

CEAD class – AI applications for CO₂ capture

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The energy sector is one of the main contributors to global warming due to the high amount of CO₂ released during the combustion of fossil fuels. Energy plants are always equipped with a CO₂ capture section to reduce the amount of CO₂ released into the atmosphere. Here, the flue gas is scrubbed using amines before releasing it into the atmosphere. The absorption process is reported in Figure 1.

An energy company would like to design a new CO₂ capture column. Over the years, they have collected a database that correlates the process variables and column dimensions with the gas-side mass-transfer coefficient (k_{Ga}) in the process absorption column and the absorption efficiency.

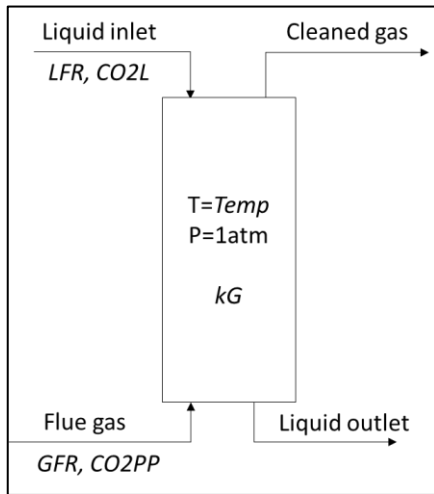


Figure 1. Absorption process schematic representation

The variable space is represented by:

- The liquid flow rate of the stripping stream (LFR in the dataset), in L/(m²·h).
- The gas flow rate of the stripped stream (GFR in the dataset), in m³/(m²·h).
- The stripping temperature (Temp in the dataset), in °C.
- The CO₂ loading inside the stripping stream at the column inlet (CO₂alpha in the dataset), in CO₂mol/mol Amine.
- The CO₂ loading of the flue gas at the column inlet (CO₂pp in the dataset), in kPa.
- The column height (Height in the dataset), in m.
- The mass-transfer coefficient gas-side (k_{Ga} in the dataset), in kmol·m⁻²·h⁻¹·kPa⁻¹.
- The efficiency of the column (eta in the dataset), in mol CO_{2, recovered} / mol CO_{2, inlet}.

It is possible to hypothesize that the flow rates vary within the column are constant.

Generate a model of the column by answering the following questions:

- Load and visualize the dataset, selecting the input and output variables of your system.
- Prepare the data for the training, scaling them using a standard scaler and generating a test set for the performance evaluation. The test set must contain 20% of the original data randomly selected.
- Train an ANN that predicts the K_{Ga} and η variables. The network has 3 hidden layers of 10 nodes each. The internal activation function is ReLU, while the output one is linear.
- Evaluate the training performance on the test set using mean squared error (MSE) and coefficient of determination (R^2) metrics.

After the generation of the model, you want to design a column that can process flue gas with the characteristics reported in Table 1. Define the diameter, height of the column, and process conditions.

Table 1. Flue-gas physical characteristics

Gas Flowrate	20 000 m ³ /h
P _{CO₂} inlet	10 kPa
Inlet CO ₂ loading	0.1 molCO ₂ /molAmine

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