Democratizing Digital Twins: Hybrid Modeling Approach for Cosmetic Process Innovation

Rohit Jain[a], Guillaume Bruneau[a], Lucie Doutrelant[a]

[a]L'Oréal Research & Innovation, France

rohit.jain@loreal.com

Background & Objective: In the evolving landscape of cosmetic manufacturing, the ability to accurately predict product quality across different production scales is a critical lever for agility and innovation. Traditional "black-box" Machine Learning (ML) models often require vast datasets and struggle with extrapolation. This work presents a "Hybrid Modeling" approach—combining first-principles mechanistic models with data-driven AI solutions —to create a robust predictive framework for L'Oréal's manufacturing processes. Another objective of this work is also to demonstrate how chemists and process engineers (Subject Matter Experts) can collaborate with digital specialists to build models rooted in physical reality rather than pure data correlation.

Methodology: The study explores the potential of hybrid modeling for manufacturing process predictions, beginning with initial **simplex formulations** and extending to complex emulsion formula. This research was conducted in partnership with **BaseTwo** , a specialist in hybrid modeling for manufacturing processes. By integrating physico-chemical principles—such as Population Balance Equations (PBE) with empirical data, we developed below workflow to predict product quality attributes as a function of process parameters:

Step 1: Manufacturing experimental batches followed by Physico-chemical characterization (Particle Size Distribution (PSD), Rheology) of product quality.

Step 2: Building the model using a training dataset

Step 3: Evaluating model performance on "unseen" conditions (data points excluded from model construction) and comparing predictive results with experimental outcomes.

Step 4: Depending on predictive accuracy, performing further iterations by either incorporating additional data or fine-tuning the mechanistic equations using the initial training dataset.

Final Step: Model validation once the targeted accuracy thresholds are achieved.

Results: Initial results demonstrated that the hybrid modeling approach accurately predicts PSD for both simple and complex emulsions across various manufacturing scales, even under unseen conditions. A second study focused on fine-tuning these models, enabling a transition from PSD to robust rheology predictions by introducing the physic-chemical "Packing Factor" parameter.

Conclusion & Impact: This collaboration between L'Oréal and Basetwo AI demonstrates that hybrid models provide a "decoded" and deployable solution for lab researchers. By leveraging previously solved parameters, we can achieve predictive scale-up without additional data, directly accelerating the transition from lab to production. Future work will focus on scaling this collaborative framework at bigger scales and other cosmetic socles to establish a new standard for inclusive process digitalization.

Keywords:

Hybrid Modeling, Digital Twin, Cosmetic Process Engineering, Emulsions, Scale-up Optimization, Physics-Informed Machine Learning

References:

A review and perspective on hybrid modeling methodologies" by Artur M. Schweidtmann, Dongda Zhang, and Moritz von Stosch, published in Digital Chemical Engineering in 2024