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Modeling the BZ reaction in gels with chemo-responsive crosslinks VICTOR V. YASHIN, OLGA KUKSENOK, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA, 15261 — We model chemo-responsive polymer gels, which expand and contract periodically in response to the ongoing oscillatory Belousov-Zhabotinsky (BZ) reaction. This behavior is due to a ruthenium catalyst, which is grafted to the polymers and affects the polymer-solvent interactions as it undergoes the redox oscillations in the course of the reaction. We consider a permanently crosslinked polymer gel that encompasses $Ru(terpy)_2$ catalytic units having both the terpyridine ligands chemically bonded to the network. It is known that oxidation of the Ru metal-ion from Ru(II) to Ru(III) results in the dissociation of the $Ru(terpy)_2$ complexes since the Ru(III) ions form only mono-complexes with terpyridine. Hence, the grafted $Ru(terpy)_2$ units would effectively create crosslinks that break and re-form in the response to the BZ reaction. We modified the Oregonator model for the BZ reaction and took into account that the re-formation of $Ru(terpy)_2$ complexes is frustrated by the gel network. The time-dependent elastic contribution of the $Ru(terpy)_2$ crosslinks was described by the BKZ-type constitutive equation. We report on the results of simulations in 1D. We show, in particular, that compression of the sample leads to stiffening of the gel due to an increase in the crosslink density.

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