

Paper Code	Title / Authors
Modeling and Simulation	
1007	Optimization of the Heat Exchanger Network in a Methanol Synthesis Plant Using Pinch Analysis J. Mahboubnasab, A. A. Azemati*, N. Hajiabdollah
1020	From Entropy Masks to U-Net: An Image Processing and Machine Learning Approach for Flare Flame Detection H. Hayer
1048	A Machine Learning Framework for Estimating Drug Solubility A. Pilehvar Meibody, M. Amani*, D. Nekoonam
1073	Effect of electrolyte chemistry on the electrochemical performance of LFP, NMC, and NCA cathodes: A simulation-based study M. J. Tavakkoli Heravi, A. Arab, E. Yasari*
1087	Advanced two-dimensional Modeling and Genetic Algorithm-Driven Optimization of Industrial Ammonia Synthesis R. Ghani, D. Iranshahi*
1090	Modeling of catalytic reforming unit and evaluation of catalyst activity by genetic algorithm A. Hedayati
1091	Predicting Biomass Yield Using Extreme Gradient Boosting (XGB) Algorithm of Machine Learning Methods R. Mohammadrezaei, R. Beigzadeh*
1112	Microfluidic Electrocoalescence Mechanisms of Moving Droplets under a DC Electric Field A. Mohammadi*, A. Behnam Bilondi
1115	Investigating the effect of voltage and increasing production volume in an ion concentration polarization desalination microfluidic system using numerical simulation A. Mohammadi*, M. Nasiri Avanaki
1121	Enhancing cement production capacity and mitigating erosion through CFD-based calciner burner redesign N. Salahi, A. Sheikhi Darani, M. S. Karimi*
1135	Molecular dynamics Study of Concentration Effects on the Structure and Dynamics of Ethyl Acetate–Lithium Bis(trifluoromethanesulfonyl)imide Electrolytes for Lithium-ion Batteries H. Akbari, B. Ghalami Choobar*, N. Gilani
1138	Plug Flow Reactor Modeling of Catalytic Phenol Oxidation in Supercritical Water A. Hedayati
1140	Modeling and genetic algorithm optimization of supercritical extraction of glycyrrhizic acid from licorice plant root A. Hedayati
1144	A Recurrence CFD Framework for Fast Simulation of Species Transport in Batch Cavity Flows M. Shariatifar, R. Sotudeh-Gharebagh*, R. Zarghami, N. Mostoufi
1145	An Efficient rCFD Approach for High-Speed Simulation of Scalar Transport in Continuous Cavity Flows M. Shariatifar, R. Sotudeh-Gharebagh*, R. Zarghami, N. Mostoufi
1157	Evaluation and Selection of the Optimal Objective Function for Heat Exchanger Network Retrofitting Problems H. Soltani*, M. M. Payamani
1158	Technical Feasibility and Optimization of Air Preheater Installation for a Furnace Utilizing NSGA-II H. Soltani*, M. M. Payamani, M. Bahari
1165	Simulation and Optimization of the Separation Process in the Medium-Pressure Separator of Parsian Gas Refinery Using Computational Fluid Dynamics (CFD) M. Solati, M. Nasr-Esfahani*
1171	Bubbling Twin Reactor for Photocatalytic CO₂-to-Methanol D. Iranshahi*, A. Norouzi Sohrabvand

Paper Code	Title / Authors
Modeling and Simulation	
1187	A Physics-based Multilayer Perceptron Model for Surrogate Simulation of Methane Oxidation Kinetics S. Firouznia, H. R. Norouzi*
1206	Investigation of Heat and Mass Transfer Phenomena in the Natural Gas Dehydration Process Using Aspen Adsorption R. Parichehreh*, Sh. Dabaghi
1221	Optimization of Well Production Using Gas Lift and ESP: A Nodal Simulation Approach for Enhanced Artificial Lift Performance F.Khalili*, I. Khonsha
1226	PEGylation Effects on Fibrinogen Binding to Dual Stimuli-responsive Star-shaped Copolymer Drug Nanocarrier: A Molecular Dynamics Investigation D. Lotfi-Moghaddam, K. Bastani, P. Zahedi*, H. Azizpour
1243	CFD Analysis of Combustion and Heat Transfer in an Industrial Boiler M. Bagheri, A. Parvareh*
1244	Comparative Analysis of Fluid Dynamics in Simple and Baffled Pipe Configurations M. Seifi, K. Keynejad*, H. Azizpour
1277	A Numerical Study on Lithium-Ion Transport in Electrodialysis: Effects of Voltage, Membrane Charge Density, Flow Velocity, and Temperature A. H. Khatibi, S. Habibzadeh*
1283	Aspen Plus-Based Simulation and Optimization of SO₂ to SO₃ Conversion in a Multi-Bed Catalytic Reactor: A Case Study of Paknam Company M. Mohammadi Nasr*, M. F. Abedini
1292	A Molecular Investigation of Enhanced Curcumin Solubility in Subcritical Water/Ethanol Solvent Mixtures M. Gazmeh, M. Khajenoori*, S. Yousefi-Nasab, A. Haghighi Asl
1329	Investigation of Parameters Affecting the Efficiency of Hydrodynamic Cavitation: A Case Study on Heavy Fuel Oil Upgrading A. Aliparast, N. Naziri*, M. Akrami
1334	Introduction of a Statistical Model for Calculating Combustion Efficiency in Furnaces and Boilers and Establishing Its Baseline Based on ISO 50006 M. Rashidi, A. Kordi*, M. Roshanaei
1344	Design, simulation, and control of a Mini LNG process H. Salehi, R. Eslamloueyan*
1347	The Effect of Plate Curvature on Heat Transfer in Plate Heat Exchangers Using Computational Fluid Dynamics M. Esperi, S. Rahbari, Sh. Ostovar, N. Eyvazi-Abhari*
1348	Numerical study of particle motion and dissolution in a shear flow using the lattice Boltzmann-smoothed profile method M. Azadpour, A. Mohebbi*, A. E. F. Monfared
1361	Simulation and Techno-Economic Evaluation of Amine-Upgraded Biogas to Power Systems M. M. Yousefi, M. Jafari*, A. H. Gorgi
1368	Simulation and Parametric Study of Electricity and Freshwater Cogeneration from Flare Gas: A Case Study of the Cheshmeh Khosh Oil Field Using MED A.-H. Gorgi, M. Jafari*, M. M. Yousefi, M. Abbasi
1373	Accelerated Discovery of High-Performance MOFs for Greenhouse Gas Adsorption via Interpretable Ensemble Learning R. Fazeli, M. Rahmani*, S. Atashrouz
1375	Role of Organic Cation Orientation in the Dynamical and Thermodynamic Stability of Hybrid Perovskites S. M. Pakzad Moghadam, F. Arabpour Roughabadi*, V. Ahmadi
1380	Packed-bed porosity prediction from rosin-rammler particle size distribution using machine-learning regression P. Rastgaran, M. Rahmani*, A. M. Rastgaran

Paper Code	Title / Authors
Modeling and Simulation	
1382	Simulation of Formaldehyde Removal from Air Stream Using a Packed-Bed Photocatalytic Column by Computational Fluid Dynamics M. Shafiee, A. Soltani Goharrizi*
1396	Machine Learning and PSO Optimization of VOC Oxidation in a High-Throughput Fixed bed Reactor: Comparison with CFD M. Haghighi, M. Rahmani*, S. Atashrouz
1403	Targeting and Design of Heat Exchanger Networks with Considering Safety and Controllability A. Sadeghikia, N. Tahouni*, M. H. Panjeshahi
1404	First Principles DFT-D2 Study of Carbon Dioxide Adsorption on Boron-Doped H₄,4,4-Graphyne Z.Asadabadi, A. Reisi-Vanani*
1411	Effect of Baffle Incorporation on Permeation Flux Enhancement in the Pervaporation Process: A Computational Fluid Dynamics Study E. Fatehi*, H. Saeidi, M. Shahbahrami, F. Ashoubi
1441	Evaluation of an Integrated Reactive Distillation Process for Biodiesel Production from Waste Cooking Oil under Feed-Quality Uncertainty A. Davoodi Nejad, H. Ahmadian Behrooz*
1443	Process Simulation and Performance Analysis of a Modular TEG Dehydration System for Shale Gas: Energy Efficiency and Cost-Effectiveness A. Goudarzi, F. Bashipour*
1459	Root Cause Analysis of Severe Uniform Corrosion in Steam Condensate Pipelines: A Multiphysics Simulation Approach P.Nasehi*, M. Zarei, F. Farhadinasab, B. Khademi, A. Ashkenani, M. Norouzi
1470	Design, Simulation, and Performance Evaluation of an Ultra-High-Temperature Milk Sterilization System Using Aspen HYSYS M. Jafari, A. Vatani*, A. Andarz, K. Bakhtiari
1477	COMSOL Validation of a Thermal Dispersion Model for Nanofluid Heat Transfer in Square Ducts F. Ardalani, A. Kazemi-Beydokhti*
1478	BC3 nano-sheet for adsorptive removal and storage of SO₂ and H₂S gases : A Theoretical quantum chemistry study M. A. Zarrini, F. Marzpour Shalmani*, M. Arabieh*
1484	CFD Simulation of Embryo Transfer Using Air-Bubble and Conventional Catheter Techniques with Injection Velocity Effects on Embryo Trajectories M. Cheraghian, E. Nabati, M.J. Abdekhodaie*
1487	From Waste to Water: A Combined Biogas Upgrading and Reverse Osmosis System A. Andarz, M. Abbasi, M. Jafari*
1503	Simulation of fluid flow in a microchannel with a trapezoidal cross-section and prediction of lift coefficient A. Adibi, M. Nasr Esfahany*, Z. Zarezade
1510	Interpretable Machine Learning for CO₂ Adsorption Prediction and MOF Screening Using Neural Networks R. Fazeli, M. Assareh*, M. Valavi
1512	Numerical Investigation of Natural Convection Heat Transfer of Al₂O₃/Water Nanofluid in an Inclined Square Cavity under the Influence of an External Magnetic Field M. H. Zare, E. Sadeghi*, L. Rostami
1545	From Second-Order Chemical Kinetics to Diffusion-Controlled Reaction: A Weibull Model Analysis of Alkali-Activated Slag Systems H. Maghsoudloord*; A. M. Vazini Athar
1582	Modeling study on the water activity for the binary mixtures of ionic liquids and water by smart paradigms E. Davoudi

Paper Code	Title / Authors
Modeling and Simulation	
1599	A Dashboard-Based System Oriented Framework for Salt Quality and Energy-Aware Analysis in Industrial Salt Washing Units M. A. Moala
1603	AI-Optimized Polymer Inclusion Membranes with Graphene Quantum Dots and Ionic Liquids for Enhanced Lithium Extraction from Brines Reza Darvishi*, Nazila Khadem*
1613	Numerical Investigation of Pressure Drop and Heat Transfer in Obstructed Microchannels S. Esmaeili, J. Rahbar Shahrouzi*
1617	CFD modeling of cavitation in an ejector for upgrading heavy oil quality G. Khodamoradi, A. Parvareh*
1620	Optimized Curved Blade Static Mixer: Design, Mixing, and Antifouling Performance in Transitional Flow H. Mahmoodi, H. Ahmadian Behrooz*, R. Alizadeh
1623	Process Simulation and Feasibility Analysis of Algae-Based Cellulose Production Using SuperPro Designer® E. Bahmani, H. Shokrkar*
1624	Mixed-Product Approach to Improving Steady-State Operability in Parallel Distillation Towers S. Toopchi Zade, A. M. Sahlodin*
1626	Design of a PI Controller for Temperature Control in a Variable-Temperature Reactor Using SIMC Tuning Method A. Mahvashian, M. Bagheri Tabar, A. Khajeh-Amiri*
1631	CFD–DOE Hybrid Modeling of Extrusion Force in the Nozzle of Fused Filament Fabrication 3D Printer H. Razzani, H. Hashemipour*
1633	Numerical Simulation of Methane Pyrolysis Process in a Bubble Column Reactor M. Mohamadi, F. Fotovat*
1641	CFD Simulation of Sieve Tray with Cylindrical Downcomer: Effects of Gas Flow Rate on Hydrodynamic Performance M. Mohseni, S. Roshdi, N. Kasiri*
1646	CFD Simulation of Sieve Tray with Cylindrical Downcomer: Effects of Gas Flow Rate on Mass transfer Performance M. Mohseni, S. Roshdi, N. Kasiri*
1647	Dynamic Simulation of South Tehran Wastewater Treatment Plant's Anaerobic Digester Using the ADM1 Model M. Sedighi*, Z. Mahdavi, M. Mollanorouzi, M. Fakhroleslam
1649	A Modeling Study of an LDPE Autoclave Reactor: Comparison Between Simulation and Experimental Results H. Haji Babaalian, V. Haddadi Asl*, H. Rostami Pour Shandi, M. M. Malekouti
1652	Hydrogen Production Transition in Refineries from Grey to Blue and Green using Machine Learning M. Ahmadi, N. Tahouni*, M. H. Panjeshahi
1675	Hydraulic Simulation of Flare Gas Transport from the Salman Gas Platform to Assaluyeh via the Crescent Pipeline M. Didari, H. Rezaei, A. Naderifar, E. Ghasemi*
1689	Thermodynamic Modeling of CH₄ Solubility in Ionic Liquids: A Study Using the SRK and PR Equations of State H. Heydari*, S. Salimi
1712	Computational Fluid Dynamics Analysis of Heat Transfer Performance in an Engine Oil–Water Plate Heat Exchanger T. Khansari, N. Noormohammadi*
1720	Neural Modeling of PVC Gelation-Fusion A. Mokhtari, A. A. Jamali*, A. Kebritchi, M. Davoodabadi

Paper Code	Title / Authors
Modeling and Simulation	
1731	Numerical Study of Particle Size Effect on Focusing Position and Force Behavior in Viscoelastic Microfluidics Z. Zarezade, N. Etesami*, M. Nasr Esfahany
1746	Machine Learning for Predicting Droplet Dynamics in Microfluidic Channels A.Majnoona, M.Mokhtarib, M.K.Moravejic, A.A.Saifoddin*
1758	Machine Learning prediction of CO₂ absorbtion capacity in ionic liquids : Role of molecular structure, pressure and temperature P. Bahrami, S. Riahi*, F. Jalali
1775	Effect of Temperature and Hydration Level on Radial Distribution Functions and Coordination Numbers in Nafion Membranes: A Molecular Dynamics Study A. Ghezi, H. Azizpour*, K. Keynejad
1782	Fluid–Structure Interaction Analysis of Mitral Valve Dynamics Using Smoothed Particle Hydrodynamics F. Mirzaei, A. Kamyabi*, A. Mohebbi
1787	Dynamic Simulation of CO₂ Capture in a Packed Bed from Air by UiO-66 Metal-Organic Framework using Aspen Adsorption H. Rahbari Asiabi, S. Masoumi, H. Aghdasinia*
1796	Hydrogen Production Reactor Modeling Using Computational Fluid Dynamics M. Farahani, M. Afzali*, M. Arshad, M. M. Amiri, M. A. Ghayour, A. Safavi
1815	Determination of Kinetic Parameters for Dibenzothiophene Desulfurization and Coupled Computational Fluid Dynamics Modeling F. Shirmohammadi, Z. Mokhtari *, M. Tabarestani
1821	Study of Sand-Induced Erosion–Corrosion in Oil Pipelines Using CFD Modeling E. Ebrahimi, F. Mohammadi*
1822	Using Genetic Algorithm to optimize steady-state process of benzene and toluene separation A. Abdollahi Zardinsofla, J. S. Moghaddas*
1824	Numerical Investigation of Active and Passive Heat Transfer Enhancement Methods in a Double-Tube Heat Exchange E. Ebrahimi, F. Mohammadi*
1843	Modeling of mass transfer in polyvinyl alcohol/montmorillonite nanocomposite hydrogel pipes S. Rahaei, M. Sirousazar*, A. Etemadi, S. Gozalzadeh
1853	A Digital Twin-Enabled Power-to-Gas System for Green Methane Production via CO₂ Methanation T. Zomorodi Soofiani, M. Rahmani*, Z. Lome Seddigh
1889	Optimal Design of Methanol Downstream Process Networks: A Case Study of Integrated Olefin-Derived Pathways M. Noori, M. Fakhroleslam*
1899	A Hybrid LSTM–SPM Model for the Prediction of Lithium-Ion Battery Voltage M.S. Ghasemi, E. Yasari*, F. Sabeti Meybod
1908	Enhancing Methanol Production via integration of captured CO₂ in Natural Gas Reforming: Process Simulation and Optimization A. Edrisi*, A.H. Rahimi
1937	Performance Analysis and prediction of the Abadan Refinery Catalytic Reforming Unit Compressor Using Artificial Intelligence I. Khoshrou, M. Nematollahi, F. Vafaei, S. M. M. Mousavi, S. M. Mousavi
1945	Multi-Objective Evolutionary Optimization of the 3E Performance of the Sulfur Recovery Process in Phases 4 and 5 of the South Pars Gas Complex M. Rezaei, Z. Bakhshi, M. H. Eghbal Ahmadi*, A. Mosayebi
1946	Dynamic Soft Sensor Development Using a Gradual Training Approach Based on Neural Networks: A Case Study of the Sulfur Recovery Unit (SRU) M. H. Eghbal Ahmadi*, M. Amani , E. Gomnam, A. Mosayebi
1952	Life cycle assessment of an extractive pressure swing distillation process for the separation of azeotropic mixtures M. A. Ghayour Najafabadi *, M. M. Amiri, S. Zeinali

Paper Code	Title / Authors
Modeling and Simulation	
1953	Exergy Analysis and Computational Fluid Dynamics Modeling in Gas Separation with Membrane A. Khadem, M. Koushikian*, F. Yadang Zavare
1960	Performance Analysis and Turndown Limit Investigation of a Gas Condensate Stabilization Unit: A Case Study of Sarkhun Refinery Unit 700 A. Darban Loghmani, A. Barzkar, M. Karimi*, A. Ghobadi, E. Bakhoda, O. Mostaghisi, H. Sayyar, Y. Hasanazade
1970	A Comparison of Large Eddy Simulation Models for Turbulent non-Newtonian Burgers' Equation F. Mahdizadeh Ghohe*, L. N. Azadani
1971	Predicting CO₂ Uptake and Working Capacity in Hypothetical MOFs with Interpretable Machine Learning and Simple Geometric Descriptors K. K. Farahani, M. Razi, F. S. Fateminia*
1976	Data-efficient Gaussian-process surrogate modeling and interpretability for multi-antibiotic degradation in a photocatalytic reactor (Bi₂WO₆/g-C₃N₄) S. Abaei, A. Gordanshekan, A. Tamimzadeh, S. Arabiyan, M. Mirzaeian, S. Safaei, O. Tavakoli*, S. Tangestaninejad, A. R. Solaimany Nazar, M. Farhadian
1979	Optimization of an Integrated Refinery Hydrogen Network Incorporating Off-Gas Streams and PSA Purification M. Sardashti Birjandi, M. M. Khalilipour*
1982	Numerical Analysis of Thermodynamic Non-Equilibrium in Near-Saturated LNG Sloshing: Effects of Excitation Parameters and Fill Ratio Y. Balouchi, M. Zivdar*, R. Rahimi, D. Mohebbi-Kalhari
1990	A Comparative Evaluation of SDP, MSDP, and LIV-based Soft Sensors for Crude Oil Distillation Column B. Bidar*, M. M. Khalilipour Langroudi
1991	Comparing Y-shaped and Arrow-Shaped Confined Liquid Impinging Jet as an Antisolvent Crystallizer using CFD modeling for Continuous Producing Loratadine Nanoparticles H. Dost Mohammadi, A. Fazeli*, M. Eftekhari, F.S. Fateminia
2000	Optimization of Hydrogen Yield in an Auto-thermal Chemical Looping Water Splitting Process R. Ghoroghi, M. Rahmani*
2011	Effect of Different Diffusion Coefficient Correlations on Mass Transfer Flux and Separation Efficiency in Pervaporation Process Using Computational Fluid Dynamics A. Hedayat, M. H. Khodabande*
2014	Comparing the Wall with/without Insulation inside a U-shaped Microchannel Reactor for Bioethanol Steam Reforming to Produce Hydrogen using CFD modeling H. Rajaei, A. Fazeli*, H. Dost Mohammadi
2024	Optimized Transition Path Design for Adsorption-Based Medical Oxygen Concentrators via First-Principles Modeling A. Ghavami, A. Memari, S. A. H. Hejazi*
2031	Development of an Operator Training Simulator (OTS) for FCC and GPTU units of Abadan Refinery I. khoshrou, M. Nematollahi, F. Vafaei*, A. Garghoul, S. M. Fallah
2053	Physics-Informed Neural Networks for Industrial-Scale Catalytic Naphtha Reforming Reactor Modeling Z. Lome Seddigh, M. Rahmani*, T. Zomorodi Soofiani
2072	Design and Technical Evaluation of Artificial Lift Methods Using PIPESIM Software for Optimum System Selection in the Azadegan Oil Field A. M. Mohammadi, M. R. Rasaei*
2074	Comparative Assessment of Machine Learning Models for CO₂ Absorption in MOF–Amine Systems R. Feizabadi, A. Shoghi, O. Tavakoli*, K. Nosrati
2089	Thermodynamic Modeling and Efficiency Improvement of an Industrial Steam Boiler F. Abbasi, S. F. Najafi, M. Roshanaei, S. Nikmanesh*
2091	Smart Thermal Management of Solar Panels with Phase Change Materials A. Esmailifard, S. H. Hashemabadi, M. Haghgoo, H. Eshaghi