Indian Institute of Technology Kanpur
Proposal for a New Course

1. Course No.:	CHE 6XX
2. Course Title:	Stochastic Simulations, Optimization, and Parameter Estimation in Chemical Engineering
3. Lectures Per Week & Total Classes:	3 [Tutorial:0, Lab:0, Additional Hours:0], 40
4. Proposing Department:	Department of Chemical Engineering
5. Other faculty members interested in teaching:	—
6. Other Departments that may be interested:	Materials Science and Engineering, Sustainable Energy Engineering, Chemistry, Mechanical Engineering, Mather and Statistics, Computer Science and Engineering
7. Proposing Instructor(s):	Raj Ganesh S. Pala (rpala@iitk.ac.in)

Course Description: This course introduces computational methods for uncertainty analysis, stochastic simulations, optimization, and parameter estimation in chemical engineering. Topics include probability distributions, Monte Carlo simulation, Markov processes, unconstrained and constrained optimization, regression, least-squares fitting, Bayesian inference, posterior prediction, and experimental design. A short supplementary unit introduces validation, regularization, and the relation between mechanistic and data-driven models in chemical engineering.

#	Title	Topics	Lec.
1	Foundations & modeling perspectives	Motivation; forward and inverse problems; deterministic versus stochastic models; mechanistic versus data-driven models.	5
2	Probability foundations	Random variables; key distributions; expectation, variance, covariance, correlation; random vectors and multivariate distributions.	5
3	Stochastic simulation & uncertainty propagation	Random sampling; Monte Carlo methods; uncertainty propagation; Markov chains and processes; Brownian motion and introductory SDE ideas.	7
4	Numerical optimization	Objective functions and constraints; simplex, gradient, Newton line-search, trust-region, and Lagrangian methods.	9
5	Parameter estimation & regression	Residuals and objective functions; linear regression; least-squares; nonlinear parameter estimation; chemical engineering examples.	6
6	Bayesian inference, MCMC & modern extension	Prior, likelihood, posterior; posterior uncertainty and prediction; experimental design; MCMC; model criticism; validation, regularization, and case studies.	8

Prerequisites: For UG (3rd and 4th year): prior exposure to calculus, linear algebra, ordinary differential equations, and introductory numerical methods, together with core chemical engineering background, is desirable. For PG: similar mathematical preparation and familiarity with MATLAB or Python are desirable.

Recommended Texts and References

1. Kenneth J. Beers, Numerical Methods for Chemical Engineering: Applications in MATLAB, Cambridge University Press.
2. Jorge Nocedal and Stephen J. Wright, Numerical Optimization, Springer.
3. Sheldon Ross, A First Course in Probability, Pearson.
4. D. S. Sivia and J. Skilling, Data Analysis: A Bayesian Tutorial, Oxford University Press.
5. Andrew Gelman et al., Bayesian Data Analysis, CRC Press.
6. Andriy Burkov, The Hundred-Page Machine Learning Book.

Proposer (Date:) DPGC Convener (Date:)

Chairman, SPGC (Date:)

The course is approved / not approved