

Abstract Submitted
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Modeling mechanochemical transduction in chemo-responsive gels. OLGA KUKSEKOK, VICTOR YASHIN, ANNA C. BALAZS, University of Pittsburgh, Pittsburgh, PA, 15261 — Using the recently developed gel lattice spring model, we study mechanochemical transduction in chemo-responsive gels undergoing the Belousov-Zhabotinsky reaction. More specifically, we examine how to harness an applied mechanical force to trigger the propagation of traveling chemical waves, which then lead to oscillations within gels that were initially non-oscillating. In our two dimensional simulations, we introduce the presence of an applied force by uniformly decreasing the thickness of the sample from its initial value. We isolate the system parameters for which the decreasing of the thickness of the sample causes the transition from the non-oscillatory to the oscillatory state. In addition, we illustrate that even if the system is not driven into the oscillatory state, the nature of the pressure-induced transient oscillations are of interest since the waves can indicate the strength of the mechanical impact. We define how this type of the mechanochemical transduction depends on the reaction parameters and on the gel's cross-link density. Our studies clarify the sensitivity of the chemo-responsive gel to mechanical deformation and indicate the extent to which the gels can be harnessed as sensors of the mechanical impact.

Olga Kuksenok
University of Pittsburgh, Pittsburgh, PA, 15261

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