW carbon capture system is designed by NETL. NETL built the corresponding CFD simulation model...
on the 1-MW carbon capture reactor and tried to increase the predictive confidence at scale by validation of the simulation model with the statistical method and laboratory-scale experimental data. The 1-MW NETL pilot-scale CO₂ capture system consists of two stages, each separated by perforated trays that allow flue gas to move upward, and then, the CO₂-loaded sorbent particles leave the adsorber system and enter the regenerator column. The whole adsorber column is arranged with cooling tubes to cool down the flue gas whose temperature increases very high because of the chemical reaction, contributing to better CO₂ adsorption ratio by the solid particles. The details of the NETL reactor system can be found in Lai, et al.

In this paper, the lower stage of the adsorber column is modeled using MFiX. A two-dimensional (2D) model is built for the 1.33 x 6.88 m adsorber column. Figure 2 shows simulation model geometry and dimensions, and initial and boundary conditions including solid and gas inlets and outlets from the conceptual design. Sorbent particles enter through the left side to the fluidized bed region, where most chemical reactions occur, and exit from the solid outlet located at the right wall side. The solids inlet is modeled as a mass flow inlet at the top-left corner of the absorber column. The solid outlet on the right side is modeled by using the constant pressure outflow boundary condition. The flue gas inlet is located at the bottom of the adsorber column and specified as a mass inflow boundary condition. The gas exits the adsorber from the top of the column where a constant pressure outlet is used. To block the adsorbent and allow the gas to flow through on the top and bottom, a semipermeable membrane is used. The solid sorbent particles have a density of 484 kg/m³ with an average size of 118 μm. The flow rates at the bottom inlet, left top fluid inlet, and left top solid inlet are 1.5, 0.0066, and 2.5394 kg/s, respectively. The details of initial and boundary conditions used in the simulation are tabulated in Tables 4 and 5, respectively. “From sim” in Table 5 means that variables at the solid and gas outlet can be computed from simulations. The other details of the NETL reactor system and simulation conditions are included in Xu, et al.

### 4.3 Verification of the 1-MW NETL reactor CFD simulation model

For the verification of the simulation model, the same reactor model developed by NETL was built using MFiX, and the results are compared to the results provided by NETL. There are some limitations in our CFD simulation for the large-scale model including heat transfer and chemical reaction like 1-MW NETL reactor. Adequately resolving the hydrodynamics and heat transfer in gas-solid flow simulations typically requires computational grids on the order of 1-10 particle sizes or some kinds of subgrid filtering method should be applied, but these are not possible at this moment because of our limited computational resources and technical ability. The current grid size is too large to implement the heat transfer in the NETL reactor including the heating effect generated by the chemical reaction and cooling effect caused by the cooling tubes. Due to these limitations, the CO₂ absorption ratio results with the flow rate obtained from our
same NETL reactor CFD model are slightly higher than the results in the published paper by NETL. However, the pattern that the CO2 capture ratio, which is defined as Equation (7), decreases when the flow rate increase is captured well. The CO2 capture ratios are 0%, 2%, and 7% greater in 0.6, 0.72, and 0.84 kg/s of flow rates, respectively, compared to the results simulated by NETL as shown in Figure 3 (NETL vs No Heat). “No Heat” means that the heat generated by the chemical reaction and the cooling effect is not included in the simulation.

These results can be further improved by entering the higher uniform temperature distribution for the entire

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**TABLE 4** Initial conditions for the computational fluid dynamic model of the nominal case

| Initial conditions 1 | Initial conditions 2 | Internal surface 1 | Internal surface 2 |
|----------------------|----------------------|-------------------|-------------------|
| Gas fraction         | 0.0                  | 0.9               | Semipermeable     |
| Gas pressure (Pa)    | Not defined          | Not defined       |                   |
| Gas temperature (K)  | 313.15               | 313.15            |                   |
| Gas-phase mass fraction |                  |                   |                   |
| N2                   | 0.93                 | 0.93              |                   |
| CO2                  | 0.05                 | 0.05              |                   |
| H2O (gas)            | 0.02                 | 0.02              |                   |
| Solid fraction       | 0.0                  | 0.1               |                   |
| Solid temperature (K)| Not defined          | 332.13            |                   |
| Solid-phase mass fraction |              |                   |                   |
| Al2O3                | Not defined          | 1.0               |                   |
| R2NH                 | 0.0                  | 0.0               |                   |
| R2NCO                | 0.0                  | 0.0               |                   |
| R2NH2                | 0.0                  | 0.0               |                   |
| HCO3                 | 0.0                  | 0.0               |                   |
| H2O (abs)            | 0.0                  | 0.0               |                   |

**TABLE 5** Boundary conditions for the computational fluid dynamic model of the nominal case

| B.C.   | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|--------|---|---|---|---|---|---|---|
| Gas flow rate (kg/s) | 1, 1.5, 2, 2.5 | 0.0066 | From sim | From sim | Free slip wall & No heat flux |
| Gas pressure (Pa)     | 1.28E + 05 | 1.01E + 05 | 1.01E + 05 | 1.01E + 05 |                   |
| Gas temperature (K)   | 316.03 | 332.13 | From sim | From sim |                   |
| Gas-phase mass fraction | N2   | 0.7709 | 0.97 | From sim | From sim |                   |
|                    | CO2 | 0.1929 | 0 |                   |                   |                   |
|                    | H2O (gas) | 0.0362 | 0.03 |                   |                   |                   |
| Solid flow rate       | Not defined | 1.0 (kg/s) | Not defined | From sim |                   |                   |
| Solid temperature (K) | Not defined | 332.13 | Not defined | From sim |                   |                   |
| Solid-phase mass fraction | Al2O3 | Not defined | 0.8515 | Not defined | From sim |                   |
|                    | R2NH | 0.1485 |                   |                   |                   |                   |
|                    | R2NCO | 0 |                   |                   |                   |                   |
|                    | R2NH2 | 0 |                   |                   |                   |                   |
|                    | HCO3 | 0 |                   |                   |                   |                   |
|                    | H2O (abs) | 0 |                   |                   |                   |                   |
reactor and the gas flow than the initial temperature of gas flow and solid sorbents. The gas temperature affects the CO₂ absorption ratio as shown in the Equations 4–6, which are chemical reaction equations. If the gas temperature increases, the chemical reaction rate decreases. The heat caused by the chemical reaction makes the gas temperature increase, but the cooling tubes arranged in the reactor prevent the temperature from increasing too high. In the steady-state condition, the temperature distribution is balanced between heating caused by a chemical reaction and cooling caused by the cooling tube. Thus, if the uniform temperature distribution which has the same effect on the CO₂ capacity as the balanced temperature distribution can be predicted in advance through the simulation results obtained by other group and entered the predicted temperature distribution to the new simulation, the more improved results of the CO₂ capacity can be obtained. Using this simplified way, the heating and cooling effect on the CO₂ absorption can be considered, albeit limited.

For this, the CO₂ capture ratio is estimated with various uniform temperature distribution for the reactor and the gas flow between 330 and 350 K without heat transfer in the simulation. Their CO₂ absorption ratio is compared to the NETL results, and the optimized temperature to make CO₂ capture ratio the same as the NETL result is identified. Figure 3 shows the CO₂ absorption ratio with the various temperatures for the reactor and the gas flow. When the temperature is 340 K, the CO₂ capture ratio is the closest to NETL results at three flow rate cases. This optimized temperature distribution will be applied to the simulation model of the PVAMU-CEES-developed PEI-PTNTs in the NETL reactor

\[ E = \left( \frac{Q_{\text{CO}_2}^{\text{in}} - Q_{\text{CO}_2}^{\text{out}}}{Q_{\text{CO}_2}^{\text{in}}} \right) \]  

(7)

### 4.4 Calibration of CFD simulation model for solid sorbents suggested by CEES in the small-scale reactor

The simulation model for the PEI-PTNTs suggested by PVAMU-CEES is calibrated by comparison of the CO₂ capture capacity results in small-scale reactors between experiment and simulation. For this, the equilibrium and kinetic parameters of chemical reaction equations are
adjusted so that CO₂ capture capacity between simulation and experiment matches with each other. Figure 4 shows that CO₂ capture capacity aligns well with the measurement value when the adjusted equilibrium parameters are entered in the simulation. The adjusted equilibrium parameter values are tabulated in Table 1. The calibrated simulation model is used for the performance of PVAMU-CEES-developed PEI-PTNTs in a 1-MW NETL reactor. In the simulation of small-scale reactor used for the PVAMU-CEES experiment, the heat transfer caused by the chemical reaction is fully included in the simulation because the ratio of grid distance to particle diameter used in the simulation for the reactor is small enough to implement the heat transfer, which is less than 10.40 The detailed information of the experiment is briefly described in Section 4.3, and the other full details are explained in the earlier paper.18

Figure 5 presents the distribution of the mass fraction of amine and ionized amines from nominal simulations at \( t = 600 \) seconds. Figure 5A shows the distribution of amine mass fraction, where the amines decrease from the initial fraction, 0.5, while \( R_2NCO^- \) and \( R_2NH^+ \) increase from zero, respectively, as shown in Figure 5B,C as the active amines are ionized with CO₂ and H₂O according to the Equations 4–6.

4.5 | Examination of PVAMU-CEES solid sorbents performance in NETL reactor

To examine the impact of gas flow rate on CO₂ capture efficiency when the PVAMU-CEES-developed solid sorbents
are applied to the same reactor developed by NETL, MFiX simulations with different flow rates are conducted using the PVAMU-CEES-developed solid sorbents. The temperature values adjusted in Section 4.3 and the calibrated equilibrium parameters for the PVAMU-CEES-developed solid sorbents are used in this simulation. Figure 6 shows the CO₂ mass fraction in the entire absorber for the four flow rates, 1.0, 1.5, 2.0, and 2.5 kg/s. At a relatively low gas flow rate, adsorption is significant at the very bottom of the absorber, which contrasts with widely spread adsorption along the absorber at a relatively high gas flow rate. Figure 7 presents the distribution of $\text{R}_2\text{NH}$, $\text{R}_2\text{NCO}_2^-$, and $\text{R}_2\text{NH}_2^+$ mass fraction, where most $\text{R}_2\text{NH}$ is used for CO₂ adsorption at the bottom of the absorber column at the given gas flow rate, 1.0 kg/s, and the ionized $\text{R}_2\text{NH}_2^+$ and $\text{R}_2\text{NCO}_2^-$ are widely spread in the reactor and flow out through the solid exit on the right side.

Figure 8 shows the transient variation of CO₂ absorption fraction with time. The steady-state CO₂ absorption fraction depends on the gas flow rate. The CO₂ capture fraction, which is calculated with Equation (7), represents the overall adsorber column performance. It can be observed that the CO₂ capture ratio initially decreases because the CO₂ included in the initial condition flows out due to the increase in pressure with the gas flow from the bottom inlet. Afterward, the CO₂ capture ratio increases with time, and its steady-state condition of absorption is reached after about 40 seconds. The steady-state CO₂ absorption fraction depends on the gas flow rate. Figure 9 shows the transient variation of CO₂ absorbed mass with time. The CO₂ absorption rate increases as the flow rate increases, but the amount of increase decreases with the flow rate. The results of the CO₂ capture ratio along with the flow rate are displayed in Figure 10. When the flow rate increases, the amount of CO₂ absorbed per second increases. However, CO₂ adsorption fraction decreases if the flow rate is over 1.5 kg/s because the amount of amine is constantly given at every flow rate case. Thus, if the user wants 100% CO₂ absorption, 1.5 kg/s is the appropriate flow rate, but if a higher absorption rate is preferable despite some loss of CO₂ absorption in the reactor, a higher flow rate than 1.5 kg/s can be selected.

5 | CONCLUSIONS

In this work, the CFD simulation model was developed by using MFiX for the PEI-PTNTs suggested in the carbon capture experiments of PVAMU-CEES. For the verification of the simulation model, the same reactor model developed by NETL was built using MFiX, and the results were compared to the results provided by NETL. The heating and cooling effect on the CO₂ absorption was considered as assuming that the temperature distribution in the reactor is uniform and entering the higher temperature than the initial temperature of gas flow. The equilibrium and kinetic parameters of the CEES-developed PEI-PTNTs are adjusted based on the comparison of CO₂ absorption capacity between simulation...
and experiment. This calibrated simulation model was employed to examine the performance of the solid sorbents and find the optimized flow rate in the reactor model developed by NETL. When the flow rate increased, the amount of CO₂ absorbed per second increased, but the CO₂ adsorption fraction decreased if the flow rate was over 1.5 kg/s.

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