

CURRICULUM VITAE

Name **Ajay Kumar Ray**
Present Position Tenured Professor, Associate and Graduate Chair
Present Employer Department of Chemical and Biochemical Engineering
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1. Education History:

Degree	University	Year
PhD - Chemical Engineering	University of Minnesota, USA	1992
M. Tech. - Chemical Engineering	Indian Institute of Technology, Kanpur	1985
B. Tech - Chemical Engineering	University of Calcutta, India	1983
B. Sc. - Chemistry	University of Calcutta, India	1980

2. Employment History:

Period	Position	Company/Institution
2005 -	Professor	University of Western Ontario
2001 - 2005	Associate Professor	National University of Singapore
1999 - 2000	Assistant Professor	National University of Singapore
1998 - 1999	Senior Lecturer	National University of Singapore
1995 - 1997	Lecturer	National University of Singapore
1993 - 1995	Scientific Investigator	Univ. of Groningen, Netherlands
1992 - 1993	Postdoctoral Fellow	West Virginia University, USA

3. Research Interests: Engineering of Chemical Reactions and Processes

Process modelling, simulation and multi-objective optimization
Simulated Moving Bed (SMB) systems for difficult or impossible separations
Band-engineered semiconductor photocatalysis
Integrated reactor-separator
Oscillatory reactor

4. Summary of Publications

1 Text book: "Mathematical Methods in Chemical and Environmental Engineering, Thomson Learning, 2 nd Edition Revised, 2005.
2 Book Chapters
1 European patent on a "Novel Photocatalytic Reactor Design"
96 Internationally Referred Journal Publications
42 Conference Papers in Proceedings, 52 Conference Presentations.

5. Professional Membership/Grade:

Member - American Institute of Chemical Engineers (AIChE)
Member - American Chemical Society (ACS)
Member – Canadian Society of Chemical Engineers (CSCChE)

6. Honours and Awards

Member of Editorial Board, International Journal of Chemical Reactor Engg., 2002 –
Member of Editorial Board, Euro-Asian Journal of Applied Sciences, 2004 –
Member of Editorial Board, Euro-Asian Journal of Scientific Research, 2004 –
Distinguished Speakers Award, Indian Inst. Chemical Engineers, 2007.
CrayQuest Award for excellence in R&D using high performance computing, 1999.
Distinguished Young Alumnus Award, University of Calcutta, India, 2001.
Teaching Commendation Certificate, National University of Singapore, 2004.
Member of Working Party, Asia Pacific Chemical Reaction Engineering (APCRE)

7. Teaching Experience and Interests

Module Code	Module Title
CBE 322 (at UWO)	Heat Transfer Operations
CBE 467 (at UWO)	Green Energy and Engineering
CBE 291 (at UWO)	Computational Methods in Engineering
CBE 425 (at UWO)	Mathematical Methods in Engineering
ES 699 (at UWO)	Mathematical Methods in Chemical Engineering
ES 700 (at UWO)	Green Energy and Engineering
CN 5010 (at NUS)	Mathematical Methods in Chemical Engineering
CN 3421 (at NUS)	Process Modeling and Numerical Simulation
TC 3111 (at NUS)	Process Dynamics and Control
TC 3411 (at NUS)	Numerical Analysis
CN 2116 (at NUS)	Chemical Kinetics and Reactor Design
EV 0007 (at NUS)	Instrumentation and Process Control
TUM (TUM-NUS joint M. Sc. Program)	Advanced Modeling and Computational Methods in Industrial Chemistry
CN 5450 (at NUS)	Application of Optimization in Chemical Engineering

8. Number of Students Supervised

	Supervised	Supervising
PhD students	7	7
M. Sc. and M. Eng. students	21	6
Research Associates / Postdoctoral Fellows	7	1
Final Year Undergraduate (FYP) projects	61	3

9. Listing of Contributions to Teaching Materials

- I have developed the graduate course "Mathematical Methods in Chemical Engineering" and in 2005 revised 2nd edition of the text book titled ""Mathematical Methods in Chemical and Environmental Engineering" was published by International Thomson Learning Publishing Company. The book is currently being used in several institutes in India, Singapore and in Korea.

Unlike many theoretical reference texts, the purpose of compiling these lectures into a book is to present the fundamental theory and applications of mathematical methods for the solution of practical engineering problems. The book describes mathematical methods for chemical and environmental engineering students or professional engineers who are interested in solving *applied* engineering problems. This book includes a broad selection of mathematical topics that are essential for a modern chemical/environmental engineer. It provides a blend of analytical and numerical techniques required for solving problems in diverse areas, e.g., heat and mass transfer, thermodynamics, fluid mechanics, reaction engineering, transport phenomena, process systems engineering, etc. It deals extensively with methods for solving systems of linear and non-linear algebraic equations and systems of linear and non-linear ordinary and partial differential equations. Concepts of linear dependence and existence of solutions, general analytical methods for solving linear differential equations, analysis of stability and convergence of numerical solutions, etc., are also discussed.

- I have developed a concept "Germinating Seed Problem: An Approach for Chemical Engineering Education", which was presented at the 2nd Symposium on Teaching and Learning in Higher Education held at National University of Singapore, September 2002. The paper also appeared in the symposium proceedings (page 206-211) under "Teaching Methodology".
- I have developed an integrated tool that interfaces HYSYS plant simulator with multi-objective optimization package based on genetic algorithm and Visual C++ code. This approach will be beneficial to practicing engineer for de-bottlenecking, revamping, retrofitting studies and to perform "Plant-wide Optimization" of the entire industrial processes. This is particularly useful in undergraduate design projects to better design a particular process.
- I was actively involved in the development of integrated teaching, an integrated approach of teaching chemical engineering modules. The idea was to use a common process flow diagram in several modules (fluid mechanics, thermodynamics, heat & mass transfer, equilibrium stage process, mass transfer operations, reaction engineering, process dynamics & control, and numerical analysis) to show the applications of the contents of these modules in a common chemical engineering process. The initiative of this integrated approach was to help the students to better appreciate the link among different modules taught at different levels of undergraduate curriculum. An article on this approach appeared in CDTL Link.
- In a world of rapidly changing technology and volatile economic environment, it is very important for engineering professionals to maintain technical knowledge and relevance and to upgrade themselves continuously. Hence, I have not limited myself to teaching courses only at the University to regular students. I have been actively involved in teaching professional short courses. I have offered two professional short courses "Applications of Optimization in Chemical Industry" and "Mathematical Methods in Engineering with Computers" to provide life-long education to practicing engineers in Singapore. I also developed a professional short course on "Spreadsheet Problem Solving" that teaches how to use spreadsheet (such as Excel) to solve non-linear equations and practical optimization problems.

10. Listing of Keynote and Invited presentations at international and local conferences.

Special Lectures, Speeches and Invited Seminars Presented

- Invited Seminar at the Polymer Science and Engineering Department, University of Akron, USA on "Optimization of polymer reactors" to be presented on 22 February 2008.
- Invited Plenary Speaker on "Design and Development of Simulated Moving Bed Systems for Industrial Applications", to be presented at the Annual Indian Institute of Chemical Engineering Conference, 27-30 December, 2007.

- Invited Keynote Speaker on “Applications of Multiobjective Optimization in the Design of Simulated Moving Bed Systems”, at the 1st International Conference on Natural Resources Engineering and Technology, Putrajaya, Malaysia, 24-25 July, 2006.
- Invited Keynote Speaker on “Experimental Investigation of Taylor Vortex Photocatalytic Reactor for Water Purification”, at the Ultrapure Water Asia 2004, Singapore, March 2004.
- Invited Speaker on “Equilibrium and Optimum: How to Kill Two Birds with One Stone?”, Department of Mathematics, National University of Singapore, 6 November 2002.
- Speaker on “Germinating Seed Problem: An Approach to Chemical Engineering Education”, at the 2nd Symposium on Teaching and Learning for Higher Education held in Singapore, 4-6 September 2002.
- Invited Seminar on “Water Purification by Semiconductor Photocatalysis”, presented at the National University of Singapore on 6 September 2002 as part of Science and Technology month celebration.
- Invited Keynote Speaker on “Major Challenges in the Design of Large-Scale Photocatalytic Reactor for Water Purification” at the Ultrapure Water Asia 2002, conference held in Singapore, 14-15 August 2002.
- Invited Seminar on "Modeling and Multiobjective Optimization of an Industrial Wiped Film Polyethylene Phthalate Reactor" presented at the Department of Chemical Engineering, Swiss Federal Institute of Technology, Zurich, Switzerland, on 13 March 2002.
- Invited Seminar on "How Genetic Algorithms Works for Optimization?" presented at the Department of Chemical Engineering, Swiss Federal Institute of Technology, Zurich, Switzerland, on 11 March 2002.
- Invited Seminar on "Applications of multiobjective optimization in the design of separators and reactor-separators based on SMB technology", presented at the Department of Chemical Engineering, University of Waterloo, Canada, on 13 March 2002.
- Invited Seminar on “Water Purification by Semiconductor Photocatalysis”, presented at the Department of Chemical Engineering, Indian Institute of Technology, Kanpur, India on 18 December 2001.
- Invited Seminar on "Applications of simulated moving bed in chemical engineering", presented at the Department of Chemical Engineering, University of Bath, UK, on 15 September 2000.
- Invited Seminar on "Multi-objective optimization of industrial chemical processes", presented at the Department of Chemical Engineering, University of Auburn, USA, on 29 October 1999.
- Invited Seminar on “Major Challenges on the Development of Photocatalytic Reactors for Water purification”, presented on 5 September 1997 jointly held by Department of Water Engineering and Centre for Water and Waste Technology, University of New South Wales, Sydney, Australia.
- Invited Seminar on “Major Challenges on the Development of Photocatalytic Reactors for Water and Air purification”, presented on 19 September 1996 as a part of celebration of Technology Month at National University of Singapore.

11. Listing of Research Prizes, Best Paper Awards, etc.

- Distinguished Speakers Award in recognition of contributions to the Chemical Engineering Profession by the Indian Institute of Chemical Engineers at the annual meeting CHEMCON 2007 and Diamond Jubilee celebrations held in Kolkata (India), December 27-30, 2007. The award carries a medal, an honorarium and a citation.
- An article on adsorption of arsenic on TiO₂ is listed as one of the top 50 most cited articles in Colloids and Interface Science Journal [278 (2004) 270] in 2005-2007 period. The article has received so far 30 citations.
- An article on arsenic removal by photocatalysis is listed as one of the top 50 most cited articles in Environmental Science & Technology [(39 (2005) 1827) in 2005-2007 period. The article has received so far 17 citations.
- An article on multi-objective optimization of chiral drug separation by SMB is listed as one of the top 50 most cited articles in AIChE Journal [48 (2002) 2800] in 2003-2005 period. The article has received so far 48 citations.

- An article on removal of toxic metal ions by photocatalysis is listed as one of the top 50 most cited articles in Chemical Engineering Science [(56 (2001) 1561) in 2002-2004 period. The article has received so far 49 citations.
- An article on optimization of industrial hydrogen plant is listed as one of the top 50 most cited articles in Chemical Engineering Science [(56 (2001) 999) in 2002-2004 period. The article has received so far 48 citations.
- An article on multi-objective optimization of industrial steam reforming process is listed as one of the top 50 most cited articles in Industrial & Engineering Chemistry Research [39 (2000) 706] in 2001-2004 period. The article has received so far 45 citations.
- An article on multi-objective optimization of SMB is listed as one of the top 100 most cited articles in Industrial & Engineering Chemistry Research [41 (2002) 3213] in 2003-2005 period. The article has received so far 19 citations.
- As recognition to my research work, I received in 1999 the CrayQuest award for excellence in research and development using high performance computing given by Silicon Graphics Inc. The work received the recognition was computer simulation of a novel photocatalytic reactor for water purification using parallel computing. I was featured in Straits Times (on October 15, 1999, page 57); Campus News (No. 140, January/February 2000, page 6-7); in the cover story of "Innovation", a magazine of research and development (July 2001, Vol. 2(2), page 19) and in ChEERs (Vol. 3, February 2000, page 3).
- Received Distinguished Young Alumnus award from University of Calcutta, India in 2001.
- One of my M. Eng. Students, Mr. Bhaskar Venkataraman, won the NSTB Gold Medal for best M. Eng. Thesis, National University of Singapore in 2000. His thesis was on modeling and multiobjective optimization of an industrial wiped-film Poly (Ethylene Terephthalate) reactor. His work resulted in four international journal publications, one article each in AIChE Journal, Computers & Chemical Engineering, Polymer Reaction Engineering, and Reviews in Chemical Engineering.
- Ms. Yeoh Simin Felicia, one of my Final Year Project students, won the best project award in 2004, given by Department of Chemical and Biomolecular Engineering, NUS.

12. Listing of Editorial Works

- Member of Editorial Board, International Journal of Chemical Reactor Engineering, 2002 - present.
- Member of Editorial Board, European Journal of Scientific Research, 2004 - present
- Member of Editorial Board, Euro-Asian Journal of Applied Sciences, 2004 - present
- Guest Editing a special issue on "Bio-energy and Green Engineering". The issue will be published in July 2008.
- Guest Edited a special issue on "Environmental reaction engineering" for Developments in Chemical Engineering and Mineral Processing Journal. The issue was published in August 2000.
- Member of Scientific committee of APCRE (Asia-Pacific Chemical Reaction Engineering) Conference to be held in Korea, June, 2005.
- Member of Scientific and Organizing committee of 2nd MaChiE (Mathematics in Chemical Kinetics and Chemical Engineering) Conference to be held in Houston, February, 2007.
- Member of Scientific and Organizing committee of Process Intensification and Innovation Process (PI)2 Conference II to be held in Christchurch, New Zealand, September, 2006.
- Reviewed a manuscript containing few chapters of a book titled "Photocatalytic Reaction Engineering" by Hugo de Lasa, Benito Serrano and Miguel Salaiques to be published by Kluwer Academic Publishers, NY in 2005.
- Reviewed a manuscript containing few chapters of a book titled "Cyclically Operated Separating Reactors" by Takashi Aida and Peter L Silveston to be published by Blackwell Publishing, Oxford, UK in 2005.
- Reviewed numerous articles (on average 20-25 per year in the last 3 years) on photocatalysis, catalytic reactors, modeling, simulation, optimization and reaction engineering for AIChE, Chemical

Engineering Science, Industrial & Engineering Chemistry Research, Journal of Catalysis, Catalysis Today, Applied Catalysis A: General, Applied Catalysis B: Environmental, Computers & Chemical Engineering, Environmental Science and Technology, Water Research, Journal of Membrane Science, Separation Science & Technology, Chemosphere, ChemTech, International Journal of Drying Technology, Journal of Applied Electrochemistry, International Journal of Chemical Reactor Engineering, Journal of Applied Polymer Science, Chemical Engineering, etc.

13. Listing of Editorial Appointments

- Member of Editorial Board, International Journal of Chemical Reactor Engineering, 2002 - present.
- Member of Editorial Board, European Journal of Scientific Research, 2004 - present
- Member of Editorial Board, Euro-Asian Journal of Applied Sciences, 2004 - present
- Guest Edited a special issue on "Environmental reaction engineering" for Developments in Chemical Engineering and Mineral Processing Journal. The issue was published in August 2000.
- Served as an external examiner for PhD thesis for
 - University of Queensland, Australia
 - Indian Institute of Technology, Kanpur, India
 - Indian Institute of Technology, Delhi, India
 - Indian Institute of Technology, Chennai, India
 - Anna University, India.
 - University of Gujrat, India
 - National University of Singapore
 - University of Teknology, Malaysia
 - Nanyang Technology Institute, Singapore

14. Listing of Research Grants:

Year	PI or Collaborator	Project title	Granting Organisation	Grant amount
1993	PI	High Intensity Photocatalytic Reactor (HIPHOCAR) Development	European Commission	750,000 ECU for 4 years
1996	PI	Development of photocatalytic reactor for destruction of toxic water pollutants by advanced oxidation process	RITE, Japan	for ¥5,000,650 per year for two years
1996	PI	Photocatalytic oxidation of polluted industrial effluents	NUS	S\$179,900 for three years
1997	PI	Water purification by semiconductor photocatalysis	Environmental Technology Enterprise, NUS	S\$100,000 for three years
1997	Co-PI	Modeling and dynamic optimization of industrial reactors	NUS	S\$50,000 for 2 years
1999	PI	Simulated countercurrent moving bed chromatographic reactor	NUS	S\$125,000 for 2 years
2000	PI	Water purification by semiconductor photocatalysis	NUS	S\$49,000 for two years
2002	PI	Synthesis of organic esters in simulated countercurrent moving bed chromatographic reactor	NUS	S\$52,900 for 2 years
2003	PI	Optimal Design of Varicol Process for Chiral Drug Separation	NUS	S\$133,232 for 2 years

2005	PI	Band-engineered photocatalysis for water purification	NUS	S\$26,000 for 2 years
2005	Co-PI	Advanced systems engineering for the pharmaceutical industry	NUS	S\$150,000 for 2 years
2005	Co-PI	Development of Semiconductor Nanostructures with Tunable Band Gaps for Advanced Technological Applications	A*STAR Singapore	S\$1,932,500
2005	Collaborator	Optimal Operation of SMB Chromatographic Processes through Wavelet and SVD Based Dynamic Modelling and Advanced Control	Australian Research Council (ARC)	A\$850,000
2005	PI	Start-up Grant	WE, Western	C\$ 64,000
2006	PI	Applications of Multiobjective optimization in the design of SMB systems	NSERC Discovery Grant	C\$ 122,500
2006	PI	Design and development of SMB systems for drug separation	NSERC Research Tools & Instruments (RTI)	C\$ 85,000
2006	PI	Development of SMB systems for Chiral drug separation	Academic Development Fund, Univ. of Western Ontario	C\$ 65,200
2006	PI	Novel Photocatalysis and SMB Technology Laboratory	CFI Leaders Opportunity Fund	C\$ 639,756
2006	Co-PI	Green Energy and Environmentally Friendly Chemical Technologies	CFI Leading Edge Fund	C\$ 18,036,200
2007	PI	Water Treatment by Photocatalysis	Foreign Affairs and International Trade Canada	C\$10,000
2007	Co-PI	Development of Reliable, efficient and economic chiral drug separation process	NSERC Strategic Grant	C\$ 202,600
2007	Co-PI	TiO ₂ Nanotube Arrays Synthesis, bandgap engineering and solar energy applications	NSERC Strategic Grant	C\$ 144,000
2008	Co-PI	Innovations in Renewable Energy Production: Biodiesel from Microalgae	NSERC Strategic Special Projects Grant	C\$ 199,400

15. Service:

Service to University, Faculty and Department

Period	Position	Organisation/Event	Brief description of activity
2005-	Associate Chair	Chemical & Biochemical Engineering, UWO	Assist department Chair in all day to day activities
2005 -	Graduate Chair	Chemical & Biochemical Engineering, UWO	Responsible for all Graduate Student matters in the department

2004 - 2005	Co-ordinator	NUS-IIT Kanpur Joint Research Program and Centre	Co-ordinating for a joint Research program & Centre and initiative for a joint PhD degree program
2004 - 2005	Chairman	Department Accreditation Committee	Co-ordinating department accreditation for IChemE in February 2006.
2004 - 2005	Chairman	Department Postgraduate Curriculum Review Committee	Reviewing current postgraduate curriculum
2001 - 2005	Chairman	Student Exchange Program (SEP) and NUS Overseas College (NOC)	Student advisor and approves application for SEP and NOC program
2002 - 2005	Member	"Mathematics", "Physics" and "Chemistry" sub-committee, FOE	Review, modification and implementation of curriculum related matters for undergraduate mathematics, physics and chemistry modules
2001 - 2005	Member	Curriculum Development Committee	Review, modification and implementation of curriculum related matters for undergraduate courses and program
2003 - 2005	Member	Task force for FOE Research Database	Involved in the development of FOE Research Database
2002 - 2005	Peer Reviewer	Peer Reviewer on Teaching of many FOE staff members	Peer review of teaching
2002 - 2005	Peer Reviewer	Peer reviewer of Mathematics lecturer	Peer Reviewing Mathematics lecturer teaching FOE students mathematics
2003 - 04	Member	"Engineering Science" program	initial development of curriculum of "Engineering Science" program
2000-2005	PhD Thesis Committee	Currently chairman or member of 11 PhD thesis committee	PhD thesis committee
1995-	Reviewer of PhD and M. Eng. thesis	Reviewed numerous PhD and M. Eng. Thesis of ChBE department as well as other departments	Reviewed thesis
1999 - 02	Member	Career Talks to Junior College Students	Explaining junior college students about chemical engineering
1998 - 02	Member	Information and Public Relations Committee	In-charge of publicity of department, corridor posters, CD-ROM, etc.
1997 - 03	Co-ordinator	Undergraduate Teaching Laboratory Year 2	In-charge of day-to-day running of undergraduate teaching laboratory
1997 - 00	Member	Professional Activity Committee	In-charge of conference organization of FOE
1997 - 00	Member	PS21 (Public Service for 21 st Century)	Represented department for development of new work improvement activities.

Service to International Academic Community

Period	Position	Organisation/Event	Brief description of activity
2002 -	Member of Editorial Board	International Journal of Chemical Reactor Engineering	Responsible for review of numerous articles

2004 -	Member of Editorial Board	Euro-Asian Journal of Applied Science	Responsible for review of numerous articles
2001 -	Member of Working Party	Asia Pacific Chemical Reaction Engineering (APCRE)	Responsible for organization of conferences and integration of reaction engineering community.
2004-	Member of Scientific Committee	Mathematics in chemical kinetic and chemical engineering (MaChiE2) Symposium	Responsible for review of numerous articles for a special issue
2002	Member of Organizing and Scientific Committee	First Asia Regional conference on UV technologies for water, wastewater & Environmental applications	Responsible for review of numerous articles and organization of the conference
2004	Member of Organizing and Scientific Committee	Process Intensification and Innovation Process Conference to be held in September, 2006	Responsible for review of numerous articles for a special issue
2000	Guest Editor	Special issue on "Environmental Reaction Engineering" for Dev. In Chem. Engg. and Mineral Processing Journal.	Entire issue was edited by myself.
2004	Reviewer	Manuscript of a book titled "Photocatalytic Reaction Engineering" by Hugo de Lasa, Benito Serrano and Miguel Salaiques	to be published by Blackwell Publishing, Oxford, UK in 2005.
2004	Reviewer	Manuscript of a book titled "Cyclically Operated Separating Reactors" by Takashi Aida and Peter L Silveston	
2000	External Examiner of PhD thesis	University of Queensland, Australia	Reviewed a PhD thesis
2000	External Examiner of PhD thesis	Anna University, India	Reviewed a PhD thesis
2001	External Examiner of PhD thesis	Indian Institute of Technology, India, Kanpur	Reviewed a PhD thesis
2002	External Examiner of PhD thesis	Anna University, India	Reviewed a PhD thesis
2004	External Examiner of PhD thesis	Gujrat University, India	Reviewed a PhD thesis
2005	External Examiner of PhD thesis	Indian Institute of Technology, India, Delhi	Reviewing a PhD thesis
2005	External Examiner of PhD thesis	University Tecknology, Malaysia	Reviewing a PhD thesis
1996-	Reviewer of research manuscripts (on average 20-25 per year in the last 3 years)	AIChE, Chem. Eng. Sci., Ind. Eng. Chem. Res., J. Catalysis, Catal. Today, Appl. Catal. A: General, Appl. Catal. B: Environ., Comp. Chem. Eng., Environ. Sci. Technol., Water Res., J. Mem. Sci., Sep. Sci. Technol., Chemosphere, ChemTech, Int. J. of Drying Technol., J. Appl.	Reviewed research manuscripts

		Electrochem., Inter. J. Chem. Reactor Engg., JAPS, etc.	
1997-	Session chair	ISCRE, AIChE, APCRE, APChE, APCAT, APSEET, WEC, Chemcon, etc.	Served as session chairs in many international and regional conferences.

Service to Profession/Industry

Period	Position	Organisation/Event	Brief description of activity
2004	Author of a textbook	Revised 2 nd Edition of a textbook titled "Mathematical Methods in Chemical and Environmental Engineering" was published by International Thomson Learning.	The book was co-authored by Professor SK Gupta of IIT, Kanpur.
2002 -	Offered short courses	A short course titled "Applications of Optimization in Chemical Industry" was offered through PAC (NUS)	The course was offered once and attended by 25 professionals.
2002-	Taught an elective module in TUM-NUS joint M. Sc program	Taught an elective module titled "Applied Modeling and Computational Methods in Industrial Chemistry"	The course was taken by 11 students.
2000 -	Offered short courses	A short course titled "Mathematical Methods in Engineering with Computers" was offered through PAC (NUS)	The course was offered twice and attended by 30 professionals.
2000-	B. Tech. modules	Teaching 50% of TC3411 and TC3111 modules for last 4 years	Teaching of B. Tech. modules

16. Research Interests and Program

Many of my research problems deals with the mathematical modeling of various complicated engineering systems with interactions between the transport processes and chemical reactions. My several past and present projects are associated with various reacting systems, such as simulated moving bed chromatographic reactors, photocatalytic reactors, oscillatory reactors, and polymer reactors. My research covers a broad range of topics in engineering of chemical reactions and processes, which can be categorized in the following areas to give a better overview:

(a) Simulated Moving Bed Systems and Integrated Reactor-Separator

Simulated Moving Bed (SMB) systems are used for separations that are either impossible or difficult using traditional separation techniques. SMB has become one of the most popular techniques finding its application in petrochemical and sugar industries, and of late, there has been an increased interest in pharmaceutical industry for enantio-separations. SMB systems can also be integrated to include reactions, which can provide economic benefit for equilibrium limited reversible reactions, such as many hydrogenation, isomerization, and esterification reactions. These are continuous flow reactors in which chemical reactions are carried out in the presence of solid adsorbents so that both separation and chemical reaction are integrated into a single process unit. In-situ separation of the products facilitates the reversible reaction to completion beyond thermodynamic equilibrium and at the same time obtaining products of high purity. Furthermore, the integration of reactor and separator can lead to considerable savings in capital and operating costs. The present investigations endeavor to determine to what extent the moving bed reactor advantages of high product purity and favorable equilibrium shifts are retained for various important chemical reactions. Our research addresses (a) experimental determination of adsorption and/or kinetic parameters, (b) modeling, experimentation and application of multi-objective optimization in the design of SMB systems, and (c) modeling, experimentation and multi-

objective optimization of Varicol (based on non-synchronous switching) process, which is a new modification of more rigid traditional SMB systems. Systems studied based on SMB technology are (a) chiral drug separation (Enantio-separation), (b) production of High Fructose Syrup by inversion of sucrose and isomerization of glucose, (c) separation of xylene isomers - industrial Parex process, (d) hydrogenation of mesitylene to tri-methyl cyclohexane, (e) synthesis of MTBE and methyl acetate, (f) oxidative coupling of methane (OCM) to ethane and ethylene, (g) transesterification of oil or animal fats with alcohol to produce biodiesel, etc.

(b) Band-Engineered Photocatalysis for Water Purification, Production of Clean Hydrogen Fuel and Self-cleaning of Building Surfaces

Photo-stimulated catalysis offers an attractive tool for applications in producing clean fuel and in degrading toxic organic pollutants (as well as removing toxic metal ions) for environmental cleanup. However, a specific problem associated with commonly used photo-catalysts is the large band-gap energy, which requires artificial light. Because of the ubiquity of sunlight the success of this technology depends on engineering of electronic bands of the catalyst for paradigm-shift to solar-based photocatalysis that could produce very large economic and social benefits. Two approaches address this issue in the on-going research. The first involves reducing the band-gap through addition of dopants, thereby permitting light absorption in the visible part of the spectrum. The second strategy involves depositing an extremely thin layer of TiO₂ on top of a metal or semiconductor whose doping level is chosen to fix the Fermi level at the solid-solid interface. Successful synthesis of chemically modified photocatalyst through molecular band engineering will enable use of sunlight for splitting water into clean hydrogen fuel, sun-powered remediation of environmental pollutants (particularly use TiO₂ tablets to get potable water), and creation of solar-driven self-cleaning and antifogging building materials. A transparent liquid form of the photocatalyst when sprayed onto building panels, glass surfaces, painted walls and (kitchen or bathroom) tiles will offer substantial self-cleaning and cost savings in maintenance.

Another thrust aims at developing a technical solution to the design of a commercial (large-scale) photocatalytic reactor that provides a high ratio of activated immobilized catalyst surface area per unit reactor volume thereby allowing for much higher specific reactor capacity. All experiments involve novel reactor configurations and catalysts to achieve high selectivity. Modeling involves simulation of the processes and description of reaction mechanisms using detailed surface reaction steps. This research involves the interplay between surface and solution chemistry, catalysis and reaction engineering, and mass transfer effects. Main contributions on photocatalysis are (a) fundamental kinetic studies for photocatalytic degradation of organics to determine true kinetic rate parameters in slurry as well as fixed catalyst systems. (b) systematic thermodynamic analysis and kinetic study for removal of toxic metal ions such as Hg(II), Cr(VI) and As(III) from wastewater, and (c) design and development of novel large-scale photocatalytic reactors for water purification such as multiple tube reactor, tube light reactor, rotating tube reactor and Taylor vortex reactor. The design specifically addressed critical issues of increasing illuminated catalyst density, uniform distribution of light and mixing of fluids. Experiments were done to show the effectiveness and efficiency of these reactors. Detailed computer simulation of photocatalytic reactors using Fluent® has also been carried out.

(c) Modeling, Simulation and Multi-objective Optimization

Our research group is pioneer to apply the concept of multiobjective optimization in the design and operation of chemical reactors and processes. Chemical reactors are often the important equipment in many process industries. Multi-objective optimizations of industrial reactors are carried out to identify the optimal conditions for producing valuable products economically using different adaptations of genetic algorithm, which usually result in an optimal Pareto set. Detailed simulation models are first developed for industrial systems. These models are verified (sometimes tuned) using industrial data. Additional control variables, important objective functions, constraints of significance, accurate kinetic schemes and practical aspects of various physical processes are considered. All these make the optimization problem more complex but the ultimate results are far more meaningful. Better (optimal) operating conditions are computed using powerful and recently developed techniques like NSGA and Simulated Annealing. These studies help optimize *several* objectives while simultaneously satisfying several real-life constraints present in industry. Significant cost savings and enhanced productivity are achieved. In addition to application of the multiobjective optimization to different industrial applications, we are also involved on improving the optimization methodologies. Industrial process studied and being studied are (a) hydrogen

production by steam reforming of hydrocarbons based on natural gas or higher hydrocarbon feed using side or top fired steam reformer, (b) industrial polymerization reactors for the production of Nylons, Polyesters, Perspex, polyethylene, polystyrene, etc., (c) beer dialysis using hollow fiber membranes, (d) industrial Styrene manufacturing process, (e) industrial Ethylene reactor, (f) catalytic membrane reactor for production of ethylene oxide and formaldehyde, and (g) multifunctional reactors such as SMBR and Varicol based on Simulated Moving Bed technology. These are continuous flow reactors in which chemical reactions are carried out in the presence of solid adsorbents so that both separation by adsorption and chemical reaction are integrated into a single process unit. Carrying out separation during chemical reaction helps to overcome reactant conversion limitation because of chemical equilibrium. Moreover, the integration of reactor and separator lead to considerable savings in capital and operating costs. Systems optimized are SMB and Varicol units for separation of chiral drugs, mixtures of C₈ hydrocarbons, glucose-fructose mixture, and reactive systems such as synthesis of methyl acetate ester, MTBE, trimethyl cyclohexane, and production of concentrated high fructose syrup by inversion of sucrose and isomerization of glucose.

(d) Performance Improvement of Chemical Reactors by Natural Oscillations

The dynamic behavior of two coupled continuous stirred-tank reactors in sequence was studied when the first reactor is operated under limit cycle regimes producing self-sustained natural oscillations. This new concept of coupling free and forced oscillation does not require any additional external energy but at times the overall performance of the system can be greatly enhanced. Systems studied are (a) wastewater treatment by activated sludge process, (b) synthesis of ethanol from glucose, (c) oxo reaction for production of aldehydes from olefins and synthesis gas, etc.

17. Journal Publication: Classification of Publications According to Journal Impact Factor

Journal Title	<i>Impact Factor</i>	<i>Half-Life</i>	<i>No. of Publications</i>
Mainstream Chemical Engineering Journal			62
AICHE Journal	2.153	> 10	6
Chemical Engineering Journal	2.034	6.7	3
Chemical Engineering Science	1.735	9.4	11
Industrial & Engg. Chem. Research	1.518	6.3	20
Computers Chemical Engineering	1.501	7.0	4
Reviews in Chemical Engineering	1.357	6.9	1
J. Chem. Technology Biotechnology	1.276	7.3	2
Chemical Engineering. Technology	0.940	4.9	3
Chemical Engineering Research Design	0.792	> 10	1
Canadian J. Chemical Engineering	0.574	> 10	1
Journal of Chemical Engineering Japan	0.594	> 10	1
Inter. J Chemical Reactor Engineering	-		5
Others	-	-	4
Specialized Engineering Journal			34
Journal of Catalysis	4.780	8.8	1
Environmental Science & Technology	4.054	6.4	1
Applied Catalysis B: Environmental	3.942	4.8	1
Journal of Chromatography A	3.554	5.8	1
J. of Membrane Science	3.442	6.4	1
Catalysis Letters	3.277	6.0	1
Water Research	3.019	7.0	1
Biotechnology & Bioengineering	2.999	7.8	2
Electrochimica Acta	2.955	6.9	1
Applied Catalysis A: General	2.728	4.7	1
Separation & Purification Technology	2.497	8.6	2
Catalysis Today	2.365	5.6	3
Chemosphere	2.297	5.6	3
J. Colloid & Interface Science	2.233	> 10	2
Biochemical Engineering Journal	1.781	6.4	2
Polymer Reaction Engineering	1.342	6.1	1
J. Applied Polymer Science	1.306	7.7	3
Polymer Engineering Science	1.076	> 10	1
J Environmental Science & Health	0.786		1
Others	-	-	5
Total Publications			96

18. Citation Analysis (as of 1 November 2007) [Scopus Database]

Most Cited Publications	Total Citation	Average Citation
Top 5	429	85.8
Top 10	652	65.2
Top 15	832	54.9
Top 20	951	47.6
Top 25	1040	41.6
Top 50	1325	26.5

Top 40 Most Cited Publications (as of 1 November 2007) [Scopus Database]

No.	Reference				Impact	No.	Topics
	Journal	Year	Vol	Page	Factor	Cited	
1	Water Research	1998	32	3223	3.442	147	Photocatalysis
2	Applied Cat B: Environ.	1999	23	143	3.942	97	Photocatalysis
3	Rev in Chem Eng	2000	16	1	2.786	88	Optimization
4	Chem. Eng. Sci.	2001	56	1561	1.735	49	Photocatalysis
5	AICHE Journal	2002	48	2800	2.153	48	SMB
6	Chem. Eng. Sci.	2001	56	999	1.735	48	Optimization
7	Catalysis Today	1998	40	73	2.365	48	Photocatalysis
8	Ind. Eng. Chem. Res.	2000	39	706	1.518	45	Optimization
9	AICHE J	1998	44	477	2.153	44	Photocatalysis
10	Chem. Eng. Sci.	1994	49	469	1.735	38	SMB
11	Chem. Eng. Sci.	1995	50	2195	1.735	38	SMB
12	Chem. Eng. Sci.	1999	54	3113	1.735	35	Photocatalysis
13	AICHE Journal	2000	46	1046	2.153	34	Optimization
14	AICHE Journal	1997	43	2571	2.153	33	Photocatalysis
15	Chem Eng Technol	1999	22	253	0.94	31	Photocatalysis
16	J Colloid Interface Sci.	2004	278	270	2.233	30	Photocatalysis
17	Chem. Eng. Sci.	1990	45	2431	1.735	27	SMB
18	Computers Chem. Eng.	2001	25	391	1.678	25	Optimization
19	AICHE Journal	2000	46	1034	2.153	24	Photocatalysis
20	J Membrane Sci.	2000	176	177	3.442	22	Optimization
21	Polymer Eng. Sci.	1986	26	1033	1.414	19	Optimization
22	Ind. Eng. Chem. Res.	2002	41	3213	1.518	19	SMB
23	Computers Chem. Eng.	2003	27	1883	1.678	18	Optimization
24	Environ. Sci. Technol.	2005	39	1827	4.054	17	Photocatalysis
25	Catalysis Today	1998	44	357	2.365	16	Photocatalysis
26	Dev. Chem. Eng.	2000	5	505	-	16	Photocatalysis
27	Ind. Eng. Chem. Res	2001	40	5305	1.518	16	SMB
28	J Applied Polymer Sci.	2000	78	1439	1.306	15	Optimization
29	Ind. Eng. Chem. Res	2003	42	4028	1.518	15	Optimization
30	Chem. Eng. Sci.	1995	50	3033	1.735	15	SMB
31	Computers Chem. Eng.	2003	27	111	1.678	15	Optimization
32	Electrochimica ACTA	2004	49	1435	2.955	15	Photocatalysis
33	J Applied Polymer Sci.	1985	30	4529	1.306	12	Optimization
34	J of Catalysis	2001	200	209	4.78	11	SMB
35	Ind. Eng. Chem. Res.	2003	42	6823	1.518	12	SMB
36	Biochemical Eng. J.	2004	21	111	1.781	12	SMB
37	Ind. Eng. Chem Res.	2003	42	2273	1.518	11	Photocatalysis
38	Catalysis Today	2001	66	475	2.365	11	Photocatalysis
39	Chemical Eng J.	2005	108	19	2.034	11	SMB
40	Chem. Eng. Sci.	2005	60	347	1.735	10	Optimization

19. Publication Record

Patent

- 1 European patent titled "A photocatalytic reactor suitable for water purification as well as a process for the purification of waste water by means of such a photocatalytic reactor", jointly with A. A. C. M. Beenackers, European Patent Number: 96200942.9-2104, 1996.

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