

Experimental Investigation and Machine Learning Study of Adsorption Isotherms and Characterization Employing Low-GWP Refrigerants

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(低 GWP 冷媒を用いた吸着等温線と特性評価に関する実験および
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論 文 内 容 の 要 旨

Adsorbents, such as activated carbon (AC), metal-organic frameworks (MOFs), silica gel, and zeolites, play critical roles in various environmental and industrial applications owing to their ability to selectively capture and store gases. The development of efficient adsorbents is essential for addressing pressing global challenges such as carbon capture, gas separation, and energy storage. In the context of climate change mitigation, adsorbents offer a promising alternative for CO₂ capture, providing high selectivity, regenerability, and energy efficiency compared with conventional separation technologies. Beyond environmental applications, adsorbents are widely used in industrial processes such as air purification, gas drying, and catalysis. Moreover, their integration into emerging technologies, such as adsorption-based cooling and heat pumps, further expands their application potential, offering energy-efficient solutions for sustainable thermal management. AC has gained significant attention for CO₂ capture among various adsorbents because of its large surface area, tunable porosity, chemical stability, and cost-effectiveness. However, AC is not only limited to CO₂ adsorption in post-combustion capture but also plays a key role in adsorption-based thermochemical energy storage systems. By pairing AC with working fluids such as CO₂, NH₃, or water, adsorption refrigeration and heat pump systems can achieve high efficiencies while operating under environmentally friendly conditions. Similarly, MOFs, silica gels, and zeolites, with their tunable pore structures and high sorption capacities, have also been widely investigated as adsorbents for these applications. The ability to optimize these materials for both gas separation and thermal management systems highlights the necessity of developing advanced adsorbents with tailored physicochemical properties. This thesis consists of six chapters.

Chapter 1 provides an overview of adsorbents, adsorption heat pumps, and machine learning (ML) and deep learning (DL) applications in material development. The motivation and aims of this study are clearly defined, highlighting the need to integrate experimental, simulation-based, and data-driven approaches to optimize adsorption performance.

Chapter 2 presents a comprehensive literature review covering the fundamentals of adsorption processes, including the classification of adsorption types and commonly used adsorption isotherm models such as Langmuir, Freundlich, D-A, Tóth, and Sun-Chakraborty. It further introduces the principles and structures of representative ML and DL algorithms, highlighting their

respective applications and advantages in adsorption research through illustrative examples. In addition, this chapter surveys recent representative studies to provide an overview of the current state and future potential of ML/DL techniques in the field of adsorption.

Chapter 3 focuses on the experimental measurement of the adsorption isotherm of the Maxsorb III/HFO1234ze (E) working pair under relatively high-pressure conditions. The obtained data were fitted using the Tóth and D-A adsorption isotherm models, and the results were used to estimate the adsorption isotherms at unmeasured temperatures. Furthermore, the heat of adsorption and COP were calculated. The limitations of conventional adsorption isotherm models are discussed, establishing the foundation for subsequent data-driven DL approaches.

In **Chapter 4**, the performance of MOF-801/water, aluminum fumarate/water, and MIL-100(Fe)/water working pairs in adsorption heat transformers (AdHTs) is investigated. The Chandra model was employed to simulate the COP of the AdHT, and the impact of the adsorption isotherm and adsorbent characteristics on temperature lifting and COP were analyzed. This study provides insights into the relationship between the physicochemical characteristics of adsorbents and AdHT performance. These simulations rely on adsorption isotherms derived from adsorption isotherm models, which serve as the foundation for the performance evaluation. This approach highlights the crucial role of accurate adsorption isotherms in AdHT performance assessment.

In **Chapter 5**, a fully connected neural network (FCNN) model trained on 19,540 adsorption isotherm data points for KOH-activated AC/CO₂ pairs is introduced. A controlled variable approach was applied to ensure consistency in data selection, limiting the dataset to ACs with comparable physicochemical characteristics. The impact of individual physicochemical characteristics on CO₂ uptake was analyzed using the Pearson correlation matrix and SHAP. The interdependence between different physicochemical characteristics was also explored to provide theoretical insights for further material optimization. External validation was conducted to assess the reliability of the model and support the conclusions.

Chapter 6 summarizes the key findings of this study and provides a comparative analysis of the experimental methods, simulation techniques, and DL approaches in CO₂ adsorption research. The strengths and limitations of each methodology are discussed, highlighting their complementary roles in guiding material design and performance predictions. Building on these insights, this chapter outlines future research directions, including investigating the pressure-dependent role of nitrogen doping, integrating structural image data into DL models, developing synthesis-to-performance prediction frameworks, incorporating cost and degradation considerations in system modeling, and extending current models to larger gas molecules via transfer learning. These recommendations aim to enhance the efficiency, accuracy, and applicability of AI-driven adsorption research.