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AI-SURSPEED - AI for faster process simulation

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Published: 26/11/2019

Document Version
Publisher's final version

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Introduction

System simulation has been used as a tool in multiple applications such as system design, optimisation and plant operator training tasks. At the same time, more powerful hardware is available all the time. This makes the simulation tools even more useful – but also makes applying AI to solve problems easier. One challenge in system simulation is that for some applications, models might be too slow to run, limiting the usability. Two kinds of applications require or benefit from accelerated simulation speed. Firstly, e.g. training simulators require at least real-time speed. Other applications are such in which huge amount of simulations are executed.

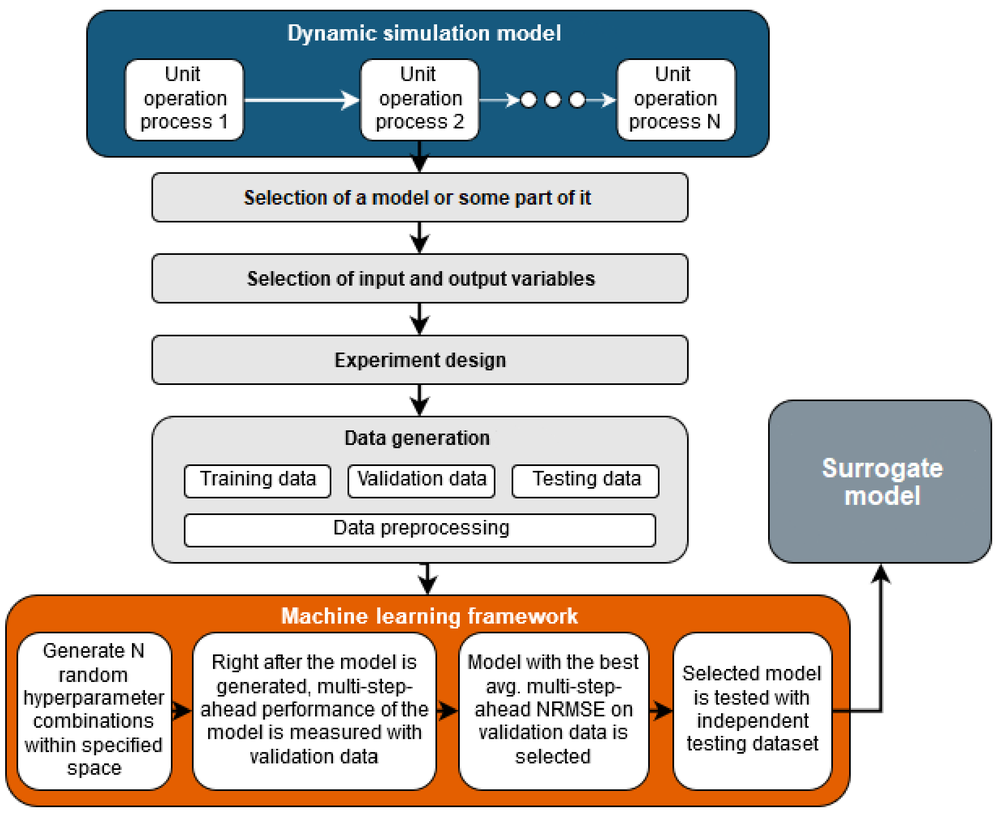

Figure 1. *Overview of the surrogate modelling pipeline.*

Machine learning in surrogate modelling

In this study, AI, or more specifically machine learning and artificial neural networks, are used to create a surrogate model of a dynamic physics-based model to accelerate simulation speed. Surrogate models in general are simplified versions of original models. Although the physics-based models in this study were built in Apros®, this method is not tied to a specific software. The used surrogate modelling pipeline is presented in Fig 1.

More details of the study and the results can be found in [1].

Neural networks in dynamic modelling

Suitability of ARX, NARX, LSTM and GRU neural networks in multi-step-ahead predicting is studied. The modelling pipeline utilises Keras Python library and has following features.

- Random hyperparameter optimisation.
- Models are instantly tested in multi-step-ahead configuration.
- Only values from one previous timestep were used.
- Models were built using data with a 5s sampling time.

[1] Tahkola, M 2019. “Developing dynamic machine learning surrogate models of physics-based industrial process simulation models”. Master’s thesis, University of Oulu. Available http://jultika.oulu.fi/files/nbnfioulu-201906042313.pdf.
[2] Götz, M *et al.* 2016. “Renewable Power-to-Gas : A Technological and Economic Review.”, Renewable Energy 2016; 85:1371–90.

Two case studies – Controlled water tank and methanation reactor in a power-to-gas process

The study included two case study models. The case 1 model is a simple water tank with an inlet and outlet pipe. The liquid level of the tank is controlled by adjusting the inlet flow with a control valve and the outlet flow is adjusted using a pump. The case 2 model was more complex – a methanation reactor 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.

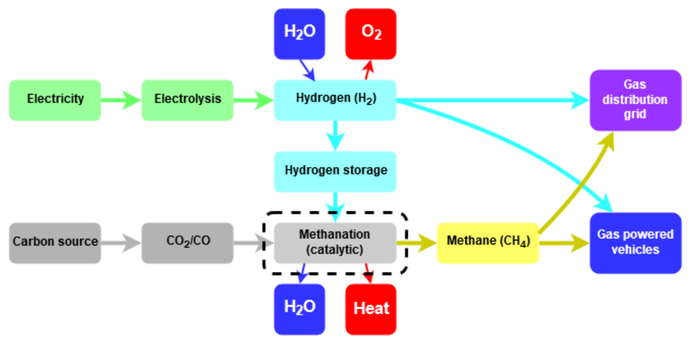

Figure 2. *Process diagram of a power-to-gas process, showing how methane is produced using H2 and CO2/CO (adapted from [2]).*

Results

Case 1:

- Both ARX and NARX had almost zero error compared to the original physics-based model (0.07 and 0.09 %, respectively).
- Good generalization ability, i.e. handled un seen situations well.

Case 2:

- Average error of the 12 predicted variables on test data:
  - ARX 2.55 %, NARX 2.41 %, **LSTM 1.94 %,** GRU 3.60 %.
  - Some variables were predicted more accurately with the linear ARX, some with nonlinear models.
- Simulation speed:
  - In Apros: 50 × real-time.
  - Surrogate: 15 000 × real-time (the Keras model).

Impact

AI methods can be used as a tool to build fast dynamic surrogate models. This makes a single physics-based model usable in wider range of applications and less work hours are needed for remodelling. Faster simulation speed also contribute to getting results faster in engineering and R&D work, potentially increasing the overall work efficiency.

Conclusions

- ✓ **High accuracy can be achieved using artificial neural networks in the modelling of 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 accuracy.**
- ✓ **300 x speed-up was achieved with the method. However, the achievable speed-up depends on the model complexity.**

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This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 723661

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