COMPLEX DYNAMICS AND CHAOS IN A HYBRID SYSTEM MODELING A CONTROLLED REVERSE FLOW REACTOR

A. BRASIIELLO
Dipartimento d’Ingegneria Chimica e Alimentare, Università di Salerno, via Ponte don Melillo, 84084, Fisciano (SA), Italy
abrasiel@unina.it

E. MANCUSI
Facoltà d’Ingegneria, Università del Sannio, Piazza Roma, 82100, Benevento, Italy

L. RUSSO
Istituto di Ricerche sulla Combustione IRC, CNR, Piazzale V. Tecchio 80, 80125 Napoli, Italy

S. CRESCITELLI
Dipartimento d’Ingegneria Chimica, Università di Napoli “Federico II”, Piazzale V. Tecchio 80, 80125 Napoli, Italy

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In this work some complex behaviors of a controlled reverse flow reactor is presented. The control system introduces discrete events making the model an infinite dimensional hybrid system. The study is conducted through continuation techniques and brute force numerical simulations. Together with standard bifurcations like pitchfork, saddle-node and Neimark-Sacker, varying the set-point parameter of the controller, several novel aspects are singled out: an unusual sequence of period-adding bifurcation phenomena, a new route to chaos and the coexistence of Zeno states with quasi-periodic and chaotic regimes. The period-adding phenomena dictate the transition between symmetric and asymmetric multiperiodic regimes and a simple rule for the occurrence of symmetry breaking and recovery is found. The new route to chaos is a transition from a quasi-periodic regime to chaos due to the presence of Zeno phenomena, typical of hybrid systems. The chaos is characterized by Zeno-like oscillations.

Keywords: Reverse flow reactor; hybrid automaton; Zeno executions; period-adding; route to chaos; impact map.

1. Introduction
Over the last decades, the analysis and design of periodically forced continuous chemical processes has been an area of intense research [e.g. Matros & Bunimovich, 1996]. It has been established that such periodic forcing may, under certain conditions, lead to the intensification of traditional processes, thus enhancing our arsenal for engineering better products and much more efficiently. For example, periodically forced tubular catalytic reactors have

*Author for correspondence
been successfully used for the combustion of volatile organic compounds concentrations of industrial exhaust gas (VOCs) [Eigenberger & Nielen, 1988; Brinkmann et al., 1999] and to improve equilibrium-limited exothermic reactions such as Methanol Synthesis [Neophytides & Froment, 1992]. The most common configuration, called Reverse Flow Reactors (RFRs), involves the periodic reversion of the flow direction. However the relative advantages of RFRs, come up with some operational problems such as the potential overheating of the catalyst and the extinction of the reaction due to external disturbances. For VOCs catalytic combustion the problems related to the use of RFRs are the reaction extinction and the hot spots formation, caused by variations of the feed temperature and/or concentration.

To deal with the problem, Barresi and Vanni [2002] proposed a simple feedback control scheme (a one point controller) for a catalytic combustor with periodical force reversion; here the flow is reversed not periodically in time but when the temperature as measured at specific points inside the reactor falls below a certain value. The closed loop system is characterized by discrete events (the inversions of the flow direction) and continuous dynamics between two successive switches. This renders the system a hybrid one [Schumacher & Van der Schaft, 2000].

Hybrid systems have been shown to exhibit a rich dynamical behavior and several peculiar bifurcations that cannot be studied with standard bifurcation theory for smooth systems [di Bernardo et al., 2002]. The topic is reaching wider and wider interest because the dynamics of many problems of current engineering, physical and biological interest are governed by periodic events that can be considered as instantaneous ones as they deploy on very short time scales. Systems ranging from aerodynamics [Tomlin et al., 1998] to process control e.g. [Göllü & Varaiya, 1994; Moungalya & Ryali, 2001], and from biology (e.g. cellular growth or insect motion) [Lincoln & Tiwari, 2004] to discrete logic control devices [Wang, 2008] are just some few examples of hybrid systems. In the case of man-made devices, the instantaneous events are often intentionally introduced in order to improve safety or efficiency [Lygeros et al., 1997; Antsaklis & Nerode, 1998]. Hence the development of new methods for the systematic bifurcation analysis of hybrid systems is of outmost importance.

In the previous work, [Mancusi et al., 2007] studied the dynamics of a controlled RFR for VOCs with a control device which inverts the flow direction when the gas temperature in the first layer of the catalyst falls below a prescribed value which serves as our set-point.

Mancusi et al. [2007] showed theoretically that the system under investigation is an infinite dimensional hybrid system which can be modeled as hybrid automaton. Moreover, they showed numerically and theoretically the occurrence of Zeno phenomena and the coexistence of these phenomena with periodic regimes. In this work, the dynamics of a similar controlled RFR, which does not include the inert sections at both edges of the catalytic bed, is considered. The system exhibits unusual and intriguing dynamics which was not observed in the previous work. The main novelties are:

• A period-adding sequence not comparable to the well-studied period-doubling cascade [Feigenbaum, 1978, 1979] and those originated by frequency-locking [Cvitanovic et al., 1985],
• A novel route to chaos, different from those reported previously in the literature for continuous systems [Ott, 1993] and for hybrid ones [di Bernardo et al., 1998],
• The coexistence of Zeno state with quasi-periodic and chaotic regimes. This coexistence affects the temporal evolutions of the chaotic orbits as they are characterized by Zeno-like oscillations.

The paper is organized as follows. In Sec. 2 we present the mathematical model of the RFR as a hybrid system. The dynamical analysis of the reactor is given in Sec. 3. In particular, the periodic regimes are discussed in Sec. 3.1 and the period-adding cascade is specifically analyzed. The coexistence between quasi-periodic regimes and Zeno states are reported in Sec. 3.2. In Sec. 3.3 the coexistence between the chaotic regimes and the Zeno states are presented and the new route to chaos is eventually discussed in detail.

2. Mathematical Model
A schematic representation of a RFR is shown in Fig. 1. The reactor is a tubular fixed bed catalytic one in which a gas containing the reactants (VOCs which undergo exothermal irreversible first order reaction) flows from left to right and from right to left, alternatively according to a control law. The reversal of the position of the feed is obtained...
through the synchronized actions of the two couples of valves (\(V_1\) and \(V_2\) in Fig. 1).

This system is hybrid as it involves time-contiguous evolution of the state variables between every two consecutive switches and time discrete instantaneous events due to the feed inversions.

The mathematical model is an infinite dimensional system constructed in terms of mass and energy balances and is represented by the following dimensionless partial differential equations:

\[
\frac{\partial \theta_s}{\partial \tau} = 1 \frac{\partial^2 y_s}{\partial z^2} + (1 - 2IO) \frac{\partial \theta_s}{\partial z} + J_{in}(y_s - y_{in}) \tag{1}
\]

\[
\frac{\partial \theta_y}{\partial \tau} = 1 \frac{\partial^2 \theta_y}{\partial z^2} + (1 - 2IO) \frac{\partial \theta_y}{\partial z} + J_{in}(\theta_y - \theta_{in}) \tag{2}
\]

\[
\frac{\partial \theta_y}{\partial \tau} = 1 \frac{\partial^2 \theta_y}{\partial z^2} - J_{out}(\theta_y - \theta_{in}) + B\eta \Delta \theta \exp \frac{\theta_y}{1 + \frac{\theta_y}{\gamma}} \tag{3}
\]

Parameters and state variables are reported in Table 1. Danckwerts boundary conditions are assumed for concentration and temperature in the gas phase:

\[
\frac{\partial \theta_s}{\partial z} \bigg|_{z=0} = -IO Pe \frac{\partial \theta_s}{\partial \tau}(0, \tau) = 0 \tag{4}
\]

\[
\frac{\partial \theta_y}{\partial z} \bigg|_{z=0} = -IO Pe \frac{\partial \theta_y}{\partial \tau}(0, \tau) - \theta_{in} = 0 \tag{5}
\]

\[
\frac{\partial \theta_s}{\partial z} \bigg|_{z=1} = 0 \tag{6}
\]

\[
\frac{\partial \theta_y}{\partial z} \bigg|_{z=1} = -(1 - IO) Pe \frac{\partial \theta_y}{\partial \tau}(1, \tau) - \theta_{in} = 0 \tag{7}
\]

In the above system of equations, the flow inversion is being modeled through the discrete binary (0 or 1) variable \(IO\) that characterizes the flow direction. In particular, the discrete variable \(IO\) appears in the convective terms, inside Eqs. (1)-(4) and in the boundary conditions (5) and (6). For \(IO = 0\) the flow is assumed to evolve from the left to the right and vice versa for \(IO = 1\). The flow-direction swaps are governed by a feedback control system which measures the gas temperature at the inlet section of the reactor (at 3\% of the reactor length from the edge). The control law is the following: the flow is reversed when the measured temperature decreases (i.e. \((\partial \theta_y(IO, \tau_n^*))/(\partial z))|_{z=1} < 0\), \(\tau_n^*\) being the instant of inversion up to a fixed instant of flow inversion, \(\eta\).

![Diagram](image-url)

**Fig. 1.** Scheme of a reverse flow reactor.

**Table 1.** Dimensionless parameter definitions and values.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
<th>Value</th>
</tr>
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<tbody>
<tr>
<td>(Da)</td>
<td>(L_{in}/v_{in})</td>
<td>0.56</td>
</tr>
<tr>
<td>(\gamma)</td>
<td>(E/(RT_{in}))</td>
<td>16.68</td>
</tr>
<tr>
<td>(Pe_{in})</td>
<td>(\rho \cdot c_{p}\cdot L_{in}/k_{y})</td>
<td>644</td>
</tr>
<tr>
<td>(Pe_{in})</td>
<td>(\rho \cdot c_{p}\cdot L_{in}/k_{y})</td>
<td>1.44</td>
</tr>
<tr>
<td>(J_{in})</td>
<td>(k_{in}a_{L}/(\rho c_{p} \cdot \alpha))</td>
<td>17.15</td>
</tr>
<tr>
<td>(J_{in})</td>
<td>(k_{in}a_{L}/(\rho c_{p} \cdot \alpha))</td>
<td>17.15</td>
</tr>
<tr>
<td>(J_{in})</td>
<td>(h_{in}a_{L}/(\rho c_{p} \cdot \alpha))</td>
<td>28.4</td>
</tr>
<tr>
<td>(B)</td>
<td>(\Delta H C_{4,44}A_{\gamma}/(\rho c_{p} \cdot \alpha))</td>
<td>0.0057</td>
</tr>
<tr>
<td>(\theta_{in})</td>
<td>((\tau_{m} - \tau_{in})\gamma/\tau_{in})</td>
<td>9.6</td>
</tr>
<tr>
<td>(\theta_{in})</td>
<td>((\tau_{m} - \tau_{in})\gamma/\tau_{in})</td>
<td>1.2</td>
</tr>
</tbody>
</table>

\(\eta = \theta_{in} - \theta_{in}\)

\([\theta_{in} = 0, \theta_{in} = \tau_{m}^*]\)
The hybrid system can be represented by the hybrid automaton schematically illustrated in Fig. 2 resulting from coupling the differential equations [Eqs. (1)–(4)] with a set of logical rules. For more details on hybrid automata refer to [Johansson et al., 1999]. In Fig. 2, the state vector of the system is denoted with $x \equiv (y_g(z,\tau), \theta_g(z,\tau), \theta_s(z,\tau))$, the parameters vector (whose components are reported in Table 1) with $\lambda$ and the right-hand side of the equations governing the evolution of the system with $F \equiv ((\partial y_g(z,\tau))/\partial \tau), (\partial \theta_g(z,\tau))/\partial \tau, (\partial \theta_s(z,\tau))/\partial \tau)$. Moreover, the boundary conditions [Eqs. (5) and (6)] are written as $B(x, IO, \lambda) = 0$. With such notation, the continuous evolution of the state variables is described by the two continuous vector fields $\dot{x} = F(x, 0, \lambda)$ with the boundary conditions $B(x, 0, \lambda) = 0$ and $x = F(x, 1, \lambda)$ with the boundary conditions $B(x, 1, \lambda) = 0$ which alternate at each switch. The control law acts on these two continuous vector fields as two guard conditions $G(IO)$. For $IO = 0$ we have:

$$G(0) = \begin{cases} \theta_g(0, \tau'_n) = \theta_{sp} \\
\left.\frac{\partial \theta_g(0, \tau'_n)}{\partial z}\right|_{\tau < \tau'_n} < 0 \end{cases}$$

while for $IO = 1$ we have:

$$G(1) = \begin{cases} \theta_g(1, \tau'_n) = \theta_{sp} \\
\left.\frac{\partial \theta_g(1, \tau'_n)}{\partial z}\right|_{\tau < \tau'_n} < 0 \end{cases}$$

where $\tau'_n$ are the switch instants.

More details on the meaning of guard conditions and more in general on hybrid automaton of the system under investigation can be found in [Mancusi et al., 2007].

3. Dynamical Analysis

The solution diagram of limit cycles as the set-point temperature is varied as shown in Fig. 3. Each point of the diagram represents a fixed point of the Poincaré map of the corresponding limit cycle. The diagram is constructed through continuation

![Fig. 3. Periodic solutions diagram varying set-point temperature $\theta_{sp}$. The diagram relates to the second iterate of impact map of periodic regimes. $\theta$ is the gas temperature at last layer of the catalyst (at a distance from the edge equal to 3% of the reactor length). Four regions are located into the diagram: $R1$ is a region characterized by the symmetric period-I periodic solution; $A$ is the region in which the period-doubling phenomenon appears; $R2$ is a region in which several periodic solutions coexist; $R3$ is a region in which more complex behavior are generated from periodic solutions. In regions $R1$, $A$, $R2$ no Zeno executions occur while in region $R3$ Zeno executions coexist with ignited regimes.](image-url)
of such fixed points (via AUTO97 software [Doedel et al., 1997]). More details about the methodology for the bifurcation analysis and the numerical technique are reported in [Mancusi et al., 2007]. Stable periodic regimes are shown as solid lines, unstable ones are shown as short dashed lines. Only ignited solutions are reported. However, in all the investigated parameter range, there are non-ignited regimes. They are regimes in which the controller is not able to trap the heat of the reaction and the reactor shuts down. Such regimes can be reached either after the control is activated a finite number of times or without control activation.

The diagram is characterized by the coexistence of many dynamical regimes and bifurcational scenarios. In particular, the diagram is divided into two major zones: one with Zeno executions ($\theta_{sp} > -7.9$ i.e. the $R_3$ zone in Fig. 3) and the other without Zeno executions ($\theta_{sp} < -7.9$, i.e. $R_1, A, R_2$ zones in Fig. 3). The zone of the diagram we are interested in, and also to be studied in detail in the following are the $A$ zone characterized by the presence of the period-adding sequence and the $R_3$ zone in which both the coexistence of Zeno states with quasi-periodic and chaotic regimes occur and the novel route to chaos from the quasi-periodic regimes is observed.

A Zeno execution is an execution in which the hybrid time trajectory (see [Johansson et al., 1999])

$$T = \{[\tau_0, \tau'_0], [\tau_1, \tau'_1], \ldots, [\tau_n, \tau'_n], \ldots\}$$

is infinite but

$$\sum_i (\tau'_i - \tau_i) < \infty.$$ 

In such case $\tau_\infty = \sum_i (\tau'_i - \tau_i)$ is called Zeno time. Roughly speaking, there is a Zeno execution when an infinite number of discrete transitions (i.e. inversions) occurs in a finite time. A temporal evolution related to a Zeno execution, obtained through numerical simulation, is reported in Fig. 4. A feature of a Zeno execution is the increasing trend of switch frequency during time (see the zoom at the top in Fig. 4), differently from a non-Zeno execution in which the switch frequency admits a maximum.

For their intrinsic nature, Zeno executions cannot be detected other than by brute force numerical simulations. However, for such kind of controlled RFR’s mathematical model, the necessary conditions for the occurrence of Zeno executions [Zhang et al., 2000] can be easily verified [Mancusi et al., 2007].

### 3.1. Period-adding bifurcations

The basic periodic regime induced by the forcing term through the control law has a period twice the switch time and emerges for values of the bifurcation parameter in the interval ($-8.166, -8.112$) (the zone is denoted as $R_1$ in Fig. 3). Temporal series of gas temperatures and spatial profiles of solid temperatures, of such regimes are shown in Fig. 5. As representative of the state vector we choose the temperature at two points placed at the same distance (34% of the reactor’s length) from the ends of the catalyst (drawn in solid and dashed lines, respectively). Spatial profiles refer to two instants just before two
consecutive switches. The regime is symmetric as a consequence of the system symmetry. Indeed, two points, at the same distance from the reactor’s center, have the same temporal behavior, but with a time-shift equal to the switch time $\Delta \tau, T = 2\Delta \tau$ being the regime period. Consequently, the spatial profiles of the temperature of catalytic bed at a time $\tau$ are the mirror reflection of the spatial profiles at $\tau + \Delta \tau$. More precisely, this periodic regime shows a spatio-temporal symmetry [Russo et al., 2002], that can be expressed by the following relation:

$$x(z, \tau) = x(1 - z, \tau + \Delta \tau)$$

(7)

where $x$ is the state vector, $\tau$ is time, $\Delta \tau$ is a half of the period and $z$ is the spatial variable.

The period-adding bifurcations sequence was found in a small range of the bifurcation parameter $\theta_{p} \in (-8.112, -8.106)$ (corresponding to the hatched A zone in Fig. 3). The analysis of the period-adding phenomenon is conducted through brute force numerical simulations as a parametric continuation could not be performed because the involved bifurcations occur in a very tiny parameter range.

In the most general meaning, the term period-adding is used in the literature to denote a wide class of different phenomena (e.g. frequency-locking phenomena in [Kaneko, 1982, 1983], period-doubling phenomena in [Feigenbaum, 1978, 1979] or the novel period-adding scenario of [Elbashah et al., 2001]). They are all characterized by a series of limit cycle bifurcations leading to period changes.

In our case, the period-adding sequence consists in a series of bifurcations leading to periodic solutions with different periods and symmetry and it follows a precise rule.

Starting from the symmetric 1-periodic regime shown in Fig. 5 and increasing the bifurcation parameter we observed bifurcations causing symmetry breaking or symmetry restoration as well increasing of the period. Such phenomena are illustrated in Fig. 6 where we show the observed sequence of the temporal series. Again, temporal series correspond to two end points placed at the same distance from the bed edges (3% of the reactor’s length, drawn in solid and dash lines, respectively).

As the bifurcation parameter is increased, the first bifurcation of the sequence causes the transition from the symmetric 1-periodic regime to a couple of period-4 asymmetric conjugate periodic regimes. As can be seen in Fig. 6(a), because of the symmetry breaking, the two new periodic regimes are characterized by different temporal series in the symmetrically placed reactor points and, because of the increase of the period, by an increased number of peaks. A further increase in the value of the bifurcation parameter leads to a symmetry recovery and a period-7 symmetric periodic orbit appears [Fig. 6(b)]. As can be observed, such regime resembles the peaks of both previous period-4 asymmetric regimes. Continuing to increase the value of the bifurcation parameter, the period-7 symmetric regime breaks its symmetry, generating two conjugate period-3 asymmetric periodic regimes [Fig. 6(c)] which further, due to a symmetry recovery, originate a period-5 symmetric periodic orbit [Fig. 6(d)]. Again, when symmetry recovery is observed, the new period regime resembles the peaks of the previous asymmetric regimes. A further increase of $\theta_{p}$ causes a symmetry breaking that leads to the birth of a couple of period-2 asymmetric regimes [Fig. 6(e)]. At about $\theta_{p} = -8.11$, these asymmetric periodic regimes bifurcate into a period-3 symmetric orbit [Fig. 6(f)] that, at higher $\theta_{p}$, leads to a couple of period-1 asymmetric regimes [Fig. 6(g)].

This period-1 asymmetric periodic regimes are those shown in Fig. 3 as 63 and 63i branches. These disappear at $\theta_{p} = -7.89$. The dynamical phenomena causing the disappearance of such regimes has not yet been understood. We have observed that such event happens for a value of $\theta_{p}$ very close to that corresponding to the first detection of Zeno executions (as can be observed in Fig. 3).

The observed period-adding bifurcations phenomena produce the following period sequence: $1 - 4 - 7 - 3 - 5 - 2 - 3 - 1$. This is in agreement with the sequence rule reported by [Huang et al., 1995] and [Sanjuán, 1996] for period-adding, according to which, between a region characterized by a $n \cdot T$ periodic orbit and a region characterized by a $(n+1)T$ periodic orbit, there should lie a region characterized by oscillations of period $n + (n+1)T$.

The occurrence of symmetric and asymmetric periodic regimes can be explained from the shape of peaks characterizing each regime. At this point we should note, that all multiperiodic (i.e. period $\geq 2$) regimes appearing in the period-adding sequence are characterized by peaks whose shapes are exactly those present in the two period-1 periodic regimes (the symmetric one in Fig. 5 and the asymmetric one in Fig. 6(g)), but occurring in different ways. Each periodic regime can
then be identified through the couple \((s,a)\) which indicates how many times the period-1 symmetric periodic regime \((s)\) and the period-1 asymmetric periodic regime \((a)\) are combined together to obtain the regime itself. For example, the period-2 periodic regime, obtained combining once the period-1 symmetric periodic regime and once the period-1 asymmetric periodic regime, is identified as \((1,1)\), while the period-3 symmetric periodic regime, obtained combining period-2 and period-1 asymmetric periodic regime, is identified as \((1,2)\). In Table 2, we report the couples \((s,a)\) are for each regime. The period-1 symmetric periodic regime is obviously identified by the couple \((1,0)\), while the period-1 asymmetric periodic regime through the couple \((0,1)\). The notation admits also the graphical representation reported in Fig. 7 in which we also illustrate in a qualitative manner the values \(s/a\) related to each periodic regime against the logarithm of the distance \(\Delta \theta_{sp}\) between two consecutive periodic solutions (which can be considered as an order of magnitude of the window in which each periodic solution exists).

Using the proposed notation, the symmetry rule is the following: If the integer \(a\) in \((s,a)\), indicating how many times the period-1 asymmetric periodic regime is combined to obtain the

<table>
<thead>
<tr>
<th>(s/a)</th>
<th>1.0</th>
<th>3.1</th>
<th>5.2</th>
<th>2.1</th>
<th>3.2</th>
<th>1.1</th>
<th>1.2</th>
<th>0.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(S)</td>
<td>(A)</td>
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<td>(A)</td>
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</tr>
</tbody>
</table>

![Fig. 6. Temporal series related to the observed period-adding cascade. (a) Period-4 asymmetric orbit \(\theta_{sp} = -8.11199272\). (b) Period-7 symmetric orbit \(\theta_{sp} = -8.11199262\). (c) Period-3 asymmetric orbit \(\theta_{sp} = -8.111999\). (d) Period-5 symmetric orbit \(\theta_{sp} = -8.11198\). (e) Period-2 asymmetric orbit \(\theta_{sp} = -8.11195\). (f) Period-3 symmetric orbit \(\theta_{sp} = -8.11165\). (g) Period-1 asymmetric orbit \(\theta_{sp} = -8.10710\).](image-url)
multiperiodic regime is odd, then the multiperiodic regime will be asymmetric; if it is even the multiperiodic regime will be symmetric (see Table 2). A similar rule was reported, in [González & Piro, 1985] for a phase-locking phenomenon.

For \( \theta_{sp} \in (-8.1076, -8.0734) \) another symmetric solution branch \( b_1 \) coexists with the already mentioned asymmetric conjugate branches \( b_3 \) and \( b_5 \) (see zone \( R_2 \) in Fig. 3). It is born unstable at \( \theta_{sp} = -8.1067 \). Proceeding along the branch \( b_1 \), it becomes stable at \( \theta_{sp} = -8.1076 \) by means of the saddle-node bifurcation (see Fig. 3).

At \( \theta_{sp} = -8.0734 \) it exhibits a supercritical pitchfork bifurcation. As a consequence, two stable asymmetric periodic regimes \( (b_2 \) and \( b_4) \) appear while the symmetric periodic regime \( b_1 \) becomes unstable.

3.2. **Quasi-periodic regimes and their coexistence with Zeno state**

At \( \theta_{sp} = -7.32 \), the two asymmetric regimes \( b_2 \) and \( b_4 \) undergo Neimark–Sacker bifurcations (see Fig. 3) as two complex conjugate Floquet multipliers related to their Poincaré maps go outside the unit circle. Thus for \( \theta_{sp} > -7.32 \), we observe the appearance of two stable asymmetric quasi-periodic regimes. As an example, the projection of the Poincaré map on the plane \( \theta_{con} \), \( \theta_{con} \) related to one of the two quasi-periodic regimes is shown in Fig. 8(a). \( \theta_{con} \), and \( \theta_{con} \) refer to gas temperatures measured at a distance from each reactor’s edge equal to 10% of the reactor’s length. Obviously, because of the symmetry of the system, a conjugate asymmetric quasi-periodic regime also exists. Its Poincaré map can be obtained from Fig. 8(a) by simply inverting the axes. These asymmetric quasi-periodic behaviors coexist with Zeno executions. We note that it is the first time that this coexistence is observed in a hybrid system. The region of coexistence is reported in Fig. 3.

3.3. **A novel route to chaos**

In this section we discuss the transition of the asymmetric quasi-periodic regime to strange chaotic attractor. To our knowledge, such transition can be considered as a new route to chaos. As this scenario has never been described before, this section can be considered as the first effort towards the characterization of the phenomenon. First, we will characterize the chaotic attractor through the tools of Time Series Analysis (TISEAN Package see [Schreiber & Schmitz, 2000] and [Hegger et al., 1999]) and then we will move on to the detailed description of the transition through several numerical simulations. The quasi-periodic attractors [Fig. 8(a)], discussed in the previous section, are stable up to about \( \theta_{sp} = -7.1 \). As the set-point temperature goes beyond this parameter value, on the Poincaré section of the quasi-periodic regime (see the Poincaré map in Fig. 8(c)) the sudden appearance of new curl shape pieces of invariant sets, together with the wrinkling of the curve corresponding to the Poincaré section of the existing quasi-periodic regimes (zoom in Fig. 8(c)) are observed. Such wrinkling of the curve is a clear sign of the fractalization of the tori surfaces on which quasi-periodic regimes were evolving and thus it is a first indication that the new attractor may be chaotic.

To further characterize this new attractor, we calculated the recurrence plot before and after the transition in order to appreciate the difference between the quasi-periodic dynamical behavior and the chaotic one (see [Eckmann et al., 1987; Casdagli, 1997]). A recurrence plot is a graphical representation of the matrix of distances \( ||X_{i} - X_{j}|| \) between all pairs of vectors representing the state vector \( X_{i} = (x_1, x_2, \ldots, x_n) \) of a n-dimensional system varying time. More precisely, a dot is placed at \((i, j)\) if \( ||X_{i} - X_{j}|| < d \), where \( d \) is a prescribed number. Recurrence plots can be useful in order to identify structures in data sets and to detect transient behaviors (a transient behavior is revealed by a distribution of dots that grow around the main
diagonal as the time grows). Moreover, recurrence plots can also provide a good evaluation of the maximal Lyapunov exponent [Trulla et al., 1996].

For our system, the recurrence plots related to the quasi-periodic regime and the new attractor are shown in Fig. 9. As recurrence plots are symmetric with respect to the main diagonal, both plots can be reported on the same diagram. The upper triangle in Fig. 9 shows continuous lines parallel to the main diagonal characteristic of a periodic signal or of a quasi-periodic one, while the lower triangle is related to a chaotic signal characterized by discontinuous diagonal lines.

The length of the lines is associated to the reciprocal of the maximal Lyapunov exponent value [Eckmann et al., 1987] (the continuous lines of the quasi-periodic signal means maximal Lyapunov exponent equal to zero). The maximal Lyapunov exponent value was calculated by means of both the graphical method and the Tisean package [Hegger et al., 1999], providing a good agreement. The positive value of the maximal Lyapunov exponent of the map ($\lambda_{\text{max}} = 0.0405 > 0$) determines the chaotic nature of the attractor. This can be heuristically confirmed by checking the sensitivity to the initial conditions. Indeed taking two different initial conditions which are different from each other for a very tiny quantity (0.003 in our case),
we observe the growth of the distance \( \text{dist}(\tau) = |y_\tau - y'_\tau| \). The diagram is shown in Fig. 10. The new regime can thus be classified as chaos.

The chaotic attractor is fractal in shape. A good estimation of the fractal dimension can be obtained through the computation of the correlation sum from which the correlation dimension can be calculated [Hegger et al., 1999]. For the chaotic attractor the computed correlation dimension is \( 1.65 \).

This route to chaos cannot be classified as one of the standard classical routes to chaos from quasi-periodic regimes. In other words, to our knowledge, this chaotic transition does not correspond to any one of the well-known scenarios encountered and described in the literature for continuous dynamical systems [Ott, 1993]. To support this argument, we report the following observations.

First, the appearance of the chaotic attractor is linked to the disappearance of the quasi-periodic one because the two events take place at the same time. Moreover, strong similarities in shape between the Poincaré maps of the quasi-periodic and the chaotic attractors can be observed (see Fig. 8).

The transition towards chaos is stated by the loss of differentiability of the 2-torus surface. The temporal series of the chaotic attractor and of the quasi-periodic one are illustrated in Figs. 8(d) and 8(b) respectively. We can observe that the chaotic time series alternates between quasi-periodic like oscillations and very fast (Zeno-like) oscillations. This can also be confirmed through the comparison of the recurrence plots in Fig. 9. Analyzing the plots at fixed values of abscissa, we observe that the chaotic regime regularly alternates regions qualitatively similar to those of the quasi-periodic regime and regions which are not. It is clear from the definition of the recurrence plot’s points that these regions are characterized by Zeno-like oscillations. Zeno-like oscillations correspond, in the phase space diagram in Fig. 8(c), to the region characterized by the presence of the curls. In Fig. 11 the Zeno-like oscillations are shown in the first part of a transitory which lead to quasi-periodic regime at \( \theta_{sp} = -7.11 \), starting from suitable initial conditions. The fast oscillations lies in the region of the phase space in which will be the curls after the transition to chaos (as \( \theta_{sp} \) exceeds \( -7.1 \)). It is worth to note that chaotic regimes always coexist with Zeno executions. This excludes the fact that the observed phenomenon is merging between quasi-periodic attractor and Zeno state.

We want to underline that we verified that a regularization of the system using a suitable time delay [Johansson et al., 1999] does not affect the occurrence of the chaotic regime. For values of \( \theta_{sp} \) higher then \( \theta_{sp} = -6.9 \), the interaction between the Zeno state and the chaotic regime produces the disappearance of the chaotic behavior and only Zeno executions are found.

4. Conclusions

In this paper the complex dynamics of a controlled RFR reactor is studied. The control law introduces discrete events and thus the model is an infinite dimensional hybrid system. This study is one of the few of this kind of dynamical systems. The analysis is carried out through continuation techniques and brute force numerical simulations, varying the set-point variable of the control system (i.e. the inlet gas temperature of the reactor) which is thus considered as our bifurcation parameter.

The system admits several dynamic regimes like periodic, quasi-periodic and chaotic ones. For a wide range of the bifurcation parameter, typical hybrid
system behaviors called Zeno states are found. In this work, the coexistence of such behaviors with quasi-periodic and chaotic regimes was observed for the first time.

Moreover, we focus our attention on two complex dynamical transitions detected: a period-adding phenomenon and a new route to chaos. Periodic regimes are found to undergo a peculiar period-adding cascade, which also cause symmetry breaking and restorations. An explanation of the occurrence of the symmetric and asymmetric solutions in the period-adding cascade is provided through a symmetry rule which seems to be a very general rule.

The chaotic behavior and the new route to chaos are investigated through the analysis of time series and the recurrence plots. The chaotic attractor is fractal in shape and its correlation dimension was calculated. The chaotic transition is characterized by the sudden appearance of fractal curls in a precise region of the phase space. The curls correspond to temporal evolutions characterized by Zeno-like oscillations. We conclude that the route to chaos is thus realized when the 2-torus surface, where the quasi-periodic regime is lying, interacts to chaos is thus realized when the 2-torus surface, where the quasi-periodic regime is lying, interacts with the curls region of the phase space leading to the fractalization of the surface. The coexistence of the Zeno state and the chaotic regime exclude the occurrence of a merging between quasi-periodic regime and Zeno state.

Although the characterization of the route is not complete and further studies are needed, to our knowledge, such route to chaos from quasi-periodic regime has never been reported before in the literature.

References


