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Modeling active materials based on self-oscillating gels VICTOR V. YASHIN, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA, 15261 — The Belousov-Zhabotinsky (BZ) reaction in solution is a classical example of an active medium that demonstrates various chemical oscillations and waves, which can be observed visually. Grafting a ruthenium metal-ion complex, the catalyst to the BZ reaction, to a chemo-responsive polymer gel creates an active material (BZ gel), which exhibits periodic volumetric changes in the course of the reaction. The redox oscillations of the catalyst affect the polymer-solvent interactions and cause the periodic swelling and de-swelling of the gel, so that chemo- mechanical energy transduction occurs within the material. We consider a model that couples the polymer gel dynamics and the BZ reaction kinetics; the latter is described by the modified Oregonator model. The model equations are solved numerically in 2D. We demonstrate that the dynamical behavior of the BZ gel can be controlled by a heterogeneous distribution of the catalyst and by such structural features as the solvent-filled voids. The dynamics of an active membrane having the self-oscillating pores is considered as an example.

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