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## 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**

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## Real Life

## Professional Networks

## Social Media

## Email

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## 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.

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### 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.

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## 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.

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Under an EU Horizon 2020 Marie Skłodowska-Curie Postdoctoral Fellowship.

Read funding news [here](#).

Read outcome highlight [here](#).

## Project

Continuous Cocrystallization 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 pro-**

- cess **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.

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## 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.
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## 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 (N<sub>2</sub>) and carbon dioxide (CO<sub>2</sub>) 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 N<sub>2</sub> and CO<sub>2</sub> on moist lithium, enabling safe and efficient conversion into solid-state Li<sub>2</sub>N 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.
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