

Research on On-board CO₂ Capture Technology (3rd Report)

- Deriving System Requirements Using Machine Learning -

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KEY WORDS: heat engine, greenhouse gas, CO₂ separation and capture system [A1]

Designing a CO₂ capture system from engine exhaust gas under constraints such as vehicle packaging and minimized energy consumption requires a systematic assessment of the sensitivities of design variables and the derivation of system requirements based on those insights. However, because the design variables are numerous and mutually interacting, an exhaustive evaluation using Computational Fluid Dynamics (CFD) is computationally expensive. Therefore, machine learning trained on one-dimensional computational fluid dynamics (1D-CFD) simulation results was applied to accelerate design-space exploration and the derivation of system requirements.

The target system is a Temperature Swing Adsorption (TSA) system employing an adsorber, operated in a cycle consisting of four processes—adsorption, desorption, scavenging, and precooling. The training data were generated from 1D-CFD (GT-SUITE) simulations, and design points were selected using a D-optimal design. In this cycle, CO₂ is collected into a CO₂ tank during the desorption and scavenging processes; to mitigate overfitting, two separate prediction models for CO₂ capture amount—one for desorption and one for scavenging—were constructed. Additionally, the minimum CO₂ concentration at the adsorber outlet during the adsorption process (MinCO₂) was introduced as an indicator for estimating the breakthrough-curve shape, and a prediction model for MinCO₂ was also developed. All models exhibited high predictive accuracy (Fig. 1).

For model interpretation and validation, feature contributions were visualized using SHAP, and model validity was confirmed. Furthermore, by using these machine-learning models for exhaustive exploration and screening, design-space studies that would have required prohibitive computation time with 1D-CFD alone were executed in a matter of seconds, enabling rapid derivation of system requirements (Fig. 2).

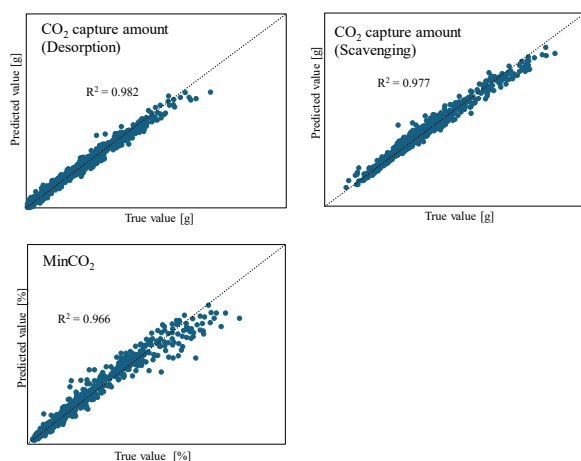


Fig. 1 Accuracy of machine learning models

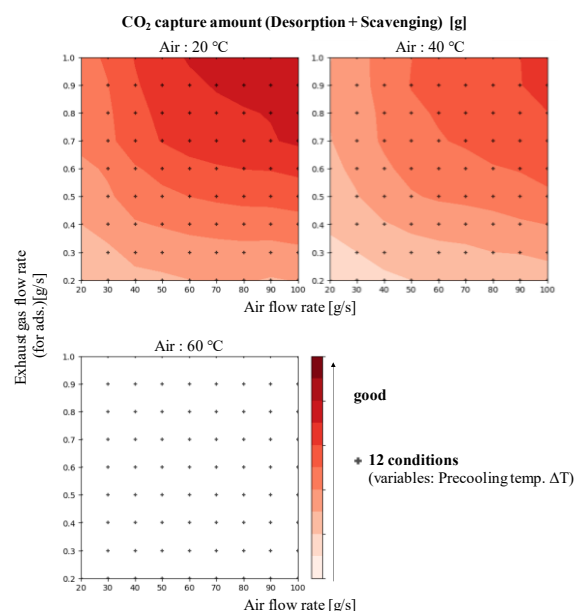


Fig. 2 CO₂ capture amount map