

# RAJIB MUKHERJEE

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## Career Objective

Pursue a career in teaching, research and development. My research was on multiscale modeling of complex material systems and its characterization using multiresolution and multivariate statistical analysis, algorithm development for optimization of multiscale process systems. My research interests includes theoretical and molecular modeling of complex mesoscale systems (self and directed assembly), find structure-property relation. I have developed the modeling skill that I would like to apply in various applications. I am also interested to do experiment for model validation.

## Summary

I have a doctorate in Chemical Engineering, graduated from the Process Systems Engineering Laboratory at Louisiana State University Department of Chemical Engineering. My recent research includes (a) developing an algorithm for chemical process sustainability evaluation and management using multivariate statistical analysis; (b) developing a MATLAB® based optimization algorithm for sensor placement with uncertainty; (c) developing an algorithm for novel polymer design using computer aided molecular design (CAMD). I am experienced in modeling from atomic to continuum scale, statistical algorithm development for multiresolution and multivariate statistical analysis, stochastic optimization algorithm development with uncertain variables and sustainability evaluation of process systems.

## Education

**Louisiana State University, Baton Rouge, LA**(2004-2010)

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PhD in Chemical Engineering

MS in Chemical Engineering

**Indian Institute of Technology (IIT Kanpur), India**(1997-1999)

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Masters in Chemical Engineering

**Andhra University College of Engineering, Visakhapatnam, India** (1993-1997)

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Bachelors in Chemical Engineering

## Work Summary

**Vishwamitra Research Institute, Chicago, IL** (May 2014 – present)

Research Scientist in the Center for Uncertain Systems: Tools for Optimization and Management

- Development of optimization algorithm for sensor placement in water network system and power plant under uncertainty
- Development of optimization algorithm for computer aided molecular design (CAMD) using group contribution method
- Application of sampling technique for efficient simulation of nano process systems.
  - Quasi Monte Carlo methods with Hammersley sequence sampling.
- Development of Better Optimization of Nonlinear Uncertain Systems (BONUS) algorithm for adaptive sensor placement
  - Use of kernel density estimation for probability density function.
  - Development of stochastic optimization algorithm with nonlinear programming solver based on sequential quadratic programming (SQP) method.
- Development of multivariate statistical algorithms for the choice of sustainable chemical process.
  - Use of PCA and PLS methods for evaluation and identification of sustainable chemical process
  - Application of multicriteria optimization for the choice of sustainable process

**US Environmental Protection Agency, Cincinnati, OH** (Nov. 2012 – Apr 2014)

ORISE postdoctoral research fellow at Office of Research and Development/National Risk Management Research Lab, Sustainable Technology Division.

- Advancing Chemical Process Engineering by integrating sustainable technologies in process design.
  - Developing a standalone software tool (GREENSCOPE) for sustainability evaluation of chemical process with indicators in the areas of environment, efficiency, energy and economics (using JAVA/C++).
- Data Analysis
  - Developing methodology for choice of sustainability indicators with multivariate statistical analysis (using MATLAB® base algorithm).
  - Using sustainability indicators for the choice of new design alternatives with multivariate statistical analysis.

**Tulane University, New Orleans, LA and Louisiana Tech University, Ruston, LA** (June 2010 – Apr. 2012)

Postdoctoral research associate of Louisiana Alliance for Simulation-Guided Materials Applications (LASiGMA) at the Center for Computational Science (CCS), Tulane University.

- Supercomputing
  - Application of novel tools for distributed high performance computing (HPC) across various supercomputers.
- Molecular Simulations
  - Molecular Dynamics (MD) simulations of biomolecular systems. Coarse graining of condensed phase and biomolecular systems.
- Data Analysis
  - Application of principal component analysis for analyzing structure and dynamics of biomolecular systems.

**Louisiana State University, Baton Rouge, LA** (Aug. 2004 – May 2010)

Dissertation Work from Process Systems Engineering Lab at the Department of Chemical Engineering.

- Statistical Process Monitoring
  - Image Analysis using multiresolution (wavelet) and multivariate (principal component analysis), cluster and Fourier analysis.
- Multiscale Modeling and Stochastic Simulation
  - Kinetic Monte Carlo (KMC) simulations to find the dynamics of phase separation of polymer solution systems.
  - Mesoscale lattice based modeling and important sampling Monte Carlo (MC) simulations of polymer solution systems.
  - KMC simulation to study adsorption/desorption on catalytic surface.
- **Graduate Teaching Assistant** in the Department of Chemical Engineering at Louisiana State University for **Advance process control, Optimization, Mathematical methods in Chemical Engineering, Advance Mathematics in Chemical Engineering, Process dynamics & control.**

**Indian Institute of Technology Bombay, India** (Aug. 2003 – June 2004)

Research Scholar

- Multiscale study of flow through microchannels
  - Molecular dynamic (MD) simulation and boundary element method to study flow through microchannels.

**National Metallurgical Laboratory, Jamshedpur, India** (Feb. 2003 – Jul. 2003)

Project Engineer

- Numerical Analysis
  - Application of Numerical Methods in solving simultaneous Partial Differential Equations (PDE) obtained from mass and energy balance inside blast furnace reactor.

**Tata Consultancy Services, India** (Aug 1999 – Feb 2003)

- Systems Engineer

Indian Institute of Technology Kanpur, India (Jan 1998 – Aug. 1999)

Masters Thesis

- Advancing Chemical Process Engineering by process intensification.
  - Experimental study of mass transfer in a centrifugal gas-liquid contactor (HIGEE).

## Publications

### JOURNALS

1. R. Mukherjee, “Selection of Sustainability Indicators: Prospective versus Retrospective Analysis” in preparation to be submitted in *Clean Technologies and Environmental Policy*
2. R. Mukherjee, U. M. Diwekar, A. Vaseastha “Optimal Sensor Placement with Mitigation Strategy for Water Network Systems under Uncertainty” required reviews completed *Journal of Water Resources Planning and Management*
3. R. Mukherjee, U. Diwekar, 2016, “Comparison of Monte Carlo and quasi Monte Carlo technique in structure and relaxing dynamics of polymer in dilute solution”, accepted, *Computers and Chemical Eng.*, 84, pp 28–35
4. R. Mukherjee, D. Sengupta, Subhas K Sikdar, 2015, “Sustainability in the context of process engineering”, *Clean Technologies and Environmental Policy*, 17(4), 833-840.
5. D. Sengupta, R. Mukherjee, Subhas K. Sikdar, 2015, “Environmental sustainability of countries using the UN MDG indicators by multivariate statistical methods”, *Env. Prog. and Sust. Energy*, 34(1), pp 198-206
6. R. Mukherjee, D. Sengupta, Subhas K Sikdar, 2013, “Parsimonious Use of Indicators for Evaluating Sustainability Systems with Multivariate Statistical Analysis”, *Clean Technologies and Environmental Policy*, 15(4), pp 699-706
7. R. Mukherjee, F.R. Hung, A. Palazoglu, J.A. Romagnoli, 2010, “Modeling and Multi-resolution Characterization for Microfabrication Applications.” *Industrial and Engineering Chemistry Research*, 49(2), pp. 548-558
8. P. Facco, F. Bezzo, M. Barolo, R. Mukherjee, and J. Romagnoli, 2009, “Monitoring Roughness and Edge Shape on Semiconductors Through Multiresolution and Multivariate Image Analysis”, *AIChE J.*, 55(5), pp. 1147-1160.
9. W. Sun\*, R. Mukherjee\*, P. Stroeve, A. Palazoglu and J.A. Romagnoli, 2009, “A Multi-Resolution Approach For Line-Edge Roughness Detection”, *Microelectronic Engineering*, 86(3), pp.340-351
10. R. Mukherjee, J.C. Flake, A. Palazoglu and J.A. Romagnoli, 2009, “A Multiresolution Spatial Correlation Approach For Line-Edge Roughness Characterization”, *J. Wavelet Theory Appl.*, 3(1), pp.103-122

\* Authors have contributed equally to this research.

### BOOK

1. S. K. Sikdar, D Sengupta, R. Mukherjee, “Measuring Progress Towards Sustainability”, in preparation, to be published by Springer

### BOOK CHAPTER

1. R. Mukherjee, D Sengupta, S. K. Sikdar, “Selection of Sustainable Processes using Sustainability Footprint Method: A Case Study of Methanol Production from Carbon Dioxide” in “*Sustainability of Products, Processes and Supply Chains*”; edited by Fengqi You, Elsevier, 2015
2. D. Sengupta, R. Mukherjee, S. K Sikdar, “Moving to a decision point in sustainability analysis” in “*Assessing and Measuring Environmental Impact and Sustainability*”; pp. 87-129, edited by Jiri Klemes, Elsevier, January 2015.
3. R. Mukherjee and T.C. Bishop. “Nucleosomal DNA: Kinked, Not Kinked, or Self-Healing Material?” in *Frontiers in Nucleic Acids*, Chapter 5, pp 69–92. Chapter DOI: 10.1021/bk-2011-1082.ch005 ACS Symposium Series, Vol. 1082 ISBN13: 9780841226234 eISBN: 9780841226289
4. R. Mukherjee, D. Deb, P. Sandilya and D. P. Rao, “Gas-Phase Mass Transfer In A Centrifugal Gas-Liquid Contactor With A Stack Of Flexible Disks As Packing”, in *Processing by Centrifugation*, pp. 51-60, DOI: 10.1007/978-1-4615-0687-4\_7 Springer US, ISBN 978-1-4613-5195-5, eISBN 978-1-4615-0687-4

### CONFERENCE PROCEEDINGS

1. R. Mukherjee, A. Thota, H. Fujioka, T. C. Bishop, S. Jha, 2012, “Running Many Molecular Dynamics Simulations on Many Supercomputers”, Proceeding XSEDE '12, Article No. 2, ACM New York, NY, USA ©2012,
2. R. Mukherjee, A. Palazoglu, J.A. Romagnoli, “A Multiresolution Multiscale computational Approach for Characterization and Analysis of Nanostructured Surfaces”, *Computer Aided Chemical Engineering*, Volume 27, 2009, pp. 1761-1766, ISBN: 978-0-444-53472-9, DOI: 10.1016/S1570-7946(09)70684-4
3. B. Zhang, R. Mukherjee, A. Abbas, J. Romagnoli, “Multi-resolution Fuzzy Clustering Approach for Image-

Based Particle Characterization”, DYCOPS2010, DOI: 10.3182/20100705-3-BE-2011.00025

4. R. Mukherjee, A. Palazoglu and J.A. Romagnoli, "Image Based Characterization And Molecular Modeling of Line-edge Roughness on Positive Resist", ESCAPE, 2008
5. R. Mukherjee, A. Palazoglu, J.A. Romagnoli, "Characterization of Different Surfaces Morphology in Heterogeneous Catalyst", NSTI-Nanotech. 2008, pp. 859 – 86

#### **CONFERENCES**

1. R. Mukherjee, U. Diwekar, "Application of Better Optimization of Nonlinear Uncertain Systems (BONUS) Algorithm for Adaptive Sensor Placement", AIChE Annual 2014, Atlanta, GA
2. R. Mukherjee, U. Diwekar, "Comparison of Monte Carlo and Quasi Monte Carlo Technique in Structure and Relaxing Dynamics of Polymer in Dilute Solution", AIChE Annual 2014, Atlanta, GA
3. R. Mukherjee, D. Sengupta, S.K. Sikdar, "Application of Sustainability Footprint and Multicriteria Optimization for the Choice of Sustainable Chemical Processes", AIChE Annual 2014, Atlanta, GA
4. R. Mukherjee, G. J. Ruiz-Mercado, R. L. Smith, M. A. Gonzalez, "Data Availability and Management for Sustainability Evaluation: GREENSCOPE", AIChE Annual 2013, San Francisco, CA
5. R. Mukherjee, G. J. Ruiz-Mercado, R. L. Smith, M. A. Gonzalez, "Data Management for Sustainability Evaluation", ICOSSE-13, Cincinnati, OH
6. R. Mukherjee, D. Sengupta, S. K. Sikdar, "Assessing Sufficiency of Sustainability Indicators With Multivariate Statistical Analyses", ICOSSE-13, Cincinnati, OH
7. R. Mukherjee, G. J. Ruiz-Mercado, R. L. Smith, M. A. Gonzalez, "GREENSCOPE: A Standalone Tool for Sustainable Chemical Process Design", ACS Summer School on Green Chemistry and Sustainable Energy
8. T. C. Bishop, R. Mukherjee, "Nucleosomal DNA: Kinked, not kinked, or self-healing material ", SWRM and SERM of ACS, Nov 30 – Dec 4, 2010, New Orleans, LA
9. R. Mukherjee, T. C. Bishop, "Computational Study of Nucleosome Positioning and Stability", Biophysical Journal, vol. 100, issue 3, pp. 67a-67a
10. R. Mukherjee, H. Fujioka, A. Thota, S. Jha, T. C. Bishop, "The Nucleosome Simulator: 100 Nucleosomes; 2 Microseconds and Counting", Albany2011, Conversation17, June 14-18 2011
11. T. C. Bishop, R. Mukherjee, H. Fujioka, A. Thota, S. Jha, "High Throughput Atomistic Simulations of the Nucleosome", CECAM-HQ-EPFL, August 30, 2011 to September 2, 2011, Lausanne, Switzerland
12. R. Mukherjee, F.R. Hung, J.J. Spivey, and J.A. Romagnoli, "DFT estimation of the adsorption energy of CO on Ni, Ru and Rh surfaces with different morphologies", AIChE Annual Meeting, Nov 16-21, 2008, Philadelphia, PA
13. R. Mukherjee, A. Palazoglu, J.A. Romagnoli, "Characterization of Different Surfaces Morphology in Heterogeneous Catalyst", NSTI-Nanotech., June 1-5, 2008, Boston, MA.
14. R. Mukherjee, A. Palazoglu and J.A. Romagnoli, "DFT Estimation of Surface Energy of Different Surface Morphology in Heterogeneous Catalyst", AIChE Spring Meeting, Apr 6-10, 2008, New Orleans, LA
15. R. Mukherjee, A. Palazoglu and J.A. Romagnoli, "Multiresolution Image Characterization of Line Edge Roughness Using Wave Cluster Technique", AIChE Annual Meeting, Nov 4-9, 2007, Salt Lake City, Utah
16. R. Mukherjee, A. Palazoglu and J.A. Romagnoli, "Wave Cluster Analysis for Image Based Characterization and Molecular Simulation of Micro/nano Surface", AIChE Annual Meeting, Nov 4-9, 2007, Salt Lake City, Utah

#### **INVITED SEMINARS**

1. Rajib Mukherjee "Modeling and Multi-resolution Characterization of Micro Surface for Tailored Nanostructures", Energy and Transport Science Laboratory, Department of Mechanical Engineering Texas A&M University, Aug 3, 2015
2. Rajib Mukherjee "Integrated Model Centric Approach for Process Development", Vishwamitra Research Institute, Nov 19, 2013, UIC
3. Rajib Mukherjee "Running many MD Simulations on many Supercomputers", 4th LBRN Computational Biology Workshop, April 18, 2011, LSU
4. Rajib Mukherjee, Thomas C Bishop, "A Preliminary Report on Computational Study of Nucleosome Positioning", New Orleans Protein Folding Intergroup, March 24, 2011

### **Technical Skills**

- Programming language: FORTRAN, Visual Basic, C, C++, JAVA, Python.
- Process simulator: Aspen Plus®, CHEMCAD.

- Database: MySQL.
- MATLAB®, R, XLStat for Statistical Analysis (Wavelet, Fourier, Cluster Analysis, Principal Component Analysis (PCA) and Partial Least Squares Variable Importance in Projection (PLS-VIP) methods).
- MATLAB® for image processing using Wavelet, Cluster Analysis and Principal Component Analysis.
- Distributed supercomputing for simulation and data analysis across various supercomputers of XSEDE and LONI.
- Developing software tool with JAVA (developed GREENSCOPE for process sustainability evaluation and optimization).
- GAMS and MATLAB® for optimization.
- Simulation package: NAMD, CPMD.
- Visualization package: VMD, RasMol.
- Operating Systems: UNIX, Linux, Mac OS X, Windows.

## Teaching Experience

Experience as teaching assistant for the following courses at IITK and LSU department of Chemical Engineering.

- Numerical Methods in Chemical Engineering (at IITK)
- Process Dynamics & Control (CHE 4198)
- Advanced Process Control (CHE 7572)
- Optimization (CHE 7314)
- Mathematical Methods in Chemical Engineering (CHE 7110)
- Advanced Mathematics in Chemical Engineering (CHE 7700)

Texas A&M University, Department of Mechanical Engineering courses I am willing to teach.

- Statics and Particle Dynamics (MEEN 221)
- Principles of Thermodynamics (MEEN 315)
- Fluid Mechanics and Fluid Mechanics Lab. (MEEN 344 and MEEN 345)
- Engineering Analysis for Mechanical Engineers (MEEN 357)
- Dynamic Systems and Controls (MEEN 364)
- Mechanical Engineering Design (MMEN 401 and MEEN 402)
- Processing and Characterization of Polymers (MEEN 458)
- Heat Transfer and Heat Transfer Lab (MEEN 461 and MEEN 464)

## Reviewer of Journal

Macromolecular Theory & Simulations

Clean Technologies and Environmental Policy

AIChE Journal

SIMIODE (Systemic Initiative for Modeling Investigations and Opportunities with Differential Equations)

ASME (IDETC/CIE 2015)

## Awards/Honors

- Graduate School Enhancement Award at Louisiana State University (2004-2008)
- Charles E. Cotes Travel Award for oral presentation at AIChE annual meeting 2007 and 2008
- Graduate School Travel Award for oral presentation at NSTI Nanotech 2008
- Teaching Assistantships from the Cain Department of Chemical Engineering at Louisiana State University (2004-2010)
- Ministry of Human Resource Development (MHRD) scholarship / assistantship for M Tech at IIT (Indian Institute of Technology) Kanpur

- Oak Ridge Institute of Science and Education Post Doctoral Fellowship.
- Scholarship to attend and present at ACS Summer School on Green Chemistry and Sustainable Energy (2013).
- Certificate of Excellence in Reviewing from Clean Technologies and Environmental Policy, 2013 and 2014