

Uncertainty quantification in deep learning frameworks for PAT

Master's Thesis

Starting date: **As soon as possible**

Real-time quality assurance in pharmaceutical manufacturing processes requires precise **process control** strategies. Herein, **Process Analytical Technology (PAT)** tools provide valuable insights into process performance, by measuring **critical quality attributes (CQAs)**. The integration of PAT data with mathematical models, then allows for **predictive control** of the process, leading to improved product quality and operational efficiency. A hybrid modeling approach, combining **mechanistic and statistical models**, could provide increased process understanding and allow for proactive process adjustments. By establishing an **integrated framework**, consisting of the operating system, the PAT sensors and a model pipeline, advances can be made towards **automated** process control in real-time.

Research Objective

The proposed project aims to introduce uncertainty quantification into data-driven process modeling. The target objectives are the prediction of cQA concentration trends throughout a chromatography unit operation. The predictive performance of the model will then be critically evaluated and a mechanistic understanding of the monitored process is to be established.

Methodology

Experimental	Computational
	<ul style="list-style-type: none"> PAT (UV/Vis, Raman, MIR,...) Data-driven modeling (Python) Uncertainty quantification Mechanistic analysis

Timeline

	Month #1	Month #2	Month #3	Month #4	Month #5	Month #6
Literature review of model theory						
Deep learning framework						
Uncertainty quantification						
Mechanistic analysis						
Thesis writing						

Requirements

- Interest in Python and statistical modeling
- Knowledge of data-driven modeling

This thesis has a strong focus on computational modeling and will be solely theoretical.

*Applications of interested applicants can be sent to **doil.yun@kit.edu***