README and Data Documentation

Leandros Paschalidis et al.

Project Information

Project Title:

The Steam Barrier as a Design Constraint in Carbon Capture: Pathways to Low-Temperature Regeneration

Related Publication:

Paschalidis, L., Kruber, K. F., Müller, S., and Skiborowski, M.
The Steam Barrier as a Design Constraint in Carbon Capture: Pathways to Low-Temperature Regeneration.
Chemical Engineering and Processing – Process Intensification, accepted for publication, 2026.
Accepted for publication on: 11 Jun 2026

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1 General Information

Data Set Title:

Python Scripts for: The Steam Barrier as a Design Constraint in Carbon Capture: Pathways to Low-Temperature Regeneration

Short Description:

This repository contains Python scripts used to investigate carbon dioxide gas-liquid equilibrium and steam exergy relevant to low-temperature solvent regeneration processes for carbon capture. The scripts calculate CO_2 loading, chemical speciation, dissolved inorganic carbon concentrations, and steam exergy under different thermodynamic assumptions. The repository also contains parameter sweep studies used to generate contour plots presented in the associated publication. The data and code can be used to reproduce figures and calculations reported in the publication and to explore the influence of activity coefficient models and thermodynamic parameters on CO_2 absorption processes.

Date of Python Code Creation:

2025–2026

Geographical Coverage:
Hamburg, Germany

Keywords:

- Carbon Capture
- CO_2 Absorption
- Low-Temperature Regeneration
- Gas-Liquid Equilibrium
- Activity Coefficient Models
- Process Intensification
- Steam Exergy
- Thermodynamics
- Python
- Chemical Engineering

2 Methodological Information

Data Collection and Processing:
The data were generated computationally using custom Python scripts. Calculations include chemical equilibrium, gas-liquid equilibrium, activity coefficient estimation, parameter sweeps, and thermodynamic property calculations. The following software packages were used:

- NumPy
- SciPy
- Matplotlib
- CoolProp

Experimental Design / Study Context:
The study investigates thermodynamic limitations imposed by steam generation requirements during solvent regeneration in post-combustion carbon capture. Three liquid-phase thermodynamic models were evaluated:

- Ideal solution model
- Davies activity coefficient model
- Extended Debye-Hückel activity coefficient model

Parameter sensitivity studies were conducted by varying pKa values and temperature dependencies. Steam exergy calculations were performed over a range of temperatures and pressures relevant to industrial carbon capture systems.

Data Validation and Quality Assurance:

Detailed parameter values and literature references are provided in the Supporting Information of the associated publication.

Validation was performed by:

- Numerical convergence checks for all equilibrium calculations.
- Comparison of ideal, Davies, and Extended Debye–Hückel activity coefficient models.
- Benchmarking against Aspen Plus simulations using the validated AMP electrolyte NRTL model reported by Morlando et al. (2025).
- Verification that the simplified screening model reproduces the qualitative CO_2 loading trends of the rigorous model shown in Figure 3 of the associated publication.

The model of Morlando et al. was made available by the authors of that publication. See the publication below:

Morlando, D., Zhang, Y., Wang, S., and Knuutila, H. K. *Development of a Validated Rate-Based Model for CO_2 Absorption in Aqueous 2-Amino-2-methyl-1-propanol and Piperazine Blends Using Aspen Plus.* Energy & Fuels, 39(40), 19350–19367 (2025). DOI: `https://doi.org/10.1021/acs.energyfuels.5c03281`

3 Data and File Overview

List of Files and Structure:

File	Description	Format
Davies	CO_2 equilibrium calculations using Davies activity coefficients	.py
Debye_Huckel	CO_2 equilibrium calculations using Extended Debye-Hückel model	.py
Ideal.py	CO_2 equilibrium calculations assuming ideal liquid phase	.py
contour_creation	Parameter sweep calculations and contour plot generation	.py
water_exergy_vs_T_vs_p	Water and steam exergy calculations	.py
README	Repository documentation	.pdf

File Naming Convention:

File names reflect the implemented thermodynamic model or analysis task. Underscores are used to separate words. Version control is managed through repository releases.

Number of Records / Observations:

Not applicable. Data are generated dynamically through numerical simulations and parameter sweeps.

4 Access and Licensing Information

Repository and Persistent Identifier:
Published via TORE.
DOI: `https://doi.org/10.15480/882.17093`

License for Use:
MIT License

Access Restrictions:
Open Access

Text for Citation:
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DOI: `https://doi.org/10.15480/882.17093`

5 Reproducibility and Software Dependencies

Software Required:

- Python
- NumPy
- SciPy
- Matplotlib
- CoolProp

Installation:

```
pip install numpy scipy matplotlib CoolProp
```

Scripts and Workflow:
Execute scripts individually:

```
python Davies.py
python Debye_Huckel.py
python Ideal.py
python contour_creation.py
python water_exergy_vs_T_vs_p.py
```

Each script automatically generates the corresponding figures and results.

Reproducibility Notes:
To reproduce the published results:

1. Install all required Python packages.
2. Execute the desired script.
3. Use the default parameter values supplied in the source code.

4. Compare generated figures with those reported in the publication.

Scientific assumptions include:

- No carbamate formation.
- Ionic strength below approximately 0.7 M.
- Temperature-independent reaction enthalpies.
- No salting-out corrections.
- Consideration of major ionic species only.

Additional details are provided in the publication Supporting Information.

6 Ethical and Legal Aspects

Data Protection:
No personal or sensitive data are contained in this repository.

Consent Statement:
Not applicable. No human participants were involved.

7 Versioning and Updates

Version Number:
v2.0

Date of Release:
[15-06-26]

Change Log:
Version 1.0: Initial public release accompanying the publication conatining all codes.
Version 2.0: The exact same thing plus the addition of this Readme file.

8 Contact Information

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