Global Analysis of a Nonlinear Model for Biodegradation of Toxic Compounds in a Wastewater Treatment Process

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Abstract The paper presents rigorous mathematical stability analysis of a dynamic model, describing biodegradation of toxic substances in a wastewater treatment plant. Numerical simulations support the theoretical results.

1 Introduction

Toxicity of 1,2-dichloroethane (DCA), in particular for aquatic and atmospheric biotic systems, has been recently recognized as a serious ecological problem [4]. DCA is difficult to remove from aquatic media by physico-chemical methods due to its very low concentration. Therefore, biodegradation remains the only available alternative. A microbial strain, recently recommended as a "novelty" and capable to degrade DCA to its complete mineralization is *Klebsiella oxytoca VA 8391* [3, 4]. This strain was isolated from active sludge from a wastewater plant at the Luckoil Neftochim Rafinery in Burgas, Bulgaria. The identification was validated by the National Bank for Industrial Microorganisms and Cultures in Sofia, Bulgaria, and the strain was registered under the code number stated above.

We consider a continuous bioreactor model for DCA biodegradation by *Klebsiella oxytoca VA 8391* immobilized on granulated activated carbon. During the microbial process the immobilized cells can detach from the solid surface and live and grow in the liquid phase. The process is irreversible, i. e. free cells can not attach again the solid particles. The model is developed and validated in [4] by authors' own experiments.

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2 Model Description

The continuous flow bioreactor model describing DCA biodegradation by *Klebsiella oxytoca VA 8391* immobilized on granulated activated carbon is presented by the following differential equations [4]

$$\dot{x}_1 = (\mu_1(s) - D)x_1 + k_{im}x_{im} \tag{1}$$

$$\dot{x}_{im} = (\mu_{im}(s) - k_{im})\, x_{im} \tag{2}$$

$$\begin{aligned}\dot{s} &= -\left(\frac{1}{\gamma}\mu_1(s) + \beta_1\right)x_1 - \left(\frac{1}{\gamma}\mu_{im}(s) + \beta_{im}\right)x_{im} \\ &\quad + D(s^{in} - s) - k_L a(1 - \mu_2(s))s\end{aligned} \tag{3}$$

$$\dot{p} = \left(\frac{1}{\gamma}\mu_1(s) + \beta_1\right)x_1 + \left(\frac{1}{\gamma}\mu_{im}(s) + \beta_{im}\right)x_{im} - Dp, \tag{4}$$

where the dot over the phase variables means $\frac{d}{dt}$. The functions $\mu_1(s)$ and $\mu_{im}(s)$ are the specific growth rates of the free and the immobilized cells respectively, $\mu_2(s)$ is related to the adsorption capacity. The following functions are proposed in [4]:

$$\mu_1(s) = \frac{m_1 s}{k_s + s + s^2/k_i}, \qquad \mu_{im}(s) = \frac{m_{im} s}{k_s + s + s^2/k_i}, \qquad \mu_2(s) = \frac{m_2 s}{k + s}.$$

The growth rate functions $\mu_1(s)$ and $\mu_{im}(s)$ exhibit inhibition, i.e. they achieve their maximum at the point $s^m = \sqrt{k_s k_i}$. The function $\mu_2(s)$ is bounded and $\mu_2(s) < m_2$ is valid for all $s \geq 0$. The definition of the phase variables x_1, x_{im}, s and p as well as of the model parameters is given in Table 1.

In the bioreactor, the free cells are expected to consume easily the substrate necessarily for their growth, but they are more keen to be carried out by the flow. On the contrary, the immobilized cells have a more difficult access to the resources of the bulk fluid, but are more resistent to detachment induced by the hydrodynamical conditions. To predict this observation by the model, we assume that the following inequality holds true (see also the hypothesis (H5) below)

(H1) $\quad m_{im} < m_1$

This inequality implies that $\mu_{im}(s) < \mu_1(s)$ for all $s > 0$.

3 Equilibrium Points of the Model and Their Lyapunov Stability

Denote by

$$\phi(s) = D(s^{in} - s) - k_L a(1 - \mu_2(s))s$$

Table 1 Definition of the model variables and parameters

	Definitions	Values
x_1	Concentration of free cells [kg m^{-3}]	–
x_{im}	Concentration immobilized cells [kg m^{-3}]	–
s	Substrate (DCA) concentration [kg m^{-3}]	–
p	Product (chloride) concentration [kg m^{-3}]	–
D	Dilution rate [h^{-1}]	5.9
k_{im}	Cell leakage factor [m h^{-1}]	0.01
s^{in}	Inlet substrate concentration s_2 [mmol/l]	0.05
β_1	Biodegradation rate constant due to free cells [h^{-1}]	0.001
β_{im}	Biodegradation rate constant due to immobilized cells [h^{-1}]	0.0015
γ	Yield coefficient for free biomass production [(kg cells)/(kg substr.)]	77.6
k	Parameter in the Langmuir isotherm	0.612
k_s	Saturation constant [kg m^{-3}]	0.26
k_i	Substrate inhibition constant [kg m^{-3}]	0.984
$k_L a$	Volumetric mass transfer coefficient for DCA for adsorption [h^{-1}]	0.51
m_1	Maximum specific growth rate for free cells [h^{-1}]	0.972
m_2	Surface concentration limit of DCA in the Langmuir isotherm [g kg^{-1}]	0.63
m_{im}	Maximum specific growth rate for immobilized cells [h^{-1}]	0.18

the function included in the right-hand side of (3) and assume that the following inequality is satisfied:

(H2) $\max\{k_L a,\ m_2\} < 1$.

It is straightforward to see, that $\frac{d}{ds}\phi(s) < 0$ for all $s \geq 0$; moreover, there exists a unique positive root ζ_0 of $\phi(s) = 0$ such that $\zeta_0 < s^{in}$ and further $\phi(s) \geq 0$ if $s \in [0, \zeta_0]$, and $\phi(s) < 0$ if $s > \zeta_0$.

The equilibrium points of the model are solutions of the form (x_1, x_{im}, s, p) of the nonlinear system, obtained from (1) to (4) by setting the right-hand sides equal to zero. We are looking for equilibrium points with nonnegative components due to physical evidence.

Proposition 1. *Under assumptions (H1) and (H2), the equilibrium points of the model are the following:*

(i) $E_0 = (0,\ 0,\ \zeta_0,\ 0)$;

(ii) $E_i = \left(\frac{\phi(\xi_i)}{\frac{1}{\gamma}D+\beta_1},\ 0, \xi_i,\ \frac{\phi(\xi_i)}{D}\right)$, $i = 1, 2$, *(with* $x_{im} = 0$*) where* ξ_i *are solutions of* $\mu_1(s) = D$; E_i *exist if and only if* $D \leq \max_{s>0} \mu_1(s) = \mu_1(s^m)$ *and* $\phi(\xi_i) > 0$.

(iii) $F_i = \left(x_1^{(i)}, x_{im}^{(i)}, \zeta_i, p^{(i)}\right)$, $i = 1, 2$, *where* ζ_i *are solutions of* $\mu_{im}(s) = k_{im}$, $x_1^{(i)} = \frac{k_{im}\phi(\zeta_i)}{\beta_{im}(D-\mu_1(\zeta_i))+k_{im}\left(\frac{1}{\gamma}D+\beta_1\right)}$, $x_{im}^{(i)} = \frac{D-\mu_1(\zeta_i)}{k_{im}} x_1^{(i)}$ *and* $p^{(i)} = \frac{x_1^{(i)}}{D}\left(\left(\frac{1}{\gamma}\mu_1(\zeta_i) + \beta_1\right) + \left(\frac{1}{\gamma}\mu_{im}(\zeta_i) + \beta_{im}\right)\frac{D-\mu_1(\zeta_i)}{k_{im}}\right)$; F_i *exist if and only if* $k_{im} \leq \max_{s>0} \mu_{im}(s) = \mu_{im}(s^m)$, $D > \mu_1(\zeta_i)$ *and* $\phi(\zeta_i) > 0$.

The point E_0 is called wash-out equilibrium. The existence of E_i corresponds to the case of free microbial culture without immobilized cells on the carrier. Practically the most important equilibria are the internal points F_i; the condition $k_{im} \leq \mu_{im}(s^m)$ describes the case of compensated immobilized cell leakage by growth within the particles.

Let $E \in \{E_0, E_1, E_2, F_1, F_2\}$ be any one of the equilibrium points, described above. Denote by $J(E)$ the Jacobian of (1)–(4) evaluated at E. The eigenvalues of $J(E)$ are the roots of the following characteristic equation (I denotes the (4×4)-unit matrix) $0 = |J(E) - \lambda I| = (-D - \lambda) \cdot (-\lambda^3 + a\lambda^2 - b\lambda + c)$, where the coefficients $a = a(E)$, $b = b(E)$ and $c = c(E)$ can be computed explicitly, using the well known invariants of the matrix $J(E)$. Obviously, $\lambda_4 = -D < 0$ is an eigenvalue of every equilibrium point $E \in \{E_0, E_1, E_2, F_1, F_2\}$. This means that there are no repelling steady states in the model. The other three eigenvalues are the roots of the cubic polynomial $g(\lambda) = -\lambda^3 + a\lambda^2 - b\lambda + c$. Using the Routh-Hurwitz criterion [5] for determining the signs of the real parts of the roots of $g(\lambda)$, we obtain the following

Proposition 2. *Let the hypotheses (H1) and (H2) be satisfied.*

(i) If $\mu_1(\zeta_0) < D$ and $\mu_{im}(\zeta_0) < k_{im}$ are fulfilled, the equilibrium point E_0 is locally asymptotically stable; otherwise E_0 is a saddle.
(ii) Let the assumptions of Proposition 1(ii) be satisfied. If $\mu_{im}(\xi_i) < k_{im}$, $i = 1, 2$, then E_1 is locally asymptotically stable and E_2 is a saddle equilibrium point. If $\mu_{im}(\xi_i) > k_{im}$, $i = 1, 2$, then E_1 and E_2 are saddle equilibrium points.
(iii) Let the assumptions of Proposition 1(iii) hold. Then F_1 is locally asymptotically stable and F_2 is a saddle equilibrium point.

4 Global Properties of the Solutions

The first three equations (1)–(3) do not depend on p. If we "compute" the solutions $x_1(t)$, $x_{im}(t)$, $s(t)$ and replace them in (4), we obtain a linear nonautonomous equation for p of the form $\dot{p} = -D\,p + \psi(t)$, which can be integrated directly. Therefore, we can omit the last equation (4) in the further considerations.

We impose additionally the following assumption on (1)–(3)

(H3) $\quad \beta_1 < \beta_{im} < \dfrac{k_L a}{\gamma}, \qquad D > 1 - k_L a(1 - m_2)$

Proposition 3. *Let the assumptions (H1)–(H3) be fulfilled. Then the set $\Omega = \left\{(x_1, x_{im}, s) : x_1 \geq 0, x_{im} \geq 0, s \geq 0, Ds^{in} \geq s + \beta_1 x_1 + \beta_{im} x_{im}\right\}$ is positively invariant for the model; all solutions are uniformly bounded for all $t \geq 0$ and thus exist for $t \in [0, +\infty)$.*

Experimental results show that the inlet substrate concentration s^{in} must be lower than the one corresponding to the maximum specific growth rate, i.e. s^{in} should be below the point s^m where substrate inhibition starts to be significant. Assume that the following inequalities are fulfilled:

(H4) $\quad s^{in} < s^m, \quad k_{im} < \mu_{im}(\zeta_0).$

It is not difficult to see that under assumptions (H1)–(H4), $s(t) < \zeta_0$ is valid for all sufficiently large $t > 0$. Moreover, since $\zeta_0 < s^{in}$ holds, assumption (H4) implies that the functions $\mu_1(s)$ and $\mu_{im}(s)$ are monotone increasing for $s \in [0, \zeta_0]$. Our last assumption is

(H4) $\quad D > \mu_1(s^{in}) + k_{im}$

The hypotheses (H1)–(H5) and Proposition 1 imply that there exist only two equilibrium points of (1)–(3) in Ω, namely E_0 and F_1; thereby F_1 is locally asymptotically stable, E_0 is a saddle equilibrium. We shall show that $F_1 = (x_1^{(1)}, x_{im}^{(1)}, \zeta_1)$ is globally asymptotically stable for the model.

Theorem 1. *Let the assumptions (H1)–(H5) be satisfied. Then the equilibrium point F_1 is globally asymptotically stable for (1)–(3) in the set Ω.*

Proof. It is enough to show that the stable manifold of E_0 lies exterior to the set Ω (cf. [6]). The negative eigenvalues of $E_0 = (0, 0, \zeta_0)$ are $\lambda_1 = \mu_1(\zeta_0) - D$ and $\lambda_2 = \frac{d}{ds}\phi(\zeta_0)$. Denote by $u = (u_1, u_2, u_3)$ and $v = (v_1, v_2, v_3)$ the corresponding eigenvectors. It is easy to see that $u_2 = 0$ and $qu_3 = -\left(\frac{1}{\gamma}\mu_1(\zeta_0) + \beta_1\right) u_1$ within $q = \mu_1(\zeta_0) - D - \frac{d}{ds}\phi(\zeta_0) > 0$. Therefore, u cannot be directed inside the positive octant. The same is valid for the eigenvector v, since the latter has the form $v = (0, 0, v_3)$ with $v_3 \neq 0$. Therefore, the stable manifold of E_0 does not intersect the interior of Ω, which implies that F_1 attracts all solutions with initial conditions in Ω, i.e. F_1 is a global attractor. This completes the proof.

5 Numerical Simulation

Consider the numerical coefficient values in Table 1 (last column). For these values, all the assumptions (H1)–(H5) are satisfied, and therefore Theorem 1 holds true.

Figure 1 visualizes results from computer experiments with an initial point $(x_1(0), x_{im}(0), s(0), p(0))$ from the set Ω, i.e. satisfying $Ds^{in} \geq s(0) + \beta_1 x_1(0) + \beta_{im} x_{im}(0)$. The solid circles correspond to experimental measurements, taken from [4].

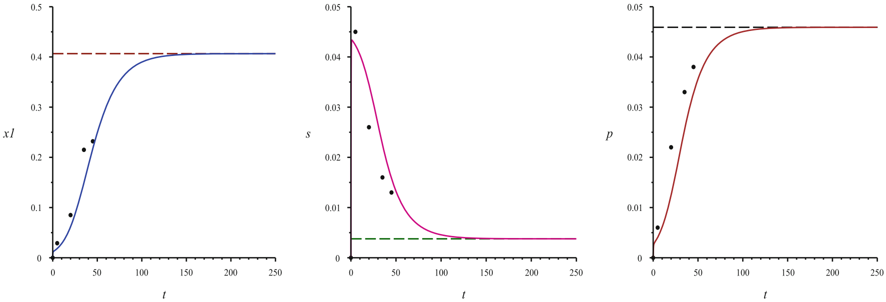

Fig. 1 Phase curves $x_1(t)$ (*left*), $s(t)$ (*middle*) and $p(t)$ (*right*); the *horizontal dashed lines* pass through the components of F_1. *Solid circles* denote experimental data

6 Conclusion

The paper presents global stability analysis of a practically validated ecological model for wastewater treatment. Most of the results are obtained and proved in [1, 2]. The proof of the above Theorem 1 is new. Here, the computer simulations are compared with experimental measurements.

The present mathematical analysis of the model (1)–(4) could be useful to outline the parameter domain for stable operation of the microbial process in a continuously stirred bioreactor.

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