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Performance and sensitivity analysis of direct air capture (DAC) model using solid amine sorbents for CO_2 capture

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Abstract

Direct Air Capture (DAC), was first proposed by Lackner and coauthors in 1999 to mitigate climate change and in the past decade, there have been significant technical advances. According to the IEA report [1], 19 DAC plants are in operation globally, capturing more than 0.01 MtCO_2/year and lately, a 1MtCO_2/year plant is under development in the United States. Also, there are commercial pioneers in the field of DAC which are Climeworks and Global Thermostat where adsorption using solid sorbent are used to capture CO_2 while Carbon Engineering has established a DAC system with a liquid solvent. DAC is also receiving huge attention in the field of academia where ETH Zurich and Twente University have studied amine solid sorbent DAC systems whereas a recent development of Moisture Swing Adsorption (MSA) to capture CO_2 has been developed by Arizona State University. However, there is currently a scarcity of literature on simulation studies of adsorption processes in the DAC field.

In this paper, a DAC model via Temperature-Vacuum Swing Adsorption (TVSA) process employing amine-functionalized adsorbent (Lewatit® VP OC 1065), is studied through the sensitivity analysis on the operating parameters and the total annual cost (TAC) of the system. In order to optimize process design and cost, it is crucial to develop detailed modeling of DAC system, and therefore, the cyclic performance of a DAC model considering CO_2-containing airflow, mass, and heat transfer with adsorption isotherm is developed using Aspen Adsorption where the time-dependent partial differential equations (PDEs) describing the DAC process are solved at each step of the process cycle. In the work of Bos et al. [2], CO_2 adsorption onto an amine-based solid sorbent, Lewatit® VP OC 1065 is described by Toth isotherm, and the isotherm parameters presented in the aforementioned paper is used in the Aspen Adsorption model used in this work. The model assumes the ideal gas law for the gaseous mixture and only carbon dioxide is adsorbed. The resistance of mass transfer in the gas phase is negligible while a constant heat of adsorption and constant adsorbent physical properties are assumed. The model is then used to optimize the entire process steps (adsorption, evacuation, desorption, and cooling) to reduce the TAC and to improve its performances in terms of energy consumptions, purity, and recovery. An example of a cyclic temperature profile obtained from a DAC process model is presented in Figure 1.

In the first part, a complete kilogram scale TVSA fixed bed Aspen adsorption model presented in Kim and Léonard [3] simulating a process similar to the DAC model of Schellevis et al. [4] is described, and model parameters (E.g. adsorption/desorption time, purge gas temperature, etc.) are varied to evaluate their impact on capital and operating costs of the DAC system. It is well known that the CO_2 equilibrium loading of solid sorbents can be affected by temperature and pressure where this characteristic will influence the performance of the DAC system. Also, cycle step

time and purge gas temperature, etc. can play an important role in achieving high purity and recovery of the CO_2 product stream. Therefore, through a detailed sensitivity analysis, optimal conditions of the Aspen Adsorption model will be identified. The energy requirement of the DAC system consists of thermal and electrical energy. The main thermal energy uses are the reaction and sensible heats of CO_2, H_2O, and purge steam while the electrical energy involves pumps and compressors. The influences of the model parameters on energy consumption are also studied to improve the existing DAC model and its CO_2 capture cost and energy requirement. IEA report [1] presented energy consumption of a solid sorbent DAC system is about 10 GJ/tCO_2 and from the preliminary study of Kim and Leonard [3], about 16 GJ/tCO_2 was reported. Through these sensitivity studies, the model's energy requirement is expected to be closer to the abovementioned IEA report value. Finally, there are various ways to regenerate solid sorbents such as steam, hot nitrogen gas, and air. Different desorption options coupled with the optimized DAC model are studied to identify trade-offs between the desorption options and key performance indicators (E.g. purity and amount of CO_2 captured per cycle). In future work, the model can serve as a basis to scale up and to study the feasibility of large-scaled DAC system deployments and its importance compared to point source CO_2 capture technologies.

Keywords: Direct Air Capture (DAC); Carbon Capture; Process Modeling; TVSA; Sensitivity Analysis

References

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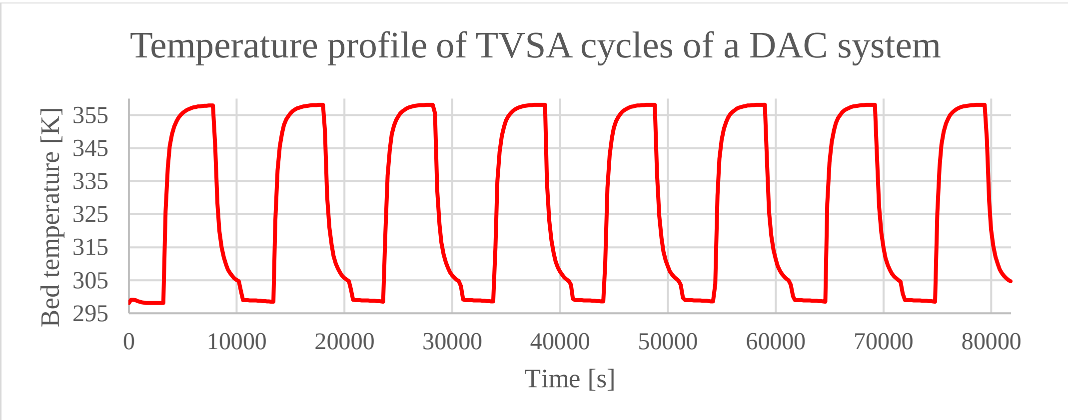

Figure 1: An example of temperature profile of a DAC system