MMK seminaras

Nuo matematikos dėstymo iki adsorbcijos modelio analizės

Teresė Leonavičienė

2019-04-30

- Pedagoginė veikla
- Mokomoji metodinė ir organizacinė veikla
- Mokslinė ir organizacinė veikla
- Adsorbcijos modelis ir jo skaitinė aproksimacija
- Linearizuotas modelis
- Rezultatai

Pedagoginė veikla

Įvairūs kursai VGTU pirmosios pakopos studijų programose Elektronikos, Fundamentinių mokslų, Mechanikos, Statybos fakultetuose.

Mokomoji metodinė ir organizacinė veikla

Darbas su kitų fakultetų studentais.

Dalyvauta rengiant Moderniųjų technologijų matematikos studijų programą, kurią sėkmingai akreditavo SKVC.

Katedros vykdomų studijų programų priežiūra (iki 2017 m. pavasario vykdyta TM studijų programa, o nuo 2017 m. rudens – MTM studijų programa).

Studijų programos viešinimas spaudoje.

Susitikimai su moksleiviais.

Mokslinė ir organizacinė veikla

Publikacijos Clarivate Analytics Web of Science duomenų bazės leidiniuose, turinčiuose citavimo rodiklį:

1. P. Baltrėnas, T. Leonavičienė, (2017). Modelling trajectories of solid particle motion in the cyclone, *Engineering Computations*, Vol. 34 Issue 6, p.1829-1848.
2. A. Bugajev, R. Čiegis, R. Kriauzienė, T. Leonavičienė, J. Žilinskas, (2017). On the Accuracy of Some Absorbing Boundary Conditions for the Schrödinger Equation, *Mathematical Modelling and Analysis*, Vol. 22 Issue 3, p.408-423.

Mokslinė ir organizacinė veikla

Publikacijos Clarivate Analytics Web of Science duomenų bazės leidiniuose, turinčiuose citavimo rodiklį:

3. T. Leonavičienė, A. Bugajev, G. Jankevičiūtė, R. Čiegis, (2016). On stability analysis of finite difference schemes for generalized Kuramoto-Tsuzuki equation with nonlocal boundary conditions, *Mathematical modelling and analysis*, Vol. 21, no. 5, p.630-643.
4. R. Čiegis, G. Jankevičiūtė, T. Leonavičienė, A. Mirinavičius, (2014). On stability analysis of finite difference schemes for some parabolic problems with nonlocal boundary conditions, *Numerical Functional Analysis and Optimization*. Philadelphia, USA : Taylor and Francis INC, Vol. 35, Issue 10, p. 1308-1327.

Mokslinė ir organizacinė veikla

Publikacija kitų tarptautinių duomenų bazių leidinyje

T. Leonavičienė, O. Suboč, (2014). Būsimų inžinierių matematinių dalykų suvokimo ypatumai, Pedagogika, Vilnius: LEU leidykla, T.113, Nr. 1, p. 159-169.

Mokslinė ir organizacinė veikla

Konferencijos

1. T. Leonavičienė, P. Baltrėnas. Removal of particles from gas in a multichannel cyclone. 19th international conference Mathematical modelling and analysis (MMA2014), Druskininkai, Lithuania, 2014.
2. T. Leonavičienė, P. Baltrėnas. Modelling of air flow in the multi-channel cyclone. 20th international conference Mathematical modelling and analysis (MMA2015), Sigulda, Latvia, 2015.
3. T. Leonavičienė, P. Baltrėnas. Effects of the parameters on the air flow in a four-channel cyclone. 7th international workshop Data analysis methods for software systems, Druskininkai, Lithuania, 2015.

Mokslinė ir organizacinė veikla

Konferencijos

4. T. Leonavičienė, A. Bugajev, G. Jankevičiūtė, R. Čiegis. On stability analysis for Kuramoto-Tsuzuki equation with nonlocal boundary conditions. 21st international conference Mathematical Modelling and Analysis (MMA2016), Tartu, Estonia, 2016.
5. T. Leonavičienė, R. Čiegis, J. Kleiza. On fluid-solid adsorption model. 23rd international conference Mathematical Modelling and Analysis (MMA2018), Sigulda, Latvia, 2018.

Mokslinė ir organizacinė veikla

Darbas projektuose

- Žmogiškųjų išteklių plėtros projektas: *Naujos kartos konstrukcijos daugiakanalis ciklonas. Akronimas DAKACIKAS*. Vykdymo terminai - 2013-2015 metai. Projekto vadovas – prof. habil. dr. P. Baltrėnas.
- Mokslininkų grupių projektas: NUMMOD *Nestandartinių netiesinių Šredingerio tipo uždavinių skaitinis modeliavimas*. Dalyvavimo terminas - 2015 - 2017 metai. Projekto vadovas – prof. habil. dr. R. Čeigis.

Mokslinė ir organizacinė veikla

Darbas projektuose

Derinamas dalyvavimo LMT projekte *Elementų singenetiškumo lignoceliuliozinėje žaliavoje įtaka adsorbcinėms bioanglies savybėms* klausimas. Projekto vadovė – prof. dr. Edita Baltrėnaitė.

Darbas rengiant MMA žurnalą.

Darbas organizuojant JMK ir MMA konferencijas.

Adsorbcijos modelis ir jo skaitinė aproksimacija

Parengta publikacija

T. Leonavičienė, R. Čiegis, E. Baltrėnaitė, V. Chemerys. Numerical analysis of liquid-solid adsorption model, *Mathematical Modelling and Analysis*, 19 p.

Formulation of the problem

Solute flux from the bulk to the liquid phase:

$$\frac{\partial C_B(t)}{\partial t} = -k_m A\Big(C_B(t) - C_L(t, r_p)\big|_{r_p=R_p}\Big), \qquad (1)$$

here k_m is the external mass transfer coefficient, $A = \frac{mS}{V}$, m is the mass of adsorbent, S is the external surface area per mass of adsorbent, V is the volume of solution, R_p is the particle radius.

[1] V. Russo, R. Tesser, M. Trifuoggi, M. Giugni and M. Di Serio. A dynamic intraparticle model for fluid-solid adsorption kinetics. *Computers & Chemical Engineering.* **74**:66-74, 2015

Formulation of the problem

Mass balance for the liquid and solid in the particle:

$$\varepsilon \frac{\partial C_L(t,r)}{\partial t} + (1-\varepsilon)\frac{\partial C_S(t,r)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\varepsilon D_P r^2 \frac{\partial C_L(t,r)}{\partial r} + (1-\varepsilon) D_S r^2 \frac{C_S(t,r)}{C_L(t,r)} \frac{\partial C_L(t,r)}{\partial r}\right), \tag{2}$$

where ε is the particle porosity, r is the particle radial direction, D_P is the pore diffusivity and D_S is the surface diffusivity.

Formulation of the problem

Langmuir isotherm:

$$C_S(t, r_p) = C_{S,*} b \frac{C_L(t, r_p)}{1 + bC_L(t, r_p)}, \tag{3}$$

where b is a Langmuir adsorption constant and $C_{S,*}$ is the saturation solute solid concentration.

Formulation of the problem

Mass balance for the liquid and solid in the particle (2) (through the liquid phase concentration)

$$\left(\varepsilon + (1-\varepsilon)\frac{\partial C_S}{\partial C_L}\right)\frac{\partial C_L(t,r)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\left(\varepsilon D_P + (1-\varepsilon)D_S\frac{C_{S,*}b}{1+bC_L(t,r)}\right)\frac{\partial C_L(t,r)}{\partial r}\right). \tag{4}$$

Formulation of the problem

Initial and boundary conditions:

$$C_B(0) = C_B^0, \quad C_L(0,r) = C_L^0, \ \ 0 \le r \le R_p, \tag{5}$$

$$r^2 \frac{\partial C_L(t,r)}{\partial r}\Big|_{r=0} = 0, \quad r^2 \frac{\partial C_S(t,r)}{\partial r}\Big|_{r=0} = 0, \tag{6}$$

$$\begin{aligned} &\Big(\varepsilon D_P + (1-\varepsilon) D_S \frac{C_S(t,r)}{C_L(t,r)}\Big) \frac{\partial C_L(t,r)}{\partial r}\Big|_{r=R_p} \\ &\quad = k_m \big(C_B(t) - C_L(t,r)\big|_{r=R_p}\big), \end{aligned} \tag{7}$$

where k_m is the mass transfer coefficient.

Formulation of the problem

In the case of the Langmuir isotherm (3) this boundary condition is defined as:

$$\left(\varepsilon D_P + (1-\varepsilon) D_S \frac{C_{S,*} b}{1 + b C_L(t,r)}\right) \frac{\partial C_L(t,r)}{\partial r}\Big|_{r=R_p} = k_m \left(C_B(t) - C_L(t,r_p)\big|_{r=R_p}\right). \tag{8}$$

Approximation of the model

Discretization in space

We divide the spatial domain in finite volume cells with centers

$$r_j = (j - 1/2)h,\ j = 1, ..., J - 1$$

and the step size

$$h = \frac{R_p}{J - 1/2}.$$

The numerical approximation for spatial derivative:

$$\frac{\partial C_L(t, r_p)}{\partial r_p} \approx \frac{C_{L,j+1} - C_{L,j}}{h}.$$

Approximation of the model

The approximation for the mass balance in the particle for $j = 1, ..., J-1$:

$$\frac{r_{j+1/2}^3 - r_{j-1/2}^3}{3}\left(\varepsilon + (1-\varepsilon)\frac{bC_{S,*}}{(1+bC_{L,j})^2}\right)\frac{\partial C_{L,j}(t)}{\partial t} \tag{9}$$

$$= r_{j+1/2}^2\left(\varepsilon D_P + (1-\varepsilon)D_S\frac{bC_{S,*}}{1+0.5b(C_{L,j+1}+C_{L,j})}\right)\frac{C_{L,j+1}-C_{L,j}}{h}$$

$$- r_{j-1/2}^2\left(\varepsilon D_P + (1-\varepsilon)D_S\frac{bC_{S,*}}{1+0.5b(C_{L,j}+C_{L,j-1})}\right)\frac{C_{L,j}-C_{L,j-1}}{h}.$$

Approximation of the model

The approximation for the boundary condition (8):

$$\frac{h}{2} r_J^2 \left(\varepsilon + (1-\varepsilon) \frac{bC_{S,*}}{(1+bC_{L,J})^2} \right) \frac{\partial C_{L,J}(t)}{\partial t} = -r_{J-1/2}^2 \times \left(\varepsilon D_p + (1-\varepsilon) D_S \frac{bC_{S,*}}{1+0.5b(C_{L,J}+C_{L,J-1})} \right) \frac{C_{L,J}-C_{L,J-1}}{h} + r_J^2 k_m (C_B(t) - C_{L,J}). \tag{10}$$

Approximation of the model

Discrete equation for the bulk concentration C_B:

$$\frac{\partial C_B(t)}{\partial t} = -k_m A(C_B(t) - C_{L,J}(t)) \tag{11}$$

The linearized and normalized mathematical model

Dimensionless variables

$$r = R_p \bar{r}, \quad t = \frac{cR_p^2}{D}\bar{t}, \quad 0 < \bar{r} < 1, \quad 0 < \bar{t} < \bar{T} = \frac{TD}{cR_p^2}, \tag{12}$$

$$c = \varepsilon + (1 - \varepsilon) f'(C_L).$$

The equilibrium isotherm

$$C_S(\bar{t}, \bar{r}) = f(C_L(\bar{t}, \bar{r}))$$

The linearized and normalized mathematical model

The combined diffusion coefficient is

$$D = \varepsilon D_p + (1-\varepsilon) D_s \frac{f(C_L)}{C_L}.$$

Mass transport parameters α and β are

$$\alpha = \frac{A k_m c R_p^2}{D}, \quad \beta = \frac{k_m R_p}{D}. \tag{13}$$

The linearized and normalized mathematical model

The simplified adsorption kinetics model

$$\frac{\partial C_B(\bar{t})}{\partial \bar{t}} = -\alpha(C_B(\bar{t}) - C_L(\bar{t},1)), \quad 0 < t < \bar{T}, \tag{14}$$

$$\frac{\partial C_L(\bar{t},\bar{r})}{\partial \bar{t}} = \frac{1}{\bar{r}^2}\frac{\partial}{\partial \bar{r}}\left(\bar{r}^2\frac{\partial C_L(\bar{t},\bar{r})}{\partial \bar{r}}\right), \quad 0 < \bar{r} < 1, \tag{15}$$

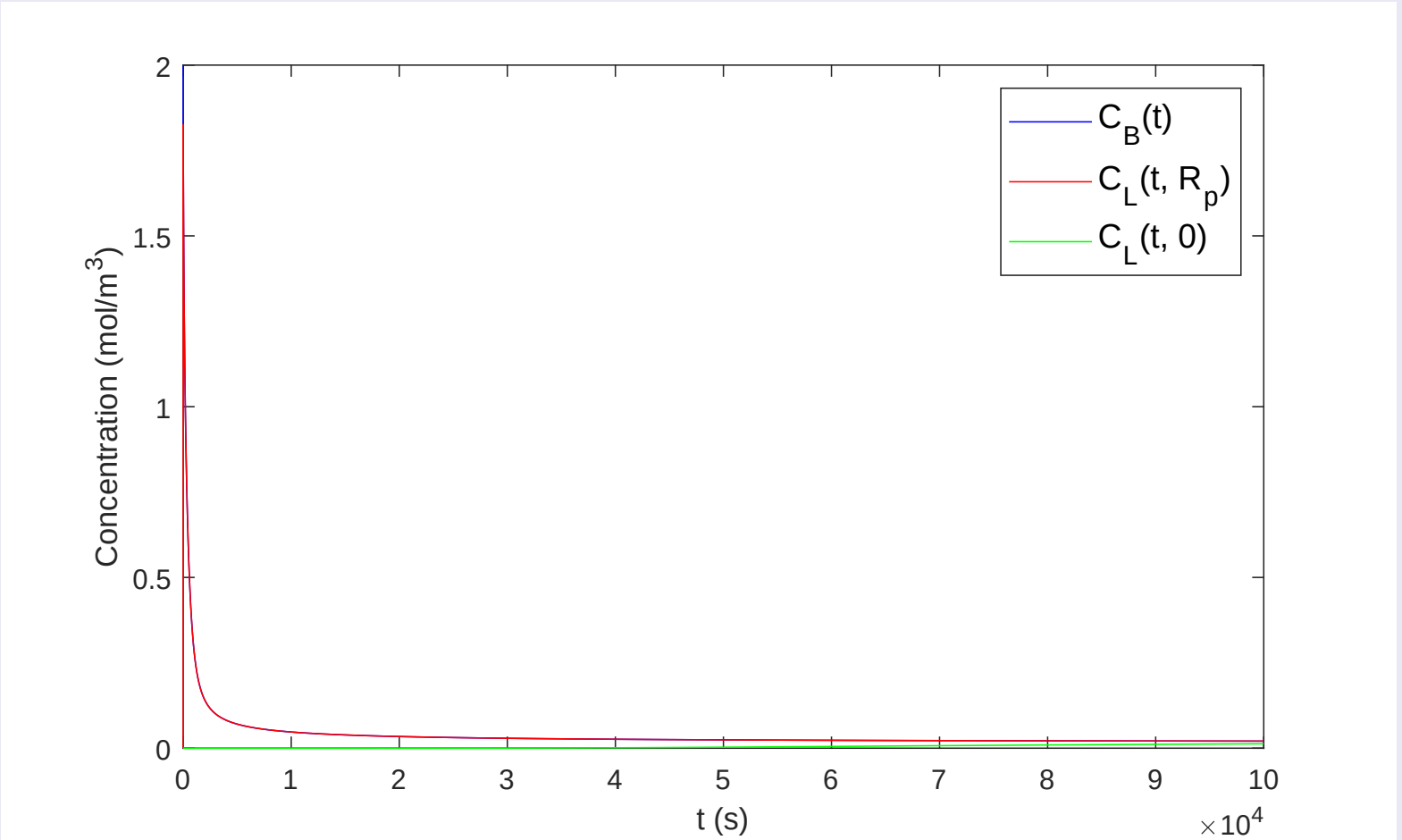
Initial and boundary conditions

$$\bar{r}^2\frac{\partial C_L(\bar{t},\bar{r})}{\partial \bar{r}}\Big|_{\bar{r}=0} = 0, \quad \frac{\partial C_L(\bar{t},\bar{r})}{\partial \bar{r}}\Big|_{\bar{r}=1} = \beta(C_B(\bar{t}) - C_L(\bar{t},1)), \tag{16}$$

$$C_B(0) = C_B^0, \quad C_L(0,\bar{r}) = C_L^0, \ \ 0 \leqslant \bar{r} \leqslant 1. \tag{17}$$

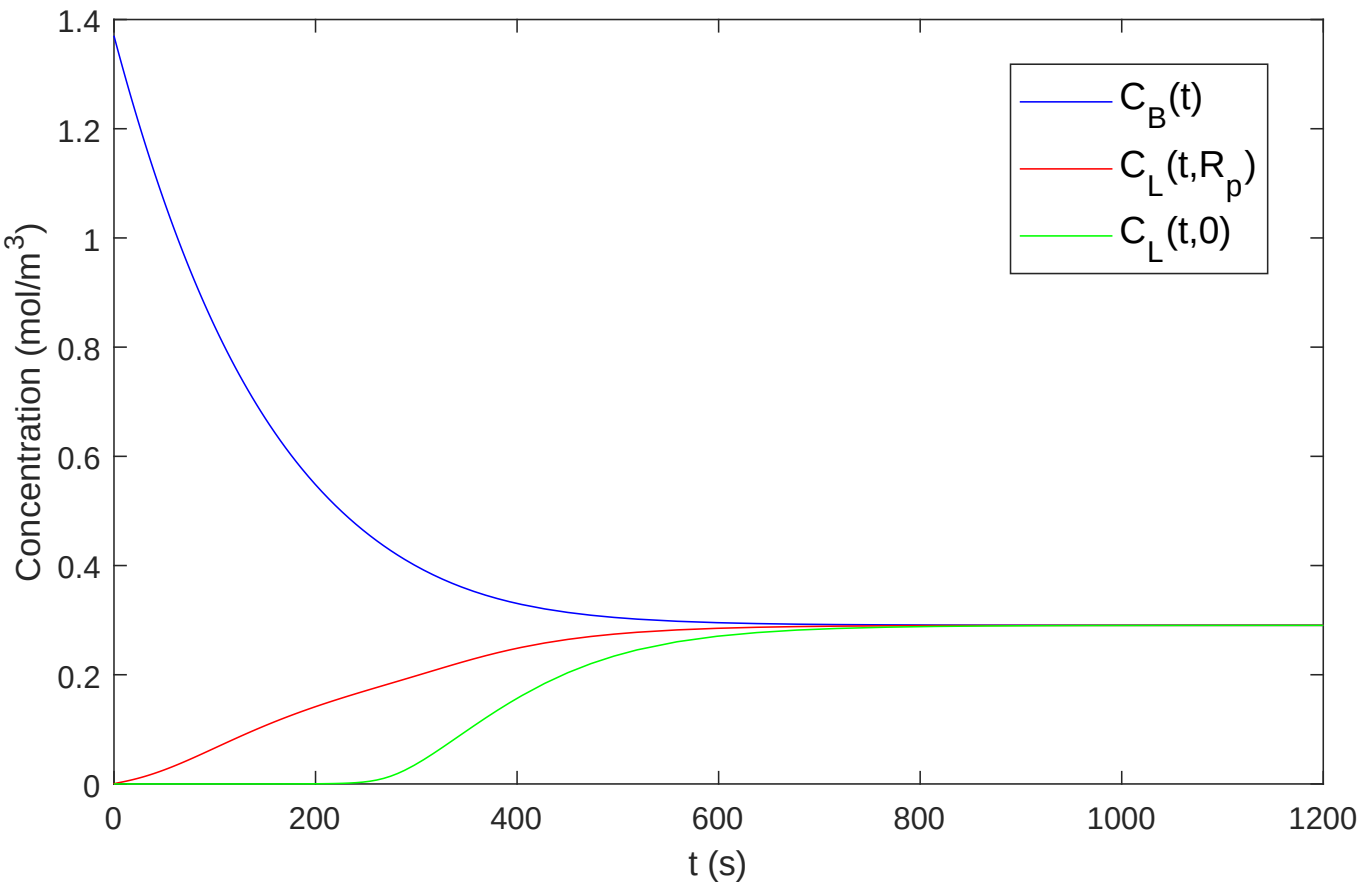
The results of numerical calculations

Concentrations for the data reported in the article by V. Russo, R. Tesser, M. Trifuoggi, M. Giugni and M. Di Serio. 2015



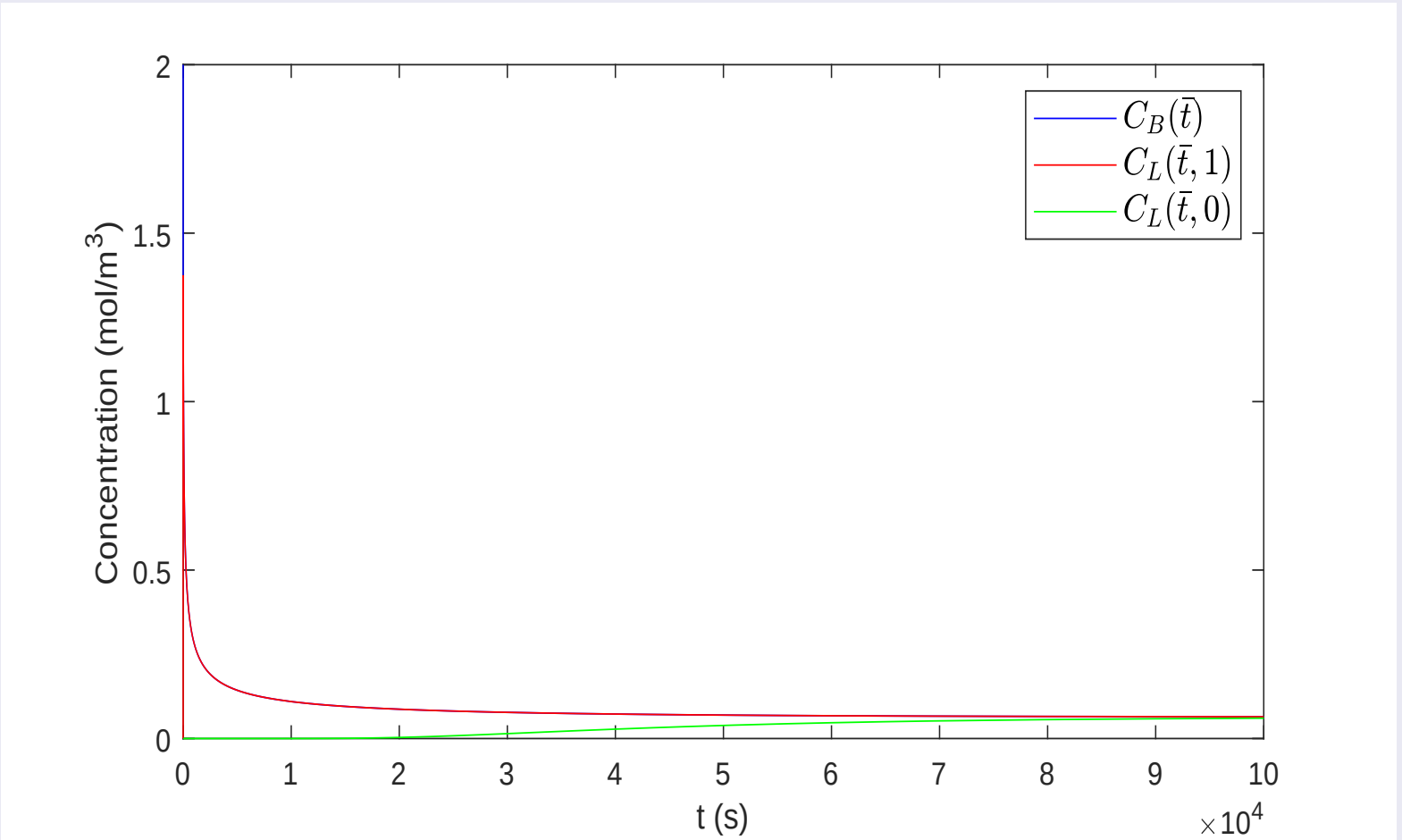
The results of numerical calculations

Concentrations for the data reported in the article by P. R. Souza, G. L. Dotto and N. P. G. Salau. 2017



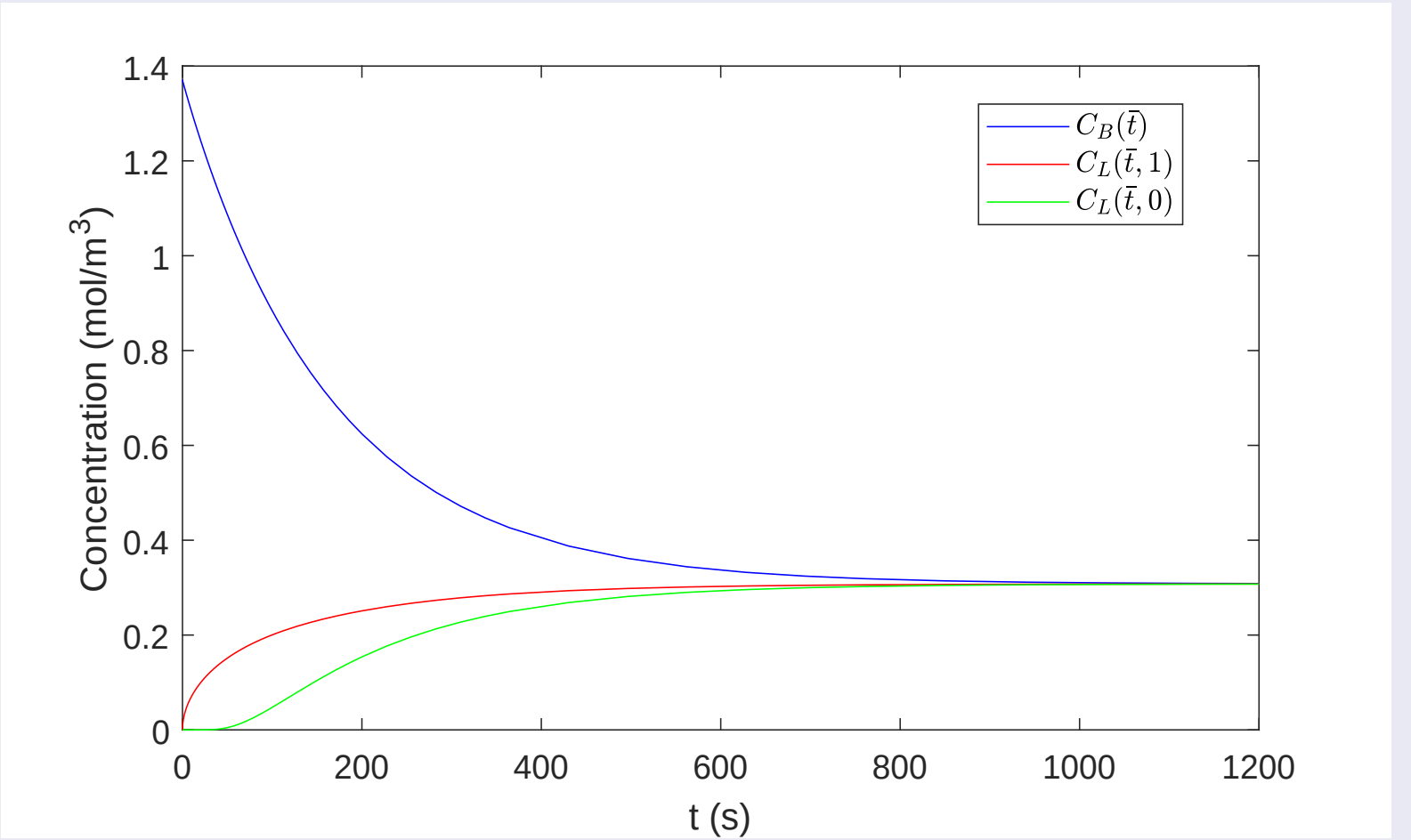
The results of numerical calculations

Dynamics of the concentrations obtained from the simplified model for the data reported by V. Russo et al. (2015)



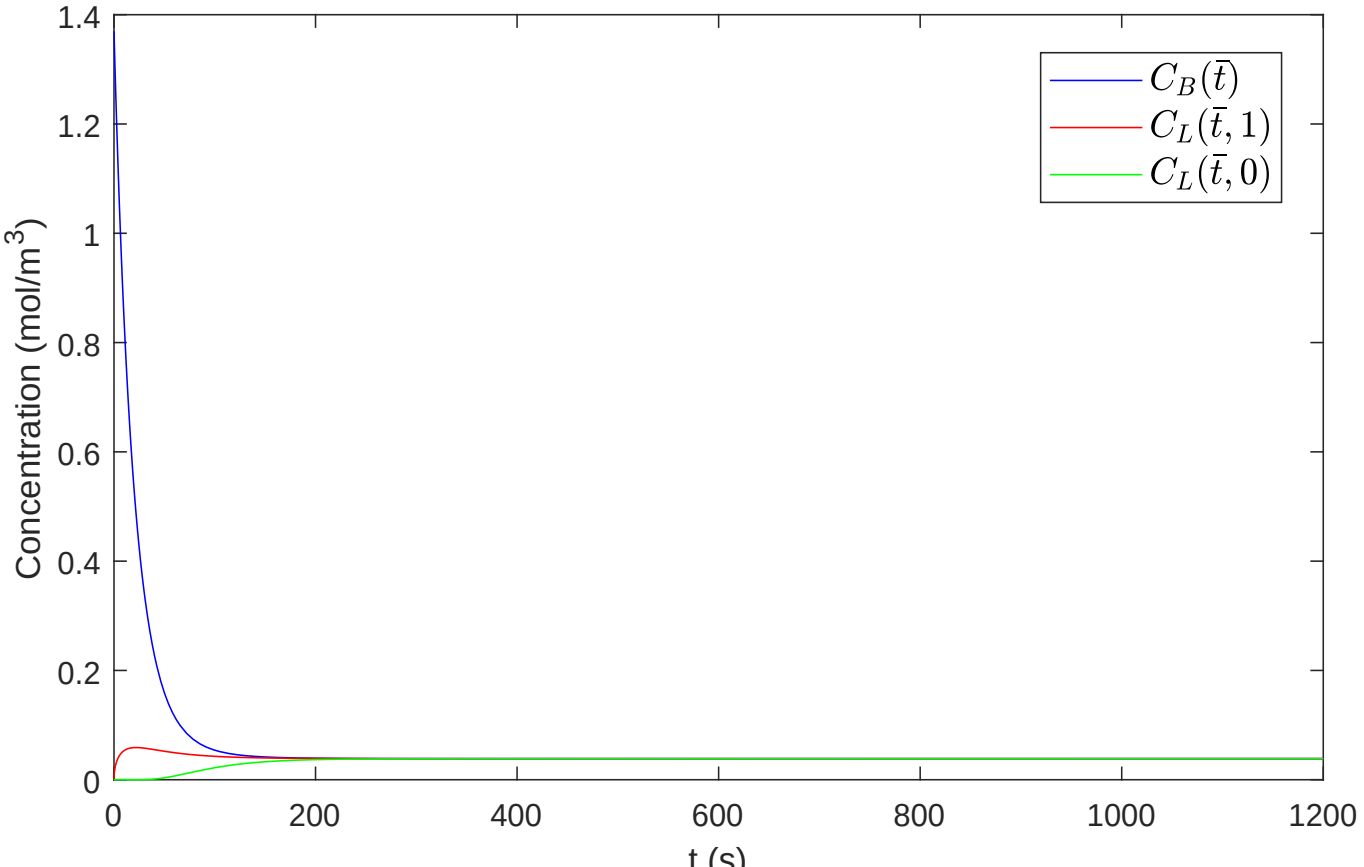
The results of numerical calculations

Dynamics of the concentrations obtained from the simplified model for the data reported by P. R. Souza et al. (2017)



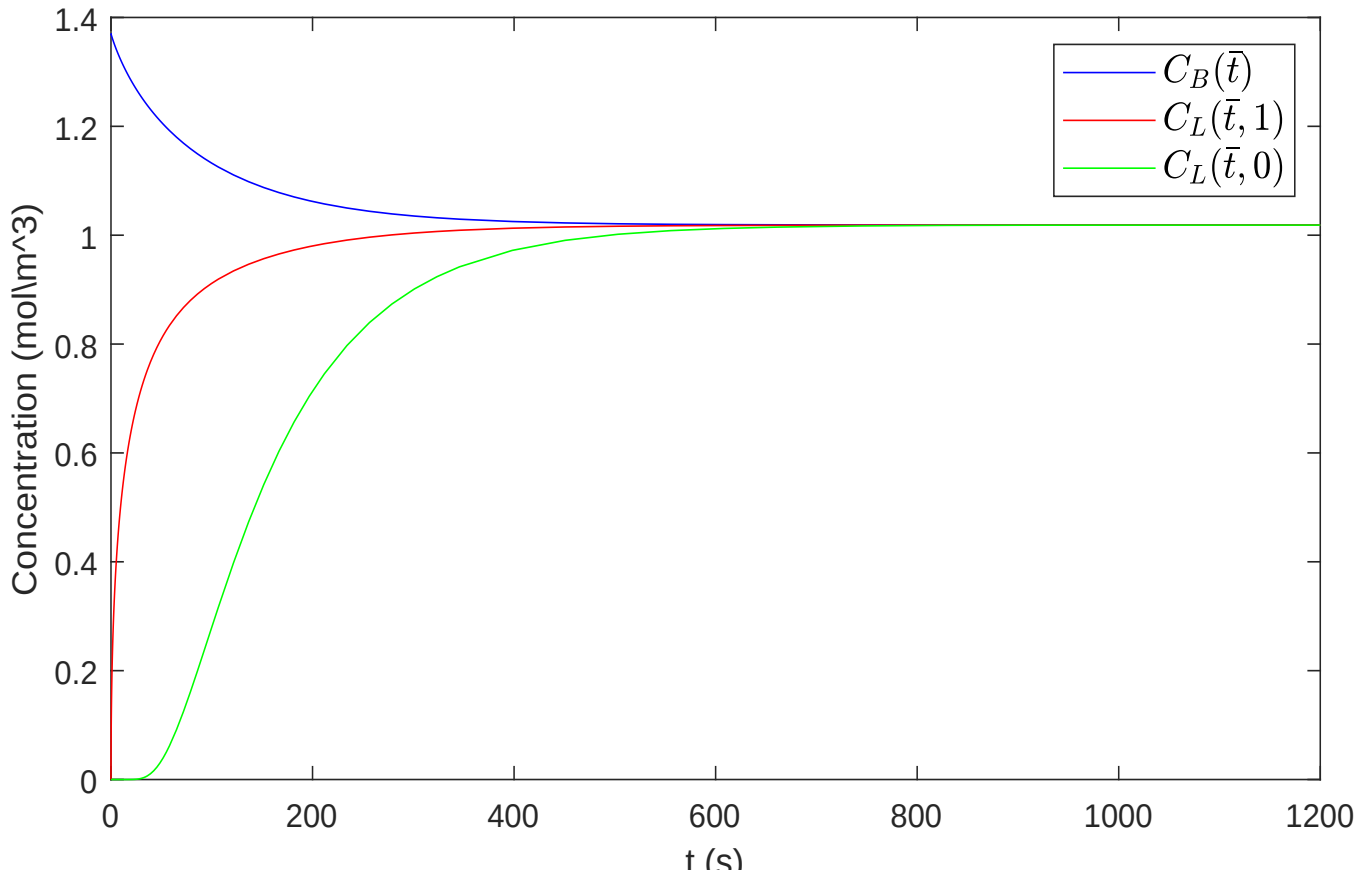
The results of numerical calculations

Dynamics of the concentrations obtained from the simplified model ($\alpha = 41.4$, $\beta = 0.4$) for the data reported by P. R. Souza et al. (2017)



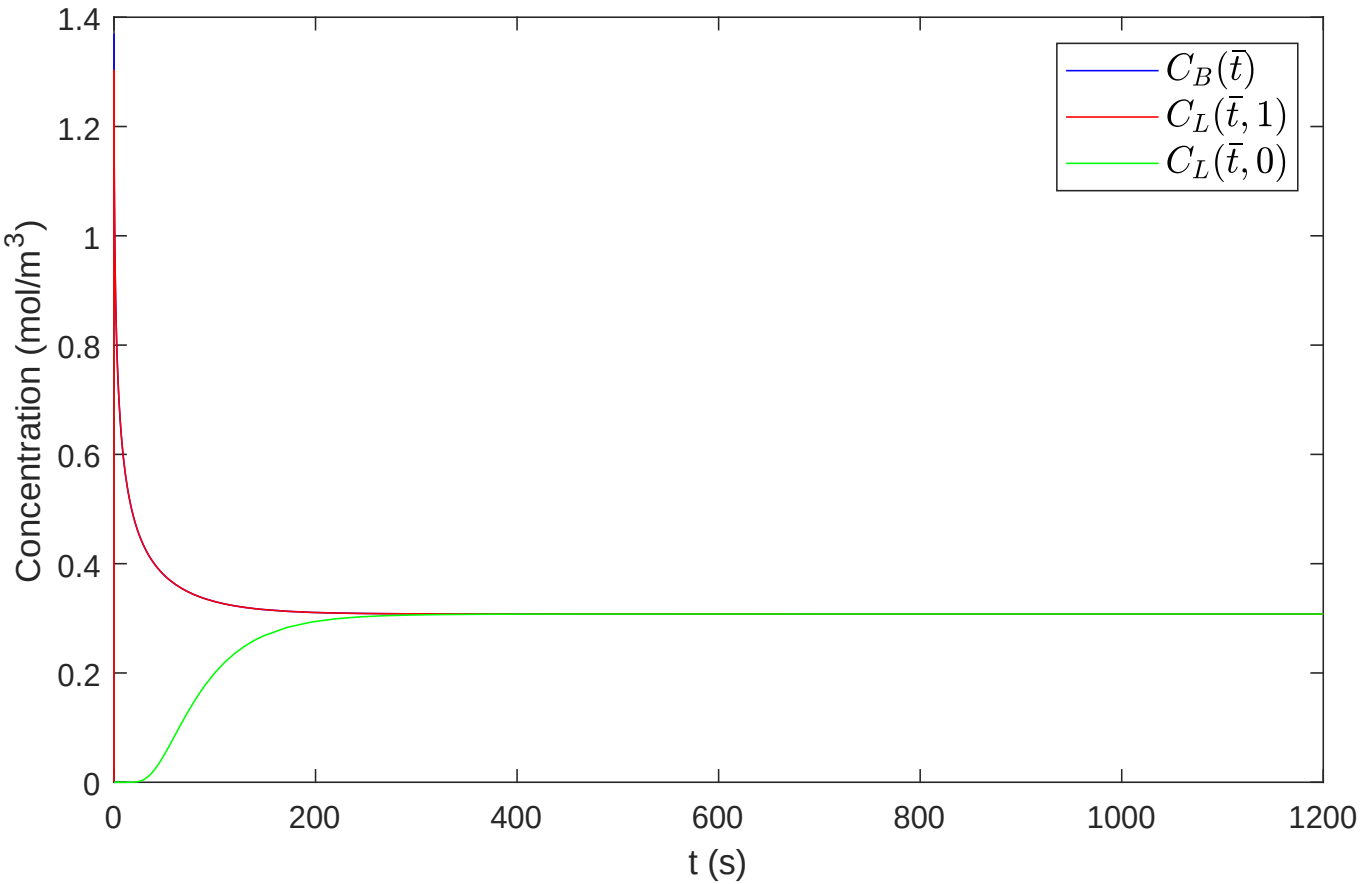
The results of numerical calculations

Dynamics of the concentrations obtained from the simplified model ($\alpha = 4.14$, $\beta = 4$) for the data reported by P. R. Souza et al. (2017)



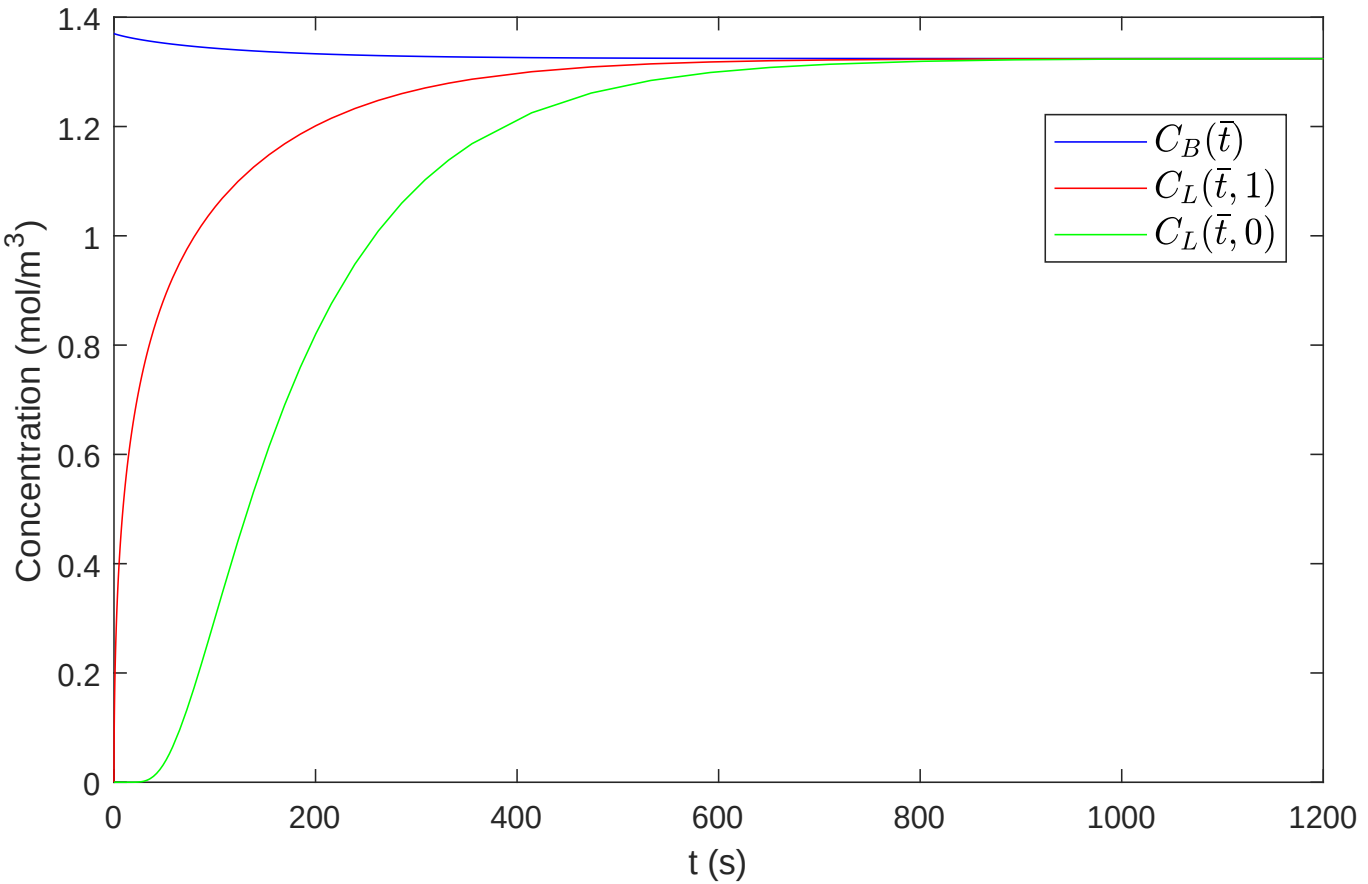
The results of numerical calculations

Dynamics of the concentrations obtained from the simplified model ($\alpha/\beta \approx 10$) for the data reported by P. R. Souza et al. (2017)



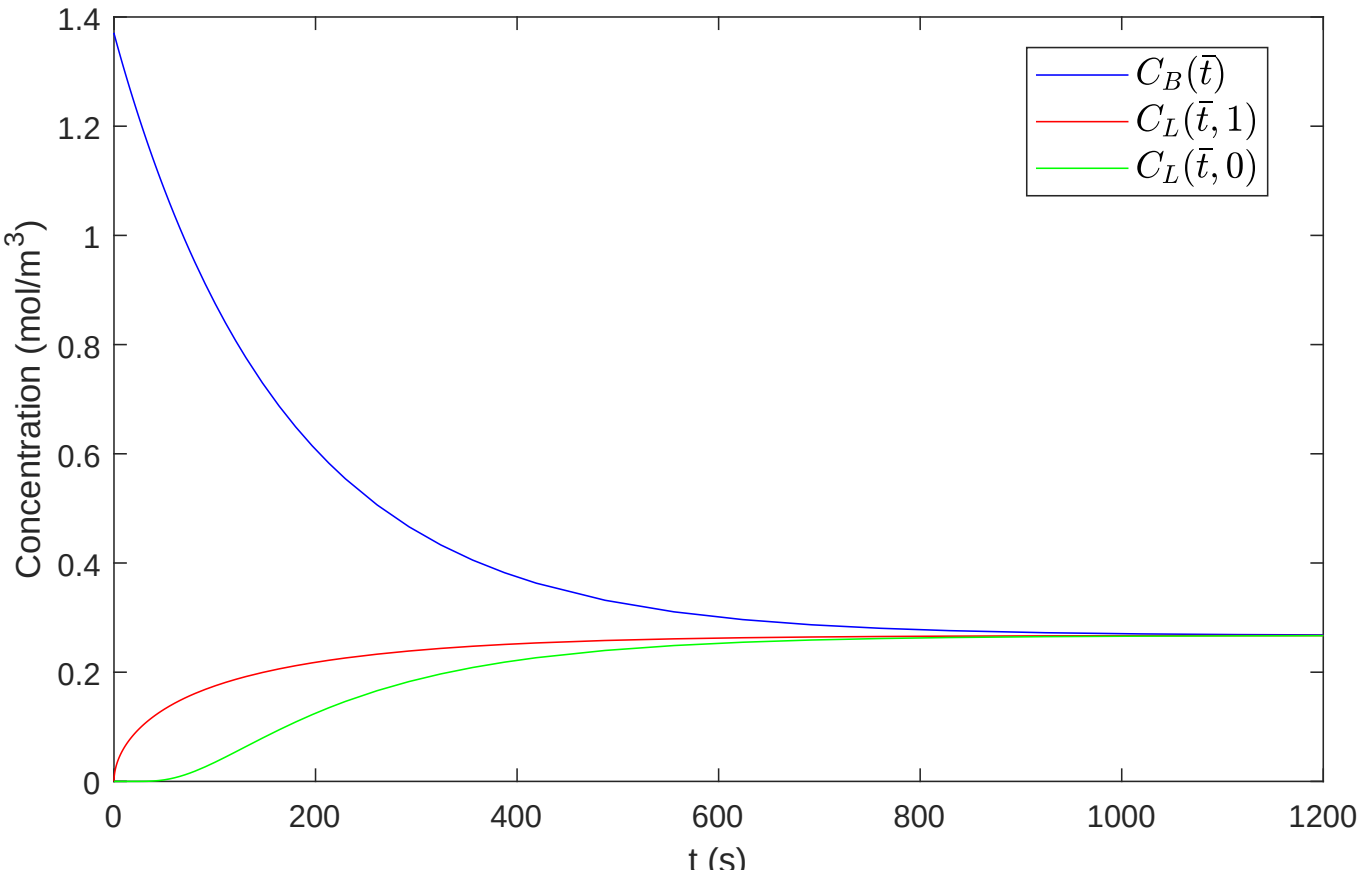
The results of numerical calculations

Dynamics of the concentrations obtained from the simplified model ($\alpha/\beta \approx 0.1$) for the data reported by P. R. Souza et al. (2017)



The results of numerical calculations

Dynamics of the concentrations obtained from the simplified model (with Langmuir isotherm) for the data reported by P. R. Souza et al. (2017)



Conclusions

1. The sensitivity of the solution with respect of main physical system parameters is analyzed using the simplified model.
2. The results obtained with the linearized and normalized mathematical model are compared with the simulations done for a full nonlinear mathematical model.
3. The results of the numerical experiments show that we can predict the main trend of the adsorption process using the proposed simplified linear model.

Dėkoju už dėmesį!