Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Modeling self-oscillation and waves in a reactive polymer gel
VICTOR YASHIN, ANNA BALAZS, Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, PA — We model the self-oscillation and wave propagation phenomena in a swollen polymer gel that participates in the Belousov-Zhabotinsky (BZ) reaction. The BZ reaction causes variations in the gel volume through reduction-oxidation changes of a metal catalyst, which is covalently bonded to the polymer chains. We employ the Oregonator model to describe the BZ reaction kinetics. The Flory and Flory-Huggins models are used to describe the gel elasticity, and the polymer-solvent interactions, respectively. We identify the model parameters that yield the oscillatory behavior, and demonstrate that the kinetics of the BZ reaction can be significantly affected by coupling the reaction to the polymer gel dynamics. To simulate the traveling waves of swelling-deswelling, we utilize the gel lattice spring model, which we have developed recently, and is equivalent to the two-fluid model. We demonstrate and discuss the effects of mechanical constraints on the generation and propagation of 1D and 2D swelling-deswelling waves in the reactive gel.

Victor Yashin

Date submitted: 22 Nov 2005 Electronic form version 1.4