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Mathematical modeling and numerical investigation of carbon capture by adsorption: Literature review and case study☆

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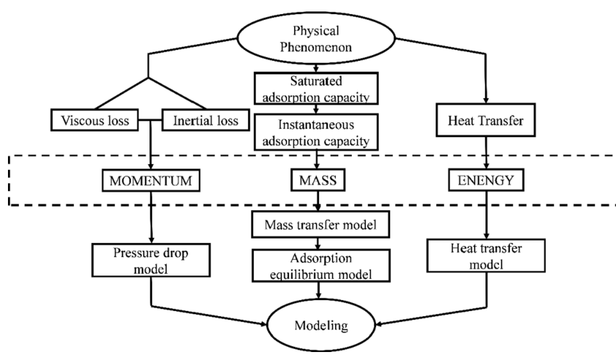
HIGHLIGHTS

- The sub-models screening of CCA is presented with the literature review.
- A pathway map is established through model group forming.
- A case study demonstrates a fluent optimal design based on the pathway map.

GRAPHICAL ABSTRACT



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ABSTRACT

The carbon capture by adsorption (CCA) is regarded as an available engineering technology because of its low energy-consumption, easy to control, and possible integration with renewable energy. The recent advances in CCA research comprises mainly about the performance improvement of adsorbents, design and optimization of engineering process. However, considering the time-consuming and intensive funding required for experimental investigation, the numerical simulation has been widely applied in CCA. In numerical simulation field of CCA, the adsorption process is commonly simplified into mathematical models group comprised of adsorption kinetics model, the adsorption equilibrium model, pressure drop model and heat transfer model. However, few studies' focus is to provide a detailed review of the research methodology of mathematical modeling in CCA simulation.

This paper presents a pathway map on CCA mathematical modeling through literature review and case study. An overview of model screening and modeling method of CCA is provided in the review part. This part also provides a short guided tour on how to combine the fundamental models about heat and mass transfer together to form a model group for various application scenarios in CCA. Then the pathway map on CCA modeling, which is summarized based on the review, is applied to a case study. In this part, the adsorption of CO_2/N_2 mixtures on activated carbon under the conditions of high temperature and low pressure is numerically investigated based on the established models. The performance indicators comprise gas temperature, mole fraction, and adsorbate amount of the fixed bed, are applied in the evaluation performance of CCA. Based on the proposed methodology, the CCA modeling demonstrates a more fluent design process relative to the real physical scenario, with a possible access to further optimization. Particularly, the simulation results showed that the optimized dimensionless velocity for the highest utilization efficiency of the fixed bed can be obtained and thus is proposed as

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