A Machine Learning Approach to Predict 3D Printability of Biopolymer-Based Ink

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Cross-Disciplinary Research Area:
Additive Manufacturing, Materials Science, Data Analytics, Process Engineering, Health Care

Abstract

The development of 3D-printed products requires significant trial and error effort. This is due to the lack of understanding of the material (i.e. polymer) used for ink development and its subsequent impact on the 3D printing outcome as variations of materials require different process parameters adjustment. This research aims to develop a machine learning model framework to predict the 3D printing outcome of biopolymer-based ink prepared for pharmaceutical applications to minimize trail-error effort and material wastage and eventually minimize the cost. As a proof of concept, we prepared 9 different ink with various polymer compositions and 67 observations considering variations of the 3D printing process parameters. The machine learning models, namely *Logistic Regression*, *Decision Tree Classifier*, *Support Vector Machine*, *Random Forest*, and *Artificial Neural Network*, were considered for the initial evaluation. Our findings show that we have achieved promising results in 3D printing prediction, with notable accuracy of 88.3%, 94.0%, 87.0%, 80.0%, and 60.0%, respectively, indicating good prediction. Based on our evaluation, Random Forest and Artificial Neural Network will be more appropriate for the complex work type we are studying for the pharmaceutical application. The F1 score for Random Forest and Artificial Neural Network is 87% and 73%, respectively, which confirms our proof of concept with limited experimental data.

Background

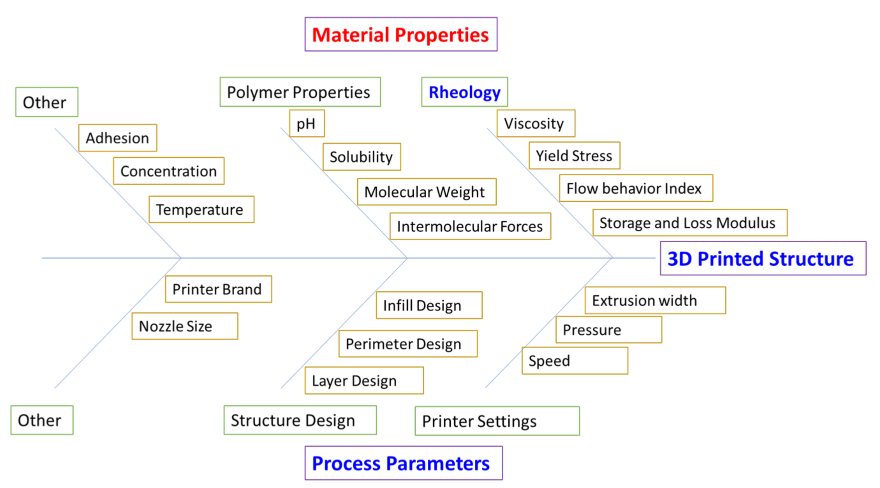


Figure 1. Fishbone diagram- essential data for 3D printing.

Stakeholders in 3D printing:

- Use case selection
- Product design
- Materials selection
- Material property analysis
- Process parameter selection
- Trial-error process

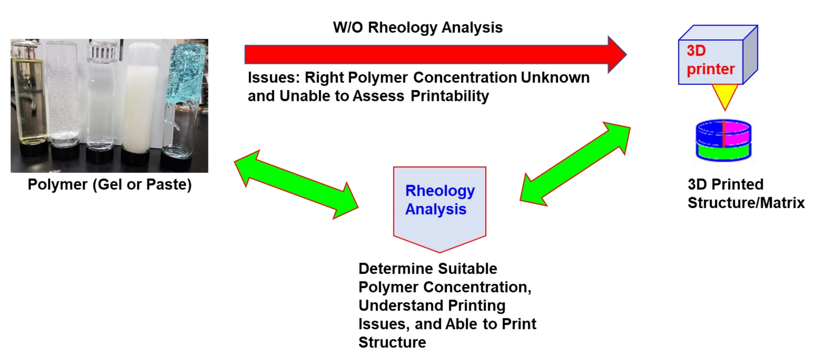


Figure 2. Current 3D printing practice.

Current research gaps:

- Only do trial & error to optimize formulation and process
- Bias research due to considering fixed material and/or conditions
- Most research considers only one aspect: Material / Rheology / Printing process
- Absence of meaningful data in the model dataset

Research Objectives and Impacts

Objectives:

- Establish a data-driven approach for predicting the printability of 3D printing processes by leveraging key insights derived from the interplay between the material's rheology and printing parameters.
- The ultimate goal is to enhance efficiency, reduce waste, and advance the precision of polymer-based additive manufacturing.

Impacts of the research

- Reduce development and manufacturing time and, eventually, the cost
- Minimize trial and error and, subsequently, material waste
- Enhance process clarity and heighten process control
- Provide the ability to incorporate variability
- Allow small-scale, low-cost production

Methodology

Table 1. Ink formulation developed for 3D printing of thin film.

Biopolymer name	Polymer	Drug	Functional excipients			Solvent
		FNB*	SSG*	Glycerin	PVP*	Water
	(g)	(g)	(g)	(g)	(g)	(g)
Sodium Alginate	0.24	6.00	0.50	3.00	1.50	18.76
	0.48	6.00	0.50	3.00	1.50	18.52
	……	……	……	……	……	……
	1.20	6.00	0.50	4.00	1.50	16.80

*FNB: Fenofibrate, *SSG: Sodium Starch Glycolate, *PVP: Poly Vinyl Pyrrolidone

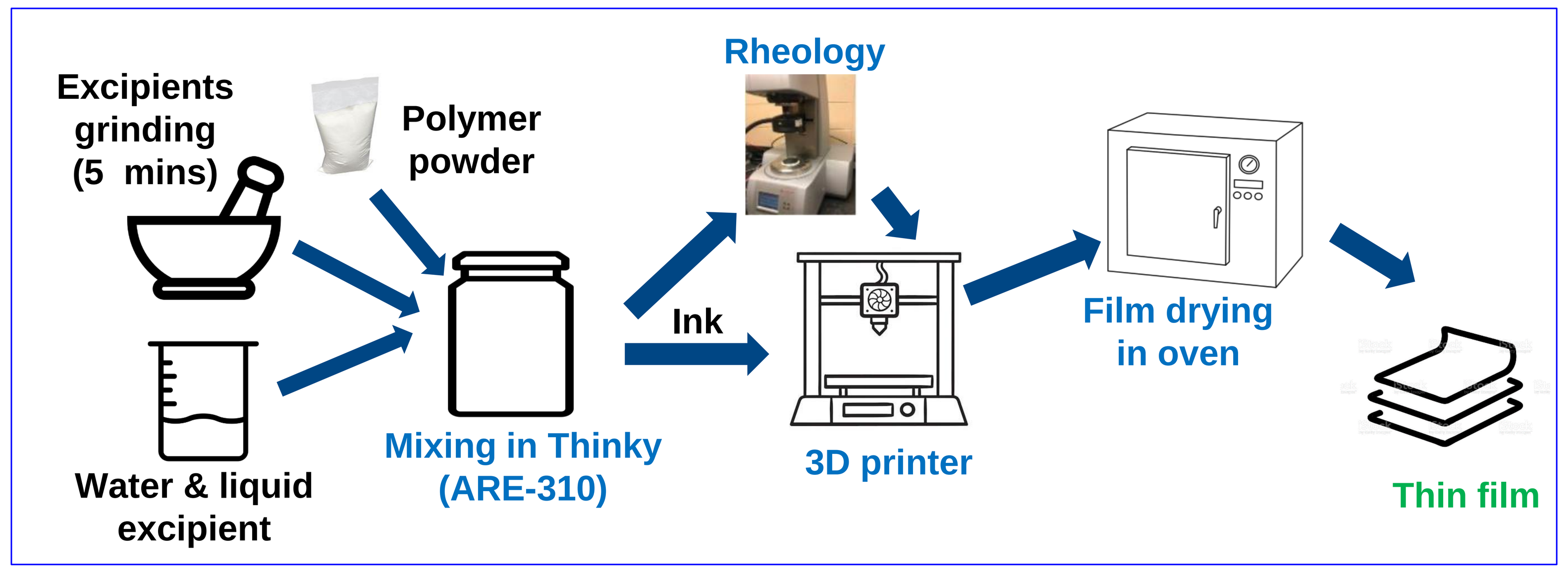


Figure 3. Schematic representation of the film 3D printing process.

Ink rheology measurement and transformation into data:

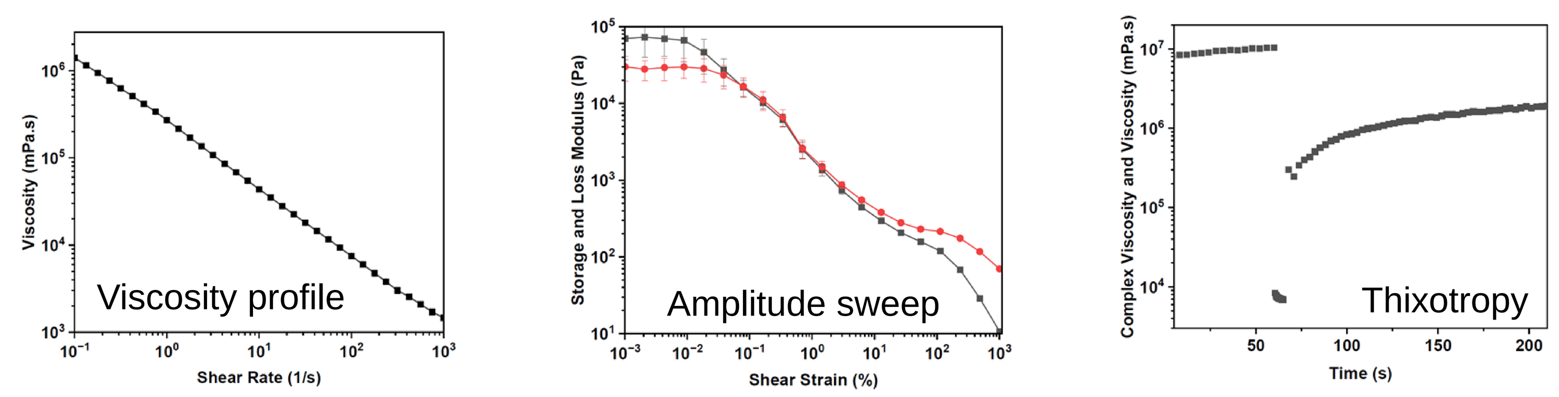


Figure 4. Rheology information of the ink.

Table 2. Rheology information transformation into quantifiable data to use in the model.

	Model Input															Model Output
	Rheology													3D Printing		
Test name	Flow test				Amplitude sweep test				Thixotropy test (Osc-Rot-Osc)							
Test Parameter	Viscosity at shear rate				Ratio of Storage and Loss modulus				Complex Viscosity or Viscosity					Print speed	Print Pressure	Print decision
Unit	[1/s]				[Pa/Pa]				[mPa·s]					[mm/s]	[kPa]	
Data point	0.1	1	…..	1000	1	3	…..	19	60s	65s	67.9s	…..	210s			
Data labeling	V0.1	V1	…..	V1000	SL1	SL3	…..	SL19	TCV60	TV65	TCV 67.9	…..	TCV210	PS	PP	PD
Observation-1																
…………….																
Observation-67																

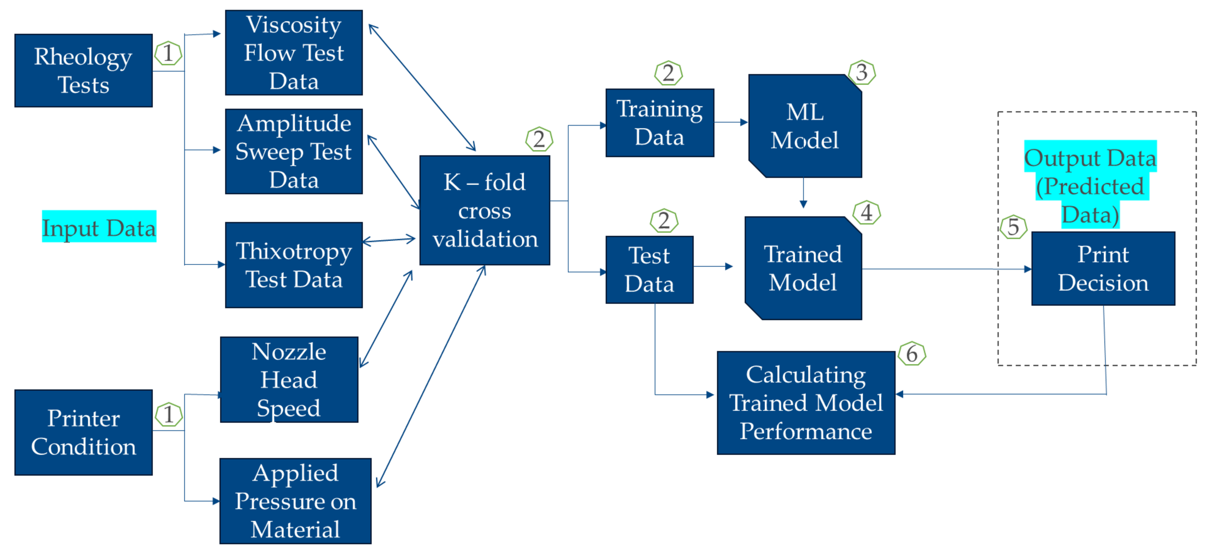


Figure 5. Developed model framework.

Methodology

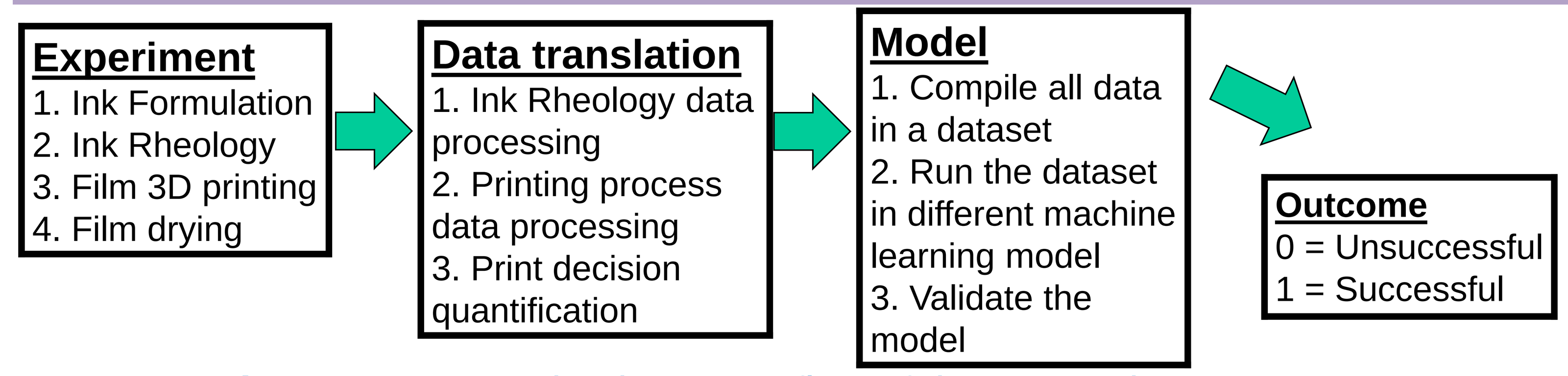
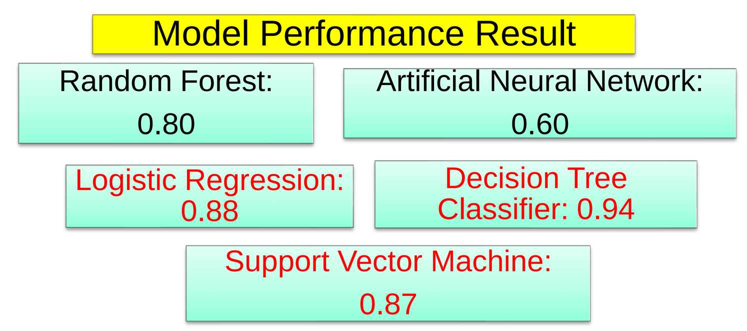


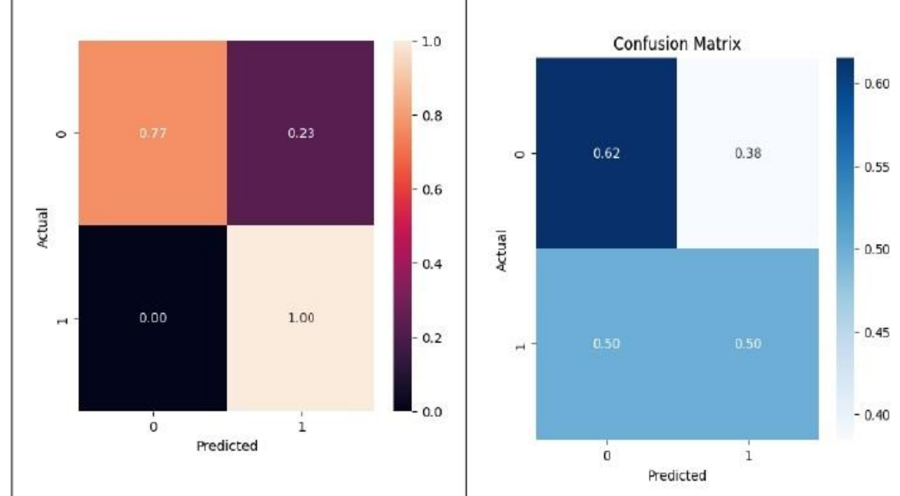
Figure 6. Summarized process flow of the research.

Results and Discussions



Models not selected and reasons:
Logistic Regression: Limited to linear relationships, assumption of independence of observations, sensitive to outliers that lead to biased results.
Decision Tree Classifier: Prone to overfitting, sensitive to small variations in training data.
Support Vector Machine: Sensitive to noise and outliers, it involves solving a quadratic optimization problem, which can become computationally intensive.

Table 3. Model performance evaluation.

Parameters	Printing Outcomes	Random Forest (RF)		Artificial Neural Network (ANN)	
Accuracy	-	0.80 (Correctly predicts the target variable 80% of the time)		0.60 (Correctly predicts the target variable 60% of the time)	
F1 Score	0	0.87	A high F1 score indicates better model performance.	0.73	A high F1 score indicates better model performance.
	1	0.57		0.25	
Confusion matrix					

RF and ANN models get selected:
Random Forest: Provides high accuracy in prediction, robust to overfitting.
Artificial Neural Network: Can model highly complex and nonlinear relationships in data, are adaptable to large and diverse datasets, automatically extracting relevant features from raw data using end-to-end learning.

Conclusions and Future Work

Models show satisfactory performance results. It represents two outcomes:

I. The selected features are able to represent the model condition.
II. The model may falsely represent that it is working well due to insufficient data variety. Hence, there are more data required.

Future work:

- Generate more data by using the current methodology.
- Consider more controlling parameters.
- Rank effective parameters to improve model efficiency.

References

M. Azad, D. Olawuni, G. Kimbell, A. Badruddoza, M. Hossain, T. Sultana. Polymers for extrusion-based 3D printing of pharmaceuticals: A holistic materials–process perspective. Pharmaceutics. 2020;12(2):124.

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