# Multi-step-ahead simulation of dynamic chemical processes using machine learning models

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## Introduction

Apros® is a dynamic physics-based process modelling and simulation software developed by VTT and Fortum. Physics-based models in Apros® can be computationally heavy when high amount of details are included in large models. One solution to make the model less heavy could be replacing computationally heavy parts of the physics-based model with a machine learning model. This study focuses on the data-driven modelling of simulated data from Apros®. In addition, the workflow to implement the models in Apros® is defined. Overall workflow to implement data-driven models is presented in Fig 1.

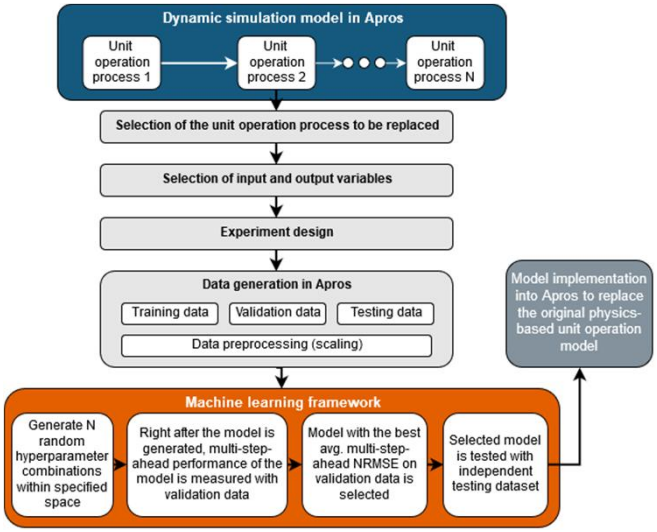


***Figure 1.*** *Overview of the workflow in replacing physics-based unit operation models of an Apros® model with a machine learning model.*

## Combining dynamic physics-based and machine learning models

Apros® includes Python-linking that enables the use of Python using SCL (Simantics Constraint Language). This way, machine learning models built in Python environment can be used in Apros®. However, the requirements for a machine learning model are very high when it needs to interact with the physics-based model in dynamic manner.

## Neural networks in multi-step-ahead predicting

- Suitability of ARX, NARX, LSTM and GRU neural networks in multi-step-ahead predicting is studied.
- Modelling framework utilises Keras Python library
  - Random hyperparameter optimisation
  - Models are instantly tested in multi-step-ahead configuration
  - Only values from one previous timestep was used
  - Models were built using data with a 5s sampling time.

[1] Götz, Manuel *et al.* 2016. "Renewable Power-to-Gas : A Technological and Economic Review.", Renew Energy 2016; 85:1371–90.

## Case study – methanation in a power-to-gas process

Principle of a power-to-gas process is shown in Fig 2. in which the studied methanation unit operation is marked with dashed line.

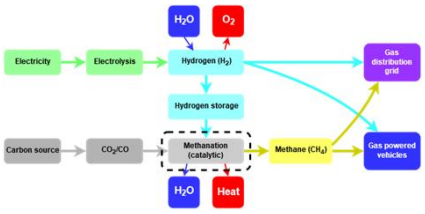


***Figure 2.*** *Process diagram of a power-to-gas process, showing how methane is produced using H2 and CO2/CO (adapted from [1]).*

Accuracies of the studied model types are presented in Fig 3. LSTM model achieved the lowest NRMSE value on test set

- Some outputs were modelled more accurately with linear ARX model and some with nonlinear models
- ARX models were faster to train as the complexity was lower than other models; also the time to make a prediction is lower (0.22ms, 0.29ms, 0.41ms, 0.39ms respectively).

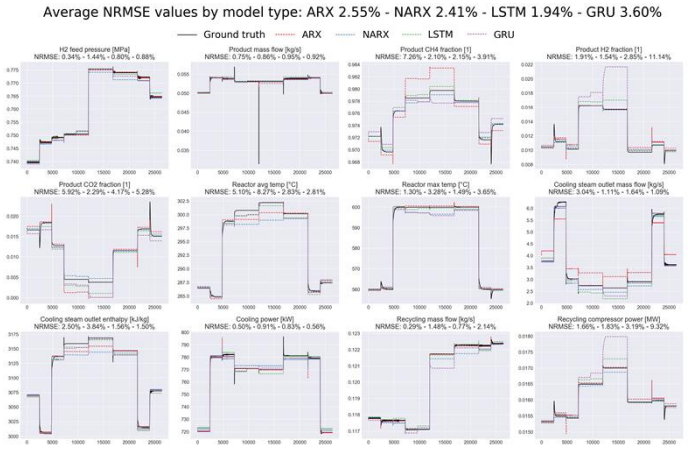


***Figure 3.*** *Results of the case study, showing the best average performance with LSTM neural network on the testing dataset.*

## Conclusions

- **Implementing machine learning models in Apros® requires them to be very accurate**
- **High accuracy can be achieved using neural networks in modelling dynamic chemical processes**
- **A modular model could increase the overall accuracy; in another case, a single model was enough for very high accuracy (avg. NRMSE: ARX 0.07%, NARX 0.09%)**
- **Generating data with higher sampling rate in the case might enhance the performance**
- **With ARX model, increasing the number of lags seem to increase the accuracy slightly**



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