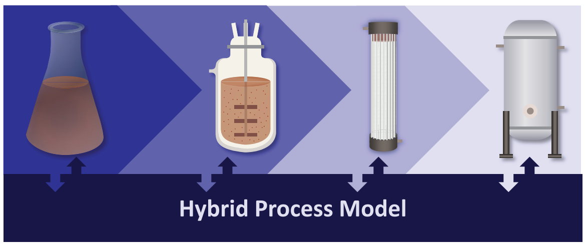
A combined probabilistic and hybrid modelling approach

Rasmus Fjordbak Nielsen[a], Nima Nazemzadeh[a], Martin Andersson[b], Krist V. Gernaey[a], Seyed Soheil Mansouri[a]

[a]*Process and Systems Engineering Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark*
[b]*Combustion and Harmful Emission Control Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark*

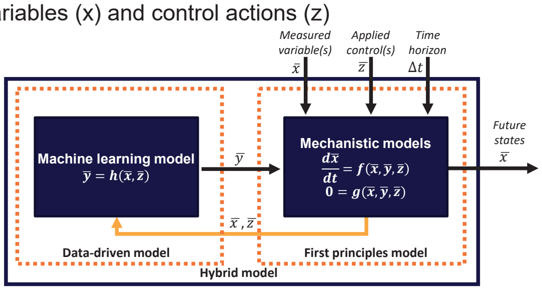
Hybrid modelling of CPPs and CQAs



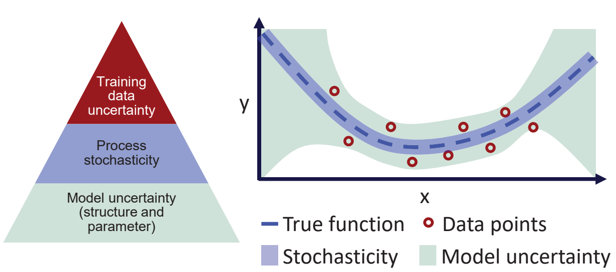
- Product variations likely to cause need for reprocessing, reduced throughput, and/or discard of product!
- Model based design of experiments for process design and/or model predictive control could potentially solve problem
- Hybrid modelling shown to be an efficient and pragmatic modelling approach if time-series measurements of CPPs and CQAs are available

Uncertainty analysis of hybrid model

- Deterministic hybrid model framework presented by Nielsen et al. [1]
- Trained using time-series data of measured process variables (x) and control actions (z)



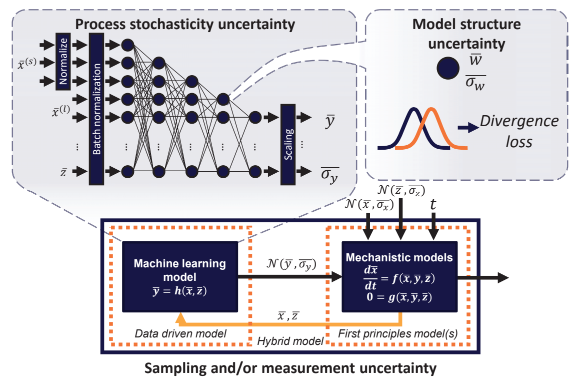
- ML model predicting kinetic rates (y), used in mechanistic model, giving predictions of future process variables (x)



- Data-driven model is the primary source to model uncertainty. A probabilistic model needed!

Probabilistic hybrid model

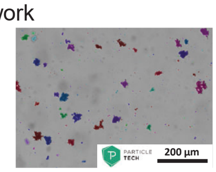
- Including uncertainty during model training on all three levels
  1. Measurement/sampling uncertainty of input and output
  2. Modelling process stochasticity with data-driven model
  3. Making data-driven model parameters stochastic

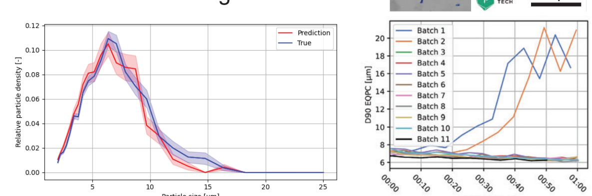


- Training model by minimizing negative log-likelihood and divergence loss between prior and posterior distribution of model parameters

Case-study: Flocculation process

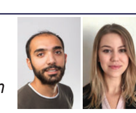
- First principles models: population and mass balance models
- Bin-specific agglomeration and breakage kinetic rates predicted using a probabilistic deep neural network
- Trained using time-series data
  - pH and PSD every 5 minutes
  - 9 batch operations (1 hour)
  - Tested on breakage-batch





- Future perspectives
  - Model based design of experiments (min. model uncertainty)
  - Extending model predictive control strategy [2] to include uncertainty (decision-making under uncertainty)

Further interested in hybrid modelling? Visit Nima Nazemzadeh and Alina Malanca at the poster *Integration of computational chemistry and machine learning in a multi-scale modeling framework: An application on flocculation*



[1] R. F. Nielsen, N. Nazemzadeh, L. W. Sillesen, M. P. Andersson, K. V. Gernaey, S. S. Mansouri, Hybrid machine learning assisted modelling framework for particle processes Comput. Chem. Eng., Elsevier, 2020, Volume 140, 106916, doi:10.1016/j.compchemeng.2020.106916
[2] R. F. Nielsen, K. V. Gernaey, S. S. Mansouri, A hybrid model predictive control strategy using neural network based soft sensors for particle processes, Comput. Aid. Chem. Eng., Elsevier, 2020, Volume 47, 1177-1182, doi:10.1016/B978-0-12-823 377-1.50197-X