BioPINNacle : Redefining Traditional Process Modelling in Bioethanol Production Through Physics Informed Neural Networks

Aditi R. Wandale, Dr. Sameer M. Wagh

Department of Chemical Engineering,Laxminarayan Innovation Technological University,Nagpur

Introduction

- Bioethanol fermentation shows strongly coupled changes in substrate, biomass, and ethanol over time.
- Accurate modelling of these dynamics is essential for improving process efficiency.
- Conventional neural networks fit data but often ignore known fermentation kinetics.
- Physics-Informed Neural Networks (PINNs) combine data with kinetic equations for reliable and interpretable modelling.

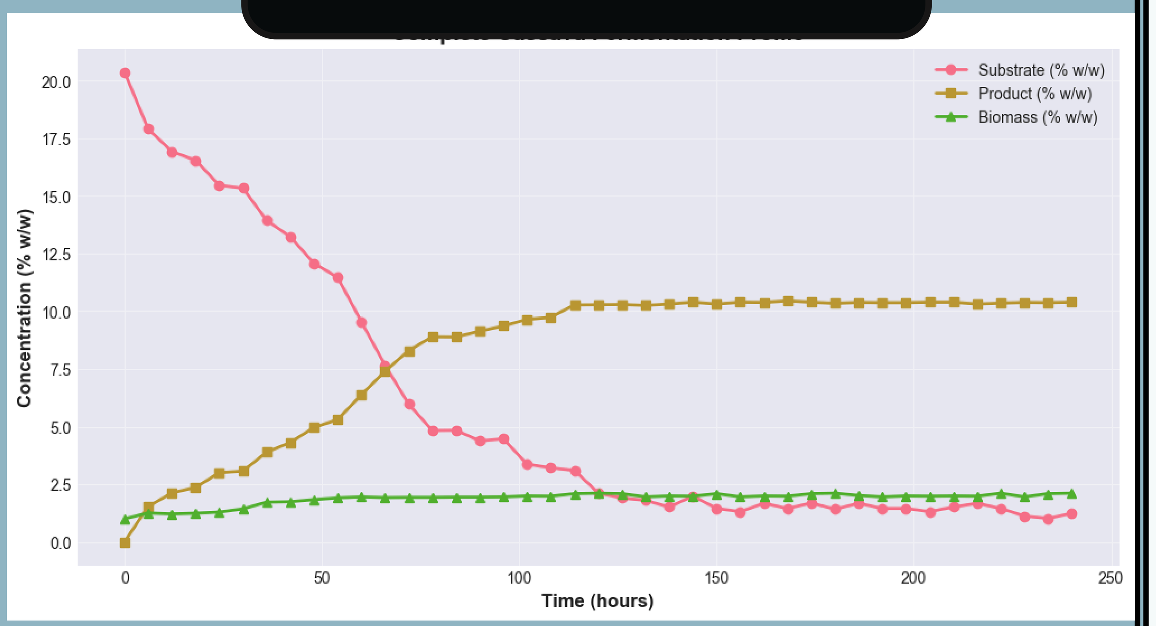
Problem Statement

- Bioethanol fermentation involves complex, time-dependent interactions between substrate consumption, biomass growth, and ethanol formation that are difficult to model accurately.
- Traditional data-driven models provide good curve fitting but often violate known fermentation kinetics and lack physical interpretability.
- There is a need for a modelling framework that can learn from limited experimental data while strictly adhering to governing biochemical laws.

References

- Raissi et al. (2019). J. Comput. Phys., 378, 686–707.
- Karniadakis et al. (2021). Nat. Rev. Phys., 3, 422–440.
- Asiedu et al. (2024). J. Eng. Appl. Sci., 71:195.

Cassava Fermentation Profile



- Substrate concentration decreases steadily over time due to microbial consumption.
- Ethanol concentration increases and eventually plateaus, indicating fermentation completion.
- Biomass exhibits initial growth followed by stabilization.
- Overall trends are consistent with Monod-based fermentation kinetics.

Governing Equations (Cassava)

- Biomass Growth

$$dX/dt = \mu(S,P)\cdot X$$

- Product Formation

$$dP/dt = q_P(S,P)\cdot X$$

- Substrate Consumption

$$dS/dt = -(1/Y_XS)\cdot\mu(S,P)\cdot X - (1/Y_PS)\cdot q_P(S,P)\cdot X$$

- Specific Growth Rate (Monod with Product Inhibition)

$$\mu(S,P) = \mu_max\cdot(S/(K_Sx+S))\cdot(1-K_ipx\cdot P)$$

- Specific Product Formation Rate

$$q_P(S,P) = q_Pmax\cdot(S/(K_Sp+S))\cdot(1-K_ipp\cdot P)$$

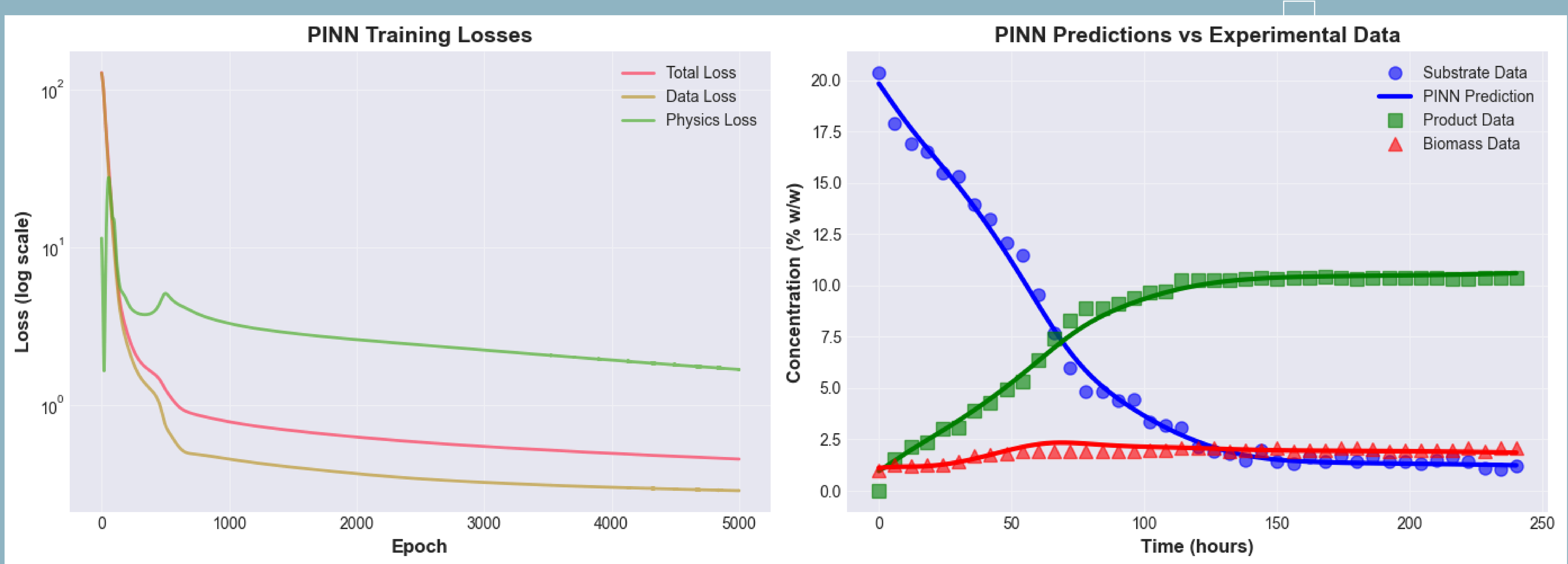
- Initial Conditions

$$X(0) = X_0 \quad S(0) = S_0 \quad P(0) = 0$$

Learned Parameters

Parameter	Value
mu_max	0.841695
q_pmax	5.58997
K_sx	-0.929824
K_sp	2.356223
K_ipx	0.102616
K_ipp	0.06313
Y_xs	0.256961
Y_ps	0.54206
M_s	-0.116052
G_s	-0.106052

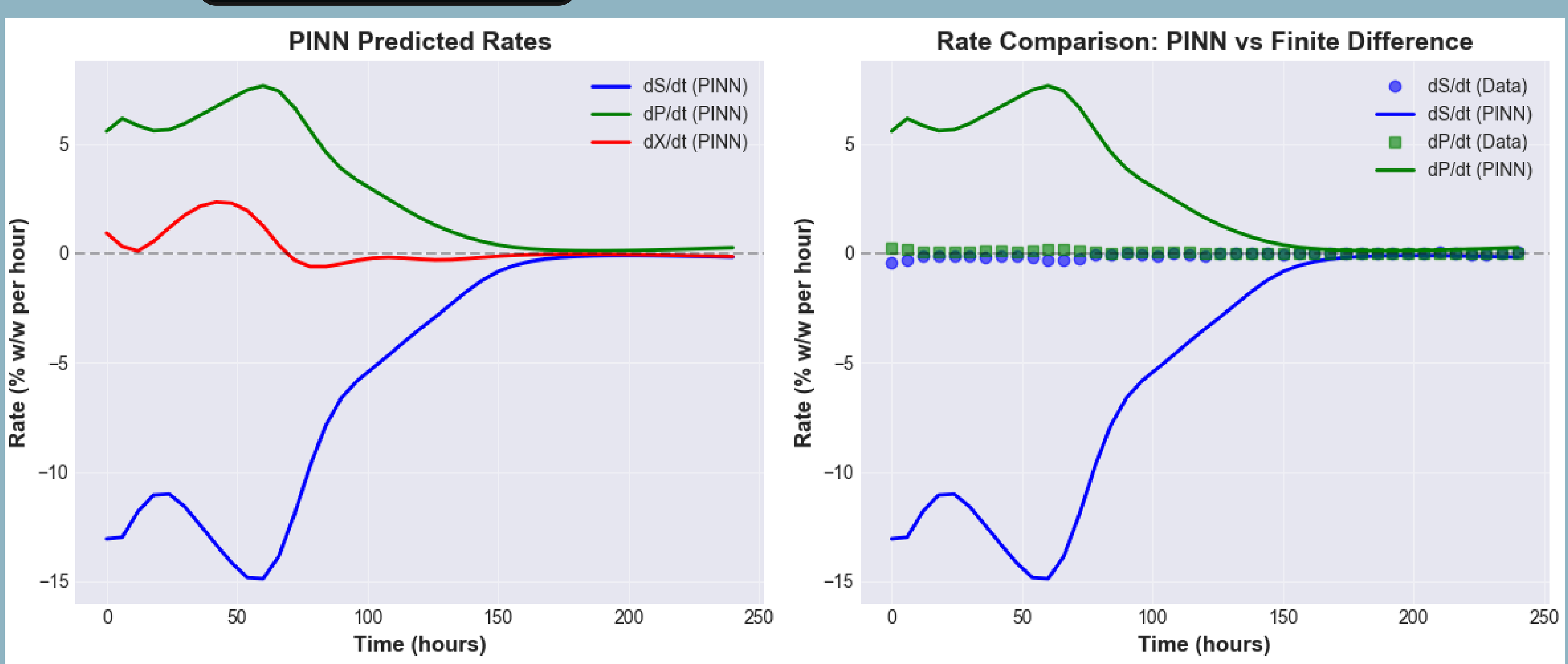
PINN Performance



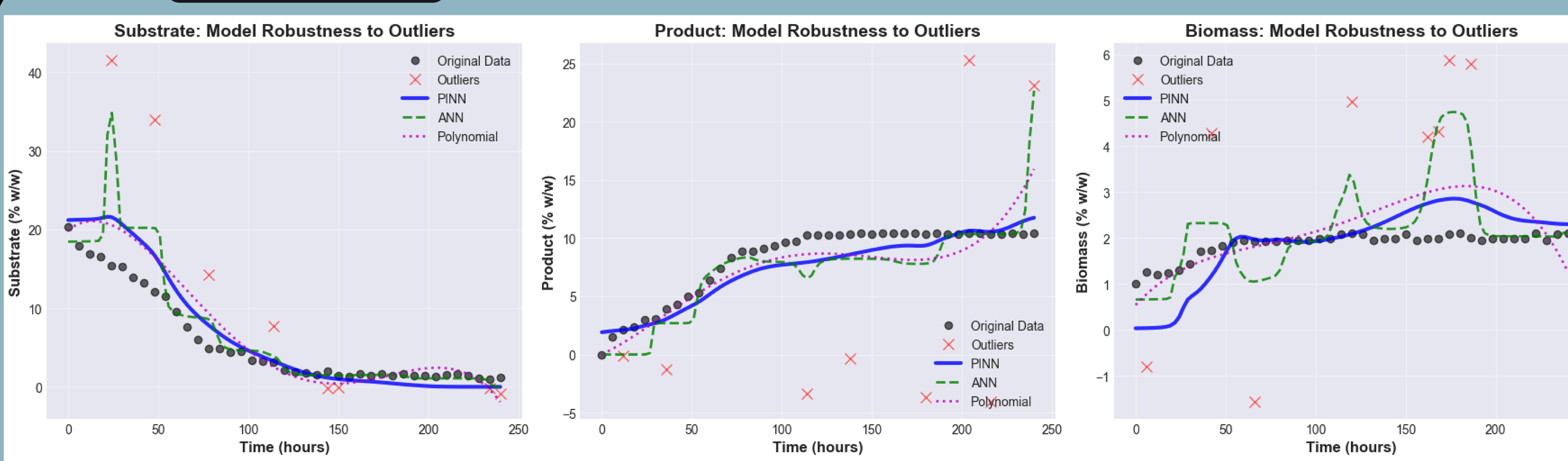
BioPINNacle App

The BioPINNacle appwas created to provide a user interface and act as a digital twin for the bioethanol fermentation process.

Saliency Plot



Outlier Scenario



R^2 Result For Outlier Scenario

Model	Substrate	Product	Biomass
PINN	0.8075	0.823	-3.3067
ANN	0.5748	0.3261	-9.6572
Polynomial	0.7903	0.6837	-3.6555