DATA RESEARCH meetup by MagIC

Deep Hybrid Modelling of a Supercritical CO2 Extraction Process

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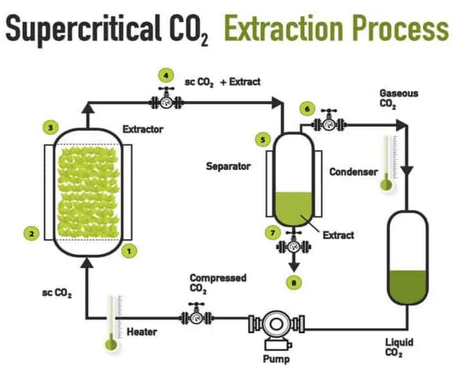
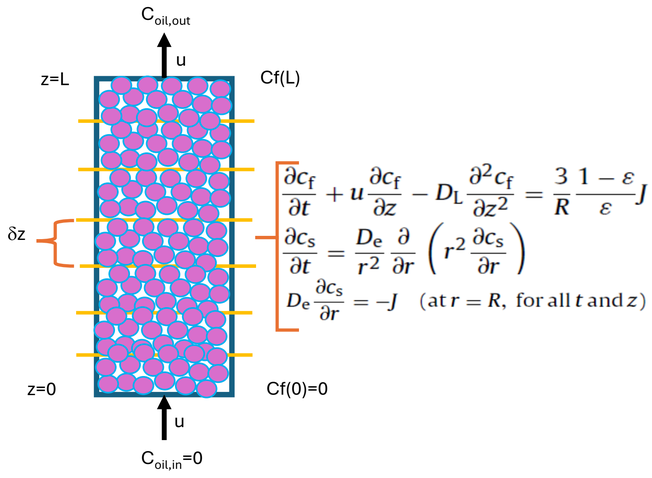
INTRODUCTION

Integrating deep learning and big data has the potential to significantly enhance efficiency in biomanufacturing.
However, the industry currently faces a challenge due to inadequate big data infrastructure.
A promising solution to this issue is the development of a **hybrid neural network (HNN)** that combines deep neural networks (DNN) with existing process knowledge [1].

This approach could improve **Supercritical Carbon Dioxide (scCO2)** extraction processes within biomanufacturing, thereby contributing to a more sustainable environment, even in the absence of robust big data infrastructure.
The scCO2 extraction process is a safe, solvent-free method for extracting active materials in biomanufacturing. CO2 is favored for its safety, availability, low cost, and possibility of extraction of heat-sensitive substances[2].

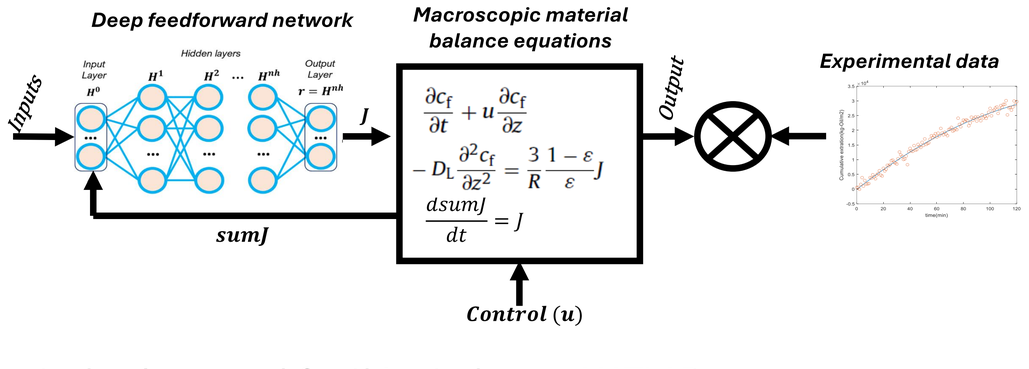




Modeling the scCO2 extraction column typically involves combining intraparticle and macroscopic material balance equations with mass transfer laws. The most challenging parts are understanding the relationships between mass transfer coefficients, flow conditions, scCO2 properties, and solute physiochemical properties[3].

METHODS AND MATERIALS

To overcome the problems discussed, a deep HNN model was developed for the scCO2 extraction process. A deep HNN model integrates a deep feedforward neural network with intraparticle and macroscopic material balance equations represented as a system of Partial Differential Equations (PDEs), incorporating parameters based on the raw material's physiochemical properties.
It was developed to predict the amount of extracted lipids from biomass.



The technology used for this study was MATLAB
- *Inputs: T, P, SC CO2 flow rate, Initial oil content*
- *Output: Oil extraction rate*

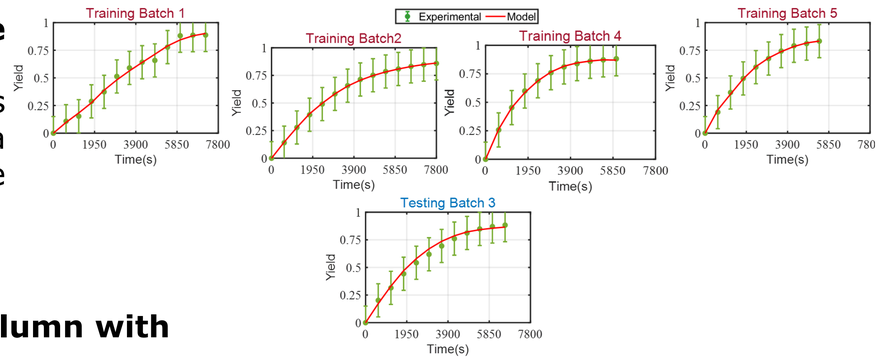
RESULTS & DISCUSSION

Step1 **Model for synthetic data**
- Solving partial differential equations (PDEs) to account for mass transfer

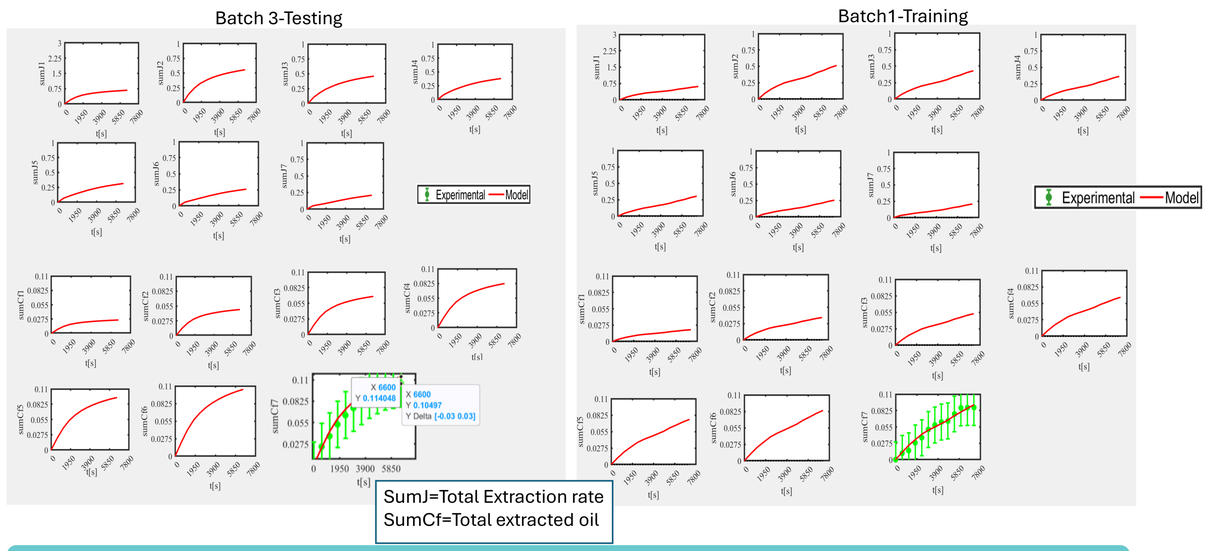
Step2 **Model for experimental data for whole column**

Step3 **Model for experimental data by dividing the column into 7 levels**
- Solved PDEs for each level were added to the model.

Modeling for the whole column:
The model shows good training and a good prediction in the test batch.



Modeling for the column with separated levels:
Results from the model indicate the following trends:
- The total extraction rate (sumJ) decreases along the column.
- The total extracted oil (sumCf) increases along the column and over time.
- Good training and a good prediction in the test batch



CONCLUSION

As discussed, the use of CO2 offers safety, accessibility, affordability, and a low critical temperature (304.25 K), making it ideal for extracting heat-sensitive substances.
This study presents **The First Application** of a Hybrid Neural Network (HNN) model to simulate the supercritical carbon dioxide (scCO2) extraction process.
The whole column model demonstrates strong optimization potential.
The separated level model effectively predicts extraction yield with tinny deviation from laboratory data (8.5%) and provides valuable insights into the processes occurring at different levels within the column.
Key improvements include:
- reduced data requirements,
- suitability for extrapolation,
- accurate predictions,
- Process optimization.

This study shows this approach not only enhances process efficiency but also promotes sustainability.

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