IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Complex fluid dynamics of viscoelastic polymer solutions**	
Project Number	**IMURA0966**	
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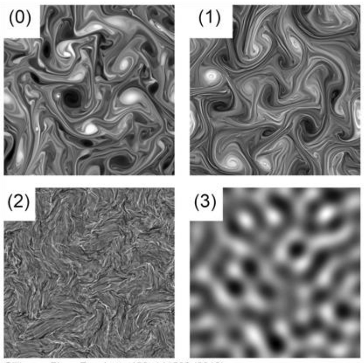
Research Clusters:

Research Themes:

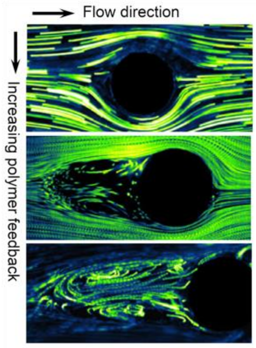
Highlight which of the Academy's CLUSTERS this project will address? *(Please nominate JUST **one.** For more information, see www.iitbmonash.org)*		**Highlight which of the Academy's Theme(s) this project will address?** *(Feel free to nominate more than one. For more information, see www.iitbmonash.org)*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

The research problem

Adding even a miniscule amount of dissolved polymer into a fluid can have a dramatic impact on the way it flows. If the flow is turbulent (high-Reynolds-number) to begin with, then the polymer can strongly modify the turbulent eddies and reduce the drag force (in flow through pipes) or even make the flow laminar. The vorticity snapshots on the right show the increasing effect of polymers (0: no polymer) on a 2D turbulent flow; notice the change in the large vortices and the eventual laminarization (panel 3). The drag-reduction effect greatly reduces the cost of transporting oil through pipelines.



Gillissen, Phys. Rev. Lett., 123, 144502 (2019)



Qin et. al., J. Fluid Mech., 864, R2 (2019)

Polymers can also destabilize a low-Reynolds-number steady flow and make it unsteady and chaotic. This effect is illustrated by the experimental visualizations of flow past a micro-scale cylinder, shown on the left. Such instabilities can produce elastic turbulence, which can greatly increase mixing in microchannels and enhance oil-recovery from underground porous reservoirs.

Due to their many applications, a lot of research has been done on these complex fluid dynamic phenomena. Yet, we currently have only a partial, qualitative understanding and are still far from being able to make accurate quantitative predictions. Dissolved polymer molecules behave like nano-springs; they get stretched-out by fluid drag forces and then exert an equivalent feedback force when they relax and contract. Modelling this flow-polymer coupling is very challenging due to the multi-scale nature of the problem. The polymers extend over nano- to micro- scales while turbulent flow eddies can span meters. Thus far, computational fluid dynamics (CFD) simulations have used very simple models of the additional stresses exerted by these nano-springs suspended in the fluid. These simulations have led to important insights but fail to make accurate predictions when compared with experiments.

Project aims

We know today that to make further progress on many important problems in polymer fluid dynamics we need improved models that actually account for the complex interactions within, and between, the polymeric nano-springs. Recently, a new class of these models have been developed that are also computationally tractable. Applying such models in CFD simulations remains an outstanding challenge. In this project, we aim to tackle this task and take the first step towards a deeper understanding of polymer fluid flows.

The key steps that the student will have to take in their journey towards this goal are:

1. Understand models for the contribution of polymers to stresses in flowing polymer solutions.
2. Understand basic fluid dynamics and turbulence theory. Become familiar with past work on viscoelastic fluid dynamics that is based on simple models.
3. Combine the knowledge gained from both fields and apply the intermediate-level, new models to study a specific fluid dynamical phenomenon (e.g.: drag reduction in turbulence).
4. Compare the new predictions with experiments, as far as possible, and reveal the role played by the newly incorporated polymer-scale effects on the macroscopic dynamics.

PhDs in this project will be provided training in the following theoretical, computational and analytical areas: Newtonian and viscoelastic fluid mechanics, statistical mechanics, stochastic processes, advanced CFD (spectral methods), numerical methods for stochastic differential equations, tensor analysis, stability analysis.

Expected outcomes

- This project will break new ground by presenting simulations of complex flows of polymer solutions that go beyond toy models and incorporate hitherto-neglected effects such as hydrodynamic interactions.
- The simulations will not only lead to new understanding of the role of polymer-scale physics on macroscopic dynamics, but also go beyond qualitative effects and allow for quantitative comparison with experiments
- The new methodologies and simulation algorithms developed will represent an important first step towards accurately predicting polymer flows in a wide range of industrial applications.
- On obtaining her PhD, the student will be an expert in both rheological modelling as well as computational fluid dynamics (CFD). This skill set is in high demand in research groups across the world, as well as at research and development wings of companies involved in polymer processing (e.g. Saint-Gobain, Chennai), as well as at CFD consultancy and software companies (ESI Group, Bangalore and Pune; SankhyaSutra Labs, Bangalore).

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

<u>Major theme: Advanced computational engineering, simulation and manufacture</u>

The project will produce new computational methods and simulation software that will significantly improve our ability to predict the flow of polymer solutions, with a wide range of possible applications, from transport of oil in pipelines to underground oil recovery, and from microchip reactors to polymer processing.

Potential RPCs from IITB and Monash

IITB:

1. Prof. Rochish Thaokar (instabilities, elasto-hydrodynamics)
2. Prof. Partha Goswami (turbulent flow of suspensions, CFD)

Monash:

1. Prof. Murray Rudman (CFD of non-Newtonian fluids)
2. Prof. Greg Sheard (spectral-element methods and CFD of thermal convection and magneto-hydrodynamic flows)
3. Prof. Ravi Jagadeeshan (statistical mechanics and Brownian Dynamics simulations of polymer solutions)

Capabilities and Degrees Required

The ideal candidate for this project should meet the following criteria:

1. Strong foundation in fluid dynamics, mathematical and numerical methods, evidenced by having high grades in the corresponding courses, or by having done projects in these areas.
2. Done an undergraduate-level (or higher) project involving fluid dynamics, or soft matter, or mathematical modelling and simulation. Preferably, this project should have led to a concrete outcome, in the form of a thesis, submitted or published research paper, etc.
3. Be comfortable with either C/C++, or Fortran, or Python, and have written code for a project. If not, then the candidate should at least have used software like Matlab or Mathematica. Use of COMSOL, FLUENT, etc., does not count.
4. Good verbal and written communication skills, as demonstrated by a written undergraduate thesis, or paper, or blog, etc. We will also consider this aspect during the interview.
5. Qualifications: BTech, BE (or higher) in Chemical or Mechanical Engineering, or allied disciplines. Students from a physics (BSc + MSc) or mathematics background are also welcome, provided they have the required capabilities.

Necessary Courses

CL601	Advanced Transport Phenomena	(6 credits)
CL602	Mathematical and Statistical Methods in Chem Engg.	(6 credits)
CL701	Computational Methods in Chem Engg.	(8 credits)

Potential Collaborators

The work is envisioned as a collaboration between Prabhakar Ranganathan (Monash), Jason Picardo (IITB) and Dario Vincenzi (Université Côte d'Azur, Nice, France: https://math.unice.fr/~vincenzi/). Dario Vincenzi has contributed extensively to our current understanding of how polymer molecules behave in a turbulent flow. We will explore the possibility of obtaining separate funding for the student to visit Dario Vincenzi in France in order to benefit from his expertise and guidance.

Select up to **(4)** keywords from the Academy's approved keyword list **(available at http://www.iitbmonash.org/becoming-a-research-supervisor/)** relating to this project to make it easier for the students to apply.

Computational Fluid Dynamics and Mechanics; Maths; Computer Simulation; Modelling and Simulation