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НАУКА И ОБРАЗОВАНИЕ ЗА ИНТЕЛИГЕНТЕН РАСТЕЖ

ПРОЕКТ

BG05M2OP001-1.001-0003

„ЦЕНТЪР ЗА ВЪРХОВИ ПОСТИЖЕНИЯ ПО ИНФОРМАТИКА И ИНФОРМАЦИОННИ И КОМУНИКАЦИОННИ ТЕХНОЛОГИИ“

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ИКТ

ЦЕНТЪР ЗА ВЪРХОВИ ПОСТИЖЕНИЯ ПО ИНФОРМАТИКА И ИНФОРМАЦИОННИ И КОМУНИКАЦИОННИ ТЕХНОЛОГИИ

Stability Analysis of a Mathematical Model for Phenol and Cresol Mixture Degradation

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Проект BG05M2OP001-1.001-0003 „Център за върхови постижения по Информатика и информационни и комуникационни технологии“, финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

Introduction

- Organic chemical mixtures are among the most persistent environmental pollutants. Different aromatic compounds such as phenol, cresols, nitrophenols, benzene, etc. coexist as complex mixtures in wastewaters from petroleum refineries, coal mining and other industrial chemical sources.
- Biological degradation has recently become a viable green technology for remediation of organic pollutants in comparison to other chemical and physical methods.
- We propose a mathematical model for biodegradation of phenol and 4-methylphenol (p-cresol) in a continuously stirred tank bioreactor. The biodegradation kinetics is described by a sum kinetics with interaction parameters (SKIP) model and involves inhibition effects.
- The bioreactor model presents an extension of the batch model from [*Yemendzhiev, Gerginova, Zlateva et al, 2008*], developed on laboratory experiments for degradation of phenol and *p*-cresol mixture by *Aspergillus awamori* microbial strain.

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1. Bioreactor model for phenol and *p*-cresol degradation

$$\frac{dX(t)}{dt} = \left(\mu\left(S_{ph}, S_{cr}\right) - D\right)X(t)$$

$$\frac{dS_{ph}(t)}{dt} = -k_{ph}\mu\left(S_{ph}, S_{cr}\right)X(t) + D\left(S_{ph}^{0} - S_{ph}(t)\right) \qquad (1)$$

$$\frac{dS_{cr}(t)}{dt} = -k_{cr}\mu\left(S_{ph}, S_{cr}\right)X(t) + D\left(S_{cr}^{0} - S_{cr}(t)\right)$$

$\mu\left(S_{ph}, S_{cr}\right)$ is the specific biomass growth rate , presented by *sum kinetics with interaction parameters* (SKIP) model

$$\mu\left(S_{ph}, S_{cr}\right) = \frac{\mu_{\max(ph)} S_{ph}}{k_{s(ph)} + S_{ph} + \frac{S_{ph}^2}{k_{i(ph)}} + I_{cr/ph} S_{cr}} + \frac{\mu_{\max(cr)} S_{cr}}{k_{s(cr)} + S_{cr} + \frac{S_{cr}^2}{k_{i(ch)}} + I_{ph/cr} S_{ph}}$$

$I_{cr/ph}$, $I_{ph/cr}$ indicate the degree to which each one of *p*-cresol and phenol affects the biodegradation of the other.

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$$\frac{dS_{cr}(t)}{dt} = -k_{cr}\mu\left(S_{ph}, S_{cr}\right)X(t) + D\left(S_{cr}^{0} - S_{cr}(t)\right)$$

X is biomass concentration [g/dm^3]

S_{ph} is phenol concentration [g/dm^3]

S_{cr} is *p*-cresol concentration [g/dm^3]

S_{ph}^{0} is influent phenol concentration [g/dm^3]

S_{cr}^{0} is influent *p*-cresol concentration [g/dm^3]

D is dilution rate [h^{-1}] – **the control parameter**

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Model variables and parameters

S_{ph}^{0}	influent phenol concentration [g/dm^3]	0.7
S_{cr}^{0}	influent *p*-cresol concentration [g/dm^3]	0.3
k_{ph}	metabolic coefficient [S_{ph}/X]	11.7
k_{cr}	metabolic coefficient [S_{cr}/X]	5.8
$k_{i(ph)}$	inhibition constant for cell growth on phenol [g/dm^3]	0.61
$k_{i(cr)}$	inhibition constant for cell growth on p-cresol [g/dm^3]	0.45
$I_{ph/cr}$	interaction coefficient indicating the degree to which phenol affects the *p*-cresol biodegradation	0.3
$I_{cr/ph}$	interaction coefficient indicating the degree to which *p*-cresol affects the phenol biodegradation	8.6
$\mu_{max(ph)}$	maximum specific growth rate on phenol as a single substrate [h^{-1}]	0.23
$\mu_{max(ph)}$	maximum specific growth rate on *p*-cresol as a single substrate [h^{-1}]	0.17
$k_{s(ph)}$	saturation constant for cell growth on phenol [g/dm^3]	0.11
$k_{s(cr)}$	saturation constant for cell growth on *p*-cresol [g/dm^3]e	0.35

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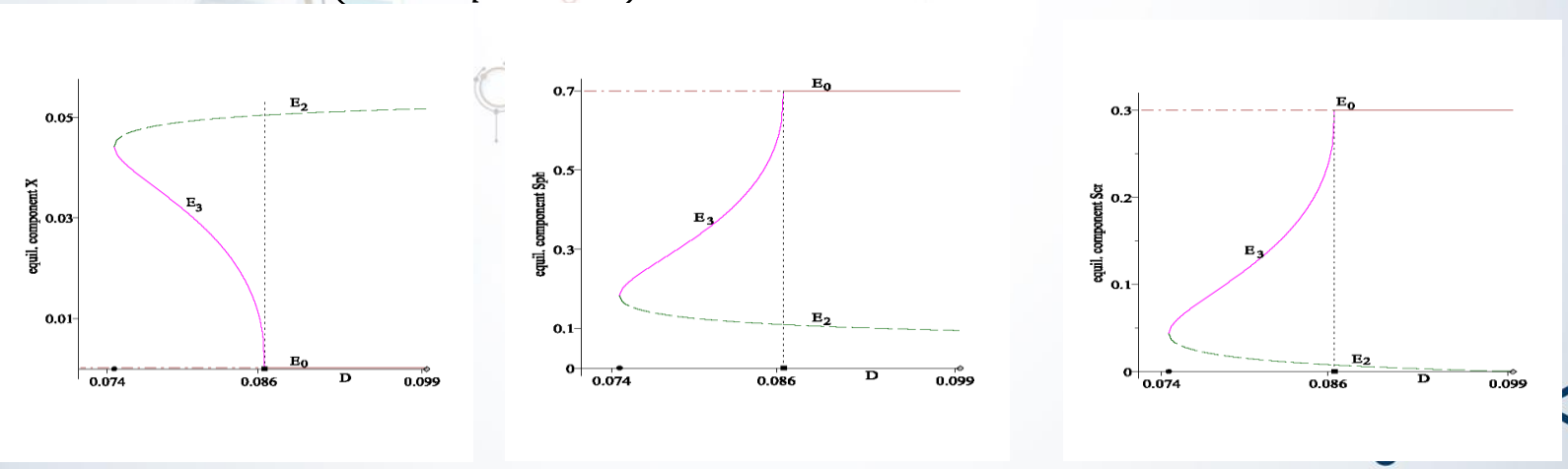
1. Bioreactor model for phenol and *p*-cresol degradation

Existence and stability of model equilibrium points are investigated in dependence of the control parameter $D > 0$

- The wash-out equilibrium $E_0=\left(0, S_{ph}^0, S_{cr}^0\right)$ (with $X = 0$) exists for all $D>0$.
- There exist values $0 < D_1 < D_2 < D_3$ such that two interior (coexistence) equilibrium points do exist:

$$E_2 = E_2(D) = \left(X^{(2)}, S_{ph}^{(2)}, S_{cr}^{(2)}\right),\ D \in (D_1, D_3)$$

$$E_3 = E_3(D) = \left(X^{(3)}, S_{ph}^{(3)}, S_{cr}^{(3)}\right),\ D \in (D_1, D_2),\ S_{cr}^{(3)} > S_{cr}^{(2)}$$



1. Bioreactor model for phenol and *p*-cresol degradation

(i) If $D < D_2$ then the equilibrium $E_0 = \left(0, S_{ph}^0, S_{cr}^0\right)$ is locally asymptotically unstable (a saddle).

(ii) If $D > D_2$ then E_0 is locally asymptotically stable (a node).

(iii) The interior equilibrium E_2, $D \in (D_1, D_3)$, is locally asymptotically unstable (a saddle).

(iv) The interior equilibrium E_3, $D \in (D_1, D_2)$, is locally asymptotically stable.

Two types of bifurcations of the equilibrium points:

- $E_2(D_1) \equiv E_3(D_1)$, thus E_2 and E_3 undergo a *saddle-node bifurcation* at $D = D_1$.
- $E_3(D_2) \equiv E_0$ and exchange stability for $D > D_2$, thus E_3 and E_0 undergo a *transcritical bifurcation* at $D = D_2$.

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1. Bioreactor model for phenol and *p*-cresol degradation

Theorem 1.1 (Existence, uniqueness)

Assume that $X(0) \geq 0,\ S_{ph}(0) \geq 0, S_{cr}(0) \geq 0.$

(i) If $X(0) = 0$ then all model solutions tend to the equilibrium point $E_0 = (0, S_{ph}^0, S_{cr}^0)$.

(ii) If $X(0) > 0$ then $(X(t), S_{ph}(t), S_{cr}(t)) > 0$ for all $t > 0$.

(iii) All solutions are uniformly bounded for all $t \geq 0$ and thus exist for all time t.

Theorem 1.2 (Global stability results)

(i) For any $D \in (D_1, D_2)$ and any initial point $X(0) > 0,\ S_{ph}(0) \geq 0, S_{cr}(0) \geq 0,$ the corresponding solution converges asymptotically towards the coexistence equilibrium E_3.

(ii) For any $D > D_2$ and any initial point $X(0) > 0,\ S_{ph}(0) \geq 0, S_{cr}(0) \geq 0,$ the corresponding solution converges asymptotically towards the wash-out equilibrium $E_0 = (0, S_{ph}^0, S_{cr}^0)$.

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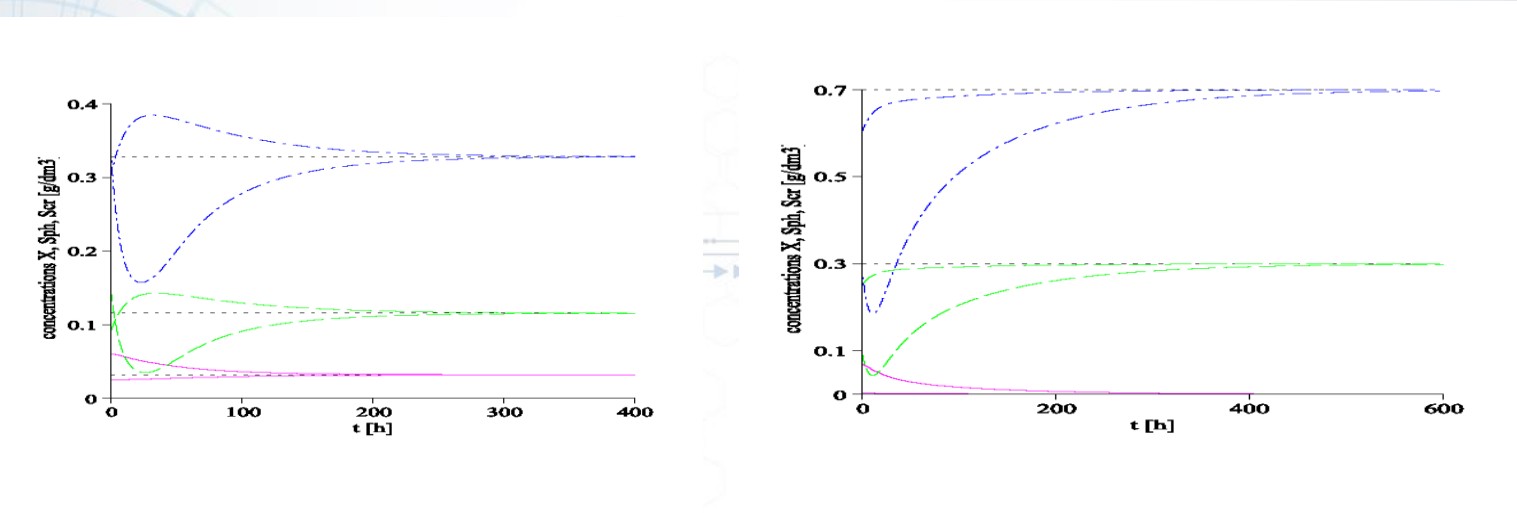
1. Bioreactor model for phenol and *p*-cresol degradation

Numerical simulations confirm the theoretical results.



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2. The bioreactor model involving discrete time delay

$$\frac{dX(t)}{dt} = e^{-D\tau}\mu\big(S_{ph}(t-\tau), S_{cr}(t-\tau)\big)X(t-\tau) - DX(t)$$

$$\frac{dS_{ph}(t)}{dt} = -k_{ph}\mu\big(S_{ph}(t), S_{cr}(t)\big)X(t) + D\left(S_{ph}^{0} - S_{ph}(t)\right) \qquad (2)$$

$$\frac{dS_{cr}(t)}{dt} = -k_{cr}\mu\big(S_{ph}(t), S_{cr}(t)\big)X(t) + D\big(S_{cr}^{0} - S_{cr}(t)\big)$$

The constant $\tau > 0$ stands for the time delay in the conversion of the consumed substrate into viable biomass.

The term $e^{-D\tau}\,X(t-\tau)$ represents the biomass of microorganisms that consumes nutrient at time $(t-\tau)$ and survives in the bioreactor for τ units of time.

C_τ^+ Banach space of continuous functions $\varphi : [-\tau, 0] \to \mathrm{R}^+$

Initial data for (2) belong to

$$C_\tau^3 = \{\varphi = (\varphi_X, \varphi_{ph}, \varphi_{cr}) \in C_\tau^+ \times C_\tau^+ \times C_\tau^+\}$$

2. The bioreactor model involving discrete time delay

Existence and stability of equilibrium points of (2) are investigated in dependence of $D > 0$ and $\tau > 0$.

Denote

$$K = \frac{k_{ph}}{k_{cr}}, \quad S^0 = S^0_{ph} - KS^0_{cr} > 0$$

$$S_{ph} = S^0 + KS_{cr}$$

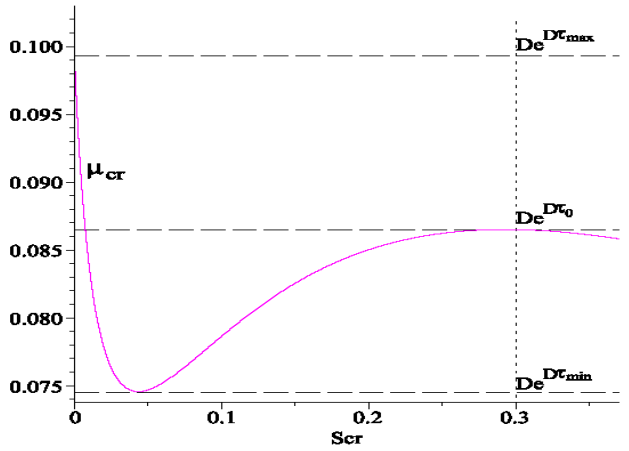
$$\mu_{cr}(S_{cr}) = \mu(S^0 + KS_{cr}, S_{cr})$$

For any $D > 0$ define

$$\tau_{min} = \tau_{min}(D) = \frac{1}{D}\ln\frac{\mu_{cr}(S^{min}_{cr})}{D}$$

$$\tau_{max} = \tau_{max}(D) = \frac{1}{D}\ln\frac{\mu_{cr}(0)}{D}$$

$$\tau_0 = \tau_0(D) = \frac{1}{D}\ln\frac{\mu_{cr}(S^0_{cr})}{D}$$



Graph of $\mu_{cr}(S_{cr})$

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Existence and stability of equilibrium points of (2) are investigated in dependence of $D > 0$ and $\tau > 0$.

- The wash-out equilibrium $E_0 = \left(0, S_{ph}^0, S_{cr}^0\right)$ (with $X = 0$) exists for all $D > 0$ and all $\tau > 0$.
- There exist two interior (coexistence) equilibrium points:

$$E_1 = E_1(D;\tau) = \left(X^{(1)}, S_{ph}^{(1)}, S_{cr}^{(1)}\right),\ \tau \in (\tau_{min}, \tau_{max});$$

$$E_2 = E_2(D;\tau) = \left(X^{(2)}, S_{ph}^{(2)}, S_{cr}^{(2)}\right),\ \tau \in (\tau_{min}, \tau_0),\ S_{cr}^{(2)} > S_{cr}^{(1)};$$

$$S_{ph}^{(i)} < S_{ph}^0, S_{cr}^{(i)} < S_{cr}^0,\ i = 1, 2$$

(*i*) The wash-out equilibrium E_0 is locally asymptotically stable for $\tau > \tau_0$ and locally asymptotically unstable for $\tau \in (0, \tau_0)$;

(*ii*) The coexistence equilibrium E_2 is locally asymptotically stable for all $\tau \in (\tau_{min}, \tau_0)$;

(*iii*) The coexistence equilibrium E_1 is locally asymptotically unstable for all $\tau \in (\tau_{min}, \tau_{max})$

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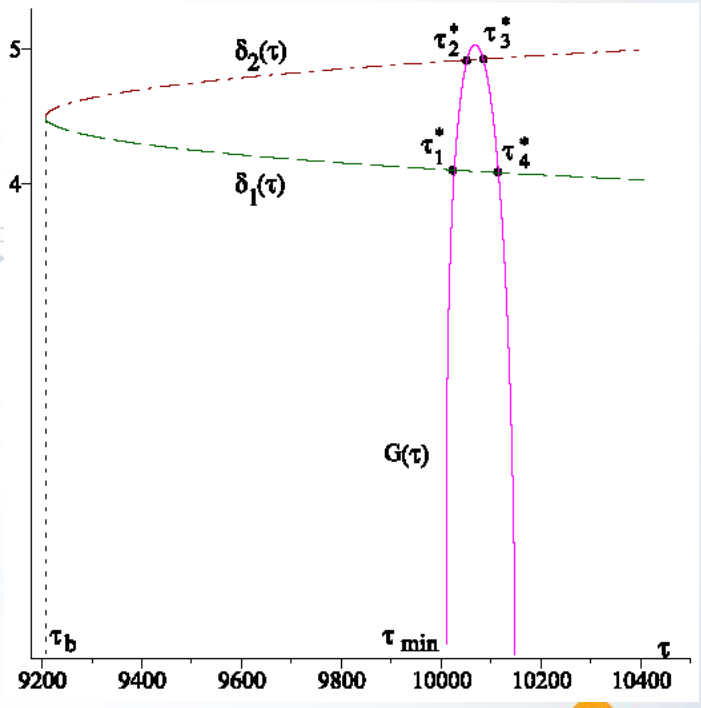
2. The bioreactor model involving discrete time delay

Hopf bifurcations of the locally unstable equilibrium point E_1 with respect to $\tau > 0$

It has been proved that under certain conditions, a finite number of critical points $\tau_i^* \in (\tau_{min}, \tau_{max})$ may exist, such that $E_1(\tau_i^*)$ undergoes Hopf bifurcations, and all bifurcating periodic solutions are unstable.



Numerical example

2. The bioreactor model involving discrete time delay

Global properties of the solutions

Theorem 2.1

(i) If $\varphi_X(\theta) = 0$ for all $\theta \in [-\tau, 0]$ then $X(t) = 0$ for all $t \geq 0$.

(ii) Let the following inequalities be fulfilled

$$0 < X(0) < \frac{DS_{cr}^0}{k_{cr}\,\mu_{cr}(0)} \qquad (3)$$

Then the solution $\Phi(\varphi; t) = \big(X(\varphi; t), S_{ph}(\varphi; t), S_{cr}(\varphi; t)\big)$ of (2) is positive for all $t \in [-\tau, +\infty]$ and is uniformly bounded.

Theorem 2.2 Let $\tau \in [\tau_{min}, \tau_0]$ and $\varphi \in C_\tau^3$ be an arbitrary element such that (3) is fulfilled. Then the corresponding positive solution $\Phi(\varphi; t)$ converges asymptotically towards E_2.

Theorem 2.3 Let $\tau > \tau_0$ and $\varphi \in C_\tau^3$ be an arbitrary element such that (3) is fulfilled. Then the corresponding positive solution $\Phi(\varphi; t)$ converges asymptotically towards E_0.

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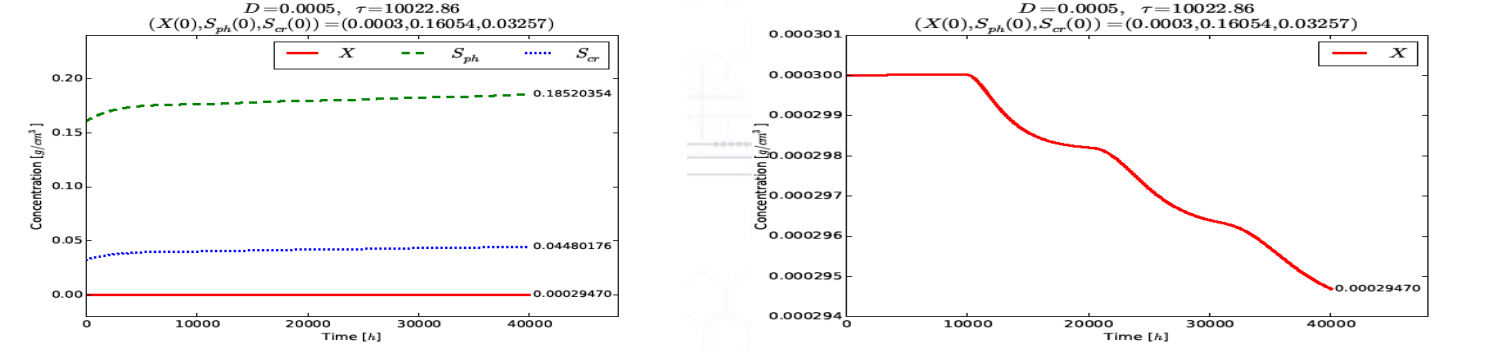
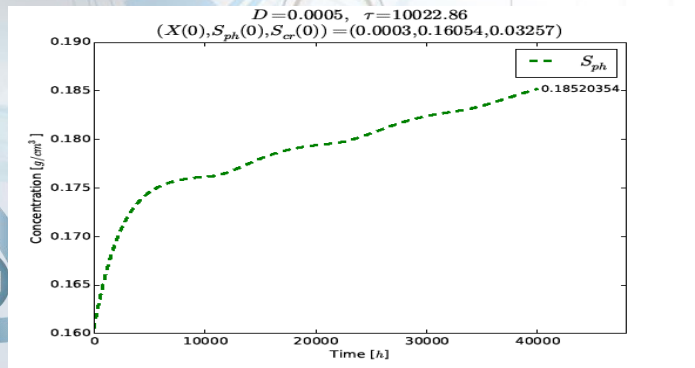
2. The bioreactor model involving discrete time delay

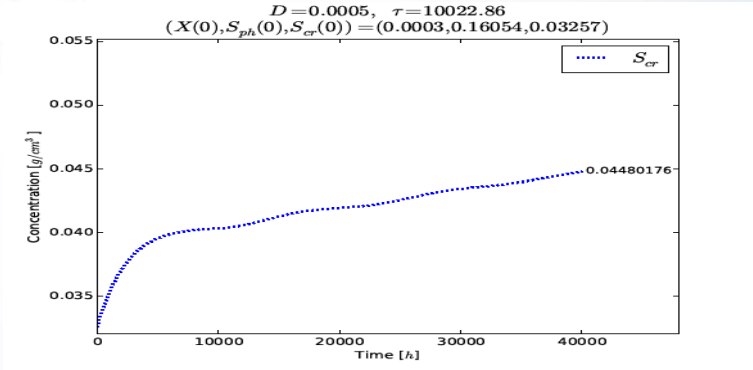
Numerical simulation

Example 1. Transient oscillations as a result of Hopf bifurcations of E_1

D=0.0005; $\tau_1^* = 10022.86$, $\tau_2^* = 10050.78$, $\tau_3^* = 10084.7$, $\tau_4^* = 10113.52$





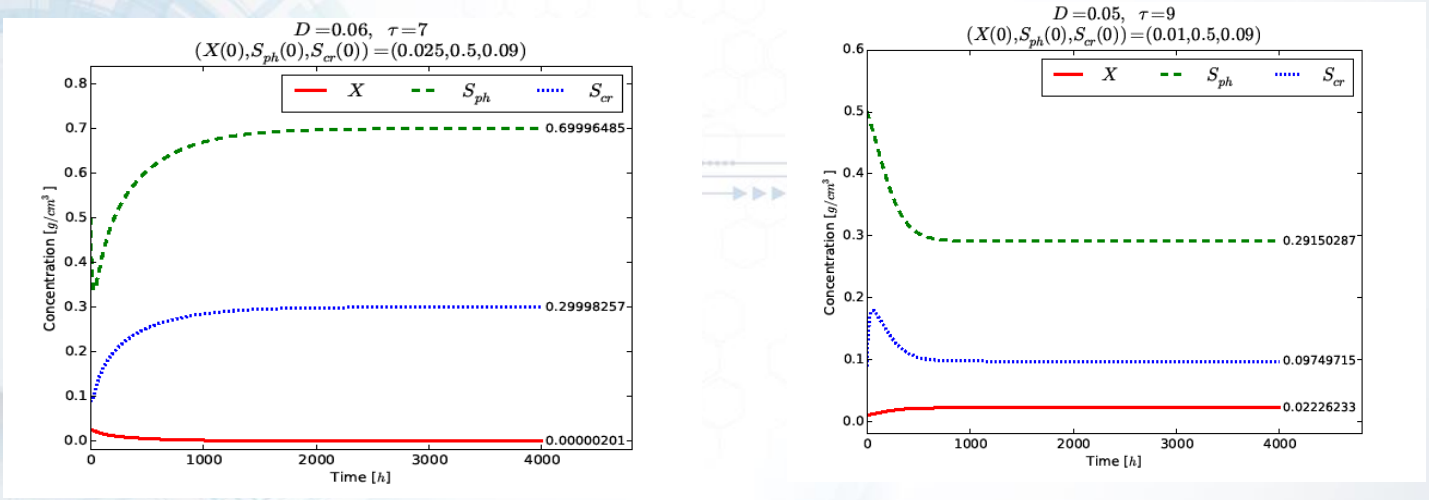


2. The bioreactor model involving discrete time delay

Numerical simulation

Example 2. The global attractors E_0 (left) and E_2 (right)

$$E_0 = (0, 0.7, 0.3), \quad E_2 = (0.02226233088, 0.2915028678, 0.09749714815)$$



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