Filippov dynamical systems

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1 Introduction

In many problems that arise in chemical engineering, a discontinuity may appear. The discontinuity may be a result of external activity, for example it is obtained by adding of a control member, or it can be directly a natural part of a model under consideration - this is the case of the closed dynamical system, more precisely an ideal gas–liquid system, which is studied in this work.

The theory of Filippov systems is applied to this system. Dependence of the solution on a given parameter set is studied namely, the dependence of the solution on the molar inflow of the gas. It is shown that the local sliding bifurcations appear on the discontinuity boundary.

All simulations are performed by making use of Maple. For numerical computations, package AUTO is used.

2 An ideal gas–liquid system

Let us start with a simple system shown in Fig. 1. Feed, that consists of a liquid and gas, is sent to the closed tank, that has only one outlet tube. If the level of liquid is above the outlet tube opening, see Fig. 1 (a), the liquid comes out of the tank. Otherwise the gas comes out, see Fig. 1 (b).

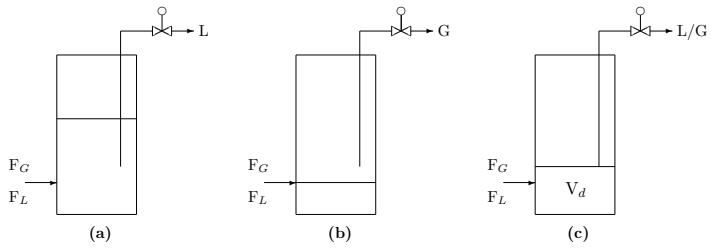

Fig. 1. An ideal gas–liquid system.

The following assumptions help to simplify the model.

1. Feed consists of an ideal gas G and an incompressible liquid L.
2. The gas and the liquid do not react.
3. The liquid has negligible vapour pressure at the operating conditions.
4. The gas does not dissolve in the liquid at the operating conditions.

5. In the liquid, there are no gas bubbles that may be leaving the tank.

6. The valve dynamics are ignored.

7. The flow rate through the valve is proportional to the diference of the tank pressure and the outlet pressure.

8. The temperature, feed flow rates, outlet pressure and the valve opening are all constant.

Let F_L and F_G be the molar inflow rate of liquid and gas, respectively. Let G and L be the molar outflow rate of liquid and gas, respectively. The following model equations of the ideal gas–liquid system were proposed by Moudgalya and Ryali [1].

If $M_L/\rho_L > V_d$ (liquid model), then:

$$\begin{aligned} \frac{\mathrm{d}\,M_G}{\mathrm{d}\,t} &= F_G, & (1)\\ \frac{\mathrm{d}\,M_L}{\mathrm{d}\,t} &= F_L - L, & (2)\\ M_G\frac{\mathrm{R}T}{P} + \frac{M_L}{\rho_L} &= V, & (3)\\ L &= k_L x(P - P_{out}). & (4) \end{aligned}$$

If $M_L/\rho_L < V_d$ (gas model), then:

$$\begin{aligned} \frac{\mathrm{d}\,M_G}{\mathrm{d}\,t} &= F_G - G, & (5)\\ \frac{\mathrm{d}\,M_L}{\mathrm{d}\,t} &= F_L, & (6)\\ M_G\frac{\mathrm{R}T}{P} + \frac{M_L}{\rho_L} &= V, & (7)\\ G &= k_G x(P - P_{out}). & (8) \end{aligned}$$

M_L and M_G are the molar hold-ups of liquid and gas, ρ_L is the molar density, T is the absolute temperature, P and P_{out} are the pressure in the tank and in the outlet, respectively. R is the gas constant, V is the volume of the tank and V_d denotes the volume of the liquid below a outlet tube opening in the tank, as is shown on Fig. 1 (c). The valve opening is denoted by x, $0 < x \leq 1$. The valve coefficients are k_L for liquid and k_G for gas flow.

F_G and F_L have to be positive constant in time. The valve opening x is constant, too.

From equations (1) and (6), one can see that dynamical system given by equations (1)–(4) and dynamical system given by equations (5)–(8) have no standard equilibrium. But are there any sliding equilibria?
From equation (3) we derive an expression for P,

$$P = \frac{M_G\mathrm{R}T}{V - M_L/\rho_L}. \quad (9)$$

Substituting this P into equations (4) and (8), we obtain

$$L = k_L x\left(\frac{M_G\mathrm{R}T}{V - M_L/\rho_L} - P_{out}\right) \quad (10)$$

and

$$G = k_G x \left(\frac{M_G \mathrm{R} T}{V - M_L/\rho_L} - P_{out} \right). \tag{11}$$

Equations (1), (2), (5) and (6) with (10) and (11) define Filippov system $\mathcal{F}$,

$$\mathcal{F}: \quad \frac{\mathrm{d}}{\mathrm{d}\, t} \begin{pmatrix} M_G \\ M_L \end{pmatrix} = \begin{cases} \mathbf{f}^{(1)}(M_G, M_L) \ , & (M_G, M_L) \in S_1, \\ \mathbf{f}^{(2)}(M_G, M_L) \ , & (M_G, M_L) \in S_2, \end{cases} \tag{12}$$

where

$$\mathbf{f}^{(1)} = \begin{pmatrix} F_G - k_G x \left(\dfrac{M_G \mathrm{R} T}{V - M_L/\rho_L} - P_{out} \right) \\ F_L \end{pmatrix}, \tag{13}$$

$$\mathbf{f}^{(2)} = \begin{pmatrix} F_G \\ F_L - k_L x \left(\dfrac{M_G \mathrm{R} T}{V - M_L/\rho_L} - P_{out} \right) \end{pmatrix}, \tag{14}$$

$$\begin{aligned} S_1 &= \{(M_G, M_L) \in \mathbb{R}^2 : \varphi(M_G, M_L) < 0\}, \\ S_2 &= \{(M_G, M_L) \in \mathbb{R}^2 : \varphi(M_G, M_L) > 0\}. \end{aligned} \tag{15}$$

The function $\varphi(M_G, M_L)$ is defined as

$$\varphi(M_G, M_L) = M_L - \rho_L V_d. \tag{16}$$

The state space of the system $\mathcal{F}$, denoted as S, is divided into two regions S_1 and S_2. The region S_1 corresponds to the case, when the gas is leaving a vessel. S_2 corresponds to the case, when the liquid is leaving a vessel. Both S_1 and S_2 can be again divided into two regions, each of them with the different qualitative behavior of the vector field. The system behavior is shown on Fig. 2 and Fig. 3 (for more details see [1]).

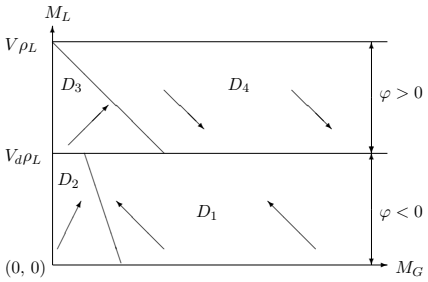

Fig. 2: The splitting of the state plane S with the qualitative directions of orbits for $M_G^L > M_G^G$

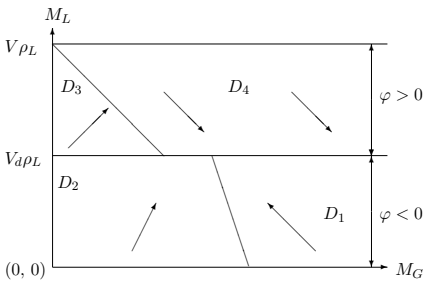

Fig. 3: The splitting of the state plane S with the qualitative directions of orbits for $M_G^L < M_G^G$

Fig. 4 show the results gained from the simulations. Parameters used for the simulations are in Table 1.

Table 1: Parameters used for the simulation of system $\mathcal{F}(F_G)$:

F_L (mol/s)	2.5
ρ_L (mol/l)	50
V (l)	10
V_d (l)	5
$T(K)$	300
P_{out} (atm)	1
R (l atm K^{-1} mol^{-1})	0.0820574587
x	0.1
k_L	1
k_G	1

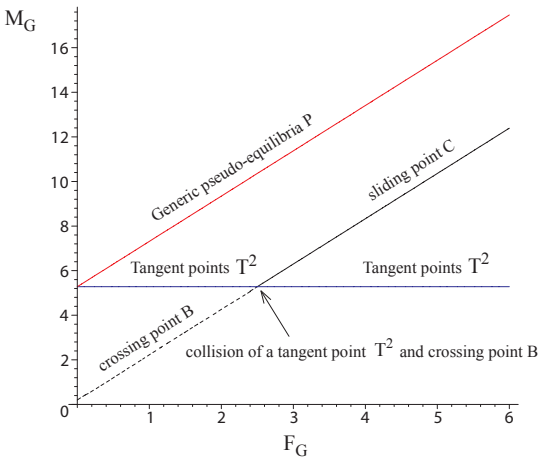

Fig. 4: Bifurcation diagram

3 Conclusion

One can see from Fig. 4, there is no possibility to collision of sliding point C and the generic pseudo-equilibrium P, because the related lines are parallel. But what if that parallelism disappear? This would require the modification of the model equations, and the ideal gas-liquid system become the non-ideal gas-liquid system.

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Computational experience with modified conjugate gradient methods for unconstrained optimization

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Conjugate gradient methods are widely used for unconstrained minimization of function $F : R^n \to R$. These methods generate a sequence of points $\{x_i\} \subset R^n$ by the formula

$$x_{i+1} = x_i + \alpha_i s_i, \quad i \in N,$$

where $s_i \in R^n$ is a direction vector satisfying a descent condition $s_i^T g(x_i) < 0$ ($g(x_i)$ is a gradient of the function F at a point x_i), and $\alpha_i > 0$ is a step-length chosen to satisfy the generalized Wolfe conditions

$$F(x_{i+1}) - F(x_i) \leq \varepsilon_1 \alpha_i s_i^T g(x_i), \tag{1}$$

$$\varepsilon_2 s_i^T g(x_i) \leq s_i^T g(x_{i+1}) \leq \varepsilon_3 |s_i^T g(x_i)|, \tag{2}$$

with $0 < \varepsilon_1 < \varepsilon_2 < 1$ and $\varepsilon_3 \geq 0$, are satisfied. The direction vector s_i is chosen in such a way that

$$s_1 = -g_1 \quad \text{and} \quad s_{i+1} = -g_{i+1} + \beta_i s_i \quad \text{for} \quad i \in N, \tag{3}$$

where parameter β_i is chosen so that the direction vectors s_i, $1 \leq i \leq n$, were mutually conjugate if we apply this method to a strictly convex quadratic function.

There is six basic conjugate gradient methods:

$$\beta_i^{HS} = \frac{y_i^T g_{i+1}}{y_i^T s_i}, \quad \beta_i^{PR} = \frac{y_i^T g_{i+1}}{g_i^T g_i}, \quad \beta_i^{LS} = \frac{y_i^T g_{i+1}}{|g_i^T s_i|} \tag{4}$$

(HS – Hestenes and Stiefel [4], PR – Polak and Ribiére [8], LS – Liu and Storey [5]),

$$\beta_i^{DY} = \frac{g_{i+1}^T g_{i+1}}{y_i^T s_i}, \quad \beta_i^{FR} = \frac{g_{i+1}^T g_{i+1}}{g_i^T g_i}, \quad \beta_i^{CD} = \frac{g_{i+1}^T g_{i+1}}{|g_i^T s_i|} \tag{5}$$

(DY – Dai and Yuan [1], FR – Fletcher and Reeves [3], CD – conjugate descent [2]). These methods can be divided into two groups by the numerator used. Methods of the first group (HS, PR, LS) are more suitable for practical computations but they are globally convergent only with necessary modifications. Methods of the second group (DY, FR, CD) are globally convergent under certain assumptions (put on a choice of a step-length) but the direction vectors stay worse conjugate if a step-length is inexact and the minimized function is not quadratic.

Relation (3) can be variously modified in order to improve effectiveness of conjugate gradient methods. One such possibility, is used in the following theorem (see also [9]).

Theorem 1 *Consider modified methods DY, FR, CD given by the rule*

$$s_1 = -g_1 \quad \textit{and} \quad s_{i+1} = -\vartheta_i g_{i+1} + \beta_i s_i \quad \textit{for} \quad i \in N, \tag{6}$$

where the values β_i^{DY}, β_i^{FR}, β_i^{CD} are determined by (5) and

$$\vartheta_i^{DY} = \frac{y_i^T s_i}{y_i^T s_i} = 1, \quad \vartheta_i^{FR} = \frac{y_i^T s_i}{g_i^T g_i}, \quad \vartheta_i^{CD} = \frac{y_i^T s_i}{|g_i^T s_i|}.$$

If a function $F : R^n \to R$ is bounded from below and has bounded second order derivatives and if we use generalized Wolfe conditions (1)–(2) with $0 < \varepsilon_1 < \varepsilon_2 < 1$ and $0 \leq \varepsilon_3 < \infty$ during a choice of a step-length, then these methods are globally convergent.

Relation (6) can also be used to improve conjugation of direction vectors in methods PR and LS.

Theorem 2 *Consider modifications of methods HS, PR, LS given by the rule*

$$s_1 = -g_1 \quad and \quad s_{i+1} = -\vartheta_i g_{i+1} + \beta_i s_i \quad for \quad i \in N,$$

where the values β_i^{HS}, β_i^{PR}, β_i^{LS} *are determined by (4) and*

$$\vartheta_i^{HS} = \frac{y_i^T s_i}{y_i^T s_i} = 1, \quad \vartheta_i^{PR} = \frac{y_i^T s_i}{g_i^T g_i}, \quad \vartheta_i^{LS} = \frac{y_i^T s_i}{|g_i^T s_i|}.$$

Then

$$y_i^T s_{i+1} = 0 \quad for \quad i \in N.$$

Efficiency of conjugate gradient methods can be improved by suitable restarts. It is very convenient to test a uniform descent condition $-g_{i+1}^T s_{i+1} \geq \varepsilon_0 \|g_{i+1}\| \|s_{i+1}\|$, where $\varepsilon_0 > 0$ is a small number. Such a modified conjugate gradient method is globally convergent without occurring restarts too often. If methods (5) are used, then it is suitable to test a conjugation of direction vectors. In this case, we perform restart if the condition

$$y_i^T s_{i+1} \leq \eta_1 \|s_{i+1}\| \|y_i\| \tag{7}$$

does not hold, where the value η_1 depends on the Wolfe conditions chosen.

Various variants of conjugate gradient methods were tested by using a collection of 60 test functions with 1000 variables. Results of these tests imply several conclusions:

- It is advantageous to use the strong Wolfe conditions with $\varepsilon_2 = \varepsilon_3 = 10^{-1}$ at a realization of conjugate gradient methods, particularly methods HS, PR, LS, and their modifications.
- In case that we use the strong Wolfe conditions, method HS gives the best results. Modification (6) improve efficiency of methods HS, PR, LS.
- In case that we use the strong Wolfe conditions, methods DY, FR, CD give worse results than methods HS, PR, LS. The properties of methods DY, FR, CD are considerably improved if they are restarted each time condition (7) is not fulfilled.
- In general, modification (6) considerably improve efficiency of methods FR and CD. This observation is independent of a choice of the Wolfe conditions which confirms a significance of Theorem 1. Moreover, if we use conjugation test (7), then the resulting methods are competitive with the best modifications of methods HS and PR.
- In case that we use the weak Wolfe conditions with $\varepsilon_2 = 0.9$ and $\varepsilon_3 = \infty$, method PR gives better results than methods HS (particularly if we use modification (6)).

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An analytical study of the effect of hydrodynamic mixing on the photosynthetic microorganism growth

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1 Introduction

The photosynthetic microorganism growth description is usually based on the so-called microbial kinetics, i.e. on the lumped parameter models (LPM) describing the photosynthetic response in small cultivation systems with a homogeneous light distribution [3, 6]. However, there is an important phenomenon, the so-called flashing light enhancement, which demands some other model than it residing in the artificial connection between the steady state kinetic model and the empiric one describing the photosynthetic productivity under fluctuating light condition. Nevertheless, even having an adequate dynamical LPM of microorganism growth, see e.g. phenomenological model of so-called photosynthetic factory [4, 5], another serious difficulty resides in the description of the microalgal growth in a photobioreactor (PBR), i.e. in a distributed parameter system.

In order to develop the distributed parameter model (DPM) of a microorganism growth, two main approaches for transport and bioreaction processes modelling are usually chosen: (i) Eulerian infinitesimal, and (ii) Eulerian multicompartmental. While the Eulerian infinitesimal approach, leading to the partial differential equations (PDE), is an usual way to describe transport and reaction systems, the multicompartmental modelling framework, resulting in a system of ordinary differential equations (ODE), is mostly used in the process engineering area. This second approach, based on balance equation among compartments with finite control volume, has been recently treated by Bezzo *et al.* [2]. The authors presented there a rigorous mathematical framework for constructing *hybrid multicompartment/CFD models*. *Hybrid* there means that the fluid flow description is resolved by a CFD code, and does not make a part of the ODE system of governing equations.

In the sequel, we adopt the first approach aiming to clarify in an analytical manner the role of hydrodynamic mixing, or more precisely, the mechanism of the photosynthetic microorganism growth enhancement due to the microbial cell transport by radial dispersion. Nevertheless, in the future work, our results should serve to develop a numerical scheme for setting up the optimal compartment size in the multicompartment/CFD models.

2 Model development

Accordingly to [7], the transport equation for microbial cells (concentration or cell density c) as the function of spatial coordinates and time gets the next form:

$$\frac{\partial c}{\partial t} + \nabla \cdot (\vec{v}c) - \nabla \cdot (D_e \nabla c) = R \ , \tag{1}$$

where R is the source term (representing microbial growth, unit: cell $\mathrm{m}^{-3}\mathrm{s}^{-1}$), $\vec{v}$ represents the velocity field, and D_e is the dispersion coefficient, which corresponds to diffusion coefficient in

microstructure description and becomes mere empirical parameter suitably describing mixing in the system. D_e is influenced by the molecular diffusion and velocity profile. When mixing is mainly caused by the turbulent micro-eddies, the phenomenon is called the turbulent diffusion and a *turbulent diffusion coefficient* is introduced e.g. in [1]. The reaction obviously depends on some variables, usually called as substrates. For our special case of photosynthetic growth in a PBR, the role of only one limiting substrate (the nutrients are supposed to be present in a sufficient amount, i.e. they do not limit the growth) fulfills the irradiance, in other words, an external forcing input u. Moreover we suppose the rectangular PBR geometry illuminated from one side, i.e. the irradiance level is decreasing from the PBR wall to PBR core. Thus, the PBR volume (our computational domain) can be divided into layers with the same irradiance level, transforming the 3D problem into the one-dimensional. Consequently, the description of cell motion in direction of light gradient, i.e. perpendicular to PBR wall and at the same time perpendicular to the direction of convective flow, is of most interest. This motion is caused by the just mentioned turbulent diffusion. Furthermore, we can introduce the dimensionless spatial coordinate x by $r := xL$, where L is the the PBR length in direction of light gradient, and the dimensionless dispersion coefficient $p(x)$ by $D_e := p(x)\ D_0$, where D_0 is a constant with some characteristic value, unit: $\mathrm{m^2 s^{-1}}$. Furthermore we introduce the dimensionless concentrations as $y := \frac{c}{c_m}$, $y_{ss} := \frac{c_{ss}}{c_m}$, where c_m is a characteristic (e.g. maximal) concentration of c.

Based on photosynthetic factory model [4, 5] we have for the reaction term R the relation

$$R = -k\ (c - c_{ss})\ , \tag{2}$$

where k is the rate (unit: $\mathrm{s^{-1}}$) associated with the dynamic process by which is the concentration approaching to some value c_{ss} depending only on the external input u.

As we are interested on the steady state solution of (1), i.e. $\frac{\partial c}{\partial t} = 0$, we obtain

$$-\left[p(x)y'\right]' + q(x)\ y = q(x)\ y_{ss}, \quad y'(0) = 0,\ y'(1) = 0\ , \tag{3}$$

where $q(x) := \frac{k(u(x))\ L^2}{D_0}$.

If we define k_0 as follows: $k := k_A(u(x))\ k_0$, then the characteristic number, so-called *Damköhler number* of second type, could be defined as $Da_{II} := \frac{k_0 L^2}{D_0}$, and the the dependence of the solution of (3) on Da_{II} could be studied.

3 Analytical solution

In fact, we do not need the solution of equation (3) in form $y = y(x)$, but we want to find the mean value of y in the interval $x \in [0.1]$, i.e. to compute the expression $\int_0^1 y(x)\ \mathrm{d}x$. Based on [8], the boundary value problem is transformed into the related initial value problem. It consists in finding solutions of two homogeneous equations, two differential equations with the right-hand side and computing a solution of a system of two algebraic equations. The result is that we obtain a function value and its derivative in an arbitrary point. The original differential equation with boundary conditions is thus transformed into a differential equation with an initial condition. As we need only a solution in several points, we can apply the above procedure repeatedly. Finally, the value $\int_0^1 y(x)\ \mathrm{d}x$ is obtained by a suitable numerical method.

4 Conclusion

An analytical study of the effect of hydrodynamic mixing on the photosynthetic microorganism growth is presented. The spatio-temporal dependence of microorganism cell concentration in our system of interest, i.e. in the photobioreactor (PBR), is reduced into a one-dimensional problem described by the second-order non-homogeneous ordinary differential equation with the non-linear continuous function on the right hand side. The impermeability of the PBR's walls imposes the Neumann boundary condition. The related initial value method is applied, and for a special case of forcing input and for the special right hand side (Haldane type kinetics), the resulting dependence of the PBR productivity (the average value of steady-state concentration) on hydrodynamic mixing is determined.

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