

An Indian-Australian research partnership

Project Title: **Dynamics of active chains of chemically-powered micromotors**

Project Number IMURA0978

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IITB Department: Department of Physics

Research Clusters:

Research Themes:

Highlight which of the Academy's CLUSTERS this project will address? <i>(Please nominate JUST one. For more information, see www.iitbmonash.org)</i>	Highlight which of the Academy's Theme(s) this project will address? <i>(Feel free to nominate more than one. For more information, see www.iitbmonash.org)</i>
1 Material Science/Engineering (including Nano, Metallurgy) 2 Energy, Green Chem, Chemistry, Catalysis, Reaction Eng 3 Math, CFD, Modelling, Manufacturing 4 CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control 5 Earth Sciences and Civil Engineering (Geo, Water, Climate) 6 Bio, Stem Cells, Bio Chem, Pharma, Food 7 Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng 8 HSS, Design, Management	1 Advanced computational engineering, simulation and manufacture 2 Infrastructure Engineering 3 Clean Energy 4 Water 5 Nanotechnology 6 Biotechnology and Stem Cell Research 7 Humanities and social sciences 8 Design

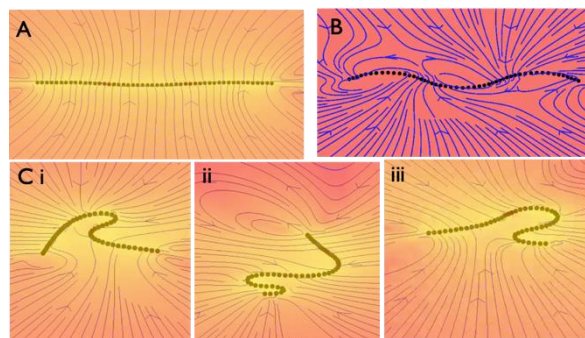
Motivation: Micromotors are micron-sized particles that are propelled by chemical reactions. Such micromotors are well known in biological cells. For instance, motors act on filamentous propellers to help many different kinds of cells to swim. The cytoskeleton in every one of our cells is a suspension of motors that drives processes such as cell division. Creating artificial micromotors driven by reactions that occur on their surfaces has emerged as an exciting new field of research. It has been observed that micromotors connected together as chains can exhibit a range of different motions from steady oscillations to chaotic, random motion. Such “active chains” could potentially be used to power swimming microrobots. Suspensions of these chains could be a new class of synthetic materials powered internally by chemical reactions. Some of these motors can be switched on or off by light and could lead to the design of interesting microfluidic applications driven by light.

The problem: To be able to design interesting new applications with active chains, we must know how their motion is related to parameters such as the chemical kinetics of the surface reactions, the size and shape of the particles, the length and flexibility of the chains, the suspending medium’s viscosity and temperature, etc. These are currently not very well understood. Not much is known either about the mechanical properties of suspensions of active chains and their dependence on the parameters mentioned above.

The approach: PhD candidates in this project will design mathematical models and simulations of active chains to explore the behaviour of single isolated chains, as well as suspensions of multiple chains interactive with one another. The force that propels a micromotor arises from the flow created adjacent to its surface by the surface reactions. This flow in turn depends on the concentration field of the reactants around the particle. In a chain of reacting particles, the concentration field depends on the instantaneous shape of the chain. The mathematical model will therefore need to account for the constantly changing flow and concentration fields as the flexible chains keep changing their shapes. The simulations will use advanced numerical techniques for mesoscale low-Reynolds-number hydrodynamics, such as Brownian Dynamics (for single-chain simulations) and Multi-Particle Collision Dynamics or Dissipative Particle Dynamics (for multiple chains). These techniques are required to correctly handle thermal and other fluctuations that are important in these systems.

Research outcomes: Simulations will study the chemo-mechanical instabilities that are known to be the underlying cause of the complex motion of active chains. We will establish the connections between the motion states of single chains and the physical parameters that govern such systems. This will enable identifying the conditions under which regular oscillatory motions can be obtained for applications such as propulsion and payload delivery. In the case of chaotic behaviour, we will study the average properties of chains and the statistics of their distributions. These states could be exploited to design self-mixing catalytic systems.

The effect of inter-chain interactions in non-dilute systems will be studied using multi-chain simulations. The rheological properties of suspensions will be predicted as functions of chain concentrations as well as the other system parameters. This will establish the foundation for the



Our simulations of active chains driven by the flow induced by chemical reactions predict the existence of various motion states e.g. (A) stable, straight state; (B) Regular waves with forward or backward chain swimming; (C i – iii) Chaotic oscillations.

use of such suspensions as self-driven materials whose flows can be turned on or off at will by, say, using light-controlled reactions.

Training outcomes

The project will train PhD candidates for long-term careers in advanced computations of mesoscale hydrodynamics. Candidates will get a firm grounding concepts, methods and analytical techniques for the theoretical and computational study of active matter, colloidal systems, and polymers. The Project can be the springboard for exciting careers in either academia or the industry in the areas of microfluidics, soft condensed matter, nanosciences, or biophysics.

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

This project will develop and implement advanced simulations of the mesoscale hydrodynamics of active flexible chains coupled with the reaction-diffusion equations for the concentration field.

Potential RPC members from IITB and Monash

IITB

Prof. Guruswamy Kumaraswamy: experiments on active colloidal chains and soft matter

Prof. Rochish Thakkar: theory and simulations of low-Reynolds number hydrodynamics and soft matter

Prof. Mahesh Tirumkudulu: theory, simulations and experiments in fluid mechanics, microswimmers, and colloids, and polymers.

Monash

Prof. Ravi Jagadeeshan: Brownian Dynamics of macromolecular hydrodynamics

Dr. Tuncay Alan: experimental and theoretical microfluidics

Prof. Murray Rudman: computational fluid dynamics

Capabilities and Degrees Required

- Bachelor's or Master's degree in either physics, or chemical or mechanical engineering, with excellent academic scores.
- A strong interest in understanding theoretical foundations, mathematical modeling and computational fluid dynamics.
- Research publications or a significant research project (e.g. final year project) involving theory and simulations.
- Significant coding experience in a scientific programming language such as C, Fortran, MATLAB. (Just using simulation packages such as FLUENT, COMSOL, etc., without coding experience is not sufficient.)
- Ability to communicate technical ideas well verbally or in writing.

Necessary Courses: TBD

Potential Collaborators: N/A

Keywords: Computational Fluid Dynamics and Mechanics, Nanotechnology/nanoscience,