Contribution ID: **1** Type: **not specified**

Enhancing Pharmaceutical Manufacturing Efficiency with End-to-End Models and Physics-Informed AI

Thursday, 29 May 2025 16:20 (20 minutes)

End-to-End (E2E) models and Digital Twins in the pharmaceutical industry enhance efficiency, improve decision-making, allow for real-time monitoring, optimization, predictive analytics, and ultimately strengthen quality control and reduce costs. A key component of E2E models is the use of Monte Carlo simulations to capture uncertainties and variability within complex processes.

Typically, E2E models rely on linear regression models due to their simplicity, ease of implementation, and high computational speed. This makes them particularly suitable for Monte Carlo simulations, which require numerous iterations to achieve statistically meaningful results. However, linear regression models may be too simplistic for accurately representing certain dynamic aspects of pharmaceutical processes. In such cases, more complex models —such as those based on Ordinary Differential Equations (ODEs) and Partial Differential Equations (PDEs) —are necessary to provide a more precise and mechanistic understanding of process dynamics.

Despite their advantages, ODE- and PDE-based models present significant computational challenges. Unlike linear regression models, solving differential equations is computationally intensive, leading to long processing times. When incorporated into Monte Carlo simulations, this results in extremely prolonged computation durations, particularly as the number of required simulations increases. Additionally, these computational demands make real-time applications nearly impossible or require compromises in prediction accuracy.

To address these limitations while maintaining the benefits of ODE and PDE solvers in Monte Carlo simulations, we have developed surrogate models leveraging Physics-Informed AI. These surrogate models significantly accelerate simulations while preserving the accuracy of mechanistic models. By integrating physics-based constraints into AI-driven approximations, we enable more efficient uncertainty quantification and process optimization without the computational burden of traditional solvers.

Our approach enhances the applicability of E2E models and Digital Twins in pharmaceutical process modeling, paving the way for faster, more accurate decision-making and real-time process optimization. This advancement has the potential to revolutionize drug development and manufacturing by making sophisticated modeling techniques more accessible and practical for industrial applications.

Type of presentation

Contributed Talk

Primary author: PRETZNER, Barbara (Körber Pharma Austria GmbH)

Presenter: BOFARULL-MANZANO, Ignasi (RWTH Aachen)

Session Classification: Session

Track Classification: Spring Meeting