

DEEP P. KOTADIA

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EDUCATION

Program	Institute	CGPA	Year
M.Tech Chemical Engineering	Indian Institute of Technology Madras, Chennai	8.71	2024-2026*
B.Tech Chemical Engineering	Pandit Deendayal Energy University, Gujarat	8.57	2019-2023
Class XII	Swami Vivekanand School, Gujarat	8.23	2017-2019
Class X	Swami Vivekanand School, Gujarat	8.08	2016-2017

WORK EXPERIENCE

Data Science Intern, Rapidrug Pvt. Ltd., Chennai, India Nov 2024 – Jan 2025

- Developed an AI-driven veterinary drug safety forecasting system integrating time-series analytics and molecular intelligence.
- Engineered molecular descriptors using RDKit and combined cheminformatics workflows with predictive modeling.
- Designed agentic AI workflows for automated drug trend analysis and veterinary pharmaceutical insights.
- Applied forecasting models and exploratory ML techniques for companion animal therapeutic analytics.

Process Technology Engineer, Zentiva Pvt. Ltd., Ankleshwar, India Jan 2023 – June 2023

- Supported safe and reliable plant operations during scale-up of Grignard reagent formation for multi-step API manufacturing, achieving 88% yield through process optimization and operational troubleshooting.
- Led continuous improvement of intermediate synthesis using phase-transfer catalysis and solvent system optimization, improving yield to 93% and enhancing process robustness and reliability.
- Developed process flow diagrams (PFDs), mass balances, and operating strategies to support technology transfer and plant readiness, ensuring smooth transition to manufacturing.

Process Design Intern, TITLIS Projects & Engineering Pvt. Ltd., Baroda, India June 2022 – July 2022

- Contributed to process design and optimization for silicon extraction from coal mining waste, achieving 85% conversion and improving product purity to 89% for downstream semiconductor applications.
- Developed process flowsheets, block flow diagrams, and preliminary design basis for silicon extraction process, aligned with industrial FEED practices.
- Performed process optimization and troubleshooting using XRF/XRD data to improve product purity and operational stability.

PROJECTS

Curated dataset on catalytic depolymerisation of polyolefin using Local Large Language Models June 2025 – Present

- Developed an end-to-end **AI-driven literature mining** pipeline using **Gemma4:e4b (Local LLM)** to automate extraction of catalytic pyrolysis data from **736+ scientific** publications.
- Curated a structured dataset containing **559 experimental datapoints** from 73 research papers, covering 120+ catalysts, 6 reactor configurations, and operating conditions for catalytic polyethylene pyrolysis.
- Built and **optimized ML models (XGBoost, Random Forest, SVR) using Optuna-TPE** for hydrocarbon product yield prediction, achieving **R² up to 0.78** for gas yield estimation.
- Engineered a fully local **GPU-accelerated scientific workflow** integrating OCR, PDF parsing, prompt engineering, and schema validation, significantly reducing manual data curation effort.

Prediction of Absorption Energies of Chemical Species on Metal Catalyst Surfaces using ML Models Jan 2025 – May 2025

- Developed and benchmarked **5 ML models** to predict adsorption energies across 8 transition metals, achieving 0.12 eV MAE, reducing computational cost of DFT-based catalyst screening by >80%.
- Engineered and automated descriptor discovery via **PCA + varimax rotation**, identifying 3 optimal physical descriptors that captured 98% dataset variance, outperforming conventional trial-and-error approaches.

De Novo Molecular Generation using AI-based Bigram Models Jan 2025 – Apr 2025

- Developed a statistical **AI language model (Bigram)** to autonomously generate chemically realistic, un-synthesized molecules.
- Trained the model on a dataset of **3,000 SMILES strings**, engineering a sampling process based on learned character transition probabilities to capture local molecular syntax and successfully generate 100 novel SMILES sequences.
- Evaluated the structural uniqueness and chemical viability of the generated molecules by calculating Tanimoto Similarity coefficients with Morgan fingerprints via **RDKit**.
- Achieved an average Tanimoto similarity score of 0.024 against the training dataset, demonstrating the generation of highly unique and distinct chemical structures.

Optimization of Steam Methane Reforming Reaction to maximize conversion using Neural Networks Aug 2024 – Dec 2024

- Engineered and trained a deep neural network (8-layer, 50-neuron) to model methane conversion, achieving <0.5% prediction

error versus numerical solvers, enabling reliable process simulations without costly experiments.

- Automated reaction optimization using grid search over 100,000 parameter combinations, identifying optimal conditions that maximized **CH₄ conversion by 71%** while significantly reducing manual iteration time.
- Optimized model architecture through systematic hyperparameter tuning, reducing weights by 80% with negligible loss in accuracy, demonstrating scalable deployment for data-driven process optimization.

Process Simulation of Ethyl Lactate - A Green Solvent

Aug 2022 – Dec 2022

- Simulated and optimized ethyl lactate production via reactive distillation using **DWSIM**, achieving 96.13% lactic acid conversion & 95.7% ethyl lactate yield.
- Designed a process flowsheet integrating fermentation, reactive distillation, and product purification, resulting in an ethyl lactate production rate of 234 g/h and energy consumption of 111.41 kJ/g.
- Applied the NRTL property to represent non-ideal mixtures and optimize operating parameters for high-purity.

PUBLICATION AND PATENTS

- **Design of Solar Panel Cleaning System**, under Intellectual Property of India, Design No.: 347167-001, filed on August 2, 2021, and issued on October 06, 2021.
- **Research Paper**: “A comprehensive study on amalgamation of sustainable solar powered distillation for arsenic and fluoride removal from groundwater.” Environmental Science and Pollution Research, 2021, 28 (48), p:67909-67924.

RELEVANT COURSEWORK

- **Key Courses**: Molecular Data Science & Informatics, Application of Machine Learning in Reaction Engineering, Artificial Intelligence in Chemistry, Chemical Reaction Engineering, Process Modelling & Optimization, Process Equipment Design, Process Simulation Laboratory, Computer Aided Process Design, Transport Phenomena.
- **Additional Courses**: Computational Methods in Catalysis, Nanotechnology & Energy Storage, Fuel & Energy Technology, Material Science & Engineering, Polymer Science & Technology.

TECHNICAL SKILLS

Programming Language: Python, OOP, MATLAB, SQL.

Library: Numpy, Pandas, Matplotlib, Seaborn, Pytorch, Keras, Tensorflow, Langchain, Langgraph, RDKit, ASE, Sci-Kit Learn.

Software: Aspen Plus, DWSIM, n8n, MS Excel, MS Powerpoint, MS Word, Diagrams.net., VS Code, Claude Code, Git, Github, Docker, Ollama, LMStudio, vLLM

Other Skills: Process Optimization, Machine Learning, Large Language Models, Statistical Modelling, Prompt Engineering, Data Analysis, Workflow Automation, Data Management, Documentation, Design of Experiments.

CERTIFICATION

BCG Data Science Job Simulation	Forage
Generative AI Foundations, GANs, VAEs and Real-World image Generation Techniques	GIAN Course
Machine Learning with Python	FreeCodeCamp
Data Analysis with Python	FreeCodeCamp
Python Certification*	FreeCodeCamp
Relational Database Certification*	FreeCodeCamp
Embedded LINUX	NIELIT Calicut
Intermediate SQL: Data Reporting & Analysis	LinkedIn
Advanced SQL for Data Science: Time Series	LinkedIn
Fundamental of Agentic AI & AI Agents	Hugging Face

POSITION OF RESPONSIBILITY

- **Graphic Design Head** of IIChe Student chapter at PDEU Aug 2022 – May 2023
Led a 6-member team for the IIChe Student Chapter with a ₹60,000+ budget, managing visual content creation for 20+ chemical engineering events annually including posters, flyers, festival greetings, conference booklets, and newsletters to strengthen engagement and event outreach.
- **Graphic Design Head** of Cretus - The Robotics & Automation Club at PDEU Jul 2021 – Jun 2022
Coordinated a 4-member design team with a ₹80,000 budget to create visual content for 10+ robotics events, designing posters, flyers, banners, and newsletters that strengthened event branding and drove Instagram growth from 920 to 1,150 followers through targeted campaigns.

*-Ongoing