Zeno Trajectories in a Non-Smooth Model of a Controlled Reverse Flow Reactor

Erasmo Mancusi[1*], Lucia Russo[2], Mario di Bernardo[1],
and Silvestro Crescitelli[2]
[1]Dipartimento d'Ingegneria, Università del Sannio, Piazza Roma, 82100, Benevento, Italy.
[2]Dipartimento di Ingegneria Chimica Alimentare Università di Salerno, Via Ponte Don Melillo, 84084, Fisciano (SA), Italy.
[3]Dipartimento d'Ingegneria Chimica, Università degli Studi di Napoli "Federico II", Piazzale Tecchio 80, 80125 Napoli, Italy.

Abstract

Controlled reverse flow reactor processes show typical hybrid phenomena due to interaction between continuous and discrete dynamics. In this paper, the dynamical behaviour of a controlled RFR is discussed within the context of hybrid system theory. We focus our attention on a typical feature of hybrid system dynamics: Zeno trajectories. Such phenomena are discussed and their influence on the dynamics of a controlled RFR is presented.

Keywords: Controlled reverse flow reactor, hybrid system, Zeno phenomena, Zeno regularization

1. Introduction

Authothermal operation in chemical reactors, in which exothermic operation are carried out, has attracted considerable interest in the last years. For this purpose the catalytic reverse flow reactor (RFR) is very efficient for treatment of industrial off-gas with low concentration of volatile organic compounds (VOC). In fact, in the RFR the hot reaction zone is trapped by a periodically inversion of the flow direction (Matros and Bunimovich, 1996).

Two problems are related to the use of RFRs for VOC treatment: the extinction of the reaction and the formation of hot spots, which could be caused by a variation of the feed temperature and/or concentration. Barresi and Vanni (2002) proposed control systems for keeping the system always close to the maximum of the combustion efficiency, even in the case of variable feed conditions. A temperature sensor is located at either end of the catalytic bed and when the prescribed condition is fulfilled the feedback controller reverses the flow direction.

In this paper we consider the simplest of control systems proposed by Barresi and Vanni (2002). This one point controller takes into account only the temperature measured by the sensor located close to the inlet of the reactor: the flow is reversed when this temperature falls below a fixed value.

[*] Author to whom correspondence should be adressed : mancusi@unisannio.it

The controlled system is characterized by discrete events (the inversions of the flow direction) and continuous dynamics between two successive switches. So this system is a hybrid (time continuous/discrete) system. Roughly speaking, a hybrid system consists of a number of modes (continuous dynamics) and modes transition rules (Scumacher and Van der Schaft, 2000). The mode transition rules specify when mode changes (called events) occur. Each mode will be active until the condition for the switch, defined by a mode transition rule, is again fulfilled.

Hybrid systems have been used successfully in a number of engineering applications and, recently, also in chemical engineering. It was found that some processes have to be modelled as hybrid systems. Indeed Moudgalya and Ryali (2001a, b) have showed that a model for an industrial slurry reactor for the production of polyethylene is a Filippov system (i.e. a system described by equations with discontinuous right-hand sides, Filippov, 1988). Hybrid systems have been shown to exhibit a rich dynamical behaviour and several peculiar bifurcations that cannot be studied with standard bifurcation theory (e.g. di Bernardo et al., 2002).

In this paper we will show that RFRs with the above mentioned control exhibit typical behaviour of hybrid systems: for many set-point temperatures Zeno phenomena (e.g. Schumacher and Van der Schaft, 2000) are detected. Such phenomena correspond to an infinite sequence of discrete transition accumultating in finite time. We will discuss these phenomena and their relationship to the usual mathematical model for these reactors.

2. The Mathematical Model

The mathematical model of a one dimensonal tubular reactor is written in terms of mass and energy balances, and is given by the following equations for the catalytic section:

$$\begin{cases} \dfrac{\partial y_g}{\partial t} = \dfrac{1}{Pe_m^g}\dfrac{\partial^2 y_g}{\partial z^2} + (1-2IO)\dfrac{\partial y_g}{\partial z} + J_m^g\left(y_s - y_g\right) \\ \dfrac{\partial \theta_g}{\partial t} = \dfrac{1}{Pe_h^g}\dfrac{\partial^2 \theta_g}{\partial z^2} + (1-2IO)\dfrac{\partial \theta_g}{\partial z} + J_h^g\left(\theta_s - \theta_g\right) - \varphi\left(\theta_g - \theta_w\right) \\ \dfrac{\partial \theta_s}{\partial t} = \dfrac{1}{Pe_h^s}\dfrac{\partial^2 \theta_s}{\partial z^2} - J_h^s\left(\theta_s - \theta_g\right) + B\eta Da\left(1-y_s\right)\exp\dfrac{\theta_s}{1+\theta_s/\gamma} \\ J_m^s\left(y_s - y_g\right) = \eta Da\left(1-y_s\right)\exp\dfrac{\theta_s}{1+\theta_s/\gamma} \end{cases} \tag{1}$$

where the parameters and states are defined as in Řeháček et al. (1998). The inert sections are described by the same equations only there is no chemical reaction in the solid phase (Barresi and Vanni, 2002). Danckwerts boundary conditions are assumed for concentration and temperature in the gas phase:

$$\begin{cases} \left.\dfrac{\partial y_g}{\partial z}\right|_0 - IOPe_m^g y_g\left(0,t\right) = 0 \\ \left.\dfrac{\partial \theta_g}{\partial z}\right|_0 - IOPe_h^g\left(\theta_g\left(0,t\right) - \theta_{feed}\right) = 0 \\ \left.\dfrac{\partial \theta_s}{\partial z}\right|_0 = 0 \end{cases} \qquad \begin{cases} \left.\dfrac{\partial y_g}{\partial z}\right|_1 - \left(1-IO\right)Pe_m^g y_g\left(1,t\right) = 0 \\ \left.\dfrac{\partial \theta_g}{\partial z}\right|_1 - \left(1-IO\right)Pe_h^g\left(\theta_g\left(1,t\right) - \theta_{feed}\right) = 0 \\ \left.\dfrac{\partial \theta_s}{\partial z}\right|_1 = 0 \end{cases} \quad (2)$$

The *IO* variable takes into account the switching rule and is equal to 0 when the flow is from the left and equal to 1 when the flow is from the right. The spatial discretization of the Eqs. (1)-(2) has been performed by reducing the infinite dimensional PDE system to a finite one by orthogonal collocation technique on finite elements. The time integration is performed connecting a standard time-step integrator (LSODE, Brown et al., 1989) with a specific event-driven subroutine (DA2CJF from the NAG toolbox) for the detection of the time value and the state of the system at the inversion, as dictated by the control rule.

Denoting with $x(z,t) \equiv \left(y_g\left(z,t\right), \theta_g\left(z,t\right), \theta_s\left(z,t\right)\right) \in \mathbb{R}^n$ the state vector state and with $\boldsymbol{\lambda} \equiv \left(\tau, Pe_m^g, J_m^g, Pe_h^g, J_h^g, \varphi, J_m^s, Da, Pe_h^s, J_h^s, B, \gamma\right)$ the parameter vector, the reactor model Eq. (1), with boundary conditions given by Eq. (2), can be written in abstract form as the following dynamical system:

$$\begin{cases} \dot{x} = F_i\left(x, \lambda, IO\right) \quad i = 1,2 \\ x\left(t_0\right) = x_0 \end{cases} \tag{3}$$

The closed loop system is described by two alternating vector fields (F_1 and F_2) and by a control law that dictates the switch from one vector field to the other. Each vector field describes the system dynamics until the inlet temperature is higher than the set point value (*Tsp* is set-point temperature). The switching action is a discrete event and is assumed to be instantaneous. So the mathematical model of this controlled catalytic combustor is a particular type of hybrid (time continuous/discrete) system. Namely, the model is characterized by a discontinuous right-hand side and hence can be classified as a Filippov system (Filippov, 1988).

A hybrid system can be effectively represented as a graph characterized by nodes and edges (e.g. see Schumacher and Van der Schaft, 2000). The continuous flow evolves according to the differential equation specified in each node of the graph. When certain conditions are fulfilled, a discrete transition takes place from one node to another if the nodes are connected by an edge. The continuous flow is then forced to satisfy the differential equation in the new node. Denoting with ϑ_1 the controlled temperature when the flow is from the left and with ϑ_2 the controlled temperature when the flow is from the right, the graph corresponding to the closed loop reactor is shown in Figure 1.

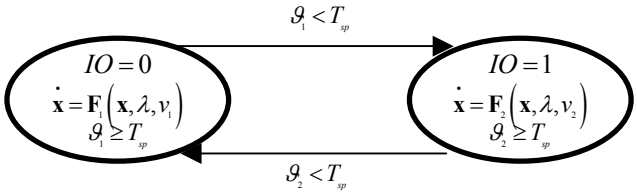

Figure 1 Schematic representation of a controlled RFR as a hybrid system.

Therefore the time evolution of the system will be over sets of the form:

$$\square = \left\{ \left[\tau_0^{'}, \tau_1 \right], \left[\tau_1^{'}, \tau_2 \right], \ldots, \left[\tau_{n-1}^{'}, t_n \right], \ldots \right\} \tag{4}$$

with $\tau_i \in \square$ and $\tau_i = \tau_i^{'} \leq \tau_{i+1}$ for all i=2,3,…,n-1. The τ_i are the times where discrete jumps of the flow occur. For every interval $\left[\tau_{i-1}^{'}, \tau_i \right]$ with $\tau_{i-1}^{'} < \tau_i$ the time evolution is continuous as dictated by the vector field (3).
Hybrid trajectories can extend to infinity if $\square$ is an infinite sequnces. A Zeno traiectories we have an infinite sequences of switches witht $\square < \infty$. Euristically , for a Zeno trajectory there is an infinite number of discrete transitions in a finite time.

3. Results

We study the influence of the feed temperature on the dynamic behaviour of the closed loop system. The set point temperature is chosen equal to the catalyst ignition temperature so that the control action forces the gas to have enough enthalpy to allow the reaction at the first catalyst layers. Varying the feed temperature, the controlled reverse flow reactor shows a very complex behaviour: multiplicity of regimes, symmetric and non-symmetric regimes (Russo et la., 2002) and Zeno trajectories. Here we focus our attention to the existence of Zeno phenomenon. These kind of trajectories are strictly related to the hybrid nature of the system and are characterized by infinitely many discrete transitions within a finite time interval. More precisely, the series $\sum_{i=0}^{\infty} \left(\tau_i^{'} - \tau_i \right)$ is finite. This is clear in the Fig.2, where a transition is reported from a periodic regime to a Zeno state. When the feed temperature is 100° C, the closed loop reactor exhibits a periodic regime. In this case the flow direction is reversed periodically. If the feed temperature is decreased to 50 °C this periodic regime looses stability and the closed loop reactor exhibits a Zeno trajectory. Now the flow direction is reversed with higher and higher frequency and an infinite number of switches occurs in a finite time value $\tau_\infty = \sum_{i=0}^{\infty} \left(\tau_i^{'} - \tau_i \right) \approx 5600$.

Note that Zeno phenomena are unfeasible in real systems. Typically they arise due to modelling abstractions or are related to the control policy (Johansson et al., 1999). In applications they are associated to high frequency switching or chattering , which is undesirable from a practical view point.

Zeno systems are hard to analyze and simulate in a way that gives a constructive information about the behaviour of the real system. Therefore, it is important to be able to determine if a hybrid system exhibits Zeno trajectories and, if this is the case, to find ways to remove Zenoness from the abstract mathematical model. In the case under study, the Zeno state corresponds to an extinction regime and thus its detection has practical relevance in spite of the numerical difficulties. This behaviour can be explained by considering that with this feed temperature the heat of reaction is not enough to sustain autothermally the process. On the other hand the control policy dictates that the inlet temperature cannot be lower than the set point value. So the extinction of the reactor is reached with an infinite number of switches.

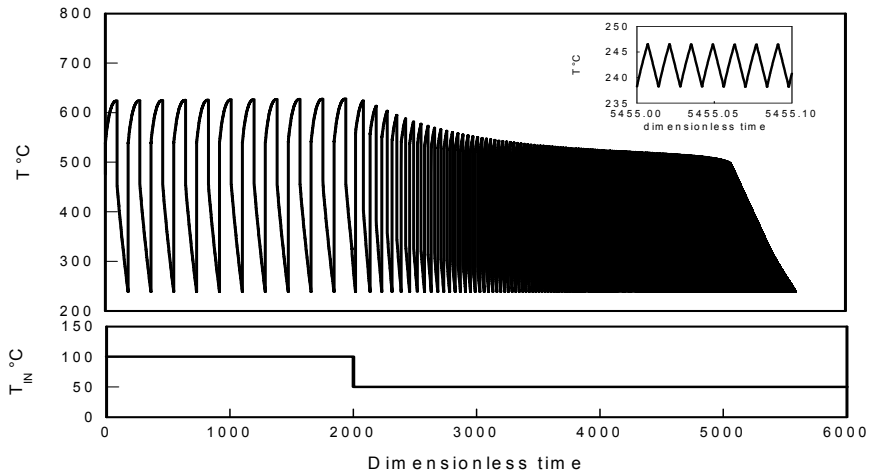

Figure 2 The uppermost plot shows the temperature evolution, and the lower most plot reports the inlet temperature imposed policy.

Generally, Zeno phenomena are due to model simplifications. In the case of the controlled reverse flow reactor, this simplification is in the assumption that the flow inversion is instantaneous. So a way to resolve the Zeno phenomena is to consider a temporal regularization (Johansson et al., 1999). In many cases, this regularization can be obtained modelling the switching action with a more realistic time delay (τ_ε) between the time at which the set point valued is reached and the time at which the flow is commanded to switch. A temporal regularization of the closed loop reactor is shown in Fig. 3.

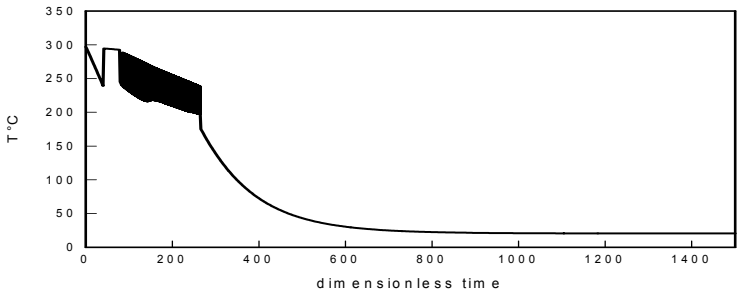

Figure 3 Time series of a temporally regularaized closed loop reactor.

In the case reported in Fig. 3 we use a time delay τ_ε=0.05. As it is apparent in Fig. 3 after a short transient that shows many high frequency switches, the inlet temperature decreases until the extinction of the reaction. The longer the time delay chosen is, the shorter the transient. It is important to stress that, though the Zenoness is removed, a wide time range exists where the closed loop system exhibits many fast switches. Note that regularization itself is a process bound with difficulties, as different regularaization methods can lead to different simulation results (Johansson et al. 1999).

4. Conclusions

In the present work, the hybrid system approach for a closed loop reverse flow reactor is adopted. With this approach the existence of Zeno phenomena is addressed. Motivated by physical considerations we have discussed the regularization of this dynamical behaviour. Introducing a time delay (τ_ε) between the time at which the set point valued is reached and the time at which the flow is commanded to switch, Zenoness is removed allowing more efficient simulation of the system behaviour. In spite of that, there is a wide range where the system exhibits high frequency oscillations. This behaviour can damage the controller and then other types of control actions have to be explored. We wish to emphasize that understanding and characterizing Zeno phenomena is essential when dealing with hybrid systems. As these models are being increasingly used in chemical engineering, we conjecture that the analysis of such phenomena will become an essential part of the design process.

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