



POLYTECHNIQUE
MONTRÉAL

LE GÉNIE
EN PREMIÈRE CLASSE

Alireza Shams, PDF

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Education

- **McGill University, Montreal, QC, Canada** (2010-2015)
Ph.D. Degree, Department of Chemical Engineering
Thesis: Theory and Simulation of Defect Dynamics in Confined Liquid Crystals

- **Sharif University of Technology, Tehran, Iran** (2004-2006)
M.Sc. Degree, Department of Chemical and Petroleum Engineering
Thesis: Determination of the Maximum Capacity of Sweetening & Drying of Molecular Sieve

- **Sharif University of Technology, Tehran, Iran** (1999-2004)
B.Sc. Degree, Department of Chemical and Petroleum Engineering
Thesis: Microbial Desulfurization of Crude Oil

Research Interests

- Mathematical modeling
- Computational materials science
- Process design and modeling & simulation
- Application of AI in chemical engineering
- Transport phenomena in chemical & biochemical systems

Expertise

- Machine Learning
- Techno-Economic Analysis (TEA)
- Life-Cycle Assessment (LCA)
- Programming: MATLAB, C, Python, R
- Process Design Software: ASPEN Plus, HYSYS, CHEMCAD, DWSIM, EES, AutoCAD
- Molecular Modeling Software: PyMOL, MODELLER, VMD, and NAMD

Certificates

- Specialization in Deep Learning (2020)
- Project Management (2020)
- Clinical Data Science (2017)
- Graduate Teaching (2013)

Work Experience

- **McGill University**, Montreal, Canada Mitacs Industrial Postdoctoral Researcher (2017-2019)
- **Sigma Energy Storage Inc.**, Montreal, Canada Senior R&D Scientist and Process Specialist (2017-2019)
- **Yale University**, New Haven, US Research Consultant (2015-2017)
- **Simon Fraser University**, Vancouver, Canada Visiting Researcher (2016)
- **University of Tromsø**, Tromsø, Norway Visiting Researcher (2016)
- **McGill University**, Montreal, Canada Research Assistant (2010-2015)
- **Mining and Metals Engineering (MME) Company**, Tehran, Iran Process Engineer (2009-2010)
- **Danesh Pajouhan Noavar Consulting Company**, Tehran, Iran Consulting Research Engineer (2007-2009)
- **Sharif University and South Pars Gas Complex Company**, Asalooyeh, Iran Consulting Engineer (2007-2008)
- **Sharif University of Technology**, Tehran, Iran Research Assistant (2004-2006)
- **Sharif Technology Studies Center**, Tehran, Iran Researcher (2004)
- **Tehran Oil Refinery Company**, Tehran, Iran Engineer Intern (2003)

Teaching Experience

- **Chemical Plant Design and Economics**, Global Innovative Campus, Canada Instructor (2019-present)
- **Transport Phenomena in Biological Systems**, McGill University Teaching Assistant (2014)
- **Process Design**, McGill University Teaching Assistant (2013, 2014)
- **Separation Processes**, McGill University Teaching Assistant (2013)
- **Material Engineering**, McGill University Teaching (2012)

	Assistant	
• Chemical Engineering Principles II , McGill University	Teaching Assistant	(2012)
• Advanced Reactor Design , Sharif University	Teaching Assistant	(2006)
• Chemical Reactor Design , Sharif University	Teaching Assistant	(2006, 2005)
• Mass and Energy Balance for Petroleum Engineering , Sharif University	Teaching Assistant	(2005)

Journal Publications

- S. Golshan, R. Rabiee, **A. Shams**, R. Hoballah, P. Maheshwari, R. Jafari, J. Chaouki, and B. Blais, On the VOF Simulation Details and Droplet Size Distribution Inside Rotating Packed Beds, *Chemical Engineering and Processing - Process Intensification*, **2021**, Under review.
- V. N.-N. Tran, **A. Shams**, S. Ascioğlu, A. Martinecz, J. Liang, F. Clarelli, R. Mostowy, T. Cohen, A. A. zur Wiesch, vCOMBAT: a Novel Tool to Create and Visualize a Computational Model of Bacterial Antibiotic Target-binding, *BMC Bioinformatics*, **2020**, Under review.
- **A. Shams** and F. Moazeni, Modeling and Simulation of the MIDREX Shaft Furnace: Reduction, Transition and Cooling Zones, *JOM: Journal of the Minerals, Metals, and Materials Society*, **2015**, 67(11), 2681-2689.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Disclination Elastica Model of Loop Collision and Growth in Confined Nematic Liquid Crystals, *Soft Matter*, **2015**, 11, 5455-5464.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Nematic Liquid Crystals under the Conical Capillary Confinement: Theoretical Study of Geometry Effects on Disclination Lines, *Molecular Crystals Liquid Crystals*, **2015**, 612(1), 56-63.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Theory and Simulation of Ovoidal Disclination Loops in Nematic Liquid Crystals under Conical Confinement, *Liquid Crystals*, **2015**, 42(4), 506-519.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Theoretical Predictions of Disclination Loop Growth for Nematic Liquid Crystals under Capillary Confinement, *Physical Review E*, **2014**, 90 (4), 042501.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Mechanisms and Shape Predictions of Nematic Disclination Branching under Conical Confinement, *Soft Matter*, **2014**, 10, 3245-3258.

- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Disclination Shape Analysis for Nematic Liquid Crystals under Micron-range Capillary Confinement, *Mater. Res. Soc. Symp. Proc.*, **2013**, 1526.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Theory and Modeling of Nematic Disclination Branching Under Capillary Confinement, *Soft Matter*, **2012**, 8, 11135-11143.
- A. Taghavi, K. Parand, **A. Shams** and H. Ghezel Sofloo, Spectral method for solving differential equation of Gas Flow through a Micro-Nano Porous Media, *Journal of Computational and Theoretical Nanoscience*, **2010**, 7, 3, 542-546.
- H. Ghezel Sofloo, **A. Shams** and R. Ebrahimi, Study of Temperature and Velocity Distribution of Gas Flow in Micro-Nano Channels, *ASME, FEDSM2009-78017* pp. 1045-1050.
- H. Ghezel Sofloo, R. Ebrahimi and **A. Shams**, A Numerical Study of the Cylindrical TAYLOR-COUETTE Flow of a Rarefied GAS, *ASME, FEDSM2009-78015* pp. 1039-1044.
- **A. Shams**, A. M. Dehkordi, I. Goodarznia, Desulfurization of Liquid-Phase Butane by Zeolite Molecular Sieve 13X in a Fixed Bed: Modeling, Simulation, and Comparison with Commercial-Scale Plant Data, *Energy Fuels J.*, **2008**, 22(1), 570-575.
- **A. Shams**, A. Rezvanpour, Study on Chalcopyrite Bioleaching, *Farayand: Iranian Chemical & Petroleum Engineering Journal*, Winter **2005**, V. 9, pp 47-52.

Conference Publications

- **A. Shams**, Estimation of Mechanical Properties of Cell Populations Using the Elasticity Theory of Liquid Crystals, XXIX Interamerican Congress of Chemical Engineering Incorporating the 68th Canadian Chemical Engineering, October 28-31, **2018**, Toronto, Canada.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, A New MATLAB Tool for Estimation of Viscoelastic Properties of Confined Liquid Crystals, XXIX Interamerican Congress of Chemical Engineering Incorporating the 68th Canadian Chemical Engineering, October 28-31, **2018**, Toronto, Canada.
- **A. Shams**, M. Najafiyazdi, R. Boudreault and J. L. Meunier, CO₂ Capturing from Exhaust of Diesel Generators by Liquefaction in Low Ambient Temperature, XXIX Interamerican Congress of Chemical Engineering Incorporating the 68th Canadian Chemical Engineering, October 28-31, **2018**, Toronto, Canada.
- **A. Shams**, J. L. Meunier and R. Boudreault, The Effect of NO_x gases on the High-Pressure Cryogenic Carbon Capture Efficiency: A Theoretical Study, XXIX Interamerican Congress of Chemical Engineering Incorporating the 68th Canadian Chemical Engineering, October 28-31, **2018**, Toronto, Canada.
- **A. Shams**, P. Abel Zur Wiesch, T. Cohen., Theoretical Estimation of Biomechanical Properties of M. Tuberculosis Cell Populations, Montreal Biomaterials Research Day, February 23, **2017**, Montreal, Canada.

- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Estimation of Viscoelastic Properties from Confined Liquid Crystal Defects, Canadian Society of Rheology, Mason Award Symposium, May 20, **2015**, McGill University, Montreal, Canada.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Disclination Loop Growth for Nematic Liquid Crystals under Capillary Confinement, Proceeding of Material Research Society Fall Meeting, November 29- December 3, **2014**, Hynes Convention Center, Boston, Massachusetts, USA.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Estimation of the Elastic Modulus of Spider Silk Using a Nematic Disclination Shape Model, 3rd CRIBIQ Student Symposium, Centre sur la biodiversité de l'Université de Montréal, September 22-23, **2014**, Montreal, Canada.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Texture Transformation Process for Confined Nematic Liquid Crystals, September 8, **2014** CSACS Student Symposium, University of Montreal, Canada.
- **A. Shams**, Rain: An Immigrant Short Story, the Tenth Biennial Iranian Studies Conference, Hilton Montreal Bonaventure, August 6-9, **2014**, Montreal, Canada.
- **A. Shams** and A. D. Rey, Nematic Liquid Crystals under the Conical Capillary Confinement: Theoretical Study of Geometry Effects on Disclination Lines, 25th International Liquid Crystal Conference, June 29-July 1, **2014**, Trinity College Dublin, Dublin, Ireland.
- **A. Shams** and A. D. Rey, Theory and Modeling of Disclination Lines in Nematic Liquid Crystals under Conical Capillary Confinement, September **2013** CSACS Student Symposium, Loyola campus, Concordia University, Montreal, Canada.
- **A. Shams**, S. Gurevich and A. D. Rey, Defect Pattern Formation in Liquid Crystals under Confinement, Canadian Association of Physicists Congress, May 27-31, **2013**, Université de Montréal, Montreal, Canada.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Disclination Shape Analysis for Nematic Liquid Crystals under Micron-range Capillary Confinement, Proceeding of Material Research Society Fall Meeting, November 25-30, **2012**, Hynes Convention Center - Boston, Massachusetts, USA.
- **A. Shams** and A. D. Rey, Modeling of Disclination Loops in Bent-core Liquid Crystals, September **2012** CSACS Student Symposium, Centre Culturel, Université de Sherbrooke, Sherbrooke, Canada.
- **A. Shams**, X. Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Estimation of Viscoelastic Properties from Time-dependent Textural Transformations for Chromonic Liquid Crystals, 24th International Liquid Crystal Conference, August 19-24, **2012**, Mainz, Germany.
- **A. Shams** and A. D. Rey, Disclination Shape Analysis for Nematic Liquid Crystals under Capillary Confinement, Liquid Crystal Mini-Symposium: Theory & Experiments, March 28, **2012**, McGill University, Montreal, Canada.

- **A. Shams** and A. D. Rey, Nematic Liquid Crystals: From Disclination Lines to Elastic Properties, CSACS 10th Annual Meeting, May 9-10, **2012**, New Residence Hall, Montreal, Canada.
- **A. Shams**, X, Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Textural transformations in lyotropic cholesteric liquid crystals under confinement, American Physics Society meeting, February 27 - March 2, **2012**, Boston, Massachusetts, USA.
- **A. Shams**, X, Yao, J. O. Park, M. Srinivasarao and A. D. Rey, Estimation of viscoelastic properties from cholesteric liquid crystals defects, September **2011** CSACS Student Symposium, McCord Museum, Montreal, Canada.
- **A. Shams**, Prediction of breakthrough curves for dehydration of tetrahydrofuran by zeolite 4A in a fixed bed, Proceeding of 85th ACS Colloid and Surface Science Symposium, June 19-22, **2011**, McGill University, Montreal, Canada, p. 242.
- H. Ghezel Sofloo, **A. Shams** and R. Ebrahimi, Study of Temperature and Velocity Distribution of Gas Flow in Micro-Nano Channels, ASME Fluids Engineering Division Summer Meeting, August 2-5, **2009**, Vail, Colorado USA.
- H. Ghezel Sofloo, R. Ebrahimi and **A. Shams**, A Numerical Study of the Cylindrical TAYLOR-COUETTE Flow of a Rarefied GAS, ASME Fluids Engineering Division Summer Meeting, August 2-5, **2009**, Vail, Colorado USA.
- H. Ghezel Sofloo, **A. Shams** and R. Ebrahimi, Estimation of Temperature and Velocity Distribution of Gas Flow in Micro-Nano Channels of Zeolites by Statistic Methods, Proceedings of the National Congress on Nanomaterials & Nanotechnology, April **2009**, Najaf Abad Azad University, Iran.
- H. Ghezel Sofloo, **A. Shams** and R. Ebrahimi, Simulation of Rarefied gas flows in Nano Electro-Mechanical Systems, Proceedings of The National Congress on Nanomaterials & Nanotechnology, April **2009**, Najaf Abad Azad University, Iran.
- **A. Shams**, Estimation of Energetic and Structural Parameters for Argon Adsorption on Nanoporous Zeolites, Proceedings of the 2nd International Congress on Nanoscience & Nanotechnology, October **2008**, University of Tabriz, Iran.
- **A. Shams**, I. Goodarznia, A. M. Dehkordi, Modeling and Simulation of Desulfurization of Liquid-Phase Butane by 13X Zeolite in a Fixed-Bed, Proceedings of First Iran International Zeolite Conference, Amir Kabir University of Technology, May **2008**, Tehran, Iran.
- **A. Shams**, A. M. Dehkordi, Modeling and Simulation of Tetrahydrofuran Recovery by Zeolite 4A in a Fixed Bed: Effect of Operating Conditions and Adsorption Scale-up, Proceedings of First Iran International Zeolite Conference, Amir Kabir University of Technology, May **2008**, Tehran, Iran.
- **A. Shams** and A. M. Dehkordi, Effect of Operating Phase and Temperature on Prediction of Breakthrough Curve in Adsorption Processes, Proceedings of the 12th Iranian Chemical Engineering Congress, October **2008**, Sahand University of Technology, Tabriz, Iran.

- **A. Shams**, I. Goodarznia, A. M. Dehkordi, Effect of Operating Conditions on Binary Adsorption in Butane Sweetening Process, Proceedings of The First National Conference of Oil, Gas & Petrochemicals, April **2008**, Ghachsaran University, Iran.
- **A. Shams**, I. Goodarznia, A. M. Dehkordi, Study on Operation of Molecular Sieve in Butane Sweetening Colum, Proceedings of 2nd Conference on Chemistry & Industry, December **2006**, Azad University, Iran.
- A. Rezvanpour and **A. Shams** Study on Viscous Behavior of Oil-Water Emulsions, Proceedings of 5th National Conference on Chemical Engineering & Petroleum Eng., February **2005**, Amir Kabir University of Technology, Tehran, Iran.

Book Chapter

- 2nd Edition of *Handbook of Iran Lubrication Industry*, Chapter 8 – *Hydraulic Oils*, Danesh Pajouhan Company, 2008.