En Route to Signal Inversion in Chemical Computing

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Extended Abstract

We investigate the Belousov-Zhabotinzky (BZ) reaction as a substrate for computation. Expanding on previous research we present a new technique that utilizes two modes of the BZ reaction, excitation and oscillation, and selective diffusive coupling. We show in simulation that this technique can be used to invert input signals, providing the logical operator, NOT. Our system can readily compute NOR, which when connected in multiples is sufficient for simulating any other logical operator. Furthermore, progress to experimentally implement these operators and to wire them into circuits using soft lithography and replica molding is presented.

To synthesize living systems the field of artificial life has explored numerous substrates, physical and virtual. Chemical substrates have been gaining in popularity with recent advances in chemical computation (Adamatzky, 2009; Gorecki, 2009) and cognition (Dale and Husbands, 2010). In Braitenberg's series of vehicles of increasing cognitive complexity a key turning point is the introduction of inhibitory threshold devices, allowing for the use of *numbers*, *logic,* and *basic memory* (Braitenberg, 1986). Though to an extent the latter two properties have been introduced in our choice substrate, the Belousov-Zhabotinzky (BZ) reaction, true inhibition in the BZ has not been achieved. Here we applied the novel concept of inhibitory coupling (Toiya et al. 2008) to design signal inverting logic gates.

Using BZ substrate, various logic gates have been implemented experimentally or by computer simulation. Gorecki has simulated the gates AND and OR, as well as the MAJORITY function. Adamatzky showed XOR and AND in a related experimental substrate. Collision dynamics of BZ waves have also been exploited to annihilate signals (de Lacy Costello, 2009). To our knowledge, binary negation-based gates such as the computationally universal gates NAND and NOR (Sheffer, 1913) have not been implemented. We simulated the computation of NOT and NOR in a heterogeneous BZ substrate and synthesized a NOT gate prototype.

We designed negation-based gates using a light-sensitive implementation of the BZ reaction (Vanag and Epstein, 2009). Our system is composed of two elements: excitatory and oscillatory domains connected through a filter. Both domains are chemically identical, but differ in the amount of projected light. The illumination was tuned such that induction of a small perturbation (input) into the excitatory domain can ignite a full excitation. The oscillatory domain follows an unsuppressed periodic trajectory.

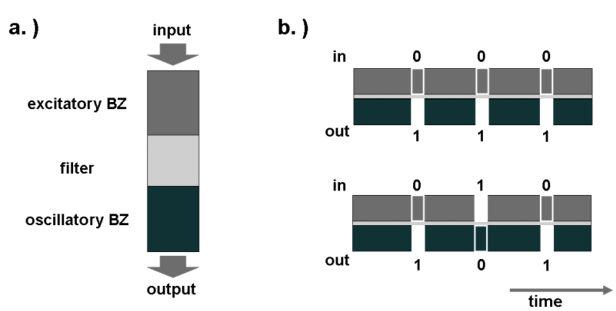

Figure 1: Inverter circuit and idealized space-time plots for signal inversion. The excitatory domain is conducting input waves into the oscillatory patch (a). Without input, the oscillatory domain transitions between oxidized (white, logic state true) and reduced (dark, logic state false) state (b, top). Due to the inhibitory coupling incoming waves will suppress and delay oscillations in the oscillatory domain into a later reading frame (b, bottom).

Using oil as a chemical filter allows for signal inversion. The filter is selective and only non-polar species such as bromine (Br_2) can permeate across (Toiya et al. 2008). Thus, a wave traveling from the excitable towards the oscillatory domain will temporarily increase the Br_2 in the oscillatory domain. Br_2 is then readily converted back to the inhibitor Br-, which will delay the oscillation in the oscillatory domain (Figure 1).

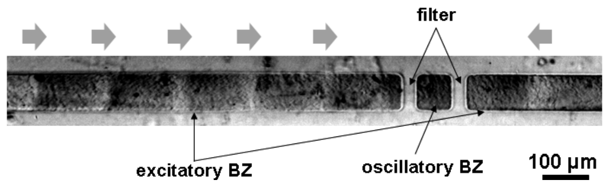

Figure 2: NOR gate prototype. Catalyst immobilized on silica gel was cast into patterned PDMS slabs. Hydrophobic PDMS walls separate BZ domains and act as chemical filters. Action potential like input waves (indicated by grey arrows) propagate towards and couple into the central oscillatory domain.

We verify our concept by simulating a simplified reaction-diffusion system of the light-sensitive BZ reaction (Vanag and Epstein, 2009). We integrate chemical turnover numerically in each BZ domain and compute the flux between compartments. Assuming fast diffusion within compartments, we reduce their size to a single point. Though a single inverter is sufficient for an inhibitory connection, we extend upon simple signal inversion to realize a NOR gate by combining two inverters. Prototypes were constructed by casting BZ catalyst immobilized on silica gel into patterned PDMS slabs (Figure 2). Hydrophobic PDMS walls were designed to separate BZ domains and act as selective chemical filters. Preliminary experimentation suggests our substrate can couple BZ domains within circuits.

The BZ reaction offers a wide range of interesting dynamics. We have described a technique capable of inverting input signals, and presented supporting simulations along with preliminary experimental results. This work suggests that the BZ reaction may be a useful substrate for the synthesis of minimally cognitive agents. Future work will utilize finite element analysis to quantitatively identify parameters for optimal input timing and delay strength. Experimental efforts will focus on increasing the robustness of single logic operators as well as connecting them into functional circuits to achieve universal computation at the microscopic scale in a chemical substrate.

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