Model Card

PSA UNIT FOR METHANE-NITROGEN SEPARATION

MODEL DETAILS:

- Pressure swing adsorption (PSA) in a bed packed with silicaliteis is an adequate tecnique for separation of N2/CH4;
- PSA is a cyclic dynamic process comprising two steps: adsorption (production) and desorption (recovery);
- ML application developed by Moura-Neto, M.H. and Monteiro, M.F., researchers from Núcleo de Pesquisa em Petróleo e Gás at Universidade Federal do Rio Grande do Norte (Brazil);
- Decission Tree Regressor model using SciKit Learning and Python lenguage were successfully applied for the calculations.

INTENDED USE

- Intended to be used for chemical engineears for calculations of stream composition obteined from a PSA unit and verify the influence of process variables in the unit outlet;
- Out-of-scope uses: the model is not adequate for PSA bed different from silicalite.

FACTORS:

- Calculate N2 mole fraction in PSA outlet stream based on 12 operational (e.g. Adsorption pressure and temperature) and design (e.g. column's length and diameter) parameters;
- Among the fixed design variables, temperature was the only variable to show small influence on the overall process performance.

TRAINING AND EVALUATION DATA:

- The data used for model development were retrieved from: Hermes R. Sant Anna et al. Machine learning model and optimization of a PSA unit for methane-nitrogen separation, Comput. Chem. Eng., 104, 2017, 377-391.
- PSA operation conditions obtained by phenomenological modeling (1300 data points);
- Separated using train test split function of sciKit Learning;
- The ratio between train and validation was set to 0.3.

METRICS:

- Mean Square Error, Root Mean Square Error, Mean Absolute Error, Mean Absolute Percetage Error and R2 metrics were considered as criterion to evaluate the quality of the split in the hyperparameters tuning;
- Mean Absolute Percetage Error was chosen as the best representative criteria to select the optmal hyperparameter configuration.
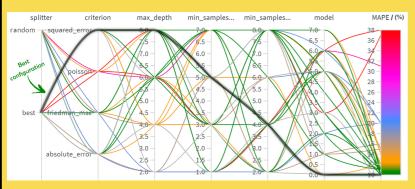
CAVEATS AND RECOMMENDATIONS:

- Verify the units of the properties inserted;
- The application was desined to consider specific ranges of the input properties, properly described in the README.md file. Those limits shall be respected in order to ensure adequate calculation results;
- May have other variables that influence the adsorpson process and were not considered for the model development.

ETHICAL CONSIDERATIONS:

- Predicted N2 conscentrations are an aproximation and must be used with caution in the development of the executive project of the industrial unit.

QUANTITATIVE ANALYSES:

- Mean Absolute Percetage Error of 11 % regarding the test dataset (390 data points).