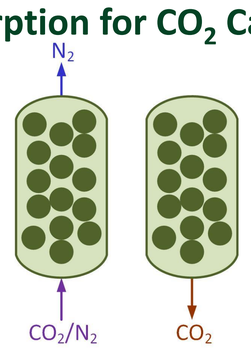
Multivariate Data Analysis of Post Combustion CO_2 Capture

Kasturi Nagesh Pai[1], Sai Gokul Subraveti[1], Arvind Rajendran[1], Vinay Prasad[1], Zukui Li[1]

BACKGROUND

Adsorption for CO_2 Capture



- Explosive growth in ability to synthesize novel solid sorbents
- Proven ability to reduce parasitic energy consumption
- Process design and optimization challenging

PSA Cycle Simulator
- Stiff PDEs
- Cyclic Process
- Convergence Complexities

≥3000 single core hours for the evaluation of 1 material

Optimizer
- Multi Objective Optimization
- Stochastic Output

AIMS AND OBJECTIVES

≥120 hours to evaluate one material on multiple core processors

Material Data + PSA Cycle Program → Parallel Computing → Evaluation and Optimization of One Solid Sorbent

Previous Data about material performance

3-4 orders of magnitude computing time saved Filtering out materials

Material Data + Machine Learning Algorithm → Single Core Computing → Evaluation and Optimization of One Solid Sorbent

≥0.12 hours to evaluate one material on a single processor

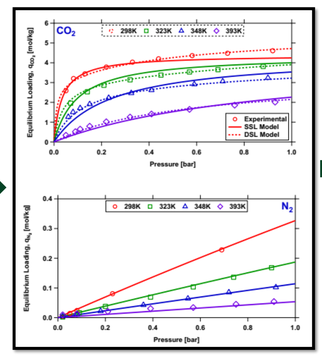
RESULTS

Machine Learning Algorithm Training

Solid Adsorbent

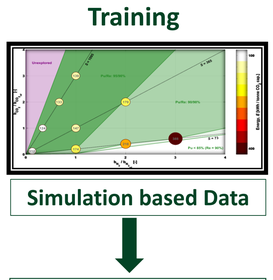
12 variables

Isotherm



4 variables

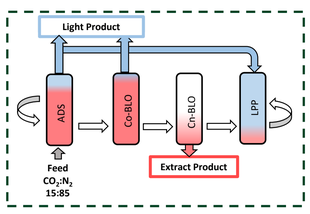
Training



Simulation based Data

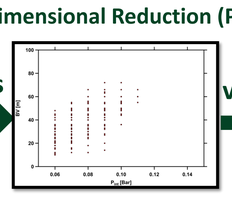
Supervised Machine Learning
- Support Vector Machines
- Ensemble Bagged

R^2_{Adj}
Purity - 0.87
Recovery - 0.92
Energy - 0.98
Productivity - 0.99



Dimensional Reduction (PCA)

6 variables

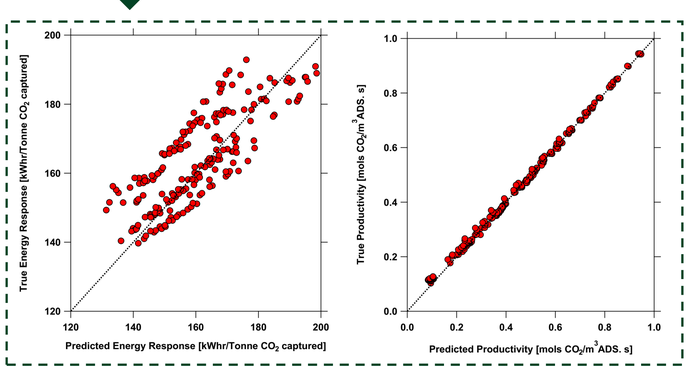


3 variables

70 Materials for Evaluation → **7 Variables** → Proxy Model

Full Model Evaluation
150000 Core Hours
- Accurate Purity, Recovery, Energy and Productivity values
- 6 operational variables 12 material parameters

Proxy Model Evaluation
1.5 Core Hours
- Accurate Filtration of Purity and Recovery
- Precise Productivity Predictions
- Limitations- Energy Predictions



Proxy Model Evaluation

Pros:
- Quick and Accurate Evaluations of Multiple Materials
- Quick Optimization of Materials
- Based on only 4 Material properties

Cons:
- Not as Accurate as Detailed Model
- Experimental Validation pending

FUTURE DIRECTIONS

Materials Engineers → Material Characterization & Tailoring Properties → Machine Learning Filters

Quick Performance Evaluation

Process Design Engineers → Process Design & Simulations → Single Column Experiments → Lab Scale Demonstration

Systems Level Optimization

Reduce Parasitic Energy → Scale up and Industrial level simulations and Implementation

PARTNERS

uOttawa

ALBERTA INNOVATES

computecanada

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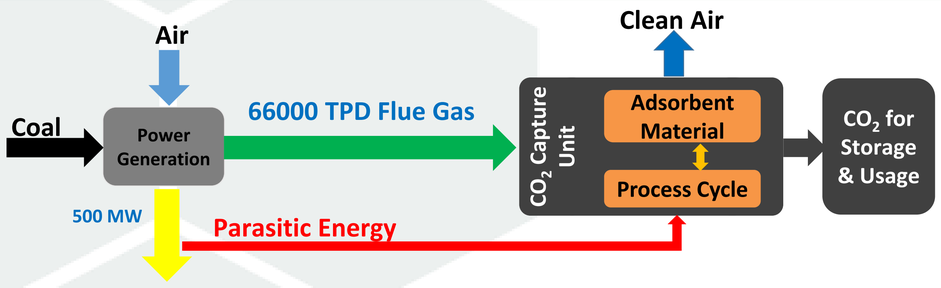
FES PROJECT OVERVIEW



Hydrocarbons will continue to serve as an essential energy source while the world transitions to a lower-carbon energy economy, but can we prevent the use of those fuels from contributing to the accumulation of CO_2 in the atmosphere? Existing technologies can capture carbon, but these methods can be costly and energy-intensive. Extracting energy without burning fuels, improving CO_2 capture efficiencies if they are burned, and finding effective ways to store or reuse captured carbon may be essential to ensuring it does not enter the atmosphere.

[1]Dept of Chemicals and Materials Engineering , 116th st 89th Ave, Edmonton, Alberta.

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FUTURE ENERGY SYSTEMS

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