CEAD class – AI applications for CO2 capture

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25th April 2024

The energy sector is one of the main contributors to global warming due to the high amount of CO_2 released during the combustion of fossil fuels. Energy plants are always equipped with a CO_2 capture section to reduce the amount of CO_2 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 CO_2 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 ($k_G a$) in the process absorption column and the absorption efficiency.

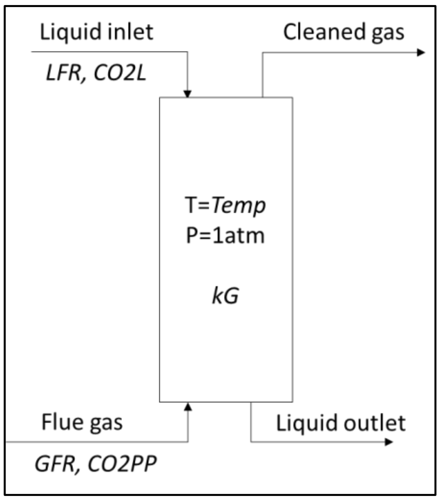

Figure 1. Absorption process schematic representation

The variable space is represented by:

- The liquid flow rate of the stripping stream (`LFR` in the dataset), in L/(m^2·h).
- The gas flow rate of the stripped stream (`GFR` in the dataset), in m^3/(m^2·h).
- The stripping temperature (`Temp` in the dataset), in °C.
- The CO_2 loading inside the stripping stream at the column inlet (`CO2alpha` in the dataset), in CO_2mol/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 (`kGa` 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 $K_G a$ and *eta* 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	2 000 m^3/h
P_{CO2} inlet	10 kPa
Inlet CO_2 loading	0.1 molCO_2/molAmine

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