Analysis of Chemical Reaction $\text{C}_6\text{H}_{12}\text{N}_6 + \text{KCLO}_4 + \text{Mg} + \text{SrSO}_4$ in Solid-phase Oscillating Combustion

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Abstract—In this paper, aiming at the chemical reaction system of solid-phase oscillating combustion, the basic dynamic behavior of laser system in terms of bifurcation diagram, Lyapunov exponent and complexity $C_0$ is analyzed by using Matlab software, and the chaotic characteristics and sensitivity to parameters of the chemical reaction system of solid-phase oscillating combustion are expounded.

1. Introduction
Chaos, which determines the internal randomness of the system, is a common phenomenon in nature. With people's understanding of nature, chaos was discovered in meteorology in 1963, and the first chaotic model was established[1]. Since then, people have begun to study chaotic systems and chaotic dynamics[2]. More than ten years ago, most researchers focused on building chaotic systems, but in recent years, people gradually found that chaos exists widely in many engineering systems, such as motor system[3], power system, DC/DC converter system[4] and chemical system[5-6].

Chemical reaction kinetics has become a very active field in chemical reaction research [7-10], and the establishment of chemical reaction models has also received extensive attention, such as the establishment and simulation of industrial chemical reaction models, and the study of biochemical dynamic systems. Nonlinear dynamics plays an increasingly important role in chemical reaction dynamics. A large number of examples show that the concentration of chemical reactants can show periodic and chaotic changes. The dynamic behavior of chemical reaction is closely related to nonlinear phenomena and its corresponding mathematical models.

Many scientists have found chaos in all kinds of chemical reactions. For a class of chemical reaction systems, the paper [5] puts forward the corresponding fractional-order chemical system, and adopts sliding mode control algorithm to control the stability of the system; In [6], a fractional order system is proposed for a chemical kinetic model without exponential term. Because the nonlinearity of the system is expressed by product, it is easier to design the controller. In [8], the classical feedback control is adopted for the solid-state oscillating combustion system of $\text{C}_6\text{H}_{12}\text{N}_6 + \text{KCLO}_4 + \text{Mg} + \text{SrSO}_4$, and the stability control of the system is realized. The chaotic behavior of chemical system is a typical nonlinear behavior, and there are few researches on the dynamic characteristics of chemical system itself. It can be seen from the above documents that most of the documents control the chemical dynamic system.

In this paper, aiming at the chemical kinetic system of solid-phase oscillating combustion, firstly, the kinetic behavior is analyzed by using phase diagram, 0-1 test and Poincare cross-section system, and secondly, the influence of parameters on the system is studied by using bifurcation diagram and complexity analysis methods. Finally, in order to further explain the mutual restraint strength of parameters on the system, the system complexity under the change of two parameters is used to study
and explain it. The simulation results show that the parameters have great influence on the system, which provides important value for the study of chemical chaotic vibration and electrochemical reaction.

2. Construction and Geometrical Dimensions of Specimens

In the chemical system, the experimental study on the reaction equation \( \text{C}_6\text{H}_{12}\text{N}_6 + \text{KCLO}_4 + \text{Mg} + \text{SrSO}_4 \) solid-state oscillating combustion shows that the reaction alternately goes on between smoldering and combustion, with uniform period and nonlinear chemical oscillating characteristics. According to the analysis of reaction mechanism, it is pointed out that the chemical oscillation phenomenon of this system is mainly caused by the competing reaction of Mg and O\(_2\), and the autocatalytic reaction of Mg(g) in gas phase leads to the appearance of multi-top-state solutions, and the flame dye SrSO\(_4\) has certain influence on the oscillation period. In this system, the reaction rate equation and heat balance equation of dimensionless steel play a key role. This equation can be described as [8]:

\[
\begin{align*}
\dot{x} &= \mu e^{x+y^2} - \varepsilon x - xy^2 + \lambda x \\
\dot{y} &= \varepsilon x + xy^2 - y \\
\dot{z} &= \delta y - yz 
\end{align*}
\]  

Where \( x \) is the oxygen \( \text{O}_2 \) concentration of dimensionless steel, \( y \) is the meteorological magnesium \( \text{Mg}(g) \) concentration of dimensionless steel, \( z \) is the temperature of dimensionless steel, \( \mu \) is the initial concentration of potassium perchlorate \( \text{KCLO}_4 \) of dimensionless steel, \( \lambda \) is the initial concentration of strontium sulfate \( \text{SrSO}_4 \) of dimensionless steel, \( \chi \) is the initial concentration of solid magnesium \( \text{Mg}(s) \) of dimensionless steel, \( \varepsilon \) is the activation energy of dimensionless steel, and the parameters \( \mu, \lambda, \chi, \varepsilon, \delta \) and \( \gamma \) control the change of reaction. Through simulation, it is found that \( \lambda=0.005, \varepsilon=0.12, \delta=0.1, \gamma=0.4, \mu=0.5 \) system (1) enters a chaotic state, that is, there is a typical chaotic attractor, as shown in Figure 1. At this time, the three Lyapunov exponents of the system are \( \lambda_1=0.12, \lambda_2=0 \) and \( \lambda_3=-3.6 \).

![Fig. 1 Chaotic attractor of chemical system](image)

Poincare cross-section is one of the important tools for analyzing chaotic dynamic systems. Therefore, this paper is applied to fractional chaotic systems. By observing the distribution of cut-off points on Poincare cross-section, we can judge whether it is chaotic. When there are some dense points with fractal structure on Poincare cross-section, the motion is chaotic. In this whole model, take the plane \( z=0.15 \), get the corresponding Poincare cross section, and get the Poincare cross section of the system as shown in Fig.2. It can be judged that the system (1) is a chaotic system.
3. 0-1 test

Recently, famous scholars Gottwald G A and Melbourne put forward an effective method to verify whether the system has chaotic characteristics, that is, binary test, also called 0-1 test. This test method establishes a random dynamic process, and then studies how the random process changes with time. 0-1 test result is p-s diagram. In any case, the trajectory in p-s plane can provide a simple visual measurement. If the trajectory is bounded in p-s plane, it is a regular cloud cluster, and if it is similar to Brownian motion, it indicates that the system is chaotic. Using this method to study the x and y sequences of chemical reaction system, its parameters are the same as those in Fig.1, and the obtained p-s diagram is shown in Fig.3, which shows that the system is a chaotic system.

4. Influence of parameters on chemical system

SE algorithm estimates complexity based on the discrete Fourier transformation, and it reflects the disorder of a time series in the frequency domain. In general, a flatter spectrum means a higher complexity of the time series. Based on SE algorithm, SE algorithm is designed here, and it is briefly described as follows.

Step 1. Coarse-grained procedure. For a one-dimensional discrete time series \( \{ x(i) : i = 0,1,\ldots,N - 1 \} \), the consecutive coarse-grained time series are constructed by \([11-13]\)

\[
y_t(j) = \frac{1}{\tau} \sum_{\ell=(j-1)\tau+1}^{j\tau} x(\ell)
\]

(2)

Where \( 1 \leq j \leq \left\lfloor N / \tau \right\rfloor \), \( \tau \) is the scale factor which represents the length of the non-overlapping window, and \( \left\lfloor \cdot \right\rfloor \) denotes the floor function.
Step 2. Calculating SE. Let \( y^\tau(i) = y^\tau(i) - \text{mean}(y^\tau) \), and the discrete Fourier transformation of this series is defined as

\[
Y(k) = \sum_{i=0}^{N-1} y^\tau(i) e^{-j\pi ik/N}
\]  

Where \( k = 0,1,\ldots,\lfloor N/\tau \rfloor - 1 \) and \( j \) is the imaginary unit. When the summation runs from \( k = 1 \) to \( k = \lfloor N/2\tau \rfloor \), the “probability” of the \( k \)-th frequency is defined as

\[
P_k = \frac{|Y(k)|^2}{\sum_{\tau=0}^{\lfloor N/2\tau \rfloor - 1} |Y(\tau)|^2}
\]  

Step 3. The normalization entropy is denoted by [13]

\[
SE(y^\tau) = \frac{\sum_{\tau=0}^{\lfloor N/2\tau \rfloor - 1} |P_k \ln(P_k)|}{\ln(\lfloor N/2\tau \rfloor)}
\]

Changing the parameter \( u \), \( \mu \in [0.2,1] \) the bifurcation diagram and complexity of the system with \( u \), \( \mu \in [0,0.6] \cup [0.75,1] \) show that it is easy to observe from the diagram that the system is in a periodic state, and the complexity of this interval is small, and the complexity \( C_0/SE \) is small; When other areas of \( q \) are in chaotic state, the complexity of the system \( C_0/SE \) is larger, as shown in Fig. 4.

![Bifurcation diagram](image1)

![SE complexity](image2)

![C0 complexity](image3)

Fig. 4 Bifurcation diagram and complexity of the system varying with \( u \)

5. Conclusion

In this paper, aiming at the chaotic system of chemical dynamics, the chaotic dynamics characteristics of the system are analyzed from the bifurcation diagram, LE index spectrum and complexity of the system. The simulation results show that the chaotic motion parameter range exists in the system, which provides a strong theoretical basis and reference value for chemical reaction time and experiment.
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