1st International Conference on Chemo and BioInformatics
ICCBIKG 2021

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BOOK OF PROCEEDINGS

October 26-27th, 2021, Kragujevac, Serbia

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Ministry of Education, Science and Technological Development of the Republic of Serbia

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APPLICABILITY OF BRAY-LIEBHAFSKY REACTION FOR CHEMICAL COMPUTING

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Abstract

The first discovered homogeneous oscillatory reaction was the Bray-Liebhafsky (BL) one, described in a paper published exactly 100 years ago. However, the applicability of oscillatory reactions in chemical computing was recently discovered. Here we intend to expose the native computing concept applied to intermittent states of the BL reaction, because we believe that this particular state may have some advantages. For this purpose, numerical simulations will be used based on the known model. Sequences of perturbations will be introduced by adding iodate (IO_3^-) and hydrogen peroxide (H_2O_2), separately, as well as in various combinations with one another. It will be shown that dynamic states obtained after perturbations with same species depend very much on the sequence in which these species were used in perturbations. Additionally, it will be shown that obtained dynamic states shift the system from chaotic intermittent dynamic state to different complex periodic states. Hence, the applicability of the BL reaction system in chemical computing was demonstrated.

Keywords: oscillatory reactions, intermittent oscillations, chemical computing

1. Introduction

The Bray-Liebhafsky (BL) [1, 2] is usually described as catalytic decomposition of hydrogen peroxide to water and oxygen, catalyzed by iodate ions in acidic medium. Concentrations of numerous intermediate compounds in this process oscillate in time. Depending on reaction conditions, form of these oscillations may be regular periodic, nearly harmonic or highly asymmetric relaxing ones, complex mixed-mode oscillations with alternating small and large amplitude oscillations, or highly irregular chaotic ones. In the BL reaction system, the intermittent chaotic oscillations were also obtained and their stochastic nature was described, indicating deterministic origin of the phenomena. [3]

The applicability of oscillatory reactions in native chemical computing was recently discovered. [4] The interest in chemical computing is often justified by applicability of parallel computing performed with spontaneous synchronization of chemical transformations between individual molecules. However, special branch in research of chemical computing is native chemical computing. This approach does not require any external elements to do the computation. To perform chemical computing an input signal in the form of sequences of reactants added to the reaction system will produce output in the form of amplitude and frequency of resulting chemical oscillations.

Here we intend to present the native computing concept applied to intermittent states of the BL reaction. Possible advantages of this reaction are complex dynamical states formed as a result of parallel existence and interaction of two distinct attractors. For this purpose, numerical simulations will be performed based on the known model. Sequences of perturbations will be introduced as separate additions of equal amounts of two reagents, iodate ions and hydrogen peroxide, which are constituents of the BL system. Perturbations will always be performed in same time intervals, but in variable sequences.

2. Model and methods

Among several variants of the model for BL reaction, one with seven reactions is selected since it is simpler than the full model but still capable to simulate all different dynamic states.

Tabela 1. The variant of the model of the Bray-Liebhafsky reaction having seven reactions [M(1-6,8)]. Dimensionless rate constant values were k_1 = 0.2250, k_{-1} = 5.1000, k_2 = 67.9725, k_3 = 100, k_{-3} = 100, k4 = 0.3375, k_{-4} = 0.0150, k_5 = 100, k_6 = 100.7000, k_8 = 0.7000

$IO_3^- + I^- + 2H^+ \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} HIO + HIO_2$	$v_1 = k_1[I^-]$ $v_{-1} = k_{-1}[HIO][HIO_2]$	(R1), (R–1)
$HIO_2 + I^- + H^+ \xrightarrow{k_2} I_2O + H_2O$	$v_2 = k_2[I^-][HIO_2]$	(R2)
$I_2O + H_2O \underset{k_{-3}}{\overset{k_3}{\rightleftarrows}} 2HIO$	$v_3 = k_3[I_2O]$ $v_{-3} = k_{-3}[HIO]^2$	(R3), (R–3)
$HIO + I^- + H^+ \underset{k_{-4}}{\overset{k_4}{\rightleftarrows}} I_2 + H_2O$	$v_4 = k_4[I^-][HIO]$ $v_{-4} = k_{-4}[I_2]$	(R4), (R–4)
$HIO + H_2O_2 \xrightarrow{k_5} I^- + H^+ + O_2 + H_2O$	$v_5 = k_5[HIO][H_2O_2]_0$	(R5)
$I_2O + H_2O_2 \xrightarrow{k_6} HIO + HIO_2$	$v_6 = k_6[I_2O][H_2O_2]_0$	(R6)
$IO_3^- + H^+ + H_2O_2 \xrightarrow{k_8} HIO_2 + O_2 + H_2O$	$v_8 = k_8[H_2O_2]_0$	(R8)

Unlike our previous papers, concentration of the hydrogen peroxide was here treated as constant (pool approximation). This way, conditions for achieving permanent steady state were attained.

The main aim of this paper is to investigate applicability of the BL reaction in native chemical computing, and therefore, perturbation technique was designed to highlight specific properties of dynamic system. It was desirable to achieve conditions where perturbations lead system to distinct dynamic states. However, standard way of perturbations having effects on instantaneous values of internal species concentrations would cause only temporary effects in present case. Hence, for achieving permanent effects, perturbations were performed with reagents iodate ions and hydrogen peroxide that are external species in any reaction system.

3. Results and Discussion

In Figure 1, three cases of intermittent oscillations are given. In all cases, iodide oscillations are given as an example. First, there is the unperturbed system. Then we have system perturbed by 10% increase in IO_3^- and finally, system perturbed by 10% increase in H_2O_2. Since only low intensity perturbation would produce only small change in oscillation amplitude here we applied excessively large intensity perturbation to demonstrate nature and intensity of produced changes. In the first case (IO_3^-) amplitude decrease was observed after perturbation while in the other case (H_2O_2) amplitude increase occurred.

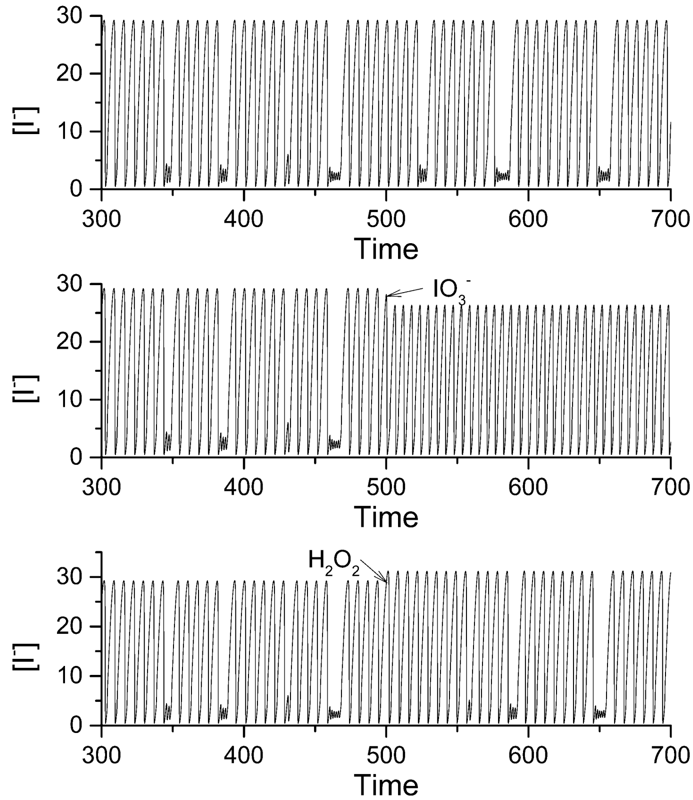

Fig.1 Iodide oscillations in case when no perturbation was applied, and in cases where perturbation with 10% increase of IO_3^- and H_2O_2 concentrations were applied after 500 time units.

Beside small amplitude changes there is also difference in dynamic state observed after the perturbation. However, this difference is more obvious when slightly longer sequences of perturbations are applied. In Figure 2, similar iodide oscillations are given for cases where small perturbations are applied in sequences of three of them with same delay period between single perturbations equal to 50 units of time. Since the effects of perturbations tend to accumulate, here we performed small intensity perturbations at the level of 1% of the initial concentration.

There is one obvious but small difference between two cases. In the first case of sequence (IO_3^- - H_2O_2 - IO_3) the amplitude was first decreased, then increased and finally again decreased. In the second case (H_2O_2 - IO_3^- - H_2O_2) the order of changes was inverted to increase, decrease and increase at the end. In both cases, initially aperiodic intermittent state was transformed to some kind of periodic or quasiperiodic state after some transient period. In the first case (IO_3^- - H_2O_2 - IO_3) final state was composed of periodic repeating of bursts with 9 large amplitude oscillations and gaps with 2 small amplitude oscillations (9^2). However, dynamic state obtained in the second case (H_2O_2 - IO_3^- - H_2O_2) was much more complex. It can be described as repeating of sequences in order $11^5 10^1 5^4 10^5$. Such a complex behaviour seems to be especially convenient for preserving information and, even more, for their codification.

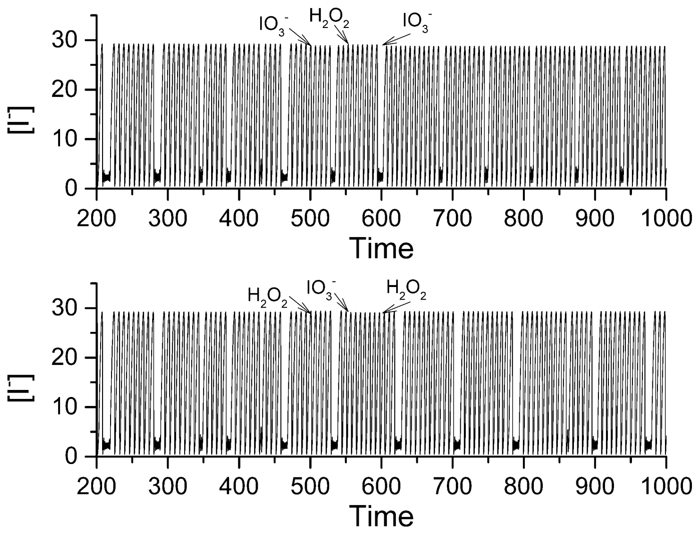

Fig.2 Iodide oscillations in cases where perturbation with 1% increase of IO_3- and H_2O_2 concentrations were applied in sequences starting from 500 and with delay of 5 time units. Used sequences were IO_3^- - H_2O_2 - IO_3^- and H_2O_2 - IO_3^- - H_2O_2

3. Conclusions

Intermittent oscillations of the BL system were perturbed by sequences of perturbations and different final states were obtained for different sequences. Hence, applicability of the BL reaction system in chemical computing was demonstrated. Information in this reaction system is preserved not only in frequency and amplitude of oscillations but moreover, in dynamic forms of oscillations.

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