IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Theoretical and computational study of polymers in the semi-dilute regime in presence of shear flow, crowding and internal viscosity**	
Project Number	**IMURA0471**	
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Research Academy Themes:

Highlight which of the Academy's Theme(s) this project will address?

(*Feel free to nominate more than one. For more information, see www.iitbmonash.org)*

1. Advanced computational engineering, simulation and manufacture
2. Infrastructure Engineering
3. Clean Energy
4. Water
5. Nanotechnology
6. Biotechnology and Stem Cell Research

The research problem

In last few years or so it has been shown using single molecule experiments that a macromolecule in aqueous solution not only experiences friction from the solvent around it but also experiences friction from within, known as "internal friction". It is believed to be a manifestation of weak interactions between different parts of the polymer, and at the single molecule level it is intra-molecular. It has also been shown that the more compact the macromolecule, higher is the "internal friction". Experiments have also shown that internal friction could profoundly affect protein-folding dynamics. Till date experiments, simulations and theoretical models to quantify internal friction have been restricted to the single molecule level and in the absence of any perturbation such as shear flow or stretching. Here, using a coarse-grained computer simulation and scaling arguments we aim at the quantification of internal friction in the semi-dilute regime where polymer molecules overlap. It is expected that in such a situation internal friction would also be present between segments of different macromolecules and will no longer be solely intra-molecular in nature. These considerations are relevant to understanding protein dynamics in a biological cell, since proteins exist in a crowded environment in cells, and experience flow.

Project aims

The specific objective of this project is to understand the dynamics of macromolecules or polymers in presence of flow in the semi-dilute regime, where other than the solvent viscosity, viscosity within or between polymer(s) is also controlling the dynamics. We would also like to see how the dynamics gets affected in presence of crowding. Recently developed Brownian dynamics (BD) simulation methods as well as simulation in presence of hydrodynamic interactions will be used to model the dynamics of polymers at the coarse-grained level. For our purpose, these methods will be used to understand the effects of crowding and internal viscosity on protein dynamics in a cell.

Expected outcomes

Specific outcomes of this project will be

1. Enhanced understanding of "internal viscosity" at intra-molecular as well as at inter-molecular level.

2. A better understanding of polymer dynamics in the semi-dilute regime, in presence of crowding and flow mimicking the cell environment.

3. A computer code to tackle long molecule dynamics in crowded environment.

How will the project address the Goals of the above Themes?

The dynamical behaviour of biopolymers such as proteins in a crowded environment is the key to understanding how biopolymers behave in cells. Using theory and simulation we ultimately aim at the understanding of protein dynamics in biological cells where solvent flow, crowding and internal viscosity are expected to play important roles. Only a combination of computer simulation and theoretical techniques can shed light onto such complex dynamical process. This project will firstly enhance our ability to understand mechanisms in biological systems such as biological cells. The outcome of this project will contribute to enabling aspects of the Strategic Research Priority "Living in a changing environment" and understanding the fundamental molecular aspects of Biodiversity—all of which is essential for harnessing biomolecular processes whether in health care or biotechnology.

Capabilities and Degrees Required

The following capabilities are essential:

1. Excellent training in mathematics and numerical methods
2. Proven experience with computer programming in high level languages
3. Ability to write and communicate fluently
4. Strong background in Engineering/Physics/Physical Chemistry
5. Candidates without this background will not be considered

Please provide a few key words relating to this project to make it easier for the students to apply.

Polymer solution dynamics, Brownian dynamics simulations, Crowding, Internal Viscosity