From Macromolecular Structure to Polymer Processing: Bridging length and time scales

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India is a significant producer of thermoplastics with an installed capacity of about 4 MMTA.[1] We are today the second largest producer of polyester and the fifth largest producer of polypropylene in the world. As petroleum prices continue to rise and the global petrochemicals industry gradually shifts to the middle-east, the Indian plastic industry is bound to make a strategic shift to the production of specialty plastics. Additionally, as demands on cleaner environment and sustainability increase the Indian plastics industry will have to focus on the production and processing of environmentally benign polymers. Development of such plastics requires a deeper understanding of the intricate relations between the structure and topology of macromolecules and their processing behavior and properties. A significant scientific challenge here is to be able to connect physical phenomena that occur over several orders of magnitudes of length and time scales (Figure 1).

To meet this challenge it is necessary to equip oneself with a tool-box of sophisticated scientific techniques that include experimental measurements of the structure and properties of polymers from molecular to macroscopic length scales, coarse-grained-mean-field theory, meso-scale simulations, continuum CFD simulations and experimental validation. Relating polymer microstructure to melt processing performance (the dotted area in Figure 1) has been a major research theme in my group at the National Chemical Laboratory. We, in collaboration with the Tata Research Design and Development Centre and the Indian Institute of Technology Bombay, have been gradually building competencies to address this scientific challenge.

In this presentation I will summarize the key historical developments in this area, present contributions from NCL, touch upon some industrially relevant problems to which we are applying our tools and give my perspective on the current state of research.

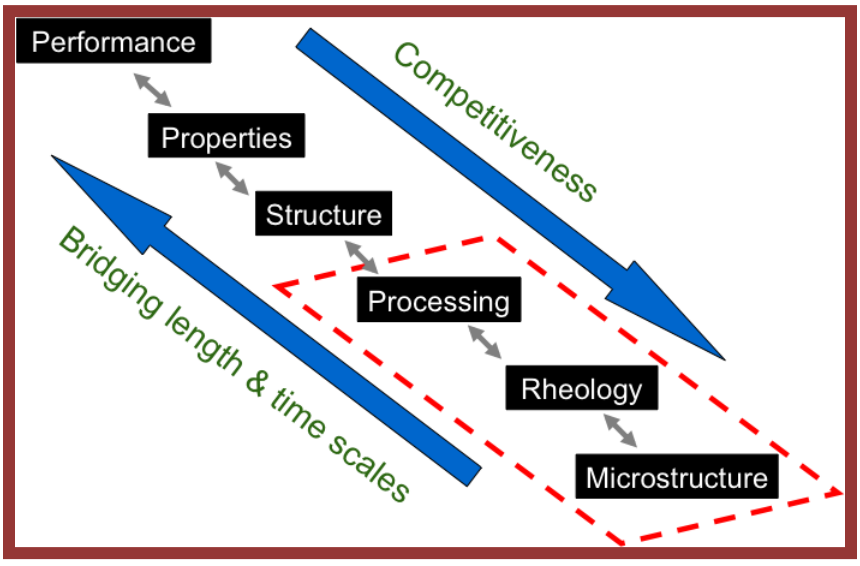

Figure 1: Structure-Property Relationships for Thermoplastics

[1] Mutha et al., *Resources, Conservation and Recycling* **2006**, *47*, 222-224.