

## PetroTel Distinguished Lecture 2023-24 in Chemical Engineering

<b>Speaker</b>	<b>Prof. K. Ganapathy Ayappa</b>
<b>Title</b>	<b>Using Molecular Dynamics to Understand Interactions of Molecules with the Bacterial Cell Envelope</b>
<b>Time</b>	<b>6: 00 PM, 19<sup>th</sup> January 2024</b>
<b>Venue</b>	<b>Outreach Auditorium</b>
	<i>Refreshments will be served at 5:30 PM</i>



### Abstract

With rising bacterial resistance there is a dire need to develop a molecular understanding of the interactions of antimicrobial molecules with the complex topology of the bacterial cell envelope. The translocation pathways associated with molecules from the extracellular environment into the bacterial cell is poorly understood. In this talk I will summarize our ongoing efforts aimed at understanding the barrier properties of the bacterial cell envelopes. We develop molecular models for peptidoglycan at atomistic as well as coarse-grained scales for the cell walls and assess several structural and mechanical properties as well as insertion free energies of small molecules. We assess the free energy of insertion of antimicrobial peptides and antimicrobial molecules with the outer lipopolysaccharide membrane and compare outer membrane insertion free energy simulations with diffusion coefficients measured using fluorescence correlation spectroscopy to rationalize the selective barrier properties. Lastly, I will talk about recent work where we study differential bacterial kill efficacy as a function of fatty acid chain length and correlate the experimental observations with molecular dynamics simulations of translocation times through the peptidoglycan layer and inner phospholipid membrane rupture tendencies deduced from electroporation simulations. Our molecular dynamics simulations can potentially open up *in silico* models for the screening and development of novel therapeutics against virulent bacterial infections.

### About the Distinguished Speaker

Professor Ayappa obtained his Bachelors degree in Chemical Engineering from Mangalore University, India in 1984, and an MS and PhD in Chemical Engineering with a Minor in Mathematics from the Department of Chemical Engineering and Materials Science at the University of Minnesota, in 1992. Professor Ayappa has held visiting positions at the University of North Carolina, the James Franck Institute at the University of Chicago and Department of Materials at ETH Zurich. He is a fellow of the Indian National Academy of Engineers and the National Science Academy. His interests lie in developing a molecular understanding of structure and dynamics of molecules at the nanoscale using molecular simulations and statistical mechanics. Current interests lie in the area of biological membranes, membrane-protein interactions implicated in bacterial and viral infections and cellular signalling and dynamics at the nanoscale.

### About the Donor

The Petro Tel Distinguished Lecture series in Chemical Engineering at IIT Kanpur has been made possible by an endowment from Dr. Anil K. Chopra (B. Tech./ChE/IITK/1976 and recipient of the IITK Distinguished Alumnus Award, 2010). Dr. Chopra obtained his PhD from the University of Houston, USA, in 1982. Currently, he is the President, CEO and Chairman of Petro Tel Inc., USA

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*All are welcome.*