

AI & Machine Learning in Biochemical Processes: From Data to Design

Vaishnavi Niranjani¹, Anirudh Singh¹, Ajay Kumar Singh^{2*}

Department of Biochemical Engineering

Harcourt Butler Technical University, Kanpur

Email: aksingh11@hbtu.ac.in

The Indian chemical and petrochemical industry market growth was US\$220–250 billion during 2024-2025, which is expected to grow US\$300 billion by 2028 as per expectation of Indian Ministry of Chemicals and Fertilizers. The contribution of new advanced methods are playing very crucial role including Artificial Intelligence (AI) and Machine Learning. Integrating Artificial Intelligence (AI) and Machine Learning is transforming biochemical engineering in various aspects by enabling data-driven approaches for designing, monitoring, and controlling biological systems, and various optimisations. Traditionally, processes of biochemical development depend heavily on experimentation and observation. AI and ML approaches offer an exemplar shift by amplifying discovery by reducing the cost of development, increasing product robustness and improving its productivity, along with pharmaceutical chemicals. A broad spectrum of machine learning is involved in innovating biochemical processes. Some supervised learning techniques, such as Decision Trees, Support Vector Machine, Random Forest, k-Nearest Neighbours, and Naïve Bayes, used for extensively predicting modeling. Artificial Neural Networks (ANNs), Convolutional Neural Networks (CNNs), and Recurrent Neural Networks (RNNs) for enhancing high-dimensional pattern recognition and data analysis at high dimensions. Some recent advances demonstrate the impact of AI in the case of biochemical research. Some Geneformer, transcriptomic foundation models, and single-cell datasets for the prediction of gene network dynamics and in the applications of therapeutic targets. Some revolutionary biomolecular structure prediction models accurately using AlphaFold3 interacting among ligands, nucleic acids, and proteins that accelerates enzyme engineering and drug discovery. In the case of developing AI-enabled bioprocess platforms that are AI enabled such as BioProfile ® FLEX2, BD FACSDiscover™ S8 integrated real-time sensing, Sartorius ambr 250 ®, and Eppendorf DASbox®. Some liquid handling systems, such as Beckman Coulter Echo ® 525, enhance throughput designs. Altogether, AI and ML are fulfilling the gap between generational biological data and process designs. Integrating biochemical engineering in new approaches enhances capabilities and manufacturing strategies.