
Introduction

A process engineer holding BAsC. & MASc. in **Chemical Engineering** and MASc. in **Mining & Minerals Engineering**, with advanced **data analytics** skills, experienced in **inspecting, designing, optimizing, and evaluating large-scale industrial systems** in conjunction with **simulation, virtual environment training and data-driven** tools to support **design, development, and decision-making** with a focus on **enhancing operational efficiency, identifying potential issues and reducing costs**.

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- **International work experience** across Asia, Europe, Middle East and North America within diverse cultural settings, built and maintained professional relationships.
 - Independent, productive and active **team player**, always met deadlines and delivered projects with high-quality results.
 - Skilled in identifying key questions with a root-cause approach, developing clear and compelling argumentation, and crafting effective **project budgets and timelines**.
 - Successfully secured **funding** from international organizations including **European Union**.
 - Authored **40+ publications** (h-index: 15) & **spoke at multiple international and national** venues.

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- **Engineering Tools**
 - **Programming**
 - **Computational Materials**

Real Life

Professional Networks

Social Media

Email

Education

Project

Microwave assisted drying of minerals, with Dr. Ali G. Madiseh.

Project Goal

Retrofitting of conventional drying unit operations at a local industrial mining partner.

Project Summary

Inspected and evaluated, experimentally and numerically (via Finite Element Modeling in COMSOL), the **feasibility and applicability** of microwave-based heating systems at a local **mining industrial partner** for the **retrofitting of conventional drying unit operations**.

Tasks Performed

- Performed experimental and numerical analysis of **mineral drying behavior under microwave exposure**.
 - Utilized **finite element modeling** (FEM) to simulate heat and mass transfer during drying at various microwave power levels and **mineral types**.
 - Conducted comprehensive **energy demand analysis** to evaluate **potential savings** compared to traditional kiln operations.
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Project

Thermo-kinetic modeling of the wet phase inversion process for polymeric membranes fabrication, with Dr. Mohammad Ali Aroon.

Project Goal

Developed a **comprehensive thermo-kinetic model** to simulate the wet phase inversion process for fabricating polymeric membranes, focusing on Multiphysics coupling and accurate prediction of **polymeric flat-sheet membrane structure evolution**.

Tasks Performed

- Constructed and solved **coupled heat, mass, and momentum transport models under non-equilibrium thermodynamics**, incorporating moving boundary conditions in multiphase, multicomponent porous systems.
- Formulated and implemented **partial and ordinary differential equation solvers (PDE/ODE)** to capture the transient dynamics of solvent-nonsolvent exchange and polymer precipitation.
- Wrote custom **code in Fortran, MATLAB, and C++** for high-fidelity numerical simulations and sensitivity analyses.
- **Validated computational results against experimental measurements**, achieving strong agreement in membrane morphology predictions.
- Gained insight into phase separation kinetics, diffusion mechanisms, and the impact of process parameters on membrane performance and structure.

Project

Simulation and cost evaluation of hot section of BIPC olefin plant, with Dr. Nasim Tahouni.

Project Goal

Used **Aspen Hysys** and **Aspen Plus** to evaluate **retrofitting** of industrial scale **petroleum refinery** complex by producing process flow diagram (**PFD**), piping/process & instrumentation diagram (**P&ID**), **cost** and **utility**, pinch and exergy.

Tasks Performed

- Simulated existing and proposed **process configurations using Aspen HYSYS and Aspen Plus**, focusing on optimizing reactor and separation systems for olefin recovery.

- Developed and **documented detailed Process Flow Diagrams (PFDs) and Piping & Instrumentation Diagrams (P&IDs)** to map unit operations, control loops, and equipment connectivity.
- Performed **equipment sizing and specification** for heat exchangers, reactors, compressors, and distillation columns based on simulated operating conditions.
- Conducted **cost estimation and utility analysis** (CAPEX and OPEX) to support retrofitting and procurement decisions.
- Applied **pinch analysis and exergy analysis** to evaluate and enhance energy integration and thermodynamic efficiency across the system.
- Assessed **retrofitting feasibility** by integrating performance data, economic viability, and process safety considerations.

Experience

Project

Fluid Bed Spray Dryer Process Monitoring and Engineering, with Dr. Marcus O'Mahony.

Project Goal

Designed and implemented a **data-driven graphical user interface** for real-time **monitoring and optimization** of a fluid bed spray drying process by integrating in-line/offline sensor data streams and advanced analytics into an interactive platform.

Tasks Performed

- Developed an interactive **graphical user interface (GUI) in MATLAB** for real-time data **visualization and diagnostics**, supporting both in-line and offline sensor data integration.
- Integrated and processed **diverse sensor types** including CCD camera feeds (image-based analysis), NIR sensors (unlabeled time-series), Raman spectroscopy probes (localized unstructured signals), and valve states (binary control signals).

- Performed extensive data preprocessing and cleansing to handle **high-dimensional and heterogeneous datasets** with missing values and sensor noise.
- Applied **pattern recognition** and signal analysis techniques to identify operational trends, detect anomalies, and support process optimization.
- Designed pipelines for real-time data ingestion and synchronization from multiple sensor sources, ensuring temporal alignment and reliable analytics under dynamic plant conditions.
- Collaborated with process engineers and control specialists to translate sensor insights into actionable process improvements and control strategies.

Under an EU Horizon 2020 Marie Skłodowska-Curie Post-doctoral Fellowship.

[Read funding news here.](#)

[Read outcome highlight here.](#)

Project

Continuous Cocrystalization via Hot Melt Extrusion in Pharmaceuticals, with Dr. Gavin Walker.

Project Goal

Developed a **data-driven digital twin framework** to address low-yield challenges in continuous crystallization, aiming to enhance product quality, optimize production, and reduce waste and operational costs in pharmaceutical manufacturing.

Tasks Performed

- Conducted detailed **root-cause analysis** of unit operations to identify inefficiencies affecting yield and product purity in **continuous crystallization systems**.
- Evaluated the influence of **critical process parameters**—temperature, residence time, screw configuration, and rotation speed—on crystallization outcomes, using both experimental data and simulation insights.
- Designed and refined **process strategies*** to maximize desired product formation, suppress by-product

generation, and reduce procurement and disposal costs.

- Built a digital twin using advanced **data analytics** and implemented a **machine learning-based process controller**, integrating both real-time (in-line) & historical (offline) **sensor data streams**-Raman spectroscopy.
- Utilized Density Functional Theory (DFT) and molecular dynamics (MD) simulations to analyze **molecular interactions**, guiding optimal cocrystal formation **pathways** and identifying **key process descriptors**.
- Integrated **Raman spectrometer** data into a live control system, enabling real-time feedback and control within a continuous manufacturing environment through predictive ML models.

Project

Machine Learning Interatomic Potentials for Materials Discovery, with Dr. Alexander Shapeev.

Project Goal

Aimed to **expedite the discovery and characterization** of hard materials for use in high-performance environments—such as aerospace, automotive, mining, and manufacturing—by developing and deploying **ML-driven interatomic potentials** for predictive modeling.

Tasks Performed

- Assessed candidate **hard materials** for industrial applications, focusing on performance under mechanical stress and durability in **extreme conditions**.
- Conducted **nanoindentation** research to evaluate **mechanical properties** such as hardness and elastic modulus of synthesized materials.
- Developed validation models to discuss experimental results with simulation predictions, extracting insights into **material failure** modes and defect behavior.
- Implemented and trained **Machine Learning Interatomic Potentials** (MLIPs) using active learning strategies to improve accuracy with minimal data.
- **Automated** molecular dynamics (MD) simulations

using LAMMPS and density functional theory (DFT) calculations using VASP for large-scale material screening **across multiple HPC clusters**.

- Wrote modular and efficient code in Python and Bash, managing environments and version control using Git.

Project

Design of Adsorptive Systems for Direct Gas Capture and Separation, with Dr. Jin Shang.

Project Goal

Developed a novel process for the direct capture, separation, and solid-state storage of nitrogen and carbon dioxide gases under ambient conditions using moist lithium as a reactive adsorbent, with an emphasis on circular material recovery for sustainable gas handling and sequestration.

Tasks Performed

- Designed and optimized gas capture protocols for ambient-condition adsorption of nitrogen and carbon dioxide on moist lithium, enabling safe and efficient conversion into solid-state lithium nitride for storage and transport.
- Applied principles of **reaction engineering** and separation to evaluate process efficiency, yield, and purity of captured products.
- Conducted Density Functional Theory (DFT) calculations to map **reaction pathways** between lithium and target gases, identifying favorable thermodynamic and kinetic conditions.
- Developed microkinetic and kinetic Monte Carlo models to simulate **reaction dynamics** and **upscale lab-scale findings for process-scale feasibility**.
- Demonstrated **on-demand recovery** of nitrogen and lithium through electrochemical regeneration, showcasing **material circularity** and long-term process sustainability.

with Dr. Carlos-Andres Palma.

Tasks Performed

- Gained hands-on expertise in **CHARMM for (bio)molecular modeling**, focusing on simulation and analysis of organic and biological matter at the atomic level.
 - Developed custom tools in **Fortran** and **Python** for simulation pre-processing and post-analysis, including data parsers, Fourier transforms, and specialized routines for trajectory and energy analysis.
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