SHORT PAPER

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A chemical chaotic system derived from Chua's circuit†

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Chua's circuit is converted into a mass action chemical system with Samardzija's nonlinear transformation method.

Keywords: nonlinear dynamics, chemical chaos, nonlinear transformation

It is well known that oscillatory and chaotic behaviour are associated with nonlinear phenomena and the corresponding mathematical models are governed by deterministic differential equations. The differential equation models for chemical systems are different from those for physical systems. This is because in the latter type of models the variables may adopt both positive and negative values while in chemistry the concentrations of molecular species can never be negative. In the past few decades, much progress have been made in nonlinear chemical dynamics. Chemical reaction systems have become one of the favourite objects for which to study nonlinear behaviour, both experimentally and theoretically. However, the number of models that can be written as a set of coupled chemical reactions and that exhibit deterministic chaos is quite small compared to the number of models that represent mechanical, electrical and hydrodynamic systems exhibiting deterministic chaos. Hence, many physical chemists and chemical physicists have tried to set up the relationship between chemical and physical systems by means of some mathematical transformation. There have been many methods[1-9] devoted to this problem, *i.e.*, transforming a physical system modeled with a polynomial differential equation into a system which can be interpreted in terms of mass action kinetics. Of these methods, Samardzija's nonlinear transformation[4] is one of the most widely used methods and has been extensively quoted[3,5,10-17]. This method succeeds in converting some famous models such as Van der Pol, Lorenz, Rössler *etc.* into mass action chemical schemes which preserve the phase space qualitative features of the original system. The "chemical Lorenz system" produced from this method has been extensively investigated in recent years.[14-17]

Chua's circuit[18] is the simplest autonomous generator of chaotic signals and is one of the most extensively studied chaotic circuits because of its simple circuit topology. Like the Lorenz model[19], Chua's circuit has played a prominent role in the modelling, investigation and understanding of new dynamic nonlinear phenomena, especially chaotic behaviour. Because they have rich nonlinear dynamical behaviour Chua's circuits can be not only used in electrical systems but also taken as a method or a tool to study complex phenomena in other fields such as chemistry, biochemistry, electrochemistry and so on. The purpose of present paper is to report an attempt in this direction, aiming to transform Chua's circuit into a mass action chemical system (here called "chemical Chua system"). Chua's circuit, also known as the Chua system, is a canonical three-dimensional nonlinear autonomous system which is governed by the following deterministic differential equations:[20, 21]

$$dX/dt = \alpha(Y - bX^3 + cX)$$

$$dY/dt = \beta(X - Y + Z)$$

$$dZ/dt = -\gamma Y \qquad (1)$$

where α, β, γ, b, c are all positive parameters. When the parameters are selected as follows: $\alpha = 10$, $\beta = 1$, $\gamma = 16$, $b = 1$, $c = 0.143$, the system exhibits chaotic attractor. The X—Y projection of the attractor is illustrated in Fig. 1.

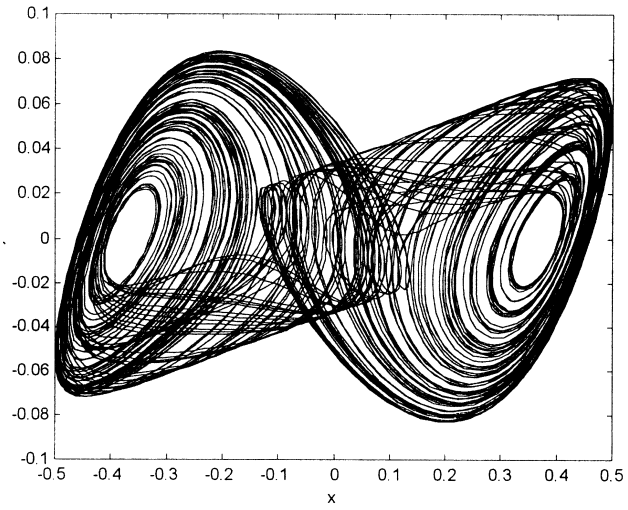

Fig. 1 Deterministic chaotic attractor produced by integrating numerically the Chua system (1). It has been projected onto $X-Y$ plane. The parameters are: $\alpha = 10$, $\beta = 1$, $\gamma = 16$, $b = 1$ and $c = 0.143$

The essence of the nonlinear transformation proposed by Samardzija *et al.*[4] is to convert an arbitrary polynomial system into an X-factorable structure (the concentration x_i as an explicit factor in the dx_i/dt equation).This is achieved by the following nonlinear transformation:

$$X = \overline{X}F[X - C]$$

where $X = [x_1, \ldots, x_m]^T$, $F[X] = [f_1(X), \ldots, f_m(X)]^T$, $\overline{X} = \mathrm{diag}(x_1, \ldots, x_m)$.

The Chua system (1) transformed into X-factorable form is

$$dX/dt = \alpha X[Y - \theta) - b(X - \phi)^3 + c(X - \phi)]$$

$$dY/dt = \beta Y[(X - \theta) - (Y - \phi) + (Z - \omega)]$$

$$dZ/dt = -\gamma Z(Y - \omega) \qquad (2)$$

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where ϕ, θ, ω are positive parameters. For simplicity these parameters are chosen as the same amount. Equation (2) can be written in the form:

$$dx/dt = k_1xy - k_2x - k_3x^4 + k_4x^3 - k_5x^2 + k_6x^2 + k_7x$$

$$dy/dt = k_8xy - k_9y - k_{10}y^2 + k_{11}y + k_{12}zy$$

$$dz/dt = k_{13}z - k_{14}yz \qquad (2a)$$

According to the mass-action law, a chemical reaction mechanism corresponding to Eqns (2a) is shown in Table 1. When parameters ϕ, θ, ω are all selected as 3000 the phase portrait obtained from numerical integration of system (2) is given in Fig.2 .It can be seen that the strange attractor is nicely in the positive space and the pattern is analogous to that of the original system (1).

Table 1

Reaction	Rate
$R_1 + X + Y \xrightarrow{k_1} 2X + Y$	$r_1 = k_1xy$
$X \xrightarrow{k_2} P_1$	$r_2 = k_2x$
$4X \xrightarrow{k_3} P_2$	$r_3 = k_3x^4$
$R_2 + 3X \xrightarrow{k_4} 4X$	$r_4 = k_4x^3$
$2X \xrightarrow{k_5} P_3$	$r_5 = k_5x^2$
$R_3 + 2X \xrightarrow{k_6} 3X$	$r_6 = k_6x^2$
$R_4 + X \xrightarrow{k_7} 2X$	$r_7 = k_7x$
$R_5 + X + Y \xrightarrow{k_8} X + 2Y$	$r_8 = k_8xy$
$Y \xrightarrow{k_9} P_4$	$r_9 = k_9y$
$2Y \xrightarrow{k_{10}} P_5$	$r_{10} = k_{10}y^2$
$R_6 + Y \xrightarrow{k_{11}} 2Y$	$r_{11} = k_{11}y$
$R_1 + Y + Z \xrightarrow{k_{12}} 2Y + Z$	$r_{12} = k_{12}yz$
$R_8 + Z \xrightarrow{k_{13}} 2Z$	$r_{13} = k_{13}z$
$Y + Z \xrightarrow{k_{14}} 2Z + P_6$	$r_{14} = k_{14}yz$

where $k_i (i = 1,2, \ldots, 14)$ are rate constants. $P_i (i = 1,2, \ldots 6)$ refer to unreactive products whose concentrations are assumed to be constant. $R_i (i = 1,2, \ldots, 8)$ denote constant reactants whose concentrations have been incorporated in the corresponding rate constants. P_i and R_i are introduced only to conserve mass in the reaction.

In this paper, we have converted a physical chaotic system into a chemical chaotic system with nonlinear transformation. The objective of this transformation is that the dynamic behaviours of physical systems can be available to chemical kinetics.

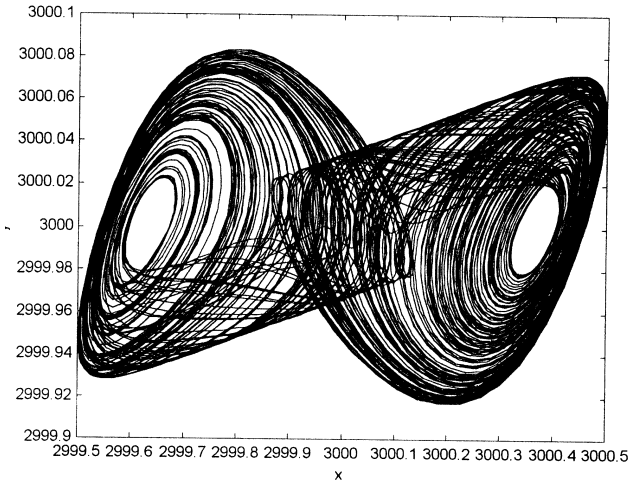

Fig. 2 Deterministic chaotic attractor obtained by integrating numerically the chemical system(2a). The rate constants k_i are: $k_1 = 10$, $k_2 = 34290$, $k_3 = 10$, $k_4 = 90000$, $k_5 = 2.7 \times 10^8$, $k_6 = 1.43$, $k_7 = 2.7 \times 10^{11}$, $k_8 = 1$, $k_9 = 6000$, $k_{10} = 1$, $k_{11} = 3000$, $k_{12} = 1$, $k_{13} = 48000$, $k_{14} = 16$.

Therefore , transforming physical systems modelled with polynomial differential equations into mass action chemical systems is interesting work and of significance.

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