Dynamic system of biological nitrogen fixation in a strange-attractor regime

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In this paper, we investigate a mathematical modeling of biochemical processes which makes it possible to determine the adaptation of a biosystem to open environmental conditions.

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A mathematical modeling of biochemical processes makes it possible to determine the adaptation of a biosystem to open environmental conditions. The mass-balance equations incorporate the nonlinear cooperative nature of the transformation processes. As a result, we have a self-regulation problem for dynamic systems far from equilibrium. The phase-portrait method, in particular the Poincare mapping, is effective for studying such nonlinear problems. In the present we wish to propose a model of this type, which is defined by the following system of nonlinear differential equations:

\[ \partial_t S = \frac{S_0 K}{K + S + \Psi} - l_1 V(S)V(S_0) - \alpha S S \] (1)

\[ \partial_t S_1 = l_1 V(S)V(S_0) - l_2 V(N^2)V(S_1^2) \] (2)

\[ \partial_t S_2 = l_2 V(N^2)V(S_1^2) - l_3 V(N)V(S_2) \] (3)

\[ \partial_t S_3 = l_3 V(N)V(S_2) - 4l_4 V(L_1 - T)V(S_3) \] (4)

\[ \partial_t S_4 = 4l_4 V(L_1 - T)V(S_3) - l_5 V(N) \frac{S_4}{1 + S_4^2 + MS_6} \] (5)

\[ \partial_t S_5 = l_5 V(N) \frac{S_4}{1 + S_4^2 + MS_6} - l_6 V(N)V(S_5) \] (6)

\[ \partial_t S_6 = l_6 V(N)V(S_5) - l_1 V(S)V(S_6) \] (7)

\[ \partial_t N = k_5 V(E_1)V(L_2 - N) - l_2 V(N^2)V(S_1^2) \] (8)

\[ -k_3 V(T^4) \frac{E_1}{1 + E_3 + O_2} - l_3 V(N) \frac{S_4}{1 + S_4^2 + MS_6} \] (9)

\[ \partial_t Q = 6k_2 V(O_2) \frac{V(L_1 - Q)}{1 + \Psi^2} - l_7 V(Q)V(L_2 - N) \] (10)

\[ \partial_t T = k_4 V(N_2)V(\Psi^4) \frac{E_1}{1 + E_4 + H_2/2} + l_8 V(L_1 - T)V(\Psi^4) - 4k_3 V(T^4) \frac{E_3}{1 + E_3 + O_2} \] (11)

\[ -2k_6 V^2(1 + K_{11})V(T^2)V(\Psi^2) \] (12)

\[ \partial_t \Psi = 4l_7 V(Q)V(L_2 - N) - 4l_8 V(L_1 - T)V(\Psi^4) - k_1 V(E_1)V(\Psi) - 4k_4 V(N_2) \] (13)

\[ -k_4 V(E_1)V(H_2) - \alpha_{E_1} E_1 \] (14)

\[ \partial_t E_1 = E_{10} \frac{A}{A + \beta_1} \frac{K_1}{K_1 + A^4} - k_1 V(E_1)V(\Psi) \] (15)

\[ +k_4 V(N_2)V(\Psi^4) \frac{E_4}{1 + E_4 + H_2/2} - k_5 V(E_1)V(L_2 - N) \] (16)

\[ +k_6 E_3 V(T^2)V(\Psi^2) - k_7 V(E_1)V(H_2) - \alpha_{E_1} E_1 \] (17)

\[ \partial_t E_2 = E_{20} \frac{K_2}{K_2 + O_2} \] (18)

where \( V(x) = x/(x + 1) \). The dynamic variables \( S(t),...,S_6(t) \) describe the Krebs cycle. The variables \( Q(t),\Psi(t),T(t),O_2(t) \) describe the respiratory chain, the kinetic membrane potential, the ATP concentration, and the concentration of molecular oxygen, respectively.

This block of the model is responsible for describing the bioenergetics of a cell. The crucial enzyme nitrogenase participates in its three forms \( E_1, E_3, E_4 \). Its activity is regulated by molecular hydrogen \( H_2 \) and molecular nitrogen \( N_2 \), while the biosynthesis is regulated by ammonia \( A \), which is present in the biosystem.

Serving as an electron donor here is \( NADH \cdot H_2 \equiv N \).

The optimal regime of the biosystem is described by the following set of parameter values:
\[
l_1 = 0.3, \quad l_2 = 0.3, \quad l_3 = 0.3, \\
l_4 = 0.03, \quad l_5 = 0.3, \quad l_6 = 0.3, \\
l_7 = 0.4, \quad l_8 = 0.2, \quad k_1 = 0.01, \\
k_2 = 0.05, \quad k_3 = 0.05, \quad k_4 = 0.06, \\
k_5 = 0.05, \quad k_6 = 0.03, \quad k_7 = 0.003, \\
L_1 = 3, \quad L_2 = 2, \quad L_3 = 2, \\
K = 0.3, \quad K_1 = 0.006, \quad K_2 = 0.3, \\
\alpha_S = 0.005, \quad \alpha_A = 0.0045, \quad O_{20} = 0.02, \\
E_{10} = 0.02, \quad \beta = 0.1, \quad N_{20} = 0.2.
\]

The kinetics of the biosystem exhibits a self-regulation. Under the open environmental conditions described by the parameters \( S_0, O_{20}, N_{20}, \alpha_S, \alpha_1, \alpha_2, \ldots \) the phase-portrait of the biosystem includes a structural adapter characterized by stable oscillations and does not dependent from a initial state of the biosystem (Cauchy data).

The presence of oscillations in the biosystem is determined primarily by the interaction of self-regulated subsystems: the Krebs cycle, the respiratory chain, and the nitrogenase complex.

Furthermore, the process of biosynthesis of nitrogenase in form of \( E_1 \) depends on the ammonia concentration in a non-monotonic way. This circumstance is expressed by the nonlinear term in (13):

\[
E_{10} \frac{A}{A + \beta_1} \frac{K_1}{K_1 + A^4}
\]

At small values of \( A \), the synthesis of \( E_1 \) is induced, while a large value of \( A \) results in a repression of \( E_1 \).

At the pumping parameter value \( S_0 = 0.07 \), a strange attractor exists in the phase space of the system. Figure 1 shows a projection of the phase portrait of a strange attractor in the coordinates \((A, \Psi)\).

The given regime forms a limiting-cycle regime through an infinite sequence of period-doubling bifurcations.\[6\]

Figure 2 shows the kinetics of simple periodic oscillations of the variables from a Krebs cycle. Figure 3 shows the kinetic behavior of the respiratory chain, of the kinetic membrane potential, of the ATP, and of molecular oxygen. Figure 4 shows the time evolution of the biosynthesis of the nitrogenase complex. We see from these figures that we have a self-regulation of the biosystem in an oscillatory regime: At high values of \( A \), we have low levels of \( E_1, E_3, E_4 \); low values of \( A \) corresponds to high values of \( E_1, E_3, E_4 \). This situation determines the kinetic behavior of the other reactants.

At the parameter value \( S_0 = 0.063 \) the attractor is a limiting cycle. At the point \( S_0 = 0.065 \) this limiting cycle undergoes a bifurcation into a limiting cycle with a period \( t \) twice the original period. The limiting cycle which is generated at \( S_0 = 0.069 \) again doubles through a period-doubling bifurcation. The next bifurcation point found is \( S_0 = 0.06932 \). After an infinite sequence of doubling bifurcations of the limiting cycle, an aperiodic oscillatory attractive regime - a strange-attractor regime - appears in the phase space.

![FIG. 1: Strange attractor in projection (A, \( \Psi \)).](image1)

![FIG. 2: Kinetics of the Krebs cycle.](image2)

![FIG. 3: Kinetics of the respiratory chain, of the ATP, of \( O_2 \), and of the kinetic membrane potential.](image3)
FIG. 4: Kinetics of the nitrogenase complex.

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