COUPLED CFD&DEM ANALYSIS OF PARTICLE-FLUID MOMENTUM AND HEAT TRANSFER AT LOW-PRESSURE REGIMES

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ABSTRACT

The detailed knowledge of particle-fluid interactions at low-pressure regimes is fundamental in fluidization processes. Fluidization at low-pressure conditions in adsorption systems dedicated to utilizing waste heat for chill production and desalination is considered one of the means of heat transfer intensification in adsorption reactors. Therefore, the paper presents a new approach to modeling the adsorption reactor, including the particle-fluid interaction at low-pressure regimes using two-way coupled Computational Fluid Dynamics (CFD) and Discrete Element Modelling (DEM). Although combined CFD&DEM analysis have already been presented in the literature, this is the first such comprehensive approach for modeling low-pressure fluidization using such a technique. It reveals great potential in optimizing the construction of adsorption reactors with numerical methods and constitutes a promising alternative for modeling particle-fluid interactions at low-pressure regimes. The developed comprehensive model incorporating CFD=&DEM techniques is validated against the experimental data collected on the test stand dedicated to experimental research of adsorption reactors operating in low-pressure regimes. The results of the presented research indicate that the coupled CFD&DEM modeling approach is a powerful and cost-effective research tool capable of effectively analyzing complicated physical phenomena occurring in low-pressure regimes. Moreover, the research will allowed to define the design and operating parameters of the adsorption systems that allow intensifying the momentum, heat, and mass transfer in the adsorption reactor and, consequently, significantly contribute to developing and popularizing the adsorption cooling technology.

1 INTRODUCTION

Combining computational fluid dynamics (CFD) with discrete element modeling (DEM) has been presented in the scientific literature. Such an approach allowed to analyze the clustering behavior in a riser applied in catalytic processes involving rapid catalyst deactivation (Ramírez et al. 2023). The authors used five drag force correlations in a combined CFD&DEM Immersed Boundary Model to predict the clustering. The simulation results were compared with experimental data obtained from a pseudo-2D riser in the fast fluidization regime. The clusters were detected based on a core−wake approach using constant thresholds. Although good predictions for the global (solids volume fraction and mass flux) variables and cluster (spatial distribution, size, and number of clusters) variables were obtained with two of the approaches in most of the simulations, all the correlations show significant deviations in the onset of a pneumatic transport regime.

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Another numerical research involving the CFD&DEM approach was carried out in (Wu, Li, and Zuo 2023) for modeling the fast fluidization of fine particles in a micro riser. A drag model that relies on the surrounding environment of particles, namely the particle circumstance-dependent drag model was applied. The simulations indicated that the local structure in a micro-fluidized bed exhibits particle aggregation, which is a natural property of fast fluidization, forming a structure where a continuous dilute phase and dispersed concentrated phase coexisted. The authors proved the strong effect of solid back-mixing in a micro-fluidized bed, leading to relatively low outlet solid flux. The gas back-mixing effect was, however, not so distinct. The axial porosity showed a monotonically increasing distribution with the bed height but did not strictly follow the single exponential distribution. The solid volume fraction at the bottom of the bed was significantly lower than the correlated value in circulating fluidized bed. The axial heterogeneous distribution of the cross-sectional average porosity in the lower half of the bed was also weakened. The radial porosity showed a higher distribution pattern in the central region and a lower one in the sidewall region. The authors considered the CFD&DEM approach an effective research tool.

Simulation of heat transfer behavior in a fluidized bed by a combined thermal model in the CFD&DEM coupling was presented in (Flamarz 2022). The numerical research implemented the CFD&DEM coupling to investigate the transport of heat energy in a fluidized bed. A numerical test compared the numerical and analytical results for a single particle in a column. The numerical results presented well adequacy with the analytical results. Three methods of column heating, including base heating, walls heating, and as well as walls and base heating, were proposed in the simulations. The results revealed that the fluid's proper inlet velocity and imposed temperature are crucial in the heating process for the fluidized beds since the particles need to provide time for the heat transport process.

Similar approach was also considered in (El-Emam et al. 2021). The authors considered CFD&DEM a promising numerical method that can model discrete particles by tracking the motion of each particle in fluid flow. They proved that DEM has been extensively used in the field of engineering, where its application is starting to gain popularity. CFD has been able to simulate complex fluid flows with a quantitative and qualitative description of the temporal and spatial change of the flow field. The paper reviewed the recent strategies and the existing applications of the CFD&DEM coupling approach in aerodynamic systems of bio-particles. It mainly represented four principal aspects: the definition of aerodynamic systems with its principles, modeling of particle motion including interaction forces of particle–particle and particle–fluid in the system, CFD&DEM coupling methodologies, and drag correlation models with theoretical developments, and the applications of aerodynamic systems related to the agricultural field.

The published literature indicates that CFD&DEM is a promising approach to studying the particulate matter behavior immersed in fluid flow, and it could benefit from developing and optimizing the device’s geometry and operations.

Therefore, the paper presents a new approach to modeling the adsorption reactor, including the particle-fluid interaction at low-pressure regimes using two-way coupled CFD&DEM. CFD generates quantitative predictions of fluid-flow phenomena based on the conservation laws (mass, momentum, and energy) governing fluid motion within the computational domain. Discrete approximations replace the mathematical equations describing flow characteristics at mesh elements that must be close enough so that the solution is independent of the mesh elements' sizes. The discrete equations are derived using finite differences or finite volumes, linking the mesh elements together. On the contrary, the DEM is a mesh-free method and does not solve the continuum equations of motion. Hence, no stress-strain constitutive law for the material is needed. Instead, a stress-strain relationship can be obtained as an output from the DEM model to be coupled with CFD. The derivation of continuous equations of state and motion for granular media is complicated, and thus, DEM aims to solve these problems by simulating the evolution of every particle in the system subjected to contact forces. Instead of numerical integration of the continuum equations of motion and state, the motion of each particle is simulated, as well as the interaction for each particle-particle and particle-fluid pair. All particles within the computational domain representing the adsorption reactor are tracked in a Lagrangian way, explicitly solving Newton’s second law that governs translational and rotational particle motion.

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2 MOTIVATION AND NOVELTY

Despite the research activities aiming to improve the adsorption cooling technology (KRZYWANSKI et al. 2021; Krzywanski et al. 2019; K. Grabowska et al. 2018; K. Grabowska, Sztekler, et al. 2021; Kulakowska et al. 2020; Karolina Grabowska et al. 2017; Sztekler, Kalawa, Nowak, et al. 2019; Krzywanski et al. 2023; Skrobek et al. 2022; Kulakowska et al. 2023; Sztekler, Kalawa, Mika, et al. 2019), further research and development are needed to optimize it and make it more cost-effective for commercial applications. Therefore, this paper aims to propose the concept of using CFD coupled with DEM to analyze the benefits of using fluidization to improve heat and mass transfer within the adsorption bed. To the best of our knowledge, the CFD&DEM approach for fluidized adsorption bed modeling has never been used by other researchers. Therefore, this approach reveals great potential for further improvement in the construction of adsorption reactors. The application of the new combined CFD&DEM approach will deliver new knowledge, especially concerning the adsorbate velocity field within the sorption reactor under low-pressure regimes (operating pressure below 3 kPa). Moreover, it will allow to design of the reactor and control of the process in a way that maximizes the heat and mass transfer within the whole volume of the adsorbent.

3 EXPERIMENTAL TEST STAND

The experimental test stand was adapted to deliver the data necessary to validate the developed CFD&DEM model of the fluidized sorption reactor. The schematic diagram and the photograph of the experimental test stand are depicted in Figure 1. The test stand consists of a bottom tank operating as an evaporator and an upper tank equipped with an interchangeable sorption reactor. Both tanks are connected to the vacuum pump and to each other via valves controlled by the data acquisition and control unit. Both tanks are equipped with electrical heating and an additional inlet/outlet to be supplied with liquid medium (water) for cooling or heating. Moreover, mass sensors, absolute and relative pressure sensors, and temperature sensors are installed in both tanks. A detailed description of the experimental test stand is provided in (K. Grabowska, Zylka, et al. 2021). The top tank can be equipped with different types of sorption reactors, which is beneficial for the validation research.

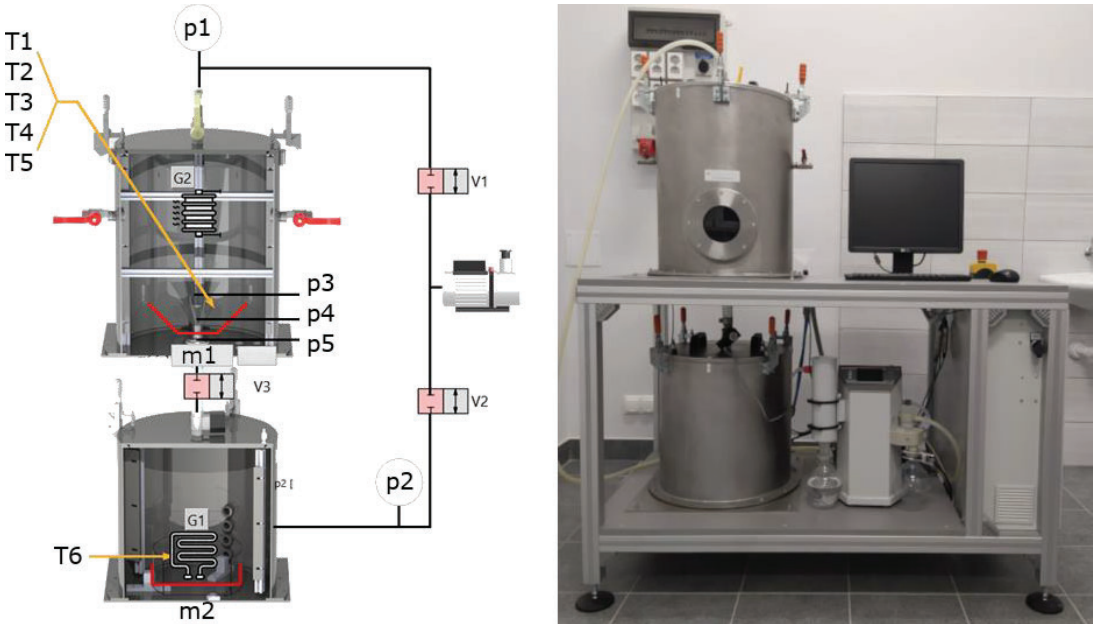

Figure 1: Experimental test stand: schematic diagram (left) and photograph (right) (Sosnowski et al. 2023)

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4 RESEARCH OBJECT

The heat and mass transfer in the sorption reactor are the main factors influencing the overall performance of the adsorption chiller. Therefore, based on the best practices and numerical models developed and validated within the previous research concerning honeycomb sorption reactor (Sosnowski et al. 2019) and multi-disc sorption reactor (Sosnowski 2019), the novel concept of a disc-shaped fluidized sorption reactor depicted in Figure 2 has been proposed to maximize the coefficient of performance of the adsorption chiller. The diameter of the reactor was 30 mm and the height was 150 mm. The fixing net was installed at the bottom and at the top of the fluidized reactor to prevent the adsorbent from leaving the reactor volume as a result of excessive adsorbate flow from the evaporator (lower chamber) to the sorption chamber (upper chamber).

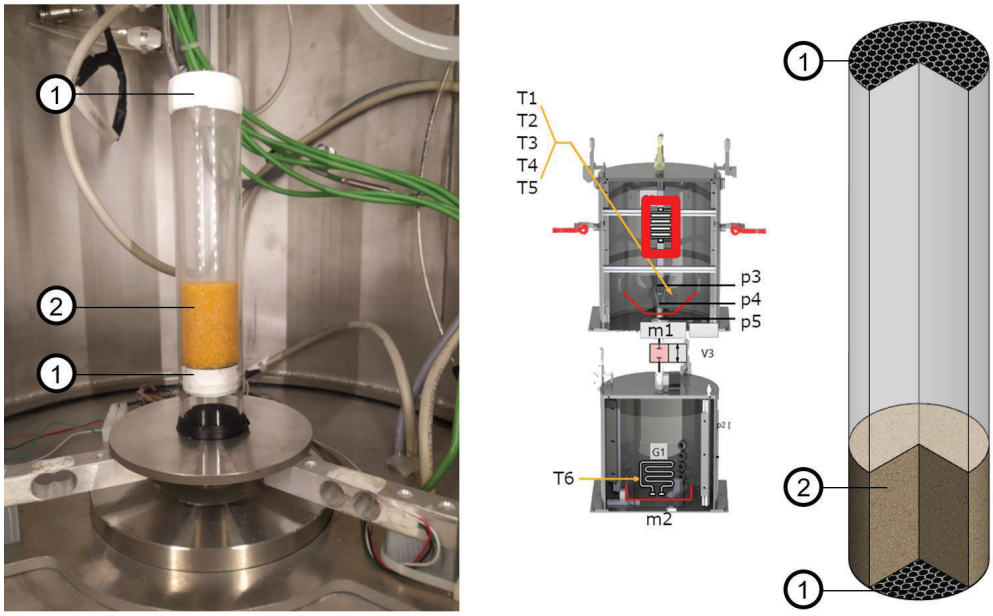

Figure 2: Disc-shaped fluidized sorption reactor: 1 – fixing net, 2 – silica gel (Sosnowski et al. 2023)

5 RESULTS AND DISCUSSION

Two-way CFD & DEM coupling, in which the fluid flow affects the particle movement, and the particle flow influences the continuous phase behavior was applied within the carried out numerical research. The CFD solver was configured as pressure-based, and the analysis was performed for the transient state. The standard k-ε viscous model was applied. Pressure velocity coupling by the COUPLED algorithm was used as a solution method. Least squares cell-based spatial discretization was chosen in case of gradients, second-order in case of pressure, second-order upwind in case of momentum as well as energy, and first-order upwind in case of turbulent dissipation rate. The model convergence was defined based on qualitative and quantitative monitoring of residuals as well as the thermodynamic stability of the model.

All the initial and boundary conditions of the two-way coupled CFD&DEM numerical analysis were consistent with the experimental data. The adsorbate was water vapor and the adsorbent was the silica gel of bulk density equal to 750 kg/m^3, specific heat equal to 920 J/kg·K, and thermal conductivity of 0.176 W/m·K. Seven granulation ranges of silica gel were applied within the research: 100 μm – 160 μm, 160 μm – 200 μm, 200 μm – 250 μm, 250 μm – 300 μm, 300 μm – 350 μm, 350 μm – 400 μm, and 400 μm – 500 μm.

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The obtained experimental and numerical results concerning pressure difference between the upper, and bottom tanks of the test stand, as well as temperature of the silica measured and calculated through the adsorption process lasting for 20 seconds and for different silica gel granulation sets are depicted in Figure 3 to Figure 9. The temperature obtained during the experimental research was measures with a thermocouple sensor located in the canter of the horizontal cross-section of the disc-shaped fluidized sorption reactor 30 mm above its bottom. The temperature obtained during the numerical research is the mean temperature of silica gel particles in the spot corresponding with the location of the thermocouple in the disc-shaped fluidized sorption reactor.

In the case of silica gel granulation 100 µm – 160 µm (Figure 3), the initial pressure difference was 1020Pa, and the initial temperature was 38.35 °C. The above values were applied as initial conditions for the CFD&DEM modeling. The correlation of the experimental and numerical results is very satisfying through the first three seconds of the process, however, some differences in measured and modeled pressure difference values start to appear in the fourth second and beyond. The modeled pressure seems to be more stable than the measured one. Such behavior is maintained until the eleventh second of the process. The above-mentioned discrepancies induce similar differences between the measured and modeled temperature of the sorption bed particularly between the sixth and tenth second of the process. The highest difference between the experimental and CFD&DEM results is 0.65 °C in the case of temperature, and 106 Pa in the case of the pressure difference.

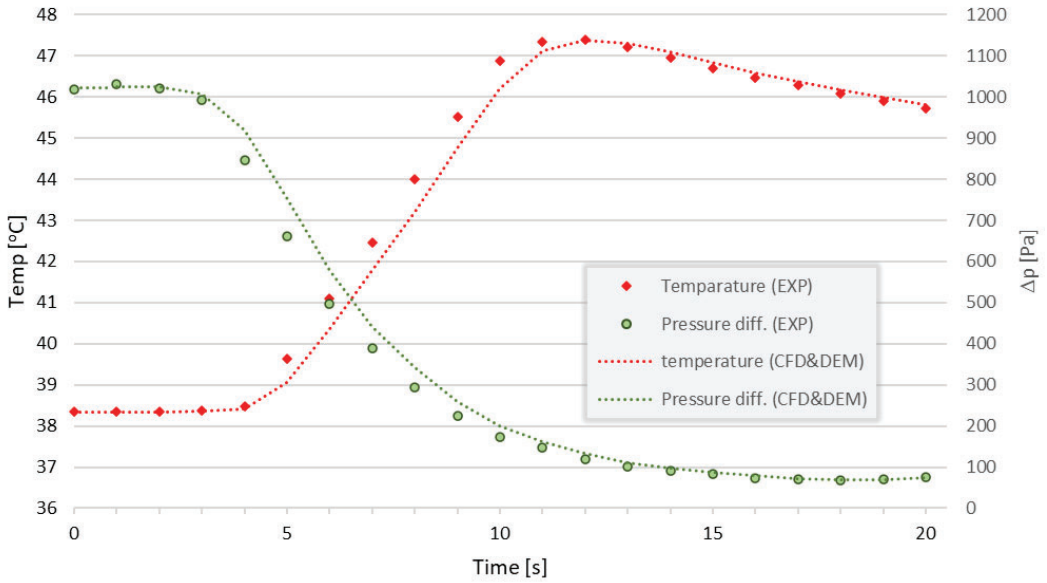

Figure 3: Experimental (EXP) and numerical (CFD&DEM) results concerning silica gel temperature and pressure difference between the tanks for granulation equal to 100µm - 160µm

In the case of silica gel granulation 160 µm – 200 µm (Figure 4), the initial pressure difference was 964 Pa, and the initial temperature was 36.63 °C. Similarly, as for the granulation of 100 µm – 160 µm, differences in measured and modelled pressure difference values start to appear in the fourth second and persist until the thirteenth second. The highest difference between the experimental and CFD&DEM results is 0.98 °C in case of temperature, and 86 Pa in case of the pressure difference.

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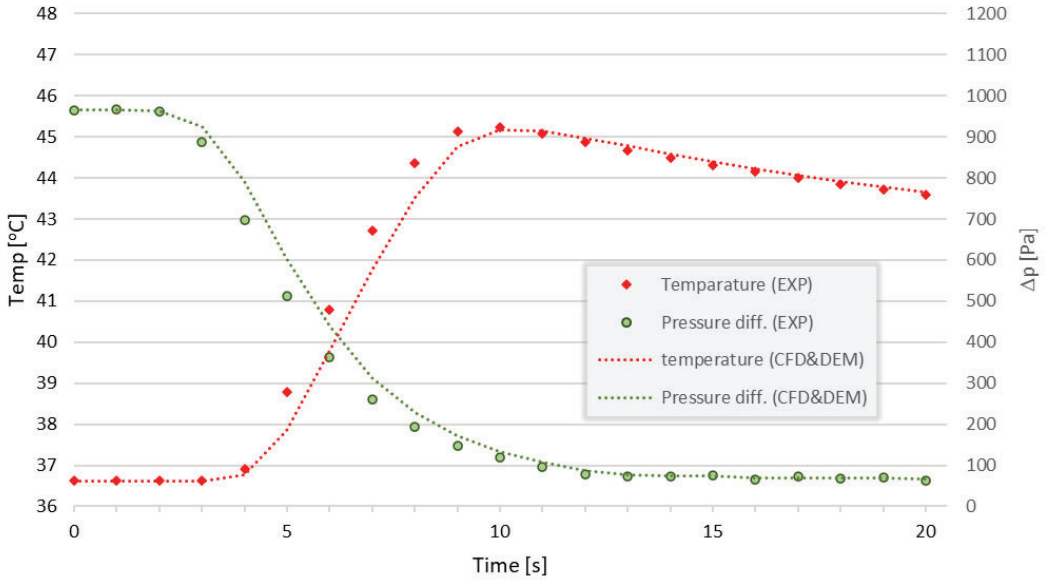

Figure 4: Experimental (EXP) and numerical (CFD&DEM) results concerning silica gel temperature and pressure difference between the tanks for granulation equal to 160 μm – 200 μm

A different temperature variation is observed for the silica gel granulation 200 μm – 250 μm (Figure 5). The initial pressure difference was 963 Pa, and the initial temperature was 38.35 °C. The above values were applied as initial conditions for the CFD&DEM modeling for this granulation set. The correlation of the experimental and numerical results is also satisfying through the first three seconds of the process, however, some differences in measured and modeled pressure difference values start to appear in the fourth second and so on. The modeled pressure difference values are slightly higher than the measured ones. Such behavior lasts until the eleventh second of the process. The temperature variation obtained in numerical research are in good agreement with the measured values.

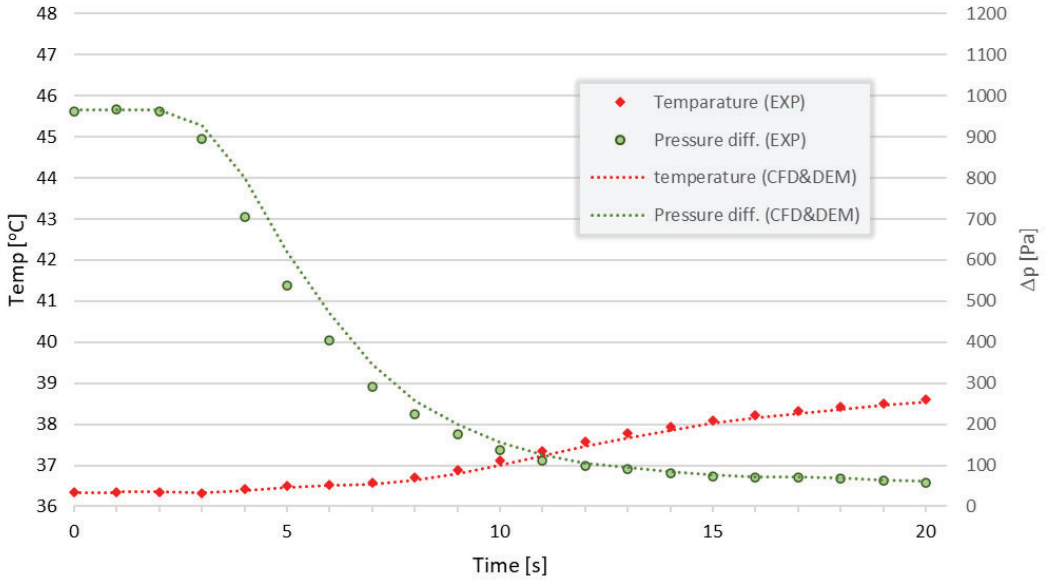

Figure 5: Experimental (EXP) and numerical (CFD&DEM) results concerning silica gel temperature and pressure difference between the tanks for granulation equal to 200 μm – 250 μm

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Very similar behavior of pressure difference and temperature to the granulation of 200 μm – 250 μm is observed for the granulation of 250 μm – 300 μm (Figure 6). The initial pressure difference was 961 Pa, and the initial temperature was 36.37 °C. Through the first four seconds of the process the correlation of the experimental and numerical results is acceptable in terms of pressure difference and in terms of temperature the correlation is very good for the first five seconds. However, some differences in measured and modeled pressure difference values start to appear in the fourth second and in the sixth second in the case of temperature. The modeled pressure difference values are higher than the measured ones and the highest difference is 76 Pa. The temperature variation obtained in numerical research is in good agreement with the measured values.

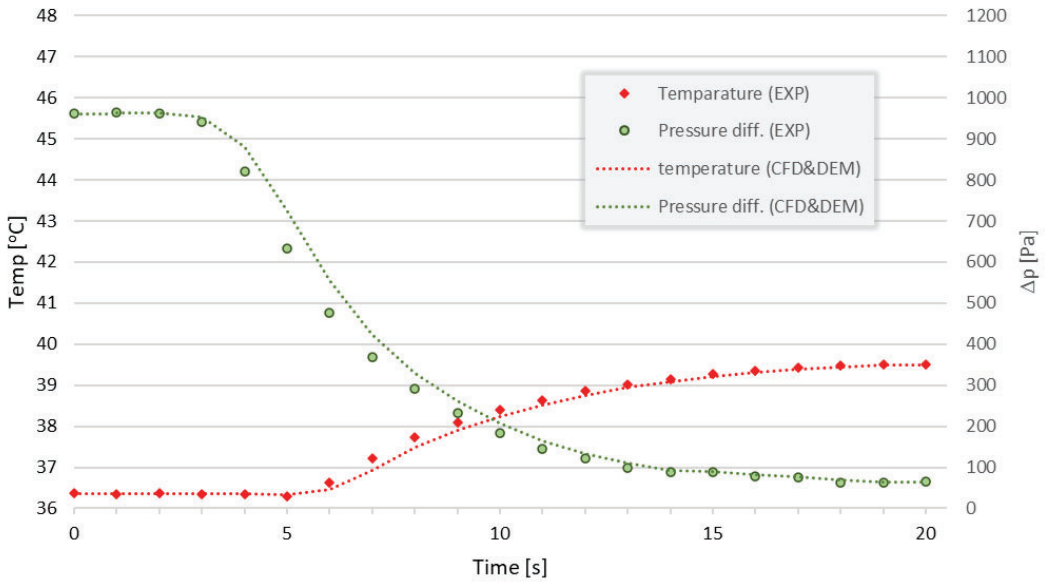

Figure 6: Experimental (EXP) and numerical (CFD&DEM) results concerning silica gel temperature and pressure difference between the tanks for granulation equal to 250 μm – 300 μm

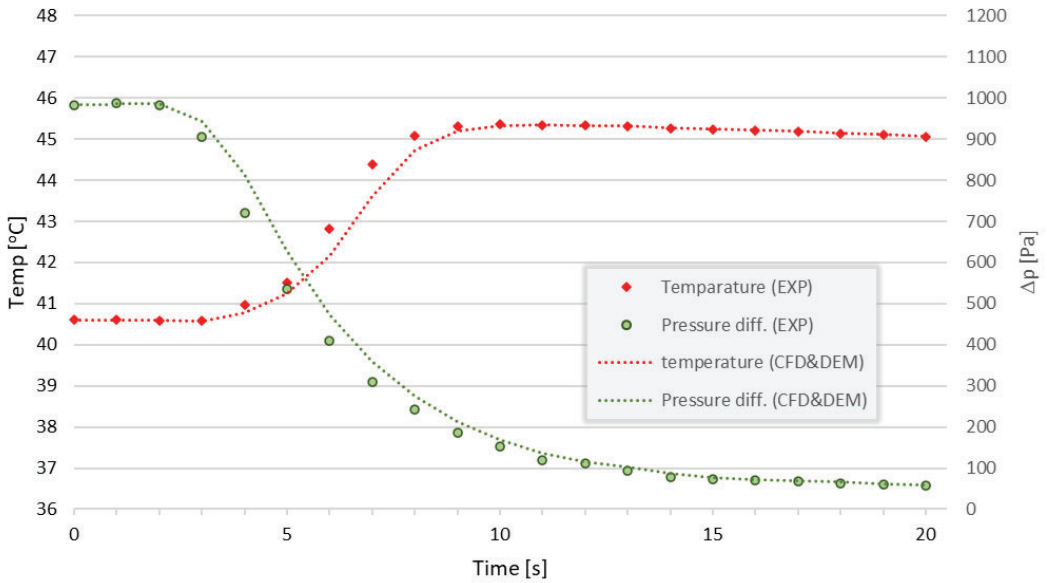

Figure 7: Experimental (EXP) and numerical (CFD&DEM) results concerning silica gel temperature and pressure difference between the tanks for granulation equal to 300 μm – 350 μm

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In the case of silica gel granulation 300µm – 350µm (Figure 7), where the initial pressure difference was 983 Pa, the initial temperature was 40.60 °C. The differences between the experimental and numerical results are insignificant until the third second of the process, when the modelled pressure difference values are starting to be overestimated by the model. However, such differences gain meaningful level after the tenth second of the process. The modelled temperature is underestimated up to 0.63 °C between the fourth and the nineth second of the analyzed process. The highest difference between the experimental and CFD&DEM results is 77 Pa.
For the granulation 350µm – 400µm (Figure 8), the initial pressure difference was 1025 Pa, and the initial temperature was 41.33 °C. Significant differences in measured and modelled temperature values start to appear after the fifth second of the process. Differences between the modeled and measured pressure difference are similar to the other analyzed granulation ranges. The highest difference between the experimental and CFD&DEM results is only 0.36 °C in the case of temperature, 91 Pa in the case of pressure difference.

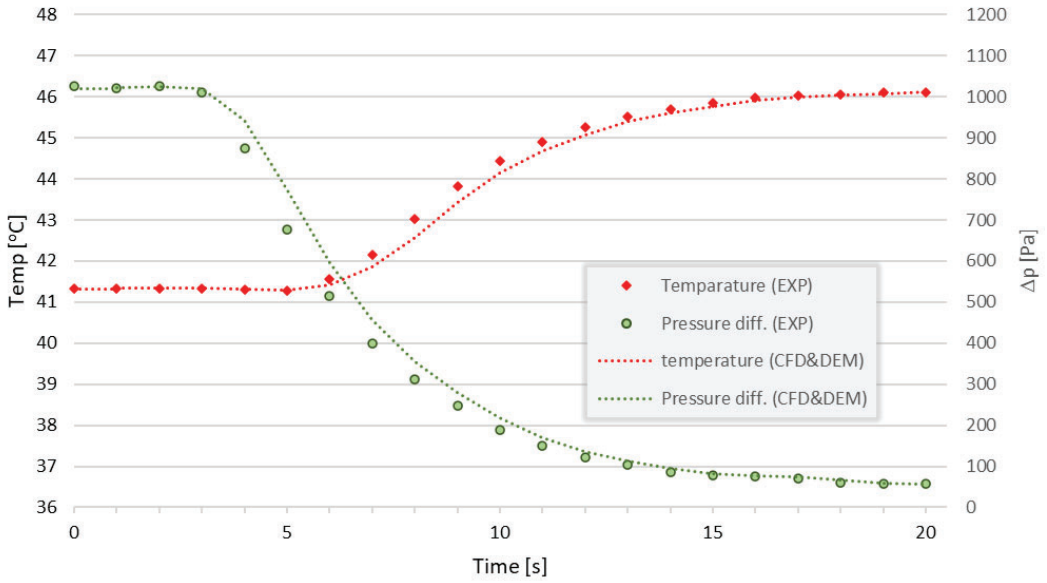

Figure 8: Experimental (EXP) and numerical (CFD&DEM) results concerning silica gel temperature and pressure difference between the tanks for granulation equal to 350 µm – 400 µm

The last analyzed silica gel granulation range was 400µm – 500µm (Figure 9). The initial pressure difference was 955 Pa, and the initial temperature was 38.96 °C. The experimental and numerical results concerning pressure difference was properly modelled for the first four seconds and last thirteen seconds, however, despite some quantitative differences, qualitatively the modelled pressures behave similarly to the measured values. The same applies to the temperature variation in the disc-shaped fluidized sorption reactor. The highest difference between the experimental and CFD&DEM results is 0.42 °C in case of temperature, 105 Pa in case of the pressure difference.

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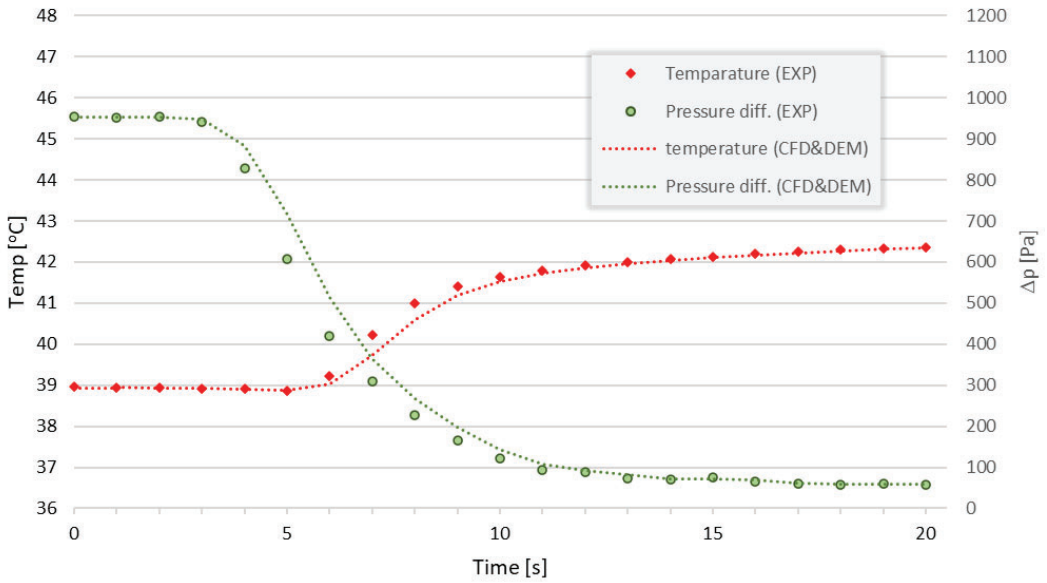

Figure 9: Experimental (EXP) and numerical (CFD&DEM) results concerning silica gel temperature and pressure difference between the tanks for granulation equal to 400 µm – 500 µm

6 CONCLUSIONS

The paper presents the concept of a fluidized disc-shaped sorption reactor dedicated to adsorption chillers. The new approach of the two-way coupled computational fluid dynamics and discrete element modelling and with sorption model was applied in the numerical analysis and the modelling results were compared to measurement data obtained on the experimental test stand.
The modelling results are qualitatively coherent with experimental data, and their quantitative error does not exceed 0.98 °C in the case of adsorbent temperature (granulation: 160µm – 200 µm), and 106 Pa in the case of pressure difference between the upper and the lower tank (granulation: 100 µm – 160 µm). These differences occur between the third and the twelfth second of the process.
However, the results of the presented research indicate that the coupled CFD&DEM modelling approach is a powerful and cost-effective research tool capable of effectively analyzing complicated physical phenomena in the proposed concept of a disc-shaped fluidized sorption reactor operating in low-pressure regimes. Such a novel approach reveals great potential for further improvement in optimizing the construction of adsorption reactors with numerical methods.

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