Chemical and Biomolecular Engineering
Fall 2009 Seminar Series

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"Using Computer Modeling to Design Smart Microcapsules and Chemo-responsive Gels"

Abstract

Using theory and simulation, we design two distinct scenarios where synthetic polymeric systems exhibit autonomous movement. In the first case, we design a "train" of N microcapsules that undergoes self-sustained, directed motion along an adhesive surface in solution. The motion is initiated by the release of nanoparticles from a single "signaling" capsule at one end of the train. The released nanoparticles can bind to the underlying surface and thereby induce an adhesion gradient on the substrate. Through the combined effects of the self-imposed adhesion gradient and hydrodynamic interactions, the N microcapsules autonomously move in a single file toward the region of greatest adhesion. At late times, this train reaches a steady-state velocity U, which decreases with train length as $N^{-1/2}$. We calculate the maximum length for which the train maintains this cooperative, autonomous movement. In the second case, we determine the effect of light on the motion of polymer gels undergoing the Belousov-Zhabotinsky (BZ) reaction. The BZ gels undergo rhythmic mechanical oscillations in response to the periodic reduction and oxidation of ruthenium catalysts that are grafted to the polymer network. The Ru-catalyzed BZ reaction is photosensitive, with light of a certain wavelength suppressing the oscillations within the gel. We exploit this property to control the self-sustained motion of millimeter-sized BZ gel "worms". By tailoring the arrangement of illuminated and non-illuminated regions, we direct the movement of these worms along complex paths, guiding them to bend, reorient and turn. Notably, the path and the direction of the gel's motion can be dynamically and remotely reconfigured. Hence, our findings can be utilized to design intelligent, autonomously moving "soft robots" that can be reprogrammed "on demand" to move to a specific target location and to remain at this location for a chosen period of time.

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