

This is a **personal** page, and all information presented here is for personal use and reference only, and I do not represent any organization or employer.

## Professional Summary

- A process engineer holding BASc. & MSc. in Chemical Engineering and MSc. 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.
- 

## Organizational Culture

- 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.
- 

## Technical Summary

### Engineering Tools

- Aspen Suite, Autodesk Plant 3D, Deswik, Vulcan, Autodesk AutoCAD, COMSOL, SolidWorks, LAMMPS, VASP, CHARMM, Biovia, Ab Initio, Gromacs, Gaussian, Microsoft Office, LaTeX, Git.

### Programming

- Python, C++, Fortran, Java, MATLAB, bash.

### Modeling Skills

- Process Flow Diagrams, Piping and Instrumentation Diagrams, CAD, equipment sizing, cost and utility estimation, exergy and pinch, OpEx and CapEx.
  - Advanced modeling skills across scales: FEM, DPD, PBM, LBM, QM/MM, MD, DFT, kMC, etc.
  - Data operations including classification, clustering, regression, segmentation, tree models, ensemble learning, temporal data correlation algorithms such as ARIMA, LSTM, CNN, PCA, via PyTorch, SciLearn, TensorFlow, SQL, Pandas, NumPy, SciPy, Scikit-Learn, Matplotlib, Seaborn, Jupyter.
- 

## Contact

- Email: [miladasgarpour@gmail.com](mailto:miladasgarpour@gmail.com)
- Mobile: 604-762-6875
- LinkedIn: <https://www.linkedin.com/in/makhansary>
- GitHub: <https://github.com/makhsry/mak>
- Google Scholar: <https://scholar.google.com/citations?hl=en&user=DZzc424AAAAJ>

## Education

**MASc. Mining and Minerals Engineering (2023 – 2025), The University of British Columbia**

### 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.
- 

**MASc. Chemical Engineering - Process Design (2012 - 2014), University of Tehran**

### 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.
- 

**BASc. Chemical Engineering (2007 - 2011), University of Tehran**

### 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

**Mineral Process Engineer: Mineral Drying (Mitacs Accelerate Internship), UBC Norman B. Keevil Institute of Mining Engineering, Canada (2023 Jan. - 2025 Dec.)**

### Project

Microwave Assisted Drying of Minerals, with [Dr. Ali G. Madiseh](#).

### Project Goal

Collaborated with a local **mining company** to electrify kiln drying processes by integrating microwave-based heating systems aimed at **reducing fossil fuel dependence** (12.25 million cubic meters of natural gas), **lowering economic expenses** (e.g., \$2.08 million carbon tax), and **minimizing greenhouse gas emissions** (e.g., 26,000 tons of CO<sub>2</sub>e annually).

## Tasks Performed

- Measured and analyzed **thermophysical** and **electromagnetic** properties of minerals subjected to **microwave heating**, providing essential data for **system design** and **process optimization**.
- Developed and validated **Finite Element Models (FEM)** of **coupled electromagnetic heating** in **COMSOL Multiphysics** to guide the design and construction of a **continuous on-site drying line**.
- Successfully compiled COMSOL Multiphysics on UBC Sockeye HPC systems, ensuring proper file access, MPI fork setup, and security configurations to facilitate large-scale simulations.
- Formulated **atomistic and molecular modeling protocols** to predict the electromagnetic properties of multicomponent materials under alternating current (AC), enhancing material design for efficient microwave heating.
- Performed **Density Functional Theory (DFT) calculations** and developed **custom Machine Learning (ML) interatomic potentials** for molecular dynamics simulations; modified **LAMMPS source code (C++)** for high-fidelity simulations of material behaviors under microwave exposure.

- Created Bash and Python scripts for post-processing of simulation results, **data visualization**, and **executive analytics** to support project planning, delivery, and presentations to stakeholders.
- 

**Mineral Process Engineer: Modelling and Simulation (Teaching Assistant), UBC Norman B. Keevil Institute of Mining Engineering, Canada (2024/2025: Sept. - Dec.)**

with [Dr. Sanja Miskovic](#) & [Dr. Scott Dunbar](#).

#### Tasks Performed

- Contributed to trainings on **methods for determining the behaviour of large-scale industrial systems** and their application to the design and analysis of such systems.
- 

**Materials Handling (Teaching Assistant), UBC Norman B. Keevil Institute of Mining Engineering, Canada (2025: Sept. - Dec.)**

with Dr. Ali Kuyuk.

#### Tasks Performed

- TBD.
- 

**Mineral Process Engineer: Process Control (Teaching Assistant), UBC Norman B. Keevil Institute of Mining Engineering, Canada (2023/2024: Sept. - Dec.)**

with [Dr. Ilija Miskovic](#).

#### Tasks Performed

- Contributed to trainings on methods for **automatic control theory**, PID control, Laplace and z-transforms, loop tuning, frequency response, stability analysis, control strategies in flotation, comminution, dewatering, reagent and bin/sump levels, automated load-haul-dump and drilling equipment, instrumentation and soft sensors.
- 

**Canada West Coordinator, Marie Curie Alumni Association, North America Chapter, Canada (2023 Sept. - 2024 Sept.)**

#### Tasks Performed

- Coordinated [MCAA North America](#) outreach activities in Canada west coast for a community of over 300 members.
- 

**Chemical Process Engineer: Modelling and Optimization (Teaching Assistant), UBC Chemical and Biological Engineering Department, Canada (2022: Sept. - Dec.)**

with [Dr. Simcha Srebnik](#).

#### Tasks Performed

- Skilled in modeling and optimizing **industrial chemical processes**, with a focus on simulating chemical reactors, emphasizing heterogeneous systems in **Aspen** environments.
-

- Applied **optimization techniques** within Aspen platforms to enhance **process performance** and **efficiency**.
  - Designed and simulated **crude oil distillation processes** using Aspen HYSYS.
  - Implemented **dynamic simulation** and **control** strategies to model **real-time** process behavior in HYSYS.
  - Created **process flowsheets** for specialty chemicals and reactions using Aspen.
  - Wrote/modified **FORTRAN subroutines** in Aspen for ad-hoc units / calculations.
- 

## Chemical Engineer: Cavitation at Nanoscale (Graduate Research Assistant), UBC Chemical and Biological Engineering Department, Canada (2022: May - Dec.)

### Project

Nanocavitation and its Mitigation in Fabricating Artificial Trees, with [Dr. Simcha Srebnik](#).

### Project Goal

Investigated nanoscale water flow mechanisms to reduce **nanobubble formation** and ensure stable, uninterrupted transport in **nanoporous channels**—critical for enhancing efficiency in advanced **evaporative cooling systems**.

### Tasks Performed

- Conducted an in-depth literature review to establish **design principles** for self-driven water transport at the nanoscale.
  - Developed algorithms to quantitatively assess the impact of **surface hydrophilicity on nanobubble nucleation and stability**.
  - Created **custom computational routines** for high-throughput molecular dynamics (MD) simulations using **LAMMPS**, tailored for complex **fluid-surface interactions**.
  - Compiled and optimized LAMMPS on UBC's Sockeye HPC environment for scalable, in-house simulation workflows.
  - Extended LAMMPS functionality with **custom C++ modules** to meet unique research needs in nanoscale flow modeling.
  - Implemented post-processing scripts in **Python** for automated extraction and visualization of simulation results, including pressure profiles, density distributions, and flow characteristics.
  - Collaborated with a **multidisciplinary team** to validate simulation results against theoretical models and experimental data, enhancing cross-domain communication and interpretation.
- 

## Chemical Process Engineer: Analytics in Fluid Bed Spray Dryer (Research Assistant), University of Limerick, Ireland (2022: Feb - May)

### 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.
- 

## Process Engineer: Continuous Crystallization (Marie Skłodowska-Curie Postdoctoral Fellow), University of Limerick, Ireland (2019 Oct. - 2022 Feb.)

Under an [EU Horizon 2020 Marie Skłodowska-Curie Postdoctoral Fellowship](#).

[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 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.
- 

## Material Engineer: AI & ML (Research Intern), Skolkovo Institute of Science and Technology (SkolTech), Russia (2018: May - Oct.)

### 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.
- 

## Process Engineer: Gas Separation and Capture (Research Assistant), City University of Hong Kong, Hong Kong (2017 Nov. - 2018 May)

### Project

Design of Adoprtive 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.
- 

## Visiting Researcher, Institute of Physics & Beijing National Lab for Condensed Matter Physics, Chinese Academy of Sciences, Beijing, China (2017: Sept. - Nov.)

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.

**Chemical Engineer: Water Quality Monitoring and Remediation (Research Assistant), Baqiyatallah University of Medical Sciences, Tehran, Iran (2015: Jan. - July)**

under [Iran National Science Foundation \(INSF\)](#).  
with [Dr. Ramezan Ali Taheri](#).

#### Tasks Performed

- Thoroughly examined presence of **biologically active matters** in hospitals **wastewater** effluents.
  - Inspected **wastewater effluent** from hospital sewage to remove biologically active materials, **hormones**, due to their wide use in patient treatments.
  - Built and performed high-throughput screening of **1k polymers** for common **estrogen**.
  - Identified relevant pairs and determined the removal capacity and routes accordingly.
- 

**Research Collaborator, Islamic Azad University, Tehran, Iran (2014 Sept. - 2017 Sept.)**

with Young Researchers and Elite Club.

#### Tasks Performed

- Managed **diverse portfolios of research and development projects**, ensuring timely delivery, quality outputs, and **cross-disciplinary collaboration**.
- Authored technical proposals, project schedules, and successfully acquired research funding for innovative environmental and industrial process solutions.
- Directed maintaining high performance across the lifecycle of **multiple concurrent projects**.

#### Sample Projects

- On-site detection and monitoring of pollutants in **water and wastewater** streams via polymeric passive samplers.
  - Translated dilation to **attenuated total reflectance Fourier-transform infrared spectroscopy (FTIR-ATR)** of polycarbonate, poly (vinyl acetate), and poly (ether urethane) induced by acetonitrile.
  - Removal mechanism of **heavy metal ions** (Pb, Cu, Cd, Zn, and Ni) by using lignin as adsorbent.
  - **Direct air capture and storage** of carbon dioxide (CO<sub>2</sub>) on biomass and polymers at ambient conditions through novel 'CO<sub>2</sub>-water-biomass' network enabling adsorption of 5–56 grams of CO<sub>2</sub> per gram of biomass.
  - Developed a detailed coated paper **process model** including convection, conduction, and radiation heat transfer in order to pave routes for optimization of industrial process through adjustments made to the air humidity, belt velocity, temperatures, as well as the distance between drying surface and the radiation heat source.
  - **Supercritical fluid extraction and purification** of high end-value products (drugs and dyes) via supercritical carbon dioxide.
- 

**Chemical / Process Engineer (Summer Internship), Research Institute of Petroleum Industry (RIPI), Iran (2011: July - Aug.)**

#### Project

Design of Separation Systems for Ethane and Methane, with [Dr. Nasim Tahouni](#).

#### Project Goal

Completed a process engineering internship focused on the **simulation and optimization** of a gas separation unit targeting high-purity ethane and methane recovery, integrating both **technical design** and **economic analysis** using industry-standard tools..

## Tasks Performed

- Designed, simulated, and optimized a separation process in **Aspen HYSYS**, achieving efficient separation of ethane and methane under various operating conditions.
  - Developed comprehensive **Process Flow Diagrams (PFDs)** to visualize and document the system configuration, **material and energy balances**, and process controls.
  - Performed **equipment sizing and selection** for distillation columns, heat exchangers, compressors, and separators based on simulated process data and vendor specifications.
  - Conducted **cost analysis**, including **capital expenditure (CAPEX)**, **operating expenditure (OPEX)**, and utility consumption, to assess **economic feasibility** and guide procurement strategies.
  - Applied **exergy analysis** and **pinch analysis** to identify thermodynamic inefficiencies and optimize energy integration, improving process sustainability and reducing waste heat.
  - Evaluated and compared equipment procurement options using technical and economic criteria to support decision-making for pilot-scale implementation.
- 

## Scientific Computing with MATLAB and C++ (Teaching Assistant), University of Tehran, Iran (2009 - 2011)

with Dr. Mohammad Ali Pourpak.

## Tasks Performed

- Developed **custom numerical algorithms** in **MATLAB** and **C++** to solve complex ordinary and partial differential equations (ODEs/PDEs), and implemented **optimization routines** for scientific and engineering applications.
  - Applied advanced computational techniques for modeling **physical systems**, performing parameter estimation, and solving **multi-variable optimization problems** with a focus on accuracy, efficiency, and scalability.
- 

## Awards

### CIM Vancouver branch's Student-Industry Night Award, amounting 2,500.00 CAD, Nov 2023

Issued by CIM | [The Canadian Institute of Mining, Metallurgy and Petroleum](#)  
one of the three recipients in 2023.

### Kashmir Singh Manhas Scholarship in Applied Science, amounting 2,700.00 CAD, Nov 2023

Issued by [The University of British Columbia](#)  
awarded on the recommendation of the Faculty of Applied Science, in consultation with the Faculty of Graduate and Postdoctoral Studies.

### Carl and Elsie Halterman Scholarship, amounting 1,675.00 CAD, March 2023

Issued by [The University of British Columbia](#)

**Marie Skłodowska-Curie Postdoctoral Fellowship, amounting 75,424.00 Euros, October 2019**

Issued by EU Horizon 2020 Research and Innovation Program and associated with University of Limerick  
qualified based on (1) having a MSc degree + (2) at least 4 years of research experience.

**Research Project Replacement to National Service, January 2015**

Issued by Iran's National Elites Foundation

---

## Talks

**Panelist, University of Ottawa, Ottawa, Canada, Nov 2023.**

Discussed EU based funding opportunities for Canadian and Marie Curie Alumni Association (MCAA) North America Chapter activities

**Panelist, The University of British Columbia, Vancouver, Canada, Jul 2022.**

Discussed how to write a successful Marie Skłodowska-Curie Action (MSCA) Fellowship proposal.

**Presenter, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany, Nov 2018.**

Discussed nanohardness from First Principles with active learning on atomic environments (MLIP)

---

## Publications

For an up-to-date list, please refer to [Google Scholar](#).

[Citation 725 | h-index 15.](#)

1. Decomposition of PFOA in IEX regeneration wastewater: Comparison of UV/sulfur-based processes, key parameters and submicellar aggregates on degradation kinetics
2. A molecularly enhanced proof of concept for targeting cocrystals at molecular scale in continuous pharmaceuticals cocrystallization
3. Nanohardness from First Principles with active learning on atomic environments
4. Molecular engineering of cocrystallization process in hot melt extrusion based on kinetics of elementary molecular processes
5. Incomplete cocrystallization of ibuprofen and nicotinamide and its interplay with formation of ibuprofen dimer and/or nicotinamide dimer: A thermodynamic analysis based on DFT data
6. Revisiting ‘penetration depth’ in falling film mass transfer
7. Physical adsorption of CO<sub>2</sub> in biomass at atmospheric pressure and ambient temperature
8. A note on the composition-dependency of the density within the mass transfer layer
9. A molecular scale analysis of TEMPO-oxidation of native cellulose molecules
10. A priority supposition for estimation of time-dependent changes in thickness and weight of polymeric flat sheet membranes fabricated by the nonsolvent induced phase separation (NIPS) technique
11. Contaminant uptake by polymeric passive samplers: A modeling study with experimental validation
12. On the search of rigorous thermo-kinetic model for wet phase inversion technique

13. Generalized similarity transformation method applied to partial differential equations (PDEs) in falling film mass transfer
  14. An enquiry on appropriate selection of polymers for preparation of polymeric nanosorbents and nanofiltration/ultrafiltration membranes for hormone micropollutants removal from water effluents
  15. Polymer-water partition coefficients in polymeric passive samplers
  16. A comparative theoretical and experimental study on liquid-liquid equilibria of membrane forming polymeric solutions
  17. Prediction of carbon dioxide sorption in polymers for capture and storage feasibility analysis
  18. Using quantum chemical modeling and calculations for evaluation of cellulose potential for estrogen micropollutants removal from water effluents
  19. Correlation of sorption-induced swelling in polymeric films with reference to attenuated total reflectance Fourier-transform infrared spectroscopy data
  20. Development and validation of a graphical sorption model: application to sorption of organic liquids into low density polyethylene polymeric membrane
  21. A quantum mechanics/molecular mechanics (QM/MM) investigation on the mechanism of adsorptive removal of heavy metal ions by lignin: single and competitive ion adsorption
  22. Lower and upper critical solution temperatures of binary polymeric solutions
  23. Theoretical modeling for thermophysical properties of cellulose: pressure/volume/temperature data
  24. Correlation of interaction parameters in Wilson, NRTL and UNIQUAC models using theoretical methods
  25. Vapor pressure and Flory-Huggins interaction parameters in binary polymeric solutions
  26. Binary mutual diffusion coefficients of polymer/solvent systems using compressible regular solutions theory and free volume theory
  27. Phase diagram of ternary polymeric solutions containing nonsolvent/solvent/polymer: Theoretical calculation and experimental validation
  28. Mathematical-thermodynamic solubility model developed by the application of discrete Volterra functional series theory
  29. Representing solute solubility in supercritical carbon dioxide: A novel empirical model
  30. On the consistency and correctness of thermodynamics phase equilibria modeling and correlation reports published in Fuel journal
  31. Reply to the comments "On the consistency and correctness of thermodynamics phase equilibria modeling and correlation reports published in Fuel journal"
  32. Development of a thermodynamic model for hydrogen and hydrogen containing mixtures
  33. Prediction of dyes solubility in supercritical carbon dioxide (CMM EOS)
  34. Using genetic algorithm (GA) and particle swarm optimization (PSO) methods for determination of interaction parameters in multicomponent systems of liquid--liquid equilibria
  35. Modeling drying of a coated paper
  36. A novel equation of state: determination and validation for dyes and drugs solubility calculations in supercritical carbon dioxide
  37. Solubility prediction of some disperse Azo dyes in supercritical carbon dioxide using equation of states (EOSs)
  38. Modeling of solubility of disperse blue dyes in supercritical carbon dioxide using equation of states (EOSs)
-