Contribution ID: **14** Type: **not specified**

Hybrid Semiparametric Modelling of the Supercritical Carbon Dioxide Extraction Process

Thursday, 29 May 2025 15:00 (20 minutes)

Keywords: Digital Twin, Hybrid Modeling, Machine Learning, Supercritical Carbon Dioxide Extraction, Process Optimization

Abstract
Supercritical carbon dioxide (ScCO2) extraction is a separation process that presents several advantages over traditional extraction methods of nonpolar solutes, eliminating the need for harmful organic solvents and costly post-processing steps required to remove solvents from extracts. Carbon dioxide is an ideal solvent due to its safety, availability, and cost-effectiveness. Its relatively low critical temperature (304.25 K) allows for the extraction of heat-sensitive substances without degradation (Couto, 2009, Mendes, 2006).
Modeling the ScCO2 extraction process typically involves a combination of intraparticle and macroscopic material balance equations alongside mass transfer laws. A significant challenge in these models lies in defining the relationships between mass transfer coefficients, flow conditions, ScCO2 properties, and the physiochemical characteristics of the target solute. The latter are typically empirical and less reliable, eventually compromising the model's predictive power.
In this study, we developed a hybrid neural network (HNN) model for the ScCO2 extraction of lipids from biomass. The developed HNN combines a feedforward neural network (FFNN) with intraparticle and macroscopic material balance equations, formulated as Partial Differential Equations (PDEs). Particularly, the FFNN is used to model the overall transfer rate of the solute from porous biomass into the bulk as function of biomass microenvironment conditions.

The study used data from ScCO2 extraction experiments (20% for testing and 80% for training the model) to extract lipids from biomass under varying temperatures (313–335 K), pressures (200–500 bar), and ScCO2 flow rates (0.00017–0.0025 kg/sec).

Initially, the extraction column was discretized into multiple levels (3–20), and a mechanistic model was developed using differential equations and empirical mass transfer laws to predict lipids extraction efficiency based on operational parameters. In the next stage, FFNNs were integrated to enhance prediction accuracy. Results showed that increasing the number of discretization elements significantly improves hybrid model predictive accuracy, reducing training and testing errors. The final hybrid model shows high predictive power, eventually supporting a digital twin of the ScCO2 extraction unit. The next step will be to optimize the ScCO2 extraction process.

References
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Type of presentation

Contributed Talk

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Session Classification: Session

Track Classification: Spring Meeting