TIRTHANKAR SENGUPTA | PhD

CONTACT DETAILS

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SKILLS AND PROFICIENCIES

- Quantitative Systems Biology
- Chemical Reaction Engineering
- Environmental Science
- Data Science
- Computer Language Proficiency: MATLAB, Python

EDUCATION

DEGREE/EXAMINATION	BRANCH/DISCIPLINE	INSTITUTE/EXAMINATION BOARD	CPI/MARKS	DURATION
PhD*	Chemical Engineering	Indian Institute of Technology Bombay (IIT Bombay), Mumbai	7.0 (10.0)	2007-2014
M.Sc. (Engineering)**	Chemical Engineering	Indian Institute of Science (IISc), Bangalore	6.3 (8.0)	2000-2002
Bachelor of Engineering***	Chemical Engineering	Jadavpur University, Kolkata	76%	1996-2000
Higher Secondary (Standard XII Examination)	Science	South Point High School (West Bengal Council of Higher Secondary Education), Kolkata	74.7%	1994-1996
Madhyamik (Standard X Examination)	-	South Point High School (West Bengal Board of Secondary Education), Kolkata	81.2%	1992-1994

[* Degree awarded in March 2015; ** Degree awarded in 2003; *** Passed with Honors]

PUBLICATIONS

- Sengupta T, Kumar V, Manokaran V, Narasimhan S, Bhatt N, Pykinemod: A Software Tool for Automated Modeling of Reaction Systems from Data, International Conference on Mathematics in (bio/food) Chemical Kinetics and Engineering (MaCKiE 2025), Cesme (Izmir), Turkey, 3-5 September, 2025. (*Accepted for oral presentation*)
- Sengupta, T., Kulasiri, D. & Swarup, S. An assessment of cumulative CO2 efflux as proxy of organic matter turnover time in the soil priming effect: analysis using the lumped parameter approach. Int. J. Environ. Sci. Technol. 21, 9867–9888 (2024). DOI: https://doi.org/10.1007/s13762-024-05569-w
- Veeramani M, Sengupta T, Narasimhan S, Bhatt N, Analysis of experimental conditions, measurement strategies and model identification approaches on parameter estimation in plug flow reactors, *Industrial & Engineering Chemistry Research,* Vol. 58, Issue 30, 2019, Page Nos. 13767-13779, DOI: 10.1021/acs.iecr.9b00266.
- Sengupta T, Bhushan M, Wangikar PP, A computational approach using ratio statistics for identifying housekeeping genes from cDNA microarray data, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, Vol. 12, Issue 6, 2015, Page Nos. 1457-1463, DOI: 10.1109/TCBB.2015.2407399.
- Sengupta T, Bhushan M, Wangikar PP, Metabolic modeling for multi-objective optimization of ethanol production in a *Synechocystis* mutant, *Photosynthesis Research*, Vol. 118, Issue 1-2, 2013, Page Nos. 155–165, DOI: 10.1007/s11120-013-9935-x.
- Sengupta T, Jain S, Bhushan M, A compressed sensing based basis-pursuit formulation of the ROOM algorithm, *12th IFAC Symposium on Computer Applications in Biotechnology*, Vol. 46, Issue 31, Mumbai, India, 16-18 December 2013, Page Nos. 238-243, DOI: 10.3182/20131216-3-IN-2044.00057.
- Ayappa KG, Sengupta T, Microwave heating in multiphase systems: An evaluation of series solutions, *Journal of Engineering Mathematics*, Vol. 44, Issue 2, 2002, Page Nos. 155-171, DOI: 10.1023/A:1020859312712.

RESEARCH AND WORK EXPERIENCE

POST-DOCTORAL WORK EXPERIENCE (2014 – Present)

- Project Officer, Web-enabled MTech in Industrial AI, IIT Madras. (February 2024-Present)
- Modeling the soil priming effect. (Consultant, NUS Environmental Research Institute (NERI), National University of Singapore, March 2021 – July 2022)
- Physiological modeling of human body weight dynamics. (Technical Project Manager, MetFlux Research Private Limited, December 2019 – May 2020)
- Identification of kinetic parameters pertaining to reaction systems using experimental data from Plug Flow Reactors. (Robert Bosch Center for Data Science and Artificial Intelligence, IIT Madras, December 2018 – November 2019)
- Modeling mitochondrial fission and fusion dynamics in the model eukaryote *Schizosaccharomyces Pombe,* the latter being also referred to, more commonly, as “Fission Yeast”. (Center for BioSystems Science and Engineering, IISc Bangalore, September 2016 – November 2017)
- Investigating how to extend Grad's moment method in the kinetic theory of gases to a bounded domain. (Engineering Mechanics Unit, JNCASR Bangalore, November 2014 – June 2016)

PhD, Chemical Engineering, IIT Bombay (2007 – 2014) (Degree awarded in March 2015)

THESIS TITLE: MODELING AND SIMULATION FOR STRAIN IMPROVEMENT

- The thesis work had three major contributions towards rational strain improvement. First, an algorithm was proposed to identify housekeeping genes from replicate microarray gene expression data. Any rational strain

improvement strategy should ideally identify housekeeping genes and exclude mutating such genes since the genes perform essential cellular functions. Second, a metabolic engineering study was performed to identify promising mutant strains, of the unicellular cyanobacterium *Synechocystis* PCC 6803, exhibiting enhanced ethanol productivity. Ethanol is a compound with several commercial applications. Finally, a reformulation of the metabolic modeling algorithm "Regulatory on/off minimization" (ROOM) was proposed. The reformulation was more computationally efficient in comparison to the original algorithm. The reformulation thus provides the advantage of requiring less computational time when a large number of ROOM simulations are performed for identifying a suitable rational strain improvement strategy.

TEACHING EXPERIENCE (2005 – 2007)

- Lecturer, Chemical Engineering Department, Heritage Institute of Technology, Kolkata.

INDUSTRIAL WORK EXPERIENCE (2002 – 2005)

- Software Engineer, Infosys.

MASTERS, Chemical Engineering, IISc Bangalore (2000 – 2002) (Degree awarded in 2003)

THESIS TITLE: HEATING IN MULTIPHASE SYSTEMS USING ELECTROMAGNETIC RADIATION

- The thesis work was related to analysis of heating arising in multiphase systems because of exposing the latter to electromagnetic radiation.

NOTE: Please refer to annexure for a synopsis of research.

AWARDS

- Received best oral presentation award in Research Scholars Symposium 2011 held at the Chemical Engineering Department, IIT Bombay.

CONFERENCES/WORKSHOPS ATTENDED

- Attended "Indian Process Systems Engineering Conference (IPSE 2019)" held at IIT Madras, Chennai, India, 18th - 19th August 2019.
- Attended workshop titled "Measurement-based Optimization in the Presence of Uncertainty" held at Robert Bosch Center for Data Sciences and Artificial Intelligence, IIT Madras, Chennai, India, 15th – 16th March 2019.
- Attended school titled "Winter School on Quantitative Systems Biology (QSB2017)" held at the International Centre for Theoretical Sciences (ICTS), Bangalore, India, December 2017.
- Attended two-week school titled "Summer Research Program on Dynamics of Complex Systems" held at the International Centre for Theoretical Sciences (ICTS), Bangalore, India, May 2016.
- Presented paper at "12th IFAC Symposium on Computer Applications in Biotechnology" held at IIT Bombay, Mumbai, India, 16th – 18th December 2013.
- Presented poster at Indo - US workshop on "Cyanobacteria: Molecular Networks to Biofuels" held at Lonavala, India, 16th - 20th December 2012.

ANNEXURE – SYNOPSIS OF RESEARCH

MASTERS THESIS: HEATING IN MULTIPHASE SYSTEMS USING ELECTROMAGNETIC RADIATION

The first part of the thesis was concerned with solving coupled electric field and heat equations for slabs in which dielectric properties vary spatially. The equations were one-dimensional. Analytical solutions involving series expansions were compared with numerical solutions obtained from the finite element method. The series solutions converged only up to a finite sample thickness. This problem of poor convergence of series solutions for large sample thicknesses was addressed by employing a proposed algorithm to improve the range of convergence. The algorithm consisted of splitting the domain of the operator and thereafter obtaining series solutions within each sub-domain. It was seen that the algorithm improved the range of convergence significantly.

The second part of the thesis modeled conditions that arise during a flooding operation in a natural oil reservoir. Typically, flooding operations are performed in an oil reservoir using water, to extract the oil from the reservoir. In such operations, heating the reservoir results in increased yield of oil. The thesis investigated the effect of heating the reservoir using electromagnetic radiation. A multilayer problem was studied. The three sections in this multilayer problem were the region richer in water having a constant saturation profile, an intermediate region in which the oil saturation varies sigmoidally with position and the region richer in oil again having a constant saturation profile. One-dimensional coupled electric field and heat equations were solved. Simulations were carried out using frequencies in the microwave range and length scales in the order of centimeters, as in the first part of the thesis. Further, an engineering analysis was also performed using radio frequencies in which the much larger actual reservoir length scale was considered. In this analysis, the oil saturation profiles were representative of an actual flooding operation in a reservoir. Different techniques of heating were compared. In one case, electromagnetic energy was introduced from the side richer in water, while in the other it was introduced from the side richer in oil. Since the length scale, pertaining to the reservoir, was such that the Lambert's law limit had been reached, it was seen that the second method preferentially heated the oil. In addition, the influence of the incident frequency was also investigated.

PhD THESIS: MODELING AND SIMULATION FOR STRAIN IMPROVEMENT

Strain improvement is the procedure of mutating a microbial strain such that there is an improved yield of some target metabolite, usually of commercial interest, in the mutant. The mutant can therefore be harnessed for commercial purposes. Traditionally, random mutagenesis has been used to achieve strain improvement. The thesis, however, was concerned with the relatively recently emerged discipline of metabolic engineering i.e., with identifying strain improvement strategies that have a rational basis.

The first contribution of the work was towards identifying housekeeping genes from microarray gene expression data. Knowledge of housekeeping genes is important in rational strain improvement. Such genes perform essential cellular functions. Therefore, housekeeping genes should ideally not be targeted for genetic alterations. Housekeeping genes were identified from microarray gene expression data by proposing an algorithm which assumes that such genes are constitutively expressed. Constitutively expressed genes were identified by statistical hypothesis testing of the data. In the hypothesis testing model, emitted intensities were assumed to be independent Gaussian random variables. This strategy for identifying housekeeping genes should ideally be applied to data with outliers, i.e., gross measurement errors, removed. Hence a technique for identifying outliers from replicate microarray experimental data was also proposed. The technique used a scoring scheme and was applicable to data sets with multiple replicates. Functions of a few predicted housekeeping genes on human gene expression data were found to be indeed vital. This result validated the proposed algorithm.

The second contribution of the work was a metabolic engineering study on cyanobacteria in the context of ethanol production. Ethanol is a compound of commercial interest. Cyanobacteria can produce ethanol via photoautotrophic metabolism. The aim of the work was to identify optimal ethanol producing mutant strains of the unicellular cyanobacterium *Synechocystis* species strain PCC 6803. Gene deletions have the potential of creating such strains. Ethanol production can be significantly enhanced due to suitable redirections in the carbon flux as a result of gene deletions. Therefore, systematic exhaustive single and double gene deletion simulations were performed on *Synechocystis* PCC 6803. Previously, model cyanobacterial strains had been engineered to produce ethanol. However, systematic gene deletion studies aimed at identifying optimal ethanol producing strains had not been performed. Hence the study. Optimization based metabolic modeling techniques, such as Flux Balance Analysis (FBA), Method of Minimization of Metabolic Adjustment (MOMA) and Regulatory on/off minimization (ROOM) were used for analysis. Pareto analysis was performed for each of single and double gene deletion MOMA and single and double gene deletion ROOM simulations with biomass and ethanol fluxes as the two objectives to be maximized. Points on the Pareto front signified maximal utilization of resources constrained by substrate uptake. Thus, these points represented an optimal trade-off between the

two fluxes. Based on these analyses, two mutants, with combined gene deletions in ethanol and purine metabolism pathways, were identified as promising candidates. The relevant genes were *adk*, *pta* and *ackA*. An ethanol productivity of approximately 0.15 mmol/ (gDW h) was predicted for these mutants. This value appeared to be reasonable based on experimentally reported values in literature for other strains.

The final contribution of the work was a reformulation, known as basis-pursuit, of the ROOM algorithm. The reformulation was based on the emerging area of compressed sensing. The advantage of the reformulation was that it did not involve any integer variables unlike the original ROOM algorithm which is a mixed integer linear programming problem. In ROOM, the number of integer decision variables is equal to the number of reactions in the metabolic network under inspection and this number is typically large. The ROOM approach thus has inherent difficulties associated with large scale integer programming problems. The proposed reformulation alleviated this issue since it could be recast as a linear programming problem. Further, it was found that the reformulation required substantially less computational time in comparison to the original algorithm. This is advantageous when performing a large number of simulations such as systematic exhaustive gene deletion simulations.

POST-DOCTORAL RESEARCH

JNCASR, Bangalore. (November 2014 – June 2016)

The Boltzmann equation describes the dynamics of dilute gases even in highly non-equilibrium conditions. Evolution equations derived from the Boltzmann equation have the property that the $(n + 1)^{th}$ moment of the velocity distribution function occurs in the evolution equation for the n^{th} moment. Thus, the evolution equations result in an infinite moment chain. In a reduced description, such as the approach suggested by Grad, only a finite number of moments are of interest. Grad's technique consists of describing the velocity distribution function by an expansion in a finite number of orthogonal Hermite polynomials around the Maxwell-Boltzmann state, with each coefficient in the expansion being a particular moment of the velocity distribution function. This method provides a consistent description of a gas in the bulk. It also achieves closure of the finite number of evolution equations pertaining to the reduced description. Closure is achieved by expressing the moment appearing in the evolution equations that is not a part of the expansion in terms of the other moments that have been considered in the expansion. However, the method fails at a solid gas boundary. Grad suggested that at the solid gas boundary, gas molecules impinging to the wall should be described by the velocity distribution function for the bulk involving the Hermite polynomials and those coming back to the gas from the wall should be described by an appropriate boundary condition. For example, in the diffusive boundary condition, the wall is assumed to act as a perfect thermal equalizer implying that the returning gas molecules have equilibrated to the wall temperature. These molecules are thus described by the Wall Maxwellian. This procedure, however, leads to an inconsistent set of algebraic equations in the moments, at the boundary. Thus, Grad's methodology fails in a bounded domain. The project involved exploring ways to remove the inconsistencies in the equations at the boundary i.e., to suitably modify Grad's methodology so that it becomes consistent in a bounded domain.

IISc, Bangalore. (September 2016 – November 2017)

Schizosaccharomyces Pombe, also referred to as fission yeast, is a model eukaryote. Mitochondrial positioning in interphase fission yeast cells is achieved by mitochondria binding to dynamic cytoplasmic microtubules via the protein mmb1p. The protein mmb1p, present at the outer mitochondrial membrane, can form ionic bonds with the lattice of a microtubule. Thus, a mitochondrion can attach to a nearby microtubule. This attachment causes the mitochondrion to be in an extended i.e., elongated state. A bound mitochondrion will become free when the microtubule to which it is attached shrinks. However, new microtubules regularly come up to which a free mitochondrion can attach. Keeping mitochondria in an extended state suffices for the local intracellular ATP requirements in fission yeast cells since the cell size is small in comparison to most eukaryotic cells. Thus, unlike in many eukaryotic cells, mitochondria are not transported by motor proteins on cytoskeletal tracks in fission yeast cells. The project involved modeling mitochondrial fission and fusion dynamics in fission yeast cells. For this, time series images of mitochondria in fission yeast cells were analyzed to determine the parameters of a proposed deterministic kinetic model. Mitochondria were modeled as "polymers", with the "monomer" being the smallest possible mitochondrial unit, composed of only a single nucleoid. The spectrum of possible fission and fusion events was constrained by the principle of conservation of mass and by invoking a closure of sizes. Here, closure of sizes implies considering a certain maximum mitochondrial size, in accordance with experimental data. Further, fission and fusion events were assumed to obey the law of mass action.

Robert Bosch Center for Data Science and Artificial Intelligence, IIT Madras. (December 2018 – November 2019)

Identification of a reaction system refers to the process of determining the stoichiometry, the rate laws, and the associated kinetic parameters of the reactions constituting the reaction system. It is an important task as it finds applications in the chemical industry and in biotechnology. It is posited here that the stoichiometry and rate laws of the reaction system under inspection are known, and the task is to only identify the kinetic parameters reliably. Assuming that the Arrhenius equation holds true, the goal, therefore, is to identify all pre-exponential factors and the activation energies of all reactions pertaining to the reaction system. Towards this end, considering the steady state Plug Flow Reactor (PFR) as a model system, experimental data generated in silico was analyzed using the simultaneous and incremental identification techniques. The experimental data was generated as follows. First, raw simulation data without noise was generated in silico by solving the design equations using specified initial conditions and known rate laws and kinetic parameter values. Thereafter, Gaussian noise was added to the raw simulation data. The data was generated and thereafter analyzed for both isothermal and non-isothermal operating conditions. The objective of the work was to analyze the efficacy of experimental conditions, measurement strategies and identification techniques, namely the simultaneous and incremental, towards parameter estimation from the generated in silico data. Here, the efficacy of experimental conditions towards parameter estimation connotes which of the two modes of operation viz. isothermal and non-isothermal is more informative in the context of parameter estimation i.e., which of the two modes of operation give a better estimate of parameter values. As regards measurement strategies, it was investigated that which among several candidate concentration and temperature measurement strategies provided reliable estimates of parameter values. A measurement strategy is characterized by the locations at which species concentrations and the temperature are measured along the length of the reactor. The locations for concentration measurements were allowed to be different from those of temperature measurements. Finally, it was examined that which of the two identification strategies, viz. the simultaneous identification approach and the incremental identification approach, is more effective in predicting accurate values of kinetic parameters.

NUS Environmental Research Institute (NERI), National University of Singapore. (March 2021 – July 2022)

The soil priming effect (PE) is an important ecological phenomenon owing to its role in the global carbon cycle. When fresh organic matter, rich in labile substrates, is introduced in soil, microbes in the soil sense that labile substrates have become available in the environment. Consequently, there is a perturbation in soil microbial respiration. This perturbation in microbial respiration leads to the soil PE, the latter being defined as an alteration in the turnover of organic matter. The soil PE can be real or apparent. An alteration in the turnover of soil organic matter is referred to as the real PE, whereas an alteration in the turnover of microbial biomass is referred to as the apparent PE. It is worth noting that soil stores a very large quantity of carbon. To cite a statistic, the top three meters of soil in the globe contains at least 2300 Pg carbon. Therefore, even a small perturbation in the turnover of soil organic matter, due to the real priming effect, will have a large impact on the global carbon cycle. The perturbation in soil microbial respiration manifests itself as altered CO_2 efflux from soil. The latter therefore acts as a proxy for organic matter turnover. Hence, the soil PE is measured in terms of CO_2 efflux. The project involved developing a lumped parameter kinetic model of the soil PE. Proposed model predictions were found to be in accordance with microbial ecological principles. The modelling framework allowed the identification of the turnover of soil organic matter and that of microbial biomass from experimental data of CO_2 efflux from soil. This therefore led to the quantification of the real and the apparent PE from experimental data. It is important to note that the CO_2 efflux from soil was not used as a proxy for organic matter turnover in the calculations. Further, certain machine learning techniques were used for analyses. For example, a Markov Chain Monte Carlo (MCMC) algorithm was implemented for model parameter estimation. Also, a global sensitivity analysis was performed using the Latin Hypercube Sampling - Partial Rank Correlation Coefficient (LHS - PRCC) procedure, for identifying sensitive model parameters. Long term model behavior was ascertained by converting the proposed model equations to dimensionless form. Also, the proposed model equations were reduced to systems of planar differential equations. For each planar system of differential equations, stream plots were constructed to investigate whether any critical points exist in the reduced system.

IIT Madras, Chemical Engineering Department (February 2024-Present)

Pykinemod is a software tool for the identification of homogeneous reaction systems from concentration data. The incremental identification technique is employed for parameter estimation from a set of rate expression candidates for each reaction. This approach is much faster in comparison to the simultaneous identification and therefore expedites the parameter estimation process. The metric for evaluating rate laws can be selected by the user and include the Akaike Information Criterion (AIC), AICC (corrected Akaike Information Criterion) and RMSE (Root Mean Square Error). Further, the module allows the user to fine tune the predictions from the incremental identification step by simultaneous identification. The k best candidate rate laws

(where the integer k can be selected by the user) for each reaction identified in the incremental identification step form the candidates in simultaneous identification. Also, parameter estimates in the incremental identification step are used as initial guesses. Overall, this dual strategy of employing both the identification strategies results in rapid and robust identification of reaction systems.