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Hybrid Physics-inspired Machine Learning for CO₂ Capture Process Modeling

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Context

Carbon Capture, Usage & Storage

How to model the absorber in the capture process?

Pure Physics

Absorber = System of physical equations

Advantage:

- Physics based → extrapolable

Disadvantage:

- Complex model, that requires lots of laboratory data to calibrate parameters

Pure Machine Learning

Absorber = Machine Learning method

Advantage:

- Fast to develop & no prior physical knowledge required

Disadvantage:

- Poor extrapolation
- Black box model
- Requires lots of industrial data

Physics Informed Machine Learning

Absorber = Machine learning method with system of physical equations

Good extrapolation, fast to develop

Application to industrial demonstrator

- IFPEN process demonstrated on ArcelorMittal site
- Available set of industrial data (~ 200 parametric test-runs)
- Various operating conditions

Operating conditions	
Gas pressure [bara]	1.15 – 2.85
Gas CO ₂ [mol/mol]	0.10 – 0.35
Liquid temperature [°C]	25 – 40
Liquid CO ₂ loading rate [mol/mol _{Amine}]	0.001 – 0.25
L/G [kg/Nm ³]	1.6 – 17.2

Contribution

Issue encountered

Whitman double film theory

Existing mechanistic simulator associated to the demonstrator

- Absorber discretized into numerical stages
- Each stage calculated by Whitman double-film theory
- Mass balance and enthalpy balance solved for every zone and stage

Problem

- Mechanistic simulator does not reproduce demonstrator data with sufficient fidelity

Proposed PiML approach

Hybrid Modeling Strategy

- Simulator discretization preserved
- Double-film model replaced by Neural Network at each stage
- Shared NN parameters across stages (*same input → same output*)
- Use of a Residual NN to learn a perturbation instead of full mapping from input to output

Training Pipeline

- Pre-train on low-fidelity simulated data
- Fine-tune on high-fidelity industrial data

Physics Integration

- Inducing physical bias via low-fidelity pretraining
- Regularization via soft constraints

Schematic workflow of the Residual Neural Network

$$loss = \sum_{i=1}^{n=480} ||y_{pred}^{(i)} - y_{true}^{(i)}||^2 + \alpha [(Q_{G,in}^{(i)} + Q_{L,in}^{(i)}) - (Q_{G,out}^{(i)} + Q_{L,out}^{(i)})]^2$$

Reconstruction loss Phys. reg. via global mass balance

Loss computation for 1 numerical stage

Pre-training results

Data processing workflow

600 Operating conditions (Range of operating conditions representative of the demonstrator) → Simulator with mechanistic model → 600 sets of profiles (Gas and liquid temperature vs Packing height from bottom [m]).

Random split: 80% for training (480), 20% for testing (120).

Model performance: parity diagrams & profiles

Metrics for model evaluation

MAE(y, \hat{y}) = $\frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$

For each type of feature

$R^2(y, \hat{y}) = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$

For each feature

Model sensitivity to regularization

		$\alpha = 0$	$\alpha = 0.25$	$\alpha = 1$
Mean Absolute Error	Liquid temperature [°C]	1.914	1.440	1.732
	Capture rate [%]	2.794	2.336	3.123
R^2 score	Average on all R^2 score	0.876	0.914	0.867

Variation of the weight of the regularization

Conclusion

- Development of a hybrid approach combining physical knowledge and machine learning for CO₂ capture by amine scrubbing
- Physical knowledge taken into account through Neural Network training on first-principles model and physics-based constraints derived from fundamental equations
- Promising preliminary results despite limited data availability (only 600 datapoints)
- Faster computation time (few seconds vs few minutes for mechanistic simulator)

Perspectives

- Implementation of stronger physical constraints (positivity, bounds, mass balance) via additional soft constraints and hard constraints
- Enrich training dataset and refine sampling strategy
- Fine-tuning of the pre-trained model using high-fidelity data via transfer learning
- Uncertainty quantification (data splits, robustness)
- Model benchmarking (alternative ML methods)
- Framework extension (other data-scarce industrial systems)