The Australian Society of Rheology, Inc.
2022 Rheology Lecture Series

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The Australian Society of Rheology is presenting a national series of lectures, which is open to anyone interested in the flow and deformation of matter. The next event in the series will be held online.

Calendar details

Date:	**Tuesday, September 06, 2022**
Time:	10:00 to 11:30 AM (Melbourne, Australia)
Event Registration Link:	https://www.eventbrite.com.au/e/australian-society-of-rheology-seminar-06-september-2022-registration-405074888897

Invited lecture

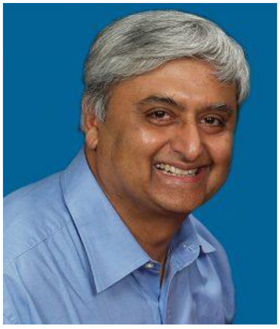
Professor Ravi Prakash Jagadeeshan

(Department of Chemical and Biological Engineering, Monash University, Australia)

Presentation Title: **Understanding the sol-gel transition of associative polymer solutions**

Abstract: Gels with thermoreversible physical crosslinks show great promise for designing materials with tuneable rheology and self-healing properties. However, many questions remain to be answered before the goal of tailoring a solution's macroscopic properties by controlling molecular scale parameters, can be achieved. We show that considerable progress in this direction can be made by examining the behaviour of physical gels near the gel transition with the help of Brownian dynamics simulations. Due to the scale-free and semidilute character of critical gels, fully capturing their structure and dynamics requires the inclusion of associative interactions between sticky monomers, solvent-mediated hydrodynamic interactions between all the monomers in a large simulation volume, and time scales spanning several orders of magnitude. We have adapted Jim Swans' algorithm for the efficient computation of hydrodynamic interactions in colloids to polymer chains, making the simulation of the dynamics of physical gels at the transition point tractable for the first time. We present simulation predictions of dynamic moduli as functions of frequency and concentration and discuss the effect of the bond dissociation time on the typical critical gel behaviour. In particular, in chemical gels, one expects the dynamic moduli to be parallel power law functions of frequency at the gel point. However, if the dissociation time is short, this power law may be cut off by the disintegration of the gel network after long times/low frequencies. We show that the typical signature of gelation can be recovered by increasing the effective strength of the associative interaction. Further, we show that the gel transition is still observable, even with weak associations, using several measurements, including the equilibrium stress autocorrelation, the instantaneous shear modulus, and zero shear rate viscosity. We also show the structural emergence of a gel as a power law distribution of chain cluster sizes, indicating a divergence of the average cluster size. Finally, we compare the prediction of the concentration at the sol-gel transition by a variety of different static and dynamic signatures of gelation.

Speaker's biography:



Professor Ravi Jagadeeshan heads the Molecular Rheology group within the Department of Chemical Engineering at Monash University. His group is focused on developing a theoretical and computational description of the flow behaviour of polymer solutions using a multiscale approach that combines molecular simulations at the mesoscopic scale with continuum simulations on a macroscopic scale. He is also interested in applying methods of soft matter physics to studying problems in biology. Professor Jagadeeshan attained his PhD in chemical engineering from the Indian Institute of Science in 1989. He undertook postdoctoral and research positions at the National Chemical Laboratory Pune (India), Cavendish Laboratory at the University of Cambridge (UK) and the Swiss Federal Institute of Technology Zurich (Switzerland). He was a Humboldt fellow at the Technical University of Kaiserslautern from 1999 to 2000, and in 2001 Professor Jagadeeshan joined Monash University.