SHORT PAPER

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Chaos in a three-variable chemical reaction model†

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A three-variable chemical reaction model that exhibits chaotic behaviour is presented.

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Nonlinear dynamics has become increasingly important in chemical kinetics. A variety of chemical systems that exhibit chaotic behaviour have been reported and reviewed.[1–6] It is well known that chaos arises from the nonlinear intrinsic nature of systems governed by deterministic differential equations. Numerical studies on differential equation models with chaotic solutions may reveal additional information unaccessible experimentally. Chemical reaction systems have become one of the favourite physical objects in which to study nonlinear behaviour, both experimentally and theoretically. So studies on dynamical behaviour (especially chaotic behaviour) in chemical models is very important and very useful. Killory[7] has investigated a four-variable chemical reaction model which has four Michaelis-Manten terms. They show that the system exhibits chaotic behaviour and has a hyperchaotic attractor. We present here a three-variable chemical reaction system which has two Michaelis-Manten reactions and it also exhibits chaotic behaviour for some values of the system parameters. This model is given in Table 1.

Table 1

Reaction	Rate
$A_1 + X \rightarrow 2X$	k_1x
$2X \rightarrow P$	k_2x^2
$X \rightarrow P$	$k_3xy/(x + K_{m1})$
$Y \rightarrow P$	k_4y
$A_2 + X + Y \rightarrow X + 2Y$	k_5xy
$Y \rightarrow P$	$k_6yz/(y + K_{m2})$
$Z \rightarrow P$	k_7z
$A_3 + Y + Z \rightarrow Y + 2Z$	k_8yz
$A_4 + Z \rightarrow 2Z$	k_9z

Where $k_i(i = 1 – 9)$ are rate constants and $K_{mi}(i = 1 – 2)$ are the Michaelis constants. $A_i(i = 1 – 4)$ refer to the species of constant concentration, P denotes the product and represents the concentration of species X, *etc*. The concentrations of species A_i have been absorbed into appropriate rate constants and the chemical reactions in Table 1 are assumed to be taking place in a well-stirred reactor under isothermal conditions. There are two Michaelis–Menten reactions: the outflux from X is catalysed by and the outflux from Y is catalysed by Z. According to the laws of chemical kinetics the rate equations for species X, Y and Z can be described by the following set of ordinary differential equations:

$$\begin{aligned} dx/dt &= k_1x - k_2x^2 - k_3xy/(x + K_{m1}) \\ dy/dt &= -k_4y + k_5xy - k_6yz/(y + K_{m2}) \\ dz/dt &= -k_7z + k_8yz + k_9z \end{aligned} \qquad (1)$$

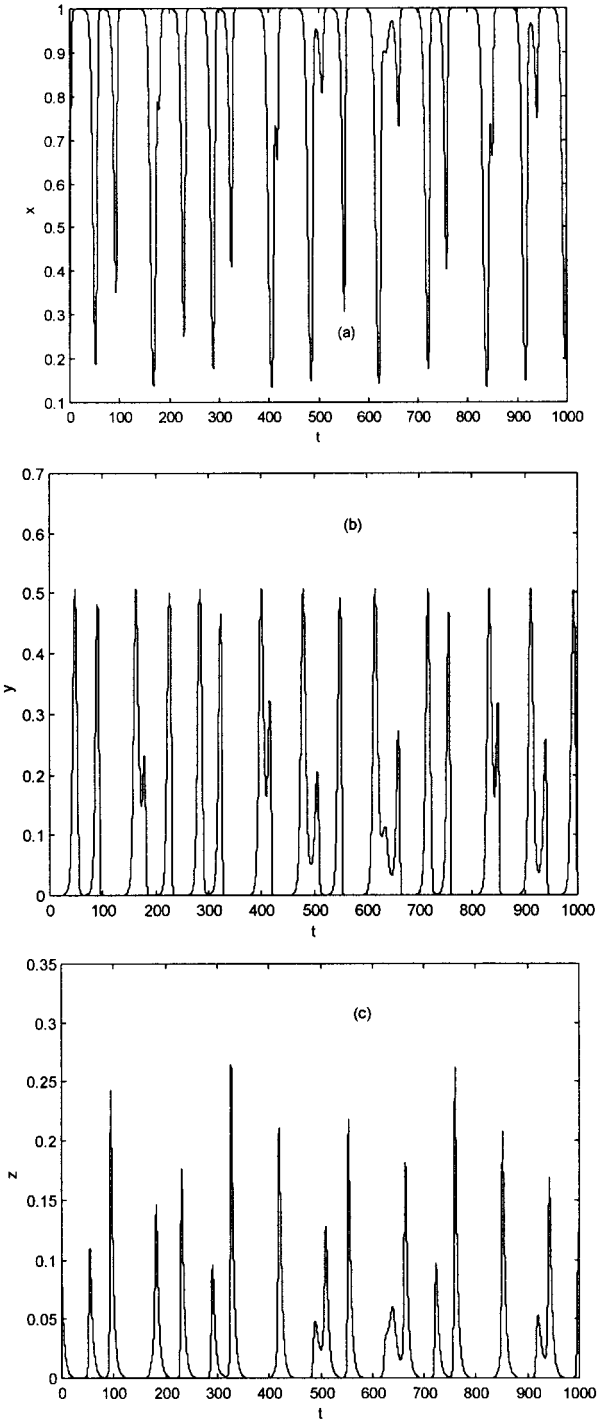

Fig. 1 Time series for the system (1) with $k_1 = 1$, $k_2 = 1$, $k_3 = 1$, $k_4 = 0.25$, $k_5 = 0.625$, $k_6 = 1$, $k_7 = 0.25$, $k_8 = 2.5$, $k_9 = 0.028$, $K_{m1} = 0.2$, $K_{m2} = 0.05$, (a) x (t) time series; (b) y (t) time series; (c) Z (t) time series.

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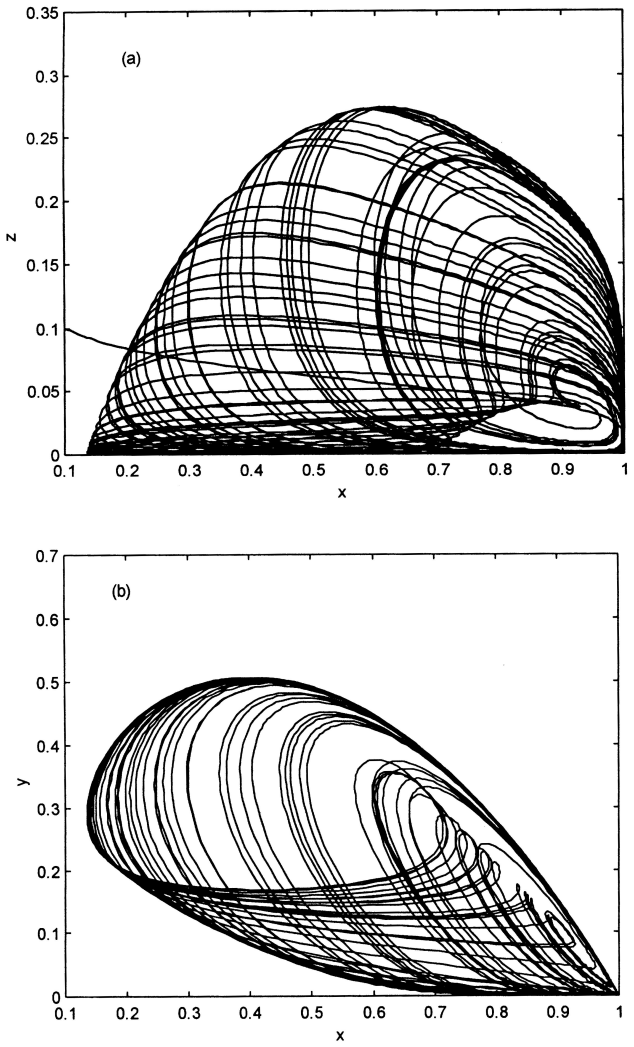

Fig. 2 Chaotic attractor produced by integrating numerically the system (1). Parameters are the same as those in Fig. 1 (a) Projection of the attractor on to *x*–*z* plane; (b) the attractor projected onto *x*–*y* plane.

When the rate constants are chosen to have the following values:

$$k_1 = 1,\ k_2 = 1,\ k_3 = 1,\ k_4 = 0.25,\ k_5 = 0.625,\ k_6 = 1$$
$$k_7 = 0.25,\ k_8 = 2.5,\ k_9 = 0.028,\ K_{m1} = 0.2,\ k_{m2} = 0.05$$

the system exhibits chaotic behaviour. Figure 1 shows three time series for the system. The strange attractor formed in concentration phase space by the chaotic motion is displayed in Fig.2.

It should be pointed out here that our system is topologically different from Hudson's model[8] (which has only one Michaelis–Manten reaction). Our system and Hasting's system[9] are also not topologically equivalent, although they appear to be so, because there is no nonsingular coordinate transformation that can convert the system of differential equations (1) to Hasting's system, or *vice versa*. Hence the system presented here is a new system.

In summary, we have presented a chaotic chemical reaction model in this paper. A good model can provide guidelines on how to synthesise chaotic systems with appropriate simple composite reactions. We believe that such a synthesis not only would increase the number of chaotic systems but also would be a decisive step toward understanding chemical chaos in simple way. How to find a simple model underlying the complex reality of a typical chemical mechanism is a very interesting but a really difficult job. Nevertheless, maybe at some distant stage in the future our experiment ability will be such that it would be possible to "design" a particular chemical reactor that fits a given scheme.[10] Chemical systems have played an important role in advancing nonlinear dynamics because they are particularly amenable to experimental and theoretical analyses and hence serve as ideal model systems. Studies of oscillations, patterns, and chaos in chemical systems constitute an exciting new frontier of chemistry. The design and development of dozens of new oscillatory and chaotic chemical reactions not only supplied dynamicists with new and different systems for characterisation, but a great deal of new chemistry has been developed in the process.[11] Therefore the work has an important significance.

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