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A numerical analysis of CO_2 storage by adsorption using ZIF-8

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In 21st century, the reduction of CO_2 concentration in the atmosphere is one of the most challenges of the humanity, specifically in the engineering. To start a possibility solution proposal, this work consisted in an analysis of carbon dioxide storage, using adsorption by ZIF-8, a material that belongs to a class called Zeolitic Imidazolate Frameworks, which have high porosity, high thermal resistance and chemical stability. The main contribution of this work is to verify which parameters are relevant in the CO2 storage capacity by adsorption. To archive this goal, the study was made through computational simulations using the open source FreeFem++ software, inputting a specified quantity of pure CO_2, entering in an 1,82 liter tank filled by the adsorbent until its internal pressure reached 1,0 MPa. First, the isothermal curve was validated with the literature, and after adjusting the parameters of adsorption model, called Dubinin Astakov (D-A). The simulations were performed, varying CO_2 inlet flow, the tank's aspect ratio with the values of 1; 1,9; 3; 5 and 7, and the external wall's heat transfer coefficient with values of 5, 700 and 1000 W/m²K. Each simulation generated at each step the tank's average and maximum temperatures, internal pressure, and the carbon dioxide adsorption density. All the simulations started with a standard temperature of 300 K and pressure of 100 kPa. Temperature and adsorption density distributions were generated to analyze in which part of the tank the adsorption is higher. The results showed that the regions where the temperatures are higher, the adsorption is lower, and in the end of the simulation, the simulations with the lower average temperatures had the higher adsorption density. The highest values of adsorption density were obtained with higher surface areas under the influence of forced convection, rather than natural convection, and with lower CO_2 inlet flow. The highest adsorption density reached was 15,67 %, in a simulation with 50% of the tank's volume per minute as CO_2 inlet flow rate, aspect ratio of 7,0; and 700 W/m²K heat transfer coefficient. The average temperature obtained in the end of this simulation was 326,20 K and it took 3644 seconds for the tank to achieve the internal pressure of 1,0 MPa.