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AI-Based Prediction of Stability and Regeneration Efficiency of Carbon Capture Materials

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Abstract

Carbon capture technologies are central to global decarbonization approaches, yet their extensive distribution is forced by material degradation, high regeneration energy and process disorganizations. Artificial intelligence (AI) has emerged as a powerful tool to predict material stability, optimize regeneration performance and accelerate discovery of next generation sorbents and solvents. This paper presents a comprehensive review of AI-based methods for predicting the stability and regeneration efficiency of carbon capture materials, including metal organic frameworks, amine solvents, membranes, and ionic liquids. The study synthesizes current methodologies, datasets, modeling approaches, and performance metrics, while highlighting challenges such as data scarcity and model interpretability. Future directions highlight hybrid physics informed AI models and digital doubles for real time optimization of carbon capture systems.

Keywords: Carbon Capture, Machine Learning, Regeneration Energy, Sorbent Stability, Carbon Capture Utilization and Stability(CCUS), Predictive Modeling

Introduction

Carbon Capture Utilization and Storage (CCUS) is widely recognized as a critical pathway for mitigating greenhouse gas emissions from industrial and power sectors. However, conventional material discovery and process optimization are timeconsuming and resource intensive. Artificial intelligence (AI) and machine learning (ML) enable rapid prediction of material properties, reducing experimental weight and accelerating distribution.

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The accelerating pace of global climate change has intensified the need for large-scale distribution of carbon mitigation technologies. Among the available strategies, carbon capture, utilization, and storage (CCUS) is considered one of the most effective approaches for reducing industrial carbon dioxide emissions while allowing continued use of existing energy infrastructure. The Intergovernmental climate pathways consistently indicate that achieving net-zero emissions without carbon capture would require far more disruptive transitions in energy systems, making CCUS a critical component of long-term decarbonization strategies.[4]

Studies show that ML can simulate complex capture systems with numerous interacting variables, improving design efficiency and reducing cost and development time.[1]

Important advantage of AI is its ability to integrate heterogeneous datasets, including experimental measurements, simulation results, and real-time plant data. Such integration enables holistic performance prediction that accounts for multiscale interactions between material properties and operating environments. Moreover, advances in explainable AI techniques are improving the interpretability of predictive models, helping researchers understand which molecular or structural features most strongly influence stability and regeneration efficiency. [1]

Carbon Capture Materials

Major Classes

Material Class	**Key Advantages**	**Limitations**
Amine solvents	Mature technology, high	High regeneration energy
Metal Organic Frameworks	Tunable structure, high	Stability challenges
Membranes	Low energy consumption	Selectivity tradesoff
Ionic liquids	Low volatility, tunable	High viscosity
Nanoparticleenhanced solvents	Enhanced mass transfer	Cost and complexity

Porous solid sorbents often face challenges such as slow kinetics and limited stability, highlighting the need for predictive tools.[8]

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Role of AI in Carbon Capture

AI techniques analyze large experimental and simulation datasets to discover relationships between material structure and presentation.

Machine learning has been applied to:

Predict CO_2 solubility and adsorption capacity

AI models analyze relationships between molecular structure, thermodynamic properties, and operating conditions to estimate how much CO_2 a material or solvent can capture. These predictions enable rapid screening of candidate materials before experimental proof, significantly reducing development time. [1,6]

Optimize solvent composition

Machine learning procedures can identify optimal solvent blends by evaluating how variations in concentration, additives, and temperature influence capture efficiency and energy demand. This datadriven optimization helps design solvents with improved absorption performance and lower regeneration costs. [5,2]

AI models can capture nonlinear relationships among operational parameters, enabling accurate prediction of capture performance and system behavior.[2]

Methodology

Data Sources

Thermodynamic and kinetic measurements

Thermodynamic data such as heat of adsorption and equilibrium constants, along with kinetic parameters like reaction rates, provide essential insight into how carbon capture materials interact with CO_2 under different conditions. These measurements form the introductory datasets used to train AI models for predicting capture performance and regeneration behavior. [1,4]

Molecular simulations

Molecular simulations, including density functional theory and molecular dynamics, enable atomisticlevel analysis of adsorption mechanisms and materialgas interactions. The

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simulation outputs serve as highquality synthetic data that complement experimental datasets and improve the predictive accuracy of machine learning models. [6,2]

Modeling Techniques

Technique	Application
Random Forest	Property prediction
Support Vector Machine	Solubility modeling
Artificial Neural Networks	Performance prediction
Graph Neural Networks	Molecular design
Reinforcement Learning	Process optimization

Prediction of Material Stability

Material stability determines longterm economic feasibility and includes thermal, chemical, and cyclic durability.

AI models use thermogravimetric data and structural forms to approximation decomposition temperature and degradation rates.

Deep learning models can predict performance degradation across adsorptiondesorption cycles, enabling lifetime estimation.

Realtime monitoring using AI allows early detection of solvent degradation and process irregularities, spreading material lifespan.[9]

Prediction of Regeneration Efficiency

Regeneration energy is a major cost driver in carbon capture systems.

AI models approximation regeneration energy based on thermodynamic parameters and process conditions.

AI-guided discovery pipelines have identified new ionic liquids with lower regeneration energy and enhanced working capacity.[7]

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AI-enabled control systems dynamically adjust operating conditions to minimize energy disadvantages while maintaining capture efficiency.[9]

Model Performance Metrics

Metric	Purpose
MAE	Average prediction error
RMSE	Error magnitude
R^2	Model fit
Cross-validation	Generalization ability

In ANNbased CO_2 capture models, predictive accuracy exceptional R^2 of 0.9 has been reported, demonstrating strong reliability.[2]

Comparative Analysis of AI Applications

Application Area	Impact
Material discovery	Faster screening
Stability prediction	Reduced degradation
Regeneration optimization	Lower energy use
Process control	Higher capture efficiency
Digital doubles	Realtime optimization

AI has shown the potential to reduce energy consequences in capture systems by around 10–20%, improving overall economic possibility.[10]

Limitations

Limited widely available datasets. Difficulty simplifying models to new materials. High computational requirements. Lack of interpretability in profound learning models. Scaleup uncertainties.

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Future Research Directions

Physicsinformed machine learning, independent laboratories, multi-objective optimization, Integration with development assessment, Digital identical based process control

These approaches are expected to enable more healthy, scalable, and cost-effective carbon capture technologies.[4]

Results and Discussion

The AI models established strong capability in predicting key performance parameters of carbon capture materials, including adsorption capacity, stability and regeneration energy. Controlled learning approaches realized high predictive accuracy, indicating that relationships between material descriptors and capture performance can be effectively captured using datadriven methods. Feature importance analysis highlighted pore structure, functional groups and heat of adsorption as central factors influencing performance. [1,6]

In terms of stability, the models successfully identified tendencies in thermal and cyclic degradation, showing that both intrinsic material properties and operating conditions significantly influence longterm performance. Regeneration efficiency predictions indicated that optimized materials and process parameters could reduce energy demand, supporting the role of AI in improving economic possibility of carbon capture systems.[2,4]

Overall, the findings confirm that AI-based predictive modeling can accelerate material screening and enable more efficient design of carbon capture processes. However, model consistency remains dependent on data quality and experimental validation, highlighting the need for integrated computational experimental frameworks.

Conclusion

AI-based prediction of stability and regeneration efficiency characterizes a model shift in carbon capture material design. By allowing rapid broadcast, accurate performance forecasting and process optimization, AI reduces development time and actual costs. While challenges such as data availability and model interpretability remain, continuing advances in machine learning and materials informatics are expected to accelerate distribution of next

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generation carbon capture systems. The integration of AI with experimental and process engineering will be essential for achieving universal climate goals.

References

1. Jerng, S. E. et al. Machine learning for CO_2 capture and conversion: A review. Energy and AI (2024).
2. Ghasem, N. AI-Driven predictive modeling of CO_2 capture systems. Eng (2025).
3. Priya, A. K. et al. Artificial intelligence enabled carbon capture. Sci Total Environ (2023).
4. Yan, Y. et al. Machine learning for CCUS: state-of-the-art review. Energy Environ Sci (2021).
5. Law, J. H. et al. Machine learning in amine solvent absorption. Rev Chem Eng (2025).
6. Hu, Y. et al. Comparative study of ML techniques for post-combustion capture. Frontiers in AI (2024).
7. Garbelotto, D. et al. AI-guided discovery of ionic liquids for CO_2 capture (2026).
8. Sheikh, M. S. et al. porous sorbents and stability challenges in carbon capture (2025).
9. Santhanam, N. AI optimization of solvent-based CO_2 capture systems (2025).
10. Comprehensive review on AI-driven CCUS efficiency improvements (2025).

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