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# Biot number calibration of an Oxy-PFBC combustor through computational particle fluid dynamic analysis

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**Abstract**−The Biot number, one of the factors of the heat transfer coefficient, is computed through computational particle fluid dynamic simulation for the development of Oxy-PFBC technology. This technology enables no additional $CO_2$ separation for its capture by injecting pure oxygen, rather than air into pressurized bubbling fluidized bed boilers. This number is a dimensionless coefficient that is affected by the structure of the combustor and its heat exchangers, determining the degree of heat diffusion in the fluidized bed. In this manner, finding the proper Biot number is important for the development of Oxy-PFBC design program since it directly affects operability and performance. First, to compute the Biot number, the model of the Grimethrope PFBC combustor was demonstrated through the KEPCO-GTI Oxy-PFBC design program. The program showed good prediction of the Grimethorpe bed temperature profile after the calibration of the Biot number. The bed temperature profile for a specific combustor structural design and operation condition was computed; it was used to calibrate the Biot number suitable for the Oxy-PFBC combustor, through 3D computational particle fluid dynamics simulation (Barracuda program). The calibrated Biot number turns out to be ten times smaller, which is from 0.002 to 0.0002. Prior to computing the Biot number, to validate the simulation program, a comparison analysis was conducted with cold-flow fluidization test data. The results showed that the simulation matched well with the actual test data.

Keywords: Oxy-PFBC, Biot Number, Barracuda Simulation

## INTRODUCTION

Recent studies in thermal power generation have mainly focused on high-efficiency and clean energy technology development. The solution for the emission of $CO_2$, the main shortcoming of fossil fuel power generation, is now moving on to carbon neutrality with $CO_2$ capture and recycling from reduction technologies. Domestically, in Korea, thermal power generation is the main cause of particulate pollution. In this matter, the need for zero-emission power generation technology without stacks is an ultimate goal. To overcome this trend, KEPRI and GTI have conducted international joint development on Oxy-PFBC technology, a combination of oxygen firing and pressurized fluidized bed combustion (PFBC). Oxy-firing has the advantage of $CO_2$ capture and storage, while PFBC has high efficiency in terms of combustion and power generation systems.

The Biot number, to be determined by CFD analysis in this study, is a dimensionless quantity used for heat transfer calculation. This parameter determines the spatial temperature gradient across the body, which is affected by a heat source. A low ratio value indicates that the heat gradient is uniform along the body or structure, and a high ratio shows the opposite trend, which is a large, deviated temperature gradient. The effect of Biot number on thermal conductivity has been generally found through conducting actual experiments [1]. However, manufacturing and conducting tests with experimental test facilities have the disadvantages of being costly and difficult to implement. There are studies that estimate the Biot number effect by experiments conjugated with CFD analysis or a newly developed algorithm in order to design the turbine and drying process [2,3]. In the field of fluidized beds, efforts have been made to determine the Biot number for composing the heat mass transfer rate in the bed [4]. The assessment of Oxy-firing is conducted through numerical study for CFB boiler [5,6]. Likewise in this study, the CFD has been widely utilized for the analysis of particle behavior in the bubbling fluidized bed [7,8].

To develop Oxy-PFBC technology, the in-house design program needs the Biot number parameter to determine the temperature gradient along the combustor height, including the structural effect of the in-bed heat exchangers located in the Oxy-PFBC combustor. To validate the program and calibrate the Biot numbers, existing PFBC plant operation data, which were obtained from the IEA-Grimethorpe PFBC facility, located in the UK and operated in the period from 1981 to 1983, was utilized [9,10]. Several designs of in-bed heat exchangers were tested at the Grimethorpe PFBC facility [11,12]. The initial values of the Biot numbers inserted into the program were adjusted to match the temperature gradient data after implanting the Grimethorpe combustor and heat exchanger structural dimensions and its operating conditions. The Biot numbers derived for the two Grimethorpe in-bed heat exchanger cases are likely applicable to other geometries and operating conditions that are similar to either of the respective Grimethorpe cases, as shown in Fig. 1. However, the Oxy-PFBC in-bed heat exchanger configuration that we are developing is denser, so it is likely to have differ-

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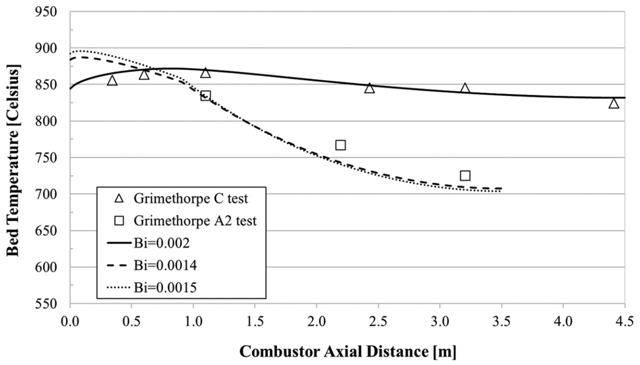


**Fig. 1. Biot number calibration with Grimethorpe PFBC cases.**

ent bed circulation characteristics; therefore, a different set of Biot numbers is needed.

One way to determine an appropriate Biot number for the Oxy-PFBC configuration is to run a non-reacting 3-D CFD analysis with heat addition in the lower portion of the combustor to simulate combustion heat release and heat removal in the upper portion of the combustor to replicate heat removal in the combustor. With the temperature gradient across the bed from the CFD analysis, the Oxy-PFBC design program can then be run to replicate the CFD case, and the Biot number can be adjusted until a match with the data can be found. The CFD model was validated before the simulation run for the Biot number.

## EXPERIMENT AND 3D SIMULATION

### 1. Minimum Fluidization Velocity (Umf) Verification

The first part of the validation process is to determine whether CFD can show appropriate Umf data under pressurized operating conditions. Therefore, we ran two simulation cases: one at atmospheric pressure and the other at 8 bar in a simple rectangular-shaped reactor. The initial and boundary conditions of the simulation are shown in Table 1 with the 3-D model shown in Fig. 2.

**Table 1. Initial and boundary condition of the simulation for the Umf verification**

| Description | Unit | Case 1 | Case 2 |
|---|---|---|---|
| Particle density | kg/m$^3$ | 2,520 | 2,520 |
| Particle diameter | mm | 1 | 1 |
| Gas temperature | °C | 870 | 870 |
| Gas pressure | Pa | 101,325 | 800,000 |
| Gas velocity | m/s | 0-0.57 | 0-0.57 |

### 2. Bed Density Verification

In the second part of the validation of the CFD model, the CFD analysis and the actual cold flow test were compared, targeting the bed density parameter. The test rig for the coal flow test is shown in Fig. 3. The cold flow test was conducted first, and then the simulation work was performed, replicating the test rig dimension into a 3-D model and the operating conditions into initial and boundary conditions, which are elaborated in Table 2. Total number of 647,325 cells was applied for the 3-D grid model with the Wen-Yu-Ergun drag model for the particles. The cold flow test was performed at six different U/Umf test points, which were calculated using pressure data from pressure transmitters. In the figure, the operating conditions of the cold flow test are shown, and according to this, the simulation condition is computed as shown in Table 3 and Fig. 4 based on air temperature and pressure at each point.

### 3. 3D Simulation for the Biot Number Calibration

Based on the prior two verification processes, the simulation for

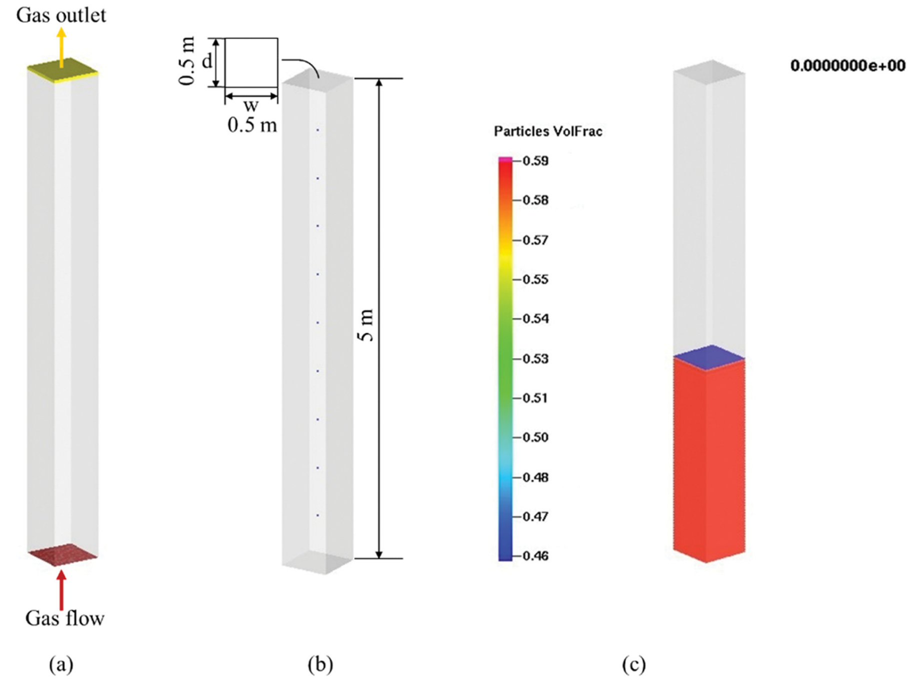


**Fig. 2. 3D model of the simulation for Umf verification ((a) gas flow direction, (b) dimension of the model, and (c) initial particle filling).**

Fig. 3. Test rig of the cold flow test.

Table 2. Initial and boundary condition of the simulation for bed density verification

| Description | Unit | Value |
|---|---|---|
| Fluidization air | | |
| Temperature | °C | 18-43 |
| Pressure | Pa | 101,325-124,106 |
| Particle diameter | mm | 1 |
| Particle density | kg/m$^3$ | 2,499 |
| Particle sphericity (Surface-volume diameter) | - | 1 |
| Initial void fraction | - | 0.479 |
| Initial bed height | m | 0.69 |

Table 3. Operation condition of the simulation for bed density verification

| Air temperature (°C) | Air pressure (Pa) | Umf (m/s) | U/Umf | Air mass flow (kg/s) |
|---|---|---|---|---|
| 36 | 106,179 | 0.83 | 0.5 | 0.03 |
| 36 | 111,006 | 0.82 | 1.0 | 0.06 |
| 36 | 114.453 | 0.81 | 1.5 | 0.09 |
| 36 | 116.521 | 0.81 | 2.0 | 0.13 |
| 36 | 118,590 | 0.8 | 2.5 | 0.16 |
| 36 | 121,348 | 0.79 | 3.0 | 0.19 |

Biot number calibration was carried out. The initial conditions for the simulation are listed in Table 4. The bed particle we employed was olivine sand 30-60 and its PSD is shown in Table 5. In Table 6 and Fig. 5, the boundary conditions for the simulation are elaborated. For heat addition, the in-bed heat exchanger tubes in section B were set to 1,200 °C, and the heat removal of section A was 250 °C for the tube surface throughout the simulation. To demonstrate the pressurized condition, the fluidization gas and combustor exit sets were set to 800 kPa of pressure as the boundary conditions. The gas composition is 81% carbon dioxide and rest for oxygen to have similar fluidization conditions as Oxy-combustion. The mass flow has 3.5 U/Umf, which is 0.471 kg/s. Six(6) transient points for recording the particle and gas temperature were placed within the 3D model.

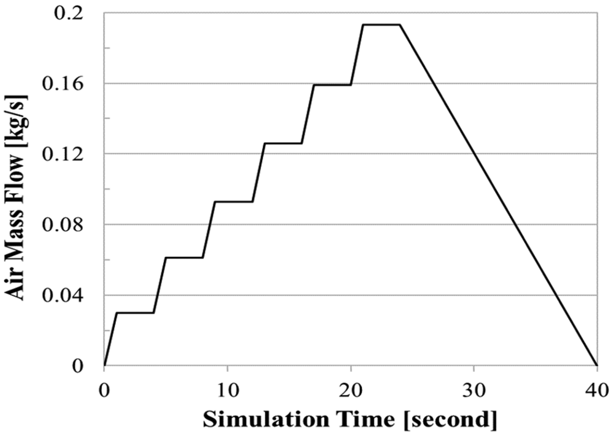


Fig. 4. Diagram showing the air mass flow for the 3D simulation of bed density verification.

Table 4. Initial condition for the simulation of the Biot number calibration

| Description | Unit | Value |
|---|---|---|
| Bed material | - | Olivine Sand 30-60 |
| Particle density | kg/m$^3$ | 3,200 |
| Particle diameter | μm | 612.6 |
| Initial particle temperature | °C | 500 |
| Initial bed height (from grid) | m | 1.33 |
| Initial bed volume fraction | - | 0.5 |
| Umf (Ergun) | m/s | 0.32 |

Table 5. Particle size distribution of particles inputted into the Biot number simulation

| Aperture size (μm) | Mass fraction |
|---|---|
| >1,180 | 0.05 |
| 850-1,180 | 0.35 |
| 600-850 | 0.35 |
| 425-600 | 0.1 |
| 300-425 | 0.025 |
| 212-300 | 0.025 |
| 0-212 | 0.025 |

## RESULTS AND DISCUSSION

### 1. Verification Process of the 3D Simulation

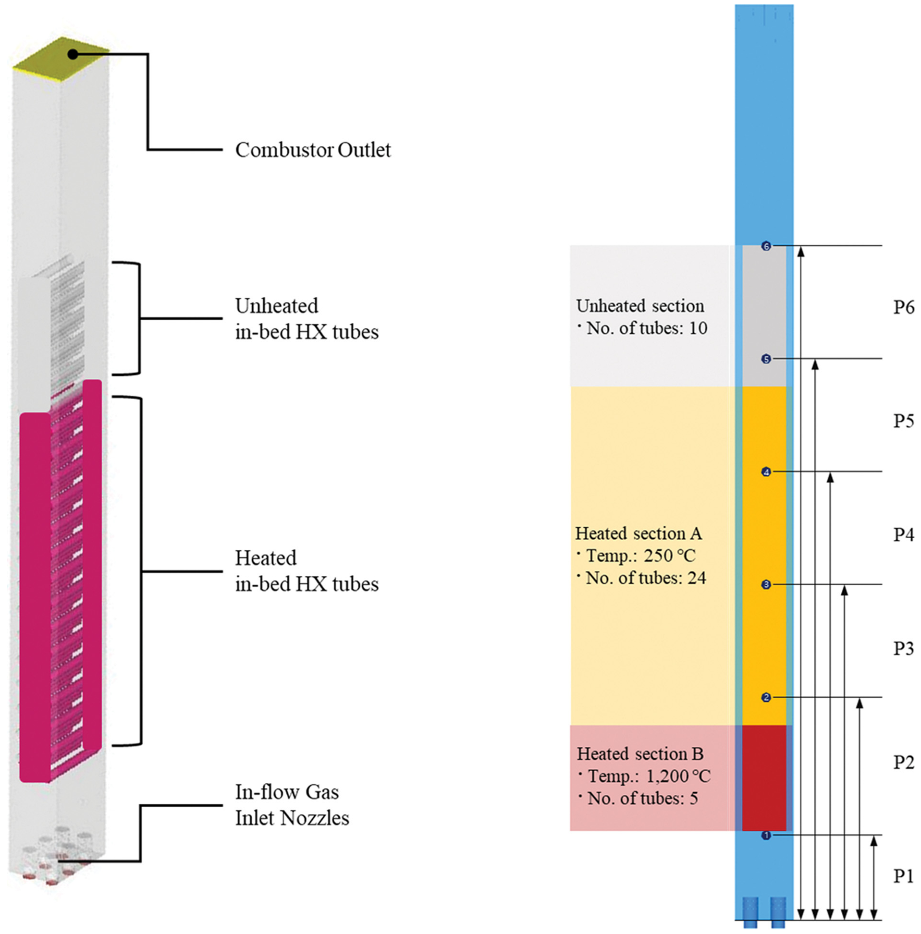
Two simulation cases were run to check the 3D simulation ability

**Table 6. Boundary condition for the Biot number simulation**

| Description | Unit | Value |
|---|---|---|
| Heated tubes | | |
| - Section A | °C | 250 |
| - Section B | °C | 1,200 |
| Unheated tubes | °C | - |
| Combustor exit | | |
| - Temperature | °C | 300 |
| - Pressure | kPa | 800 |
| Injected fluidization gas | - | |
| - Temperature | °C | 300 |
| - Pressure | kPa | 800 |
| - Composition | - | $CO_2$ 81%/$O_2$ 19% |
| - Mass flow | kg/s | 0.471 (U/Umf=3.5) |
| Ambient condition | | |
| - Temperature | °C | 20 |
| - Pressure | kPa | 1 |

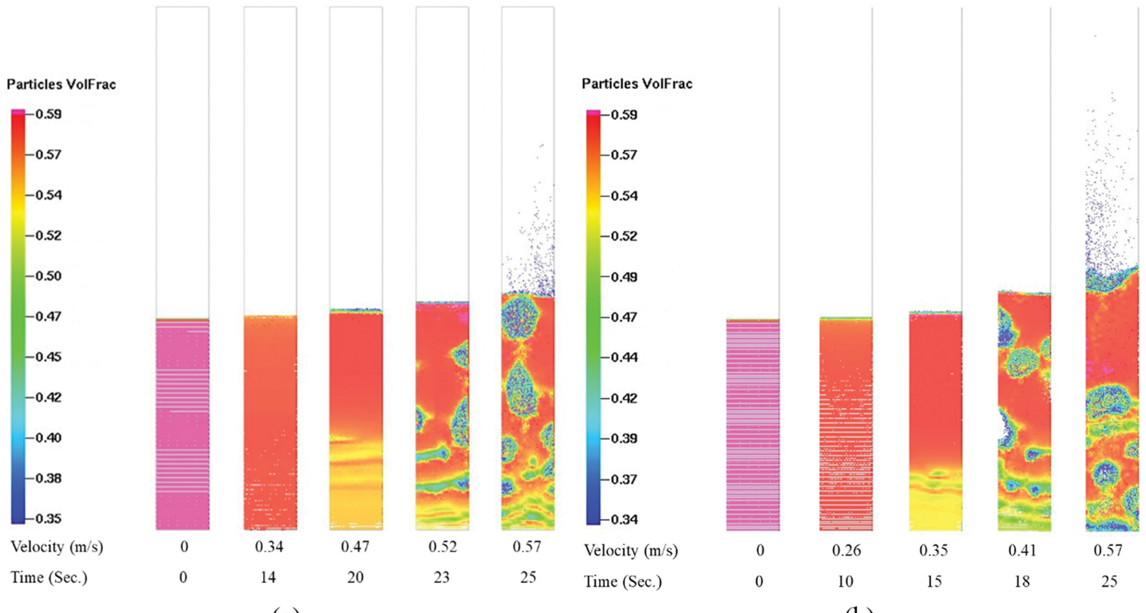
of demonstrating the bed pressure, indicating the minimum fluidization velocity, which is a basic and vital parameter in FBC. One is at atmospheric pressure and the other is at an elevated pressure of 8 bar. When we look at the volume fraction results, which are shown in Fig. 6, where case 1 of atmospheric and case 2 of 8 bar, the data point of simulation time and fluidization velocity at each fluidization behavior change is shown in the bottom part of Fig. 6. The fluidization behavior changes are bed height remaining the same, bubble creation in the bed, and injection of particles into the empty upper part of the combustor at the surface of the bed. Case 2, which is a pressurized condition, shows faster fluidization of the bed than case 1. In addition to the volume fraction image results, the pressure drop recorded at two different points in the bed throughout the simulation shows the same bed behavior, which indicates faster fluidization at a smaller fluidization velocity with a more vigorous bed fluidization environment, as shown by the larger pressure drop across the bed in Case 2, as shown in Fig. 7. To verify the Umf value, we compared the simulation-derived Umf with the pressure drop data and the literature rule-based value by Wen and Yu (1966). The error between Umf derived from CFD and Wen & Yu calculations was within 10%, as shown in Table 7.

Fig. 8 shows the particle volume fraction as the simulation time passes, and on the right side of the figures, we also tracked the fluid velocity vectors and their values because it was important to determine whether the simulation could demonstrate fluidization



(a) (b)

**Fig. 5. 3D model of the Biot number simulation showing the boundary condition ((a) Boundary condition applied 3D model, (b) Transient points and temperature of tubes in 3D model).**



(a) (b)

**Fig. 6. Simulation results of the volume fraction for the Umf verification ((a) atmospheric pressure in case 1 and (b) 8 bar pressure in case 2).**

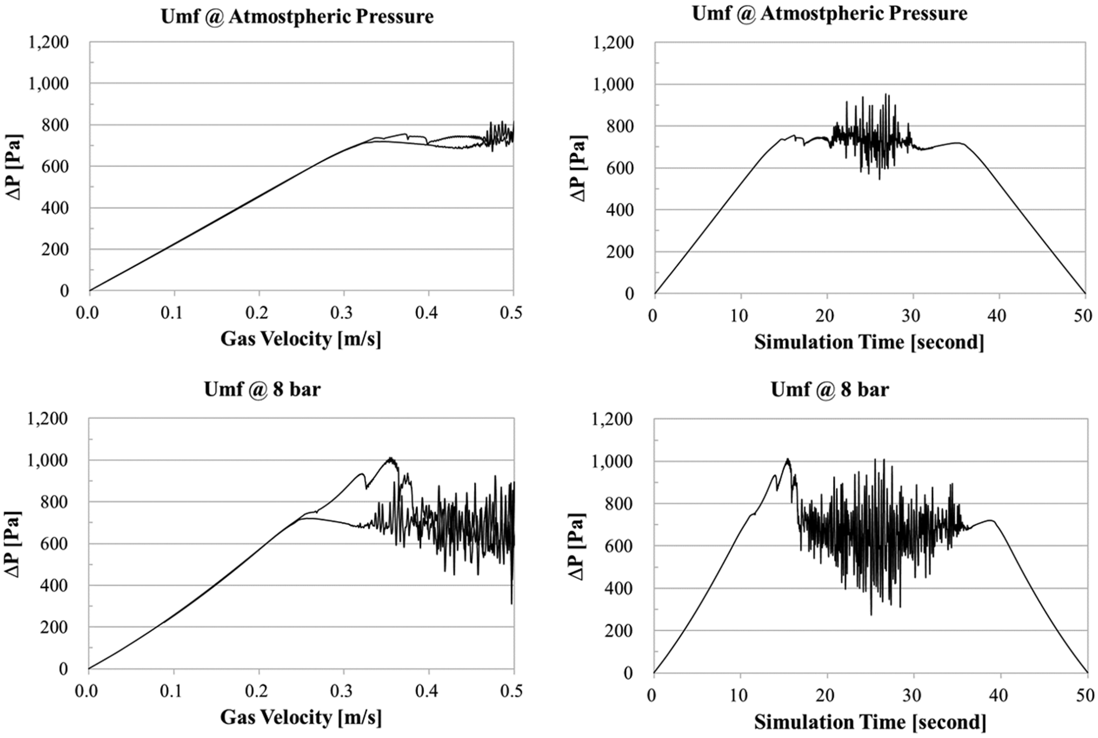


**Fig. 7. Simulation results of the pressure drop in the bed for cases 1 and 2.**

**Table 7. Comparison between the literature rule-based calculation and the simulation results on Umf**

| Simulation case | Pressure | Umf (m/s) | | Error, % |
|---|---|---|---|---|
| | | Simulation | Wen & Yu | |
| Case 1 | Atmospheric | 0.34 | 0.31 | 8.6 |
| Case 2 | 8 bar | 0.26 | 0.25 | 4.9 |

gas flow from each hole on the nozzles. It is a crucial part of the simulation to demonstrate these porous fluidization gas nozzles through the simulation in order to elaborate the bed behavior of the real cold flow test because fluidization gas flow affects the bed material behavior in a large amount. We observed that CFD showed bed behavior similar to the cold flow test. The CFD predicted a higher bed density along the walls compared to the combustor

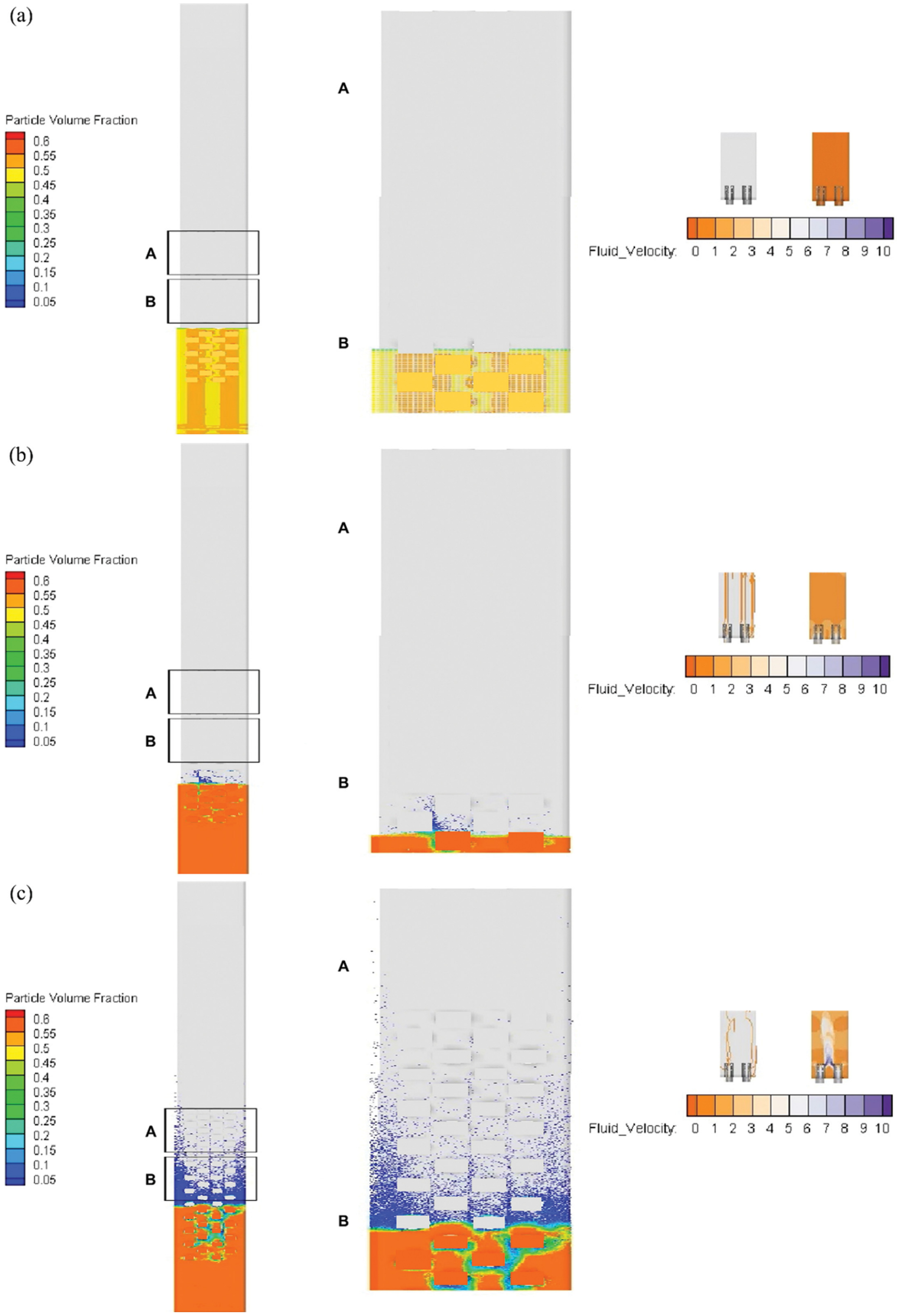


**Fig. 8. Simulation results of the volume fraction and fluidization gas velocity and its vector at different simulation times ((a) 0, (b) 3.2, (c) 7.4, (d) 11.1, (e) 15.2, (f) 18.9, (g) 23, and (h) 40 s, respectively).**

middle, as was observed during the test, and the bed material falling down along the walls. We also calculated the average bed density of the bed of the CFD results, as shown in Fig. 9. The results show that the CFD average bed density matches the bed density calculated from the cold flow test pressure data at each U/Umf data point, as shown in Fig. 9.

### 2. 3D Simulation for Biot Number and Calibration

The results of the 3D simulation for the Biot number are shown

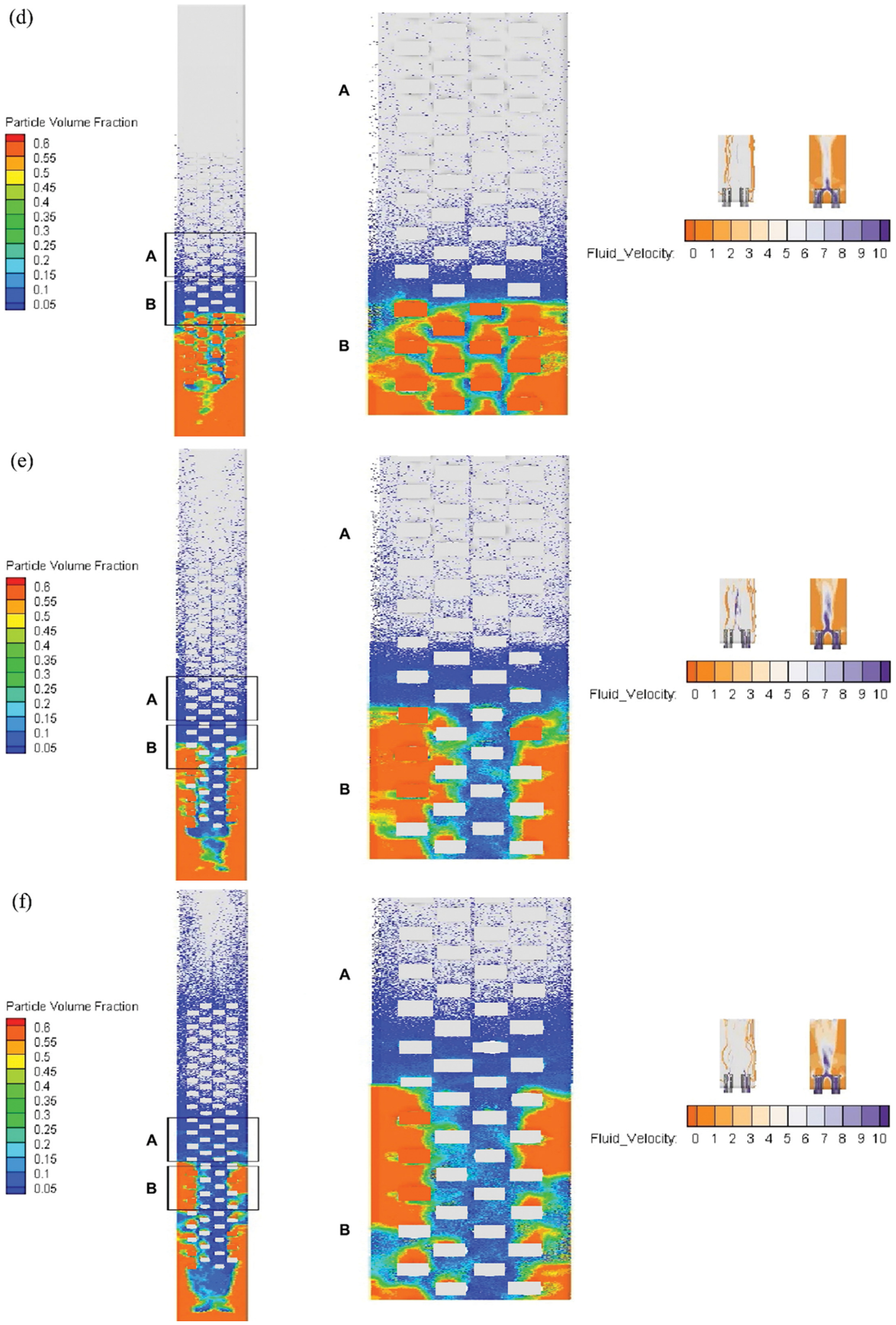


**Fig. 8. Continued.**

in Fig. 10, showing the particle temperature recorded at each of the model's transient points. As expected, P2 point, which was placed immediately after the heat addition of zone A, had the highest particle temperature. After a simulation time of 100 s, the particle temperature at each transient point appears to have a convergence region. Therefore, we extracted the bed temperature profile from this region

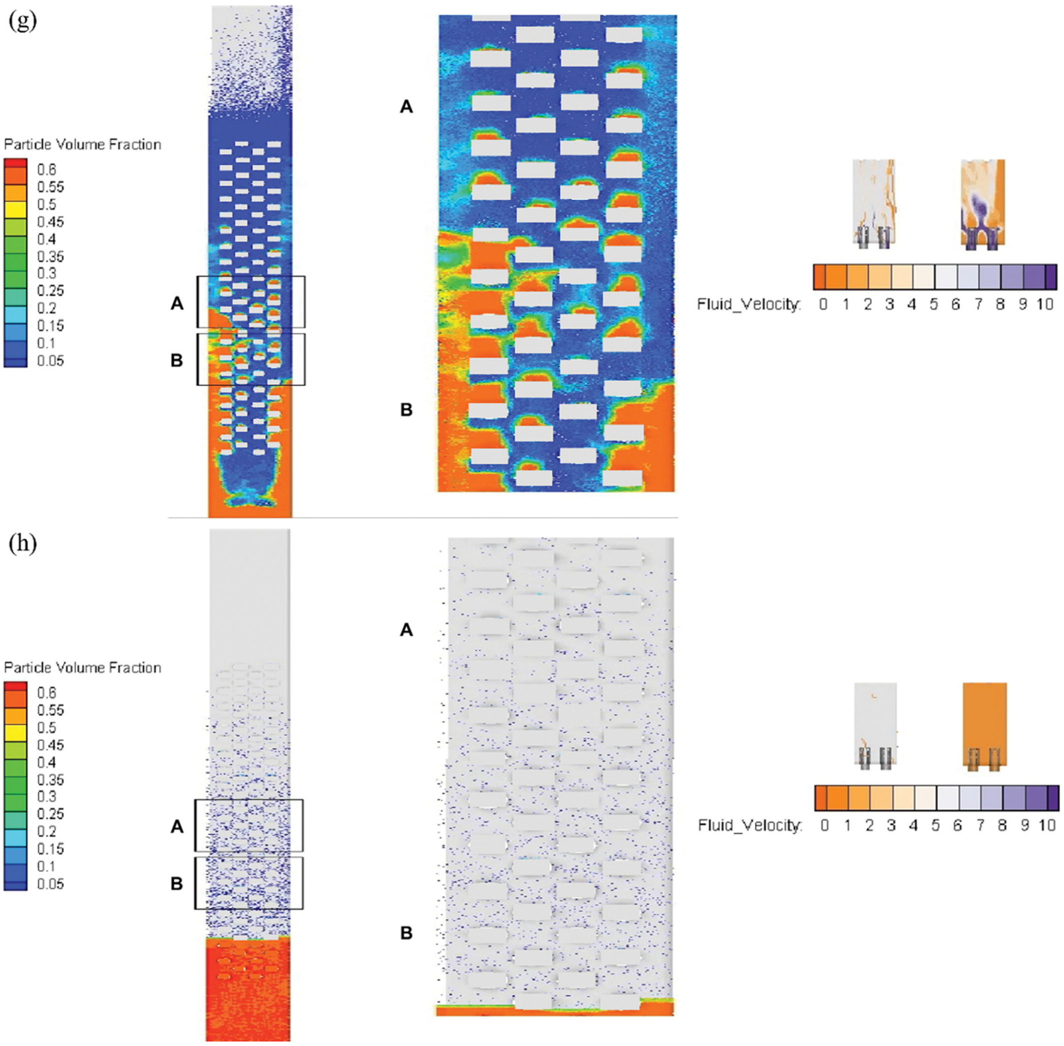


**Fig. 8. Continued.**

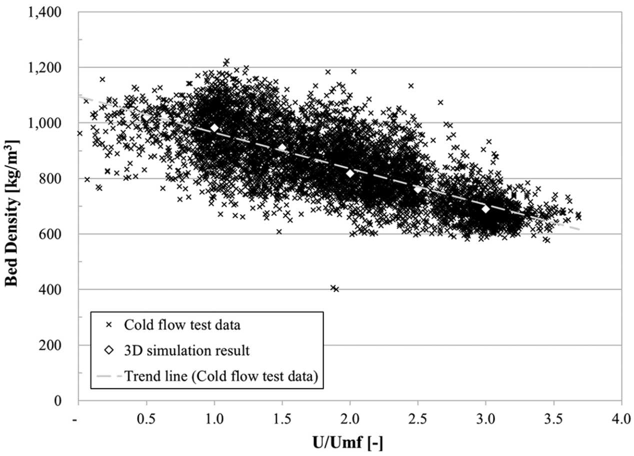


**Fig. 9. Comparison of the bed density between the cold flow test data and 3D simulation results.**

for the Biot number calibration of the Oxy-PFBC design program. The final bed temperature profile along the combustor height is shown in Fig. 11, and the gas temperature profile, which can be found in Fig. 12, is more highly affected by heat addition than the bed particle, as expected. With these bed temperature profile results, a Biot number calibration analysis was conducted to match the CFD analysis and determine a reasonable estimate for the Biot number. For this initial case, the Biot number was set to 0.002, which is the default value used to evaluate the Oxy-PFBC combustor design. The results shown in Fig. 13 indicate that the program predicted bed temperature profile (irregular dotted line) is not a particularly good match with the 3D simulation prediction (solid line). The initial bed temperature at X=0 is under-predicted by the program by 100 °C (600 °C versus 700 °C). The peak temperature was over-predicted by the program (840 °C versus 730-790 °C), but the location is approximately correct. The minimum temperature is significantly under-predicted by the program (580 °C versus 660 °C) and the location is off by 0-0.2. After several iterations with Biot number, a Biot number of 0.0002 (an order of magnitude smaller than the initial case), showed a significantly better match, as shown by the dotted line. In this case, the initial bed temperature at X=0 is approximately 700 °C and the peak temperature is close to approxi-

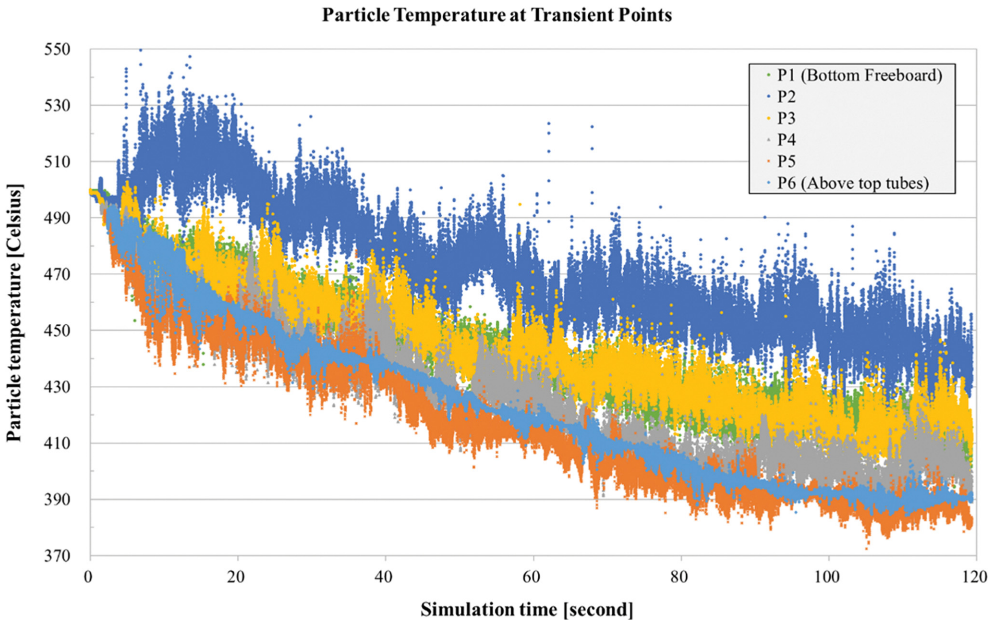


**Fig. 10. Simulation result of the particle temperature at transient data points in the 3D model.**

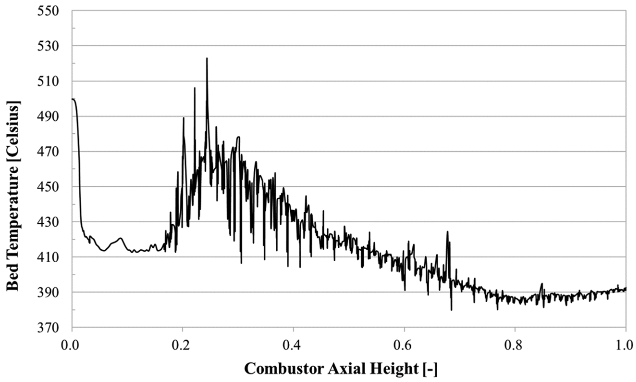


**Fig. 11. Simulation result of the bed temperature profile along the combustor axial height.**

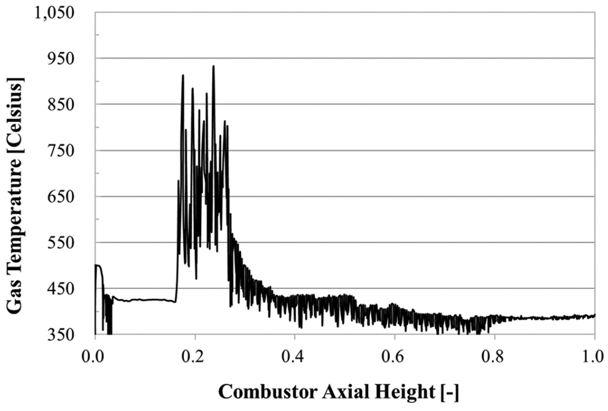


**Fig. 12. Simulation result of the gas temperature profile along the combustor axial height.**

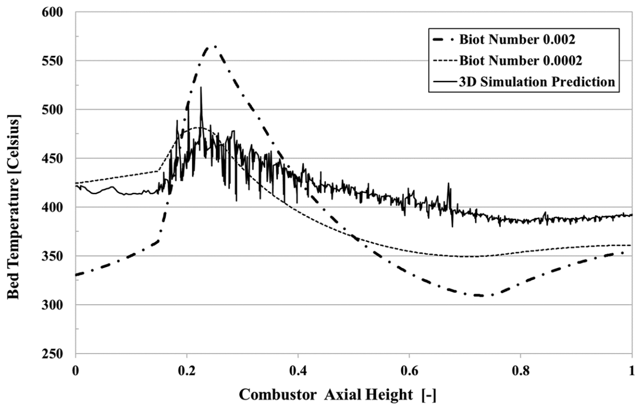


**Fig. 13. Comparison of the bed temperature profile between the Oxy-PFBC design program with Biot numbers 0.002 and 0.0002 and the 3D simulation prediction.**

mately 770 °C. The minimum bed temperature is under-predicted by the program relative to the 3D simulation (620 °C versus 660 °C); however, it is much better than the previous comparison with the initial case of Biot number.

## CONCLUSIONS

The Biot number, used in the in-house Oxy-PFBC design program to determine the amount of thermal diffusion in the bed, affects the bed temperature profiles, which also affects the operability and performance. In the Biot number calibration analysis, the preliminary analysis results indicate that the initial default value of the Biot number is likely conservative, so the actual Biot number is likely to be significantly lower and the temperature profiles in the combustor are expected to be more uniform than previous predictions based on the program results. Using CFD to resolve uncertainties with Biot number, the results show that the program with a lower Biot number shows a good match with the bed temperature profile from the 3D simulation. This means that the Oxy-PFBC combustor structural design has a more uniform heat distribution, which was determined using CFD analysis. Prior to the calibration analysis of the Biot number, the verification process of CFD was conducted, targeting two important parameters in the fluidized bed: minimum fluidization velocity and bed density. The CFD results for these parameters were compared with the literature rule-based calculated value and the cold flow test, respectively, and showed the ability of CFD analysis to predict these parameters with appropriate match.

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