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Mathematical Model of Substance Active Transport via Cytoplasmic Membrane of Microbial Cell Along Concentration Gradient

Scientific Note

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It was shown that the process of methane oxidation may be ceased by the dissipation of the electrochemical gradient across the cytoplasmic membrane of methane-oxidizing bacteria (Pinchuk and Sokolov, unpublished data). The effect observed could be explained by the existence of a mechanism of methane active transport via the cytoplasmic cell membrane (*1*). A peculiarity of this transport process is the acceleration of substance transfer along its concentration gradient.

It is possible that similar processes occur not only in methanotrophs but also in other bacteria during uptake of substrate or during the excretion of metabolites. The situation observed may occur in a case when the enzyme affinity for the substrate or the product is high or when its diffusion rate is the limiting factor. Substance transfer via the membrane along its concentration gradient could be accelerated by additional energy expenditures if necessary mechanisms exist. While in the cell itself and its environment, the substance observed is transported according to the diffusion laws.

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In this article we present the development of the mathematical model of the product active transport metabolic process across the cytoplasmic membrane of a coccoid bacterial cell along the concentration gradient with metabolic energy consumption. The model is the following initial-boundary-value task for equations in partial derivatives of the second order of parabolic type:

$$p^{-2}\frac{\partial}{\partial p}\left(D_1 p^2 \frac{\partial P(p,\tau)}{\partial p}\right) + \gamma_1 = \frac{\partial P(p,\tau)}{\partial \tau},\ 0 \le p < \alpha, \tag{1}$$

$$p^{-2}\frac{\partial}{\partial p}\left(D_2 p^2 \frac{\partial P(p,\tau)}{\partial p}\right) = \frac{\partial P(p,\tau)}{\partial \tau},\ \alpha < p \le 1, \tag{2}$$

$$P(p,0) = \begin{cases} \widetilde{P},\ 0 \le p < \alpha, \\ \overline{P},\ \alpha < p \le 1; \end{cases} \tag{3}$$

$$D_1 \frac{\partial P(p,\tau)}{\partial p}\Big|_{p=\alpha-0} = D_2 \frac{\partial P(p,\tau)}{\partial p}\Big|_{p=\alpha+0},\ \tau > 0, \tag{4}$$

$$D_1 \frac{\partial P(p,\tau)}{\partial p}\Big|_{p=\alpha-0} = h(P(\alpha+0,\tau) - P(\alpha-0,\tau)),\ \tau > 0, \tag{5}$$

$$P(0,\tau) < \infty, \qquad P(1,\tau) = \overline{P}, \tag{6}$$

where:

$P(p, \tau)$ = concentration of the metabolic product (methane for instance) transferred into the medium out of the cell;

p, τ = dimensionless coordinates:

$$p = r / R^2,\ \tau = t / t_o,\ \alpha = R_1 / R_2,\ D_j = \widetilde{D}_j t_o / R_2^2,\ j = 1, 2,$$
$$\gamma_1 = t_o \gamma,\ h = H t_o / R_2; \tag{7}$$

t_o = time unit;

r = actual coordinate;

t = time

R_1 = radius of coccoid cell;

R_2 = radius of the assumed liquid environment surrounding the cell, $R_2 >> R_1$;

γ = rate of the product P formation inside the cell, const;

$\widetilde{D}_1$, $\widetilde{D}_2$ = coefficients of the product diffusion inside the cell and in the surrounding medium, correspondingly, const;

H = permeability of the cytoplasmic membrane during the product active transport.

The following analytical solution of the task (1)–(6) was obtained:

$$P(p,\tau) = P(p) + \sum_{n=1}^{\infty} T_n p^{-1} R_n(p) e^{-\lambda_n^2 \tau}, \tag{8}$$

where:

$P(p)$ = problem solution for stationary conditions of the process duration, i.e., when

$$\frac{\partial P(p, \tau)}{\partial \tau} = 0$$

$R_n(p)$ = proper functions of Sturm-Lyuville task with piece-constant coefficients;

λ_n^2 = proper values of Sturm-Lyuville problem with piece-constant coefficients;

T_n = coefficients defined by the assumed initial condition (3)

To obtain the problem solution, the Furrier method was used (2). Thus, it is defined that:

$$P(p) = \begin{cases} A_1 p^2 + A_2, & 0 \le p < \alpha, \\ A_3 p^{-1} + A_4, & \alpha < p \le 1; \end{cases} \tag{9}$$

$$A_1 = -6^{-1} \gamma_1 D_1^{-1},$$

$$A_2 = 3^{-1} \gamma_1 \alpha [\alpha(2^{-1} D_1^{-1} + (1 - \alpha) D_2^{-1} + h^{-1}] + \bar{P},$$

$$A_3 = 3^{-1} \gamma_1 \alpha^3 D_2^{-1},$$

$$A_4 = -3^{-1} \gamma_1 \alpha^3 D_2^{-1} + \bar{P};$$

$P(p)$ = solution of the task (1)–(6) for the stationary conditions of the process duration, i.e., when

$$\frac{\partial P(p, \tau)}{\partial \tau} = 0$$

$$R_n(p) = \begin{cases} \sin(\beta_{1n} p), & 0 \le p < \alpha, \\ D_1 Q_1 D_2^{-1} Q_2^{-1} \sin(\beta_{2n}(1 - p)), & \alpha < p \le 1, \end{cases} \tag{10}$$

$$Q_1 = \sin(\beta_{1n}\alpha) - \beta_{1n}\alpha\cos(\beta_{1n}\alpha),$$

$$Q_2 = \beta_{2n}\alpha\cos(\beta_{2n}(1 - \alpha)) + \sin(\beta_{2n}(1 - \alpha)),$$

$$\beta_{1n} = (\lambda_n^2 / D_1)^{1/2}, \qquad \beta_{2n} = (\lambda_n^2 / D_2)^{1/2}.$$

The proper values λ_n^2 are defined from the characteristic equation:

$$\alpha h D_1 Q_1 \sin(\beta_{2n}(1 - \alpha)) - D_2 Q_2 Q_3 = 0, \tag{11}$$

where

$$Q_3 = D_1 \beta_{1n} \alpha \cos(\beta_{1n}\alpha) + (\alpha h - D_1)\sin(\beta_{1n}\alpha).$$

Therefore, Eq. (8) describes the product concentration distribution function by coordinate and time, taking into account Eqs. (9)–(11).

CONCLUSIONS

Considering the process of methane generation by methanogenic bacteria as an example, the model describes the distribution of methane concentration inside the cell on condition that methane active transport via the cytoplasmic membrane does exist.

The model can be used for the prediction and the evaluation of the methanogen cell metabolic efficiency. Besides, the results of the work can be applied in certain ecological studies when control of the substance bioconversion rate in the natural environment is not possible.

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