


THERMODYNAMICS FOR BIOLOGICAL SYSTEMS : CLASSICAL AND STATISTICAL ASPECTS

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PRE-REQUISITES : Undergraduate Mathematics

INTENDED AUDIENCE : Any Biological Engineering/Biological Sciences student or practitioner.

INDUSTRIES APPLICABLE TO : Biotechnology and other industries

COURSE OUTLINE :
Thermodynamics is one of the essential tools to analyze biological systems. Thus, it is essential that an undergraduate in biological engineering knows the relevant thermodynamics principles. Classical thermodynamics is suitable for analysis in the continuum domain, whereas when the number of molecules per cell is less than say 100, the principles of classical thermodynamics are invalid for that species. However, the principles of statistical thermodynamics can be used to analyze such situations, and other situations too. Therefore, this course will cover both classical and statistical aspects to provide a complete set of tools to a biological engineer to thermodynamically analyze bio-systems. Such an analysis will help in manipulation and design of bio-systems.

ABOUT INSTRUCTOR :
Prof. G. K. Suraishkumar is a Professor in the Department of Biotechnology, Indian Institute of Technology Madras (IITM). He has been at IITM as a Professor since May 2004, and was earlier a faculty member in the Department of Chemical Engineering at the Indian Institute of Technology Bombay (IITB) from April 1993 until mid-May 2004. He was also an Associate Faculty member in the erstwhile Centre for Biotechnology, which is now the Department of Biosciences and Bioengineering, at IITB, between 1995 and 2004.

He earned his Ph.D. from Drexel University, Philadelphia, USA in 1993, and his B.Tech. in Chemical Engineering from IITM in 1986. He also did his Masters work at the University of Cincinnati, USA, between 1986 and 1988.

He is passionate about improving student learning and has published papers in reputed international journals on the methods that he had developed for the same. He is the author of a book, Continuum Analysis of Biological Systems: Conserved Quantities, Fluxes, and Forces, which was published world-wide by Springer Publishing in March 2014; the foreword has been written by the reputed author of the famous textbook, Transport Phenomena, Professor R. B. Bird. Recently, he created two 10-h MOOCs on Bioreactors, and Biology for Engineers and other Non-biologists as NPTEL online certification (NOC) courses. Earlier, he created a 40-lecture NPTEL video course on Classical Thermodynamics for Biological Systems. He has also created other short videos on biochemical engineering principles.

His major area of research is reactive species – currently, the relevance of them in cancer and nanoparticle toxicity. Earlier, his research group had made significant, original contributions in the area of reactive species applied to improve bioreactor productivities and bio-oil which were financially supported through many sponsored research grants. The research contributions have been better disseminated through publications in reputed international journals– the complete list of publications is available as a link from his Department webpage, https://biotech.iitm.ac.in/faculty/suraishkumar-g-k/). He is also the inventor on 3 (granted) + 3 (under process) patents. Further, the technology developed in his group was successfully applied at Biocon industries, and has been featured in prestigious technology alerts such as the one by Frost and Sullivan. He has guided many Ph.D., and Masters theses. Some recognitions of his work by others are listed in his web-page given above.

Administratively, he played pivotal roles in the set-up of the Departments of Biotechnology, as the first formal Department Head, first at IIT Madras and later, at IIT Hyderabad. He was one of the main architects of the first postgraduate program in Clinical Engineering in India, which is a multi-Institute program, and a first of its kind in India. In addition, he contributed as the Head of the Sophisticated Analytical Instrumentation Facility, Chennai. He continues to contribute on National level faculty selection/advisory/ institution level committees in relevant areas.

Prof.Sanjib Senapati is a Professor in the Department of Biotechnology, Indian Institute of Technology Madras (IITM).His research group at I.I.T. Madras focuses on understanding the relationship between protein structure, function, and dynamics. Research is focused into two major sub-groups: 1) molecular modeling of enzyme-substrate/enzyme-inhibitor interactions and 2) structure-based drug designing. Studies are performed using computer simulation methods ranging from all-atom and coarse-grained molecular dynamics simulations, Monte Carlo simulations, protein-ligand and protein-protein docking. General properties that we address include change in protein structure and dynamics upon binding inhibitors and with mutations, ligand binding strength and specificity, and bound water structure. Our proteins of interest include: HIV-1 protease, Cyclin Dependent Kinases (CDKs), Cholesterylester transfer protein (CETP), Nicotinic Acetylcholine Receptor (nAChR) etc. Another thrust area includes the study of green solvents, ionic liquids and supercritical carbon dioxide. Here, our objective is to understand the molecular basis of increased/decreased stability of biomolecules and modulated kinetics of protein folding in these novel solvents. Subsequently, we attempt to validate our findings from computational studies usingspectroscopic and calorimetric 5 techniques. Also, with leads from our computational data we performinhibitor synthesis, enzymatic assays and drug designin our laboratory. Before joining IIT Madras in 2006, I have received my Ph.D. degree from I.I.T. Kanpur, India on Statistical Mechanics of liquids, where I had contributed on the understanding of liquid- membrane, liquid-solid interfaces, and also of liquids under confinement. Subsequently, I moved to University of North Carolina at Chapel Hill, USA to work on structure and dynamics of complex aqueous interfaces. Later I shifted to University of California San Diego (UCSD), USA, where I developed and applied a novel computational approach for drug designing, called the relaxed complex method, which allows for the direct accommodation of the receptors flexibility along with the ligands flexibility in protein-ligand docking.

COURSE PLAN :

Week 1: Review of concepts; Additional useful thermodynamic functions
Week 2: Additional useful thermodynamic functions (contd)
Week 3: Thermodynamic properties of pure fluids
Week 4: Thermodynamic properties of pure fluids (contd)
Week 5: Thermodynamics of solutions
Week 6: Thermodynamics of solutions (contd); Phase equilibria
Week 7: Phase equilibria (contd); Reaction equilibria
Week 8: Reaction equilibria (contd); Review
Week 9: Statistical Thermodynamics: Definition and Application
Week 10: Macrostates, Microstates, Partition function, Boltzmann Distribution Law
Week 11: Partition function and thermodynamic properties
Week 12: Ensemble and time average; Review