

A SEMENOV MODEL OF SELF-HEATING IN COMPOST PILES

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In this paper we model the thermal behaviour of cellulosic materials in the presence of micro-organisms undergoing exothermic reactions. For simplicity we consider a spatially uniform model which is based upon Semenov's theory for thermal explosions. The singularity theory has been used to investigate the generic properties of the model. We consider first the case in which chemical reactions are absent, which represents heat generation in low-oxygen-containing environments. Here we show that there are two generic steady-state diagrams including one in which the temperature-response curve is the standard S-shaped curve familiar from combustion problems. Thus biological self-heating can cause jumps in the steady temperature. We then investigate the full model, which is shown to have three generic steady-state diagrams. If the energy released from the chemical reaction is sufficiently small, then the steady-state diagram may contain an elevated temperature branch, which is the feature of practical interest in facilities such as industrial compost heaps and municipal tips. If the chemical reaction is too strong the energy released by biological action increases the local temperature sufficiently high that spontaneous ignition of the cellulosic material occurs. For a given degree of chemical activity it is possible to predict the biological activity at which combustion is initiated.

Keywords: self-heating; composting; biological heating; Semenov model.

INTRODUCTION

The phenomena of spontaneous ignition due to internal heating in bulk solids such as coal, grain, hay, wool wastes, etc., can be described by thermal explosion theory as developed by Semenov and Frank-Kamenetskii (Frank-Kamenetskii, 1969; Bowes, 1984). In these models heat release is represented by a single Arrhenius reaction and combustion is initiated when heat-loss is unable to balance heat generation.

In this paper we consider a simple model for the thermal response of cellulosic materials in the presence of micro-organisms (biomass) undergoing exothermic reactions. Both types of heat generation are present in any industrial process handling large volumes of bulk organic materials. Examples of such processes include the use of large-scale composting operations as a significant biorecycle process (Rynk, 2000), the storage of industrial waste fuel, such as municipal solid waste (MSW; Hogland *et al.*, 1996), and landfills. Although MSW may not seem an obvious source of combustible materials, in one set of experiments approximately 85% of industrial waste was deemed to be combustible (Hogland *et al.*, 1996). In these systems, temperature increases due to biological activity is an inherent consequence of the process and normally a goal, e.g. in composting. Elevated temperature of the order 70–90°C may be found within a few months or even a few days according to Hogland *et al.*

(1996). Although the basic theory of spontaneous combustion relating to organic materials is well understood (Frank-Kamenetskii, 1969; Bowes, 1984), there is little information regarding the mechanism of fires when biological self-heating is involved.

In addition to the industrial process mentioned previously, it has long been suspected that the initiation of haystack fires is due to biological heating under the influence of water content or air humidity, which then lifts the temperature sufficiently to trigger significant oxidation of cellulose material, consequently leading to fire. So far, however, only the influence of oxidative processes has been considered.

We model the heat release rate due to biological activity as a function which exhibits two types of behaviour: over the temperature range $0 \leq T \leq a$ it is a monotonic increasing function of temperature, whereas for $T \geq a$ it is a monotone decreasing function of temperature. This functionality represents the fact that micro-organisms die or become dormant at high temperatures.

Singularity Theory with a Distinguished Parameter

The model studied in this paper reduces to a scalar equation of the form

$$G(\theta, \lambda, \mathbf{p}) = 0 \quad (1)$$

The scalar equation contains a state variable (θ), a distinguished parameter, (λ), sometimes called the primary bifurcation parameter, and several secondary bifurcation parameters (\mathbf{p}). The graph of θ vs. λ for fixed \mathbf{p} is called a *steady-state diagram* or a *response curve*.

The parameter space \mathbf{p} consists of regions with different kinds of steady-state diagrams. The fundamental task in the study of Equation (1) is to identify the types of steady-state diagrams that occur and their location in parameter space. We refer to a figure showing where the different types of steady-state diagrams occurring in the parameter space \mathbf{p} as a *bifurcation diagram*.

In a landmark paper Golubitsky and Schaeffer proved that a qualitative change in a steady-state diagram occurs if and only if the bifurcation parameters cross the boundaries of one of three types of curves: the *cuspl*, *isola* and *double limit point* curves (Golubitsky and Schaeffer, 1979). Thus the bifurcation diagram is constructed by determining the locus of these three curves in physical parameter space. This divides parameter space into regions, each corresponding to a different steady-state diagram of the problem $G = 0$. This methodology was first systematically applied to investigate multiplicity features of chemical systems by Balakotaiah and Luss (1981, 1982, 1984).

The *cuspl variety* is the set of \mathbf{p} satisfying the equations:

$$G = G_\theta = G_{\theta\theta} = 0 \quad (2)$$

The *isola variety* is the set of \mathbf{p} satisfying the equations:

$$G = G_\theta = G_\lambda = 0 \quad (3)$$

The *double-limit variety* is the set of \mathbf{p} satisfying the four equations:

$$G(\theta_1, \lambda, \mathbf{p}) = G(\theta_2, \lambda, \mathbf{p}) = 0 \quad \theta_1 \neq \theta_2 \quad (4)$$

$$\frac{\partial G}{\partial \theta}(\theta_1, \lambda, \mathbf{p}) = \frac{\partial G}{\partial \theta}(\theta_2, \lambda, \mathbf{p}) = 0 \quad (5)$$

In addition to satisfying the above requirements along any of the curves a set of non-degeneracy conditions must also be satisfied. These can be found elsewhere (Golubitsky and Schaeffer, 1985).

A heuristic description of this theory with a focus on applications to chemical systems has been written by Balakotaiah (1986).

MODEL

The basis of our model is that developed by Semenov to explain the phenomenon of thermal explosion in well-stirred systems understood (Frank-Kamenetskii, 1969; Bowes, 1984). This model has the following features:

- (1) the heat release rate has an Arrhenius temperature dependence;
- (2) the reactant has a uniform temperature T distinct from the ambient temperature T_a ;
- (3) the heat transfer to the surroundings is convective and linked with the temperature difference solely by a constant of proportionality;
- (4) consumption of the reactants is assumed to be negligible.

The temperature dependence of the biological heat-release is parameterized in the form:

$$k(T) = \frac{A_1 \exp[-E_1/RT]}{1 + A_2 \exp[-E_2/RT]} \quad (6)$$

In this equation the biomass growth parameters A_1 and E_1 reflect that at low temperatures the metabolic activity of the cells increases with increasing temperature as activities of their own enzymes activity rise. However, when the temperature exceeds a certain level, the essential cell proteins that are heat sensitive start to denature leading to cell death. These processes are represented by the biomass deactivation parameters A_2 and E_2 . For Equation (6) to represent heat release due to biological activity it must have a global maximum on the interval $0 < T < \infty$. Differentiation of this equation leads to the requirement $E_2 > E_1$.

Equation (6) has been used to model self-heating in solid-state fermentation processes in an earlier paper (Chen and Mitchell, 1996). More details on this formulation are provided in this reference.

MODEL EQUATIONS

Dimensionalized Equations

As mentioned above we ignore depletion of the cellulosic material and biomass. Thus our model consists of an energy equation.

Energy balance for compost pile:

$$\rho c_v V \frac{dT}{dt} = Q_b V F_b \frac{A_1 \exp[-E_1/RT]}{1 + A_2 \exp[-E_2/RT]} B \left(1 - \frac{B}{B_{\max}}\right) + Q_c V A_3 \exp\left[-\frac{E_3}{RT}\right] C - \chi S(T - T_a) \quad (7)$$

Initial conditions

$$T(t = 0) = T(0) \quad (8)$$

The first term on the right-hand side of Equation (7) represents heat generation due to biological reactions, the second term is heat-generation due to oxidation of cellulosic materials and the third term is convective heat-loss.

In practice there is not a unique microbe reasonable for heat generation in a compost pile, but rather many different species, which thrive over a sequence of overlapping temperature intervals (Kubler, 1987). We do not attempt to model the temperature varying active biomass concentration but instead take a representative constant value. In some sense this temperature is implicitly incorporated into the model through the functionality of Equation (6).

Non-dimensionalized Equations

Equation (7) is non-dimensionalized using the temperature and time scales of thermal explosion theory. This leads to:

dimensionless energy balance

$$\frac{d\theta}{dt^*} = \frac{\psi_b \exp[\theta/(1 + \varepsilon\theta)]}{1 + \beta \exp[\alpha_d \theta/(1 + \varepsilon\theta)]} + \psi_o \exp\left[\frac{\alpha_o \theta}{1 + \varepsilon\theta}\right] - \theta \quad (9)$$

dimensionless initial conditions

$$\theta(t^* = 0) = \theta(0) \quad (10)$$

In this equation the condition $\psi_b = 0$ reduces the model to the standard Semenov model for thermal explosion. Note that the requirement $E_2 > E_1$ becomes $\alpha_d > 1$. We refer to the parameter β as the maximum deactivation rate.

Singularity Function

To obtain the singularity function (G) we equate the time-derivative in Equation (9) to zero and re-arrange the steady-state equation to obtain

$$G = \psi_b \exp\left[\frac{\theta}{1 + \varepsilon\theta}\right] + \left(\psi_o \exp\left[\frac{\alpha_o\theta}{1 + \varepsilon\theta}\right] - \theta\right) \times \left(1 + \beta \exp\left[\frac{\alpha_d\theta}{1 + \varepsilon\theta}\right]\right) \quad (11)$$

In the remainder of this paper we make the pre-exponential approximation ($\varepsilon=0$). This approximation is frequently made in combustion systems. Indeed it is the main reason for the standard choice of temperature scale. Note that for a typical activation energy of $E_1 \approx 80 \text{ kJ mol}^{-1}$ and an ambient temperature $T_a = 298 \text{ K}$ we have $\varepsilon = 0.03$. Thus $1 + \varepsilon\theta \approx 1$ until $\theta \approx O(30)$.

$$G = \psi_b \exp[\theta] + (\psi_o \exp[\alpha_o\theta] - \theta)(1 + \beta \exp[\alpha_d\theta]) \quad (12)$$

Note that

$$G_{\psi_b} = \exp[\theta] \neq 0 \quad (13)$$

Thus the isola singularity does not occur in our model

Numerics

The path following software program Auto 97 (Doedel *et al.*, 1998) was used to obtain steady-state diagrams. In these the standard representation is used: solid lines are stable steady states and dotted lines are unstable steady states.

RESULTS

In the next section we consider the behaviour of the model when self-heating is entirely due to the biomass, i.e. no chemical reactions occur. It is worthwhile investigating self-heating in the absence of oxidation reactions because, although oxygen promotes microbial heat generation, it is not absolutely necessary for it: some bacteria thrive under almost anaerobic, others under truly anaerobic conditions (Kubler, 1987). Additionally, this is a constructive first-step as the behaviour of the model when self-heating is entirely due to cellulosic oxidation, which is well understood (Frank-Kamenetskii, 1969; Bowes, 1984).

Following that we consider the behaviour of the model when self-heating is due to a combination of biomass activity and cellulosic oxidation. We start by summarizing the behaviour of the thermal explosion model in the absence of biological heat generation. In both sections we restrict attention to the case $\alpha_d > 1$.

Self-Heating in the Absence of Cellulosic Oxidation

The bifurcation diagram for the biomass-only model is shown in Figure 1. To obtain this figure we have treated the biomass Semenov number (ψ_b) as the primary bifurcation parameter. The secondary bifurcation parameters are then the maximum dimensionless rate of inhibition (β) and the dimensionless activation energy for inhibition (α_d). For a particular type of biomass the parameters β and α_d are fixed. However, the parameter ψ_b includes the size of the compost

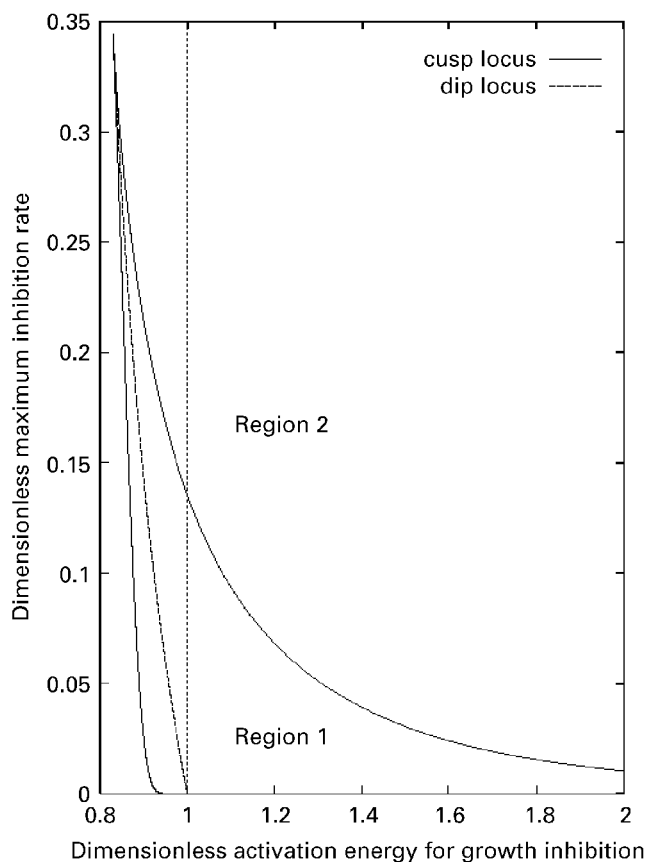


Figure 1. Bifurcation diagram for the biology-only model. Generic steady-state diagrams are shown in Figure 2.

heat and the 'concentration' of the biomass. Thus it is a controllable parameter. For specified values for the secondary bifurcation parameters, representing a specific micro-organism, Figure 1 determines the corresponding behaviour within the compost file.

Figure 1 contains a cusp curve and a double-limit point curve—as noted above, the isola variety cannot occur when ψ_b is the primary bifurcation parameter. When $\alpha_d < 1$, Figure 1 has two curves of cusp points. These curves merge at a quadratic fold singularity. At this point

$$G = G_\theta = G_{\theta\theta} = G_{\theta\theta\theta} = 0 \quad (14)$$

$$G_{\theta\theta\theta} \neq 0, \quad G_{\psi_b} \neq 0 \quad (15)$$

Observe that the double-limit point curve does not occur in the feasible region ($\alpha_d > 1$). In the feasible region the cusp locus divides the bifurcation diagram into two regions. Thus the model has two generic steady-state diagrams; these are shown in Figure 2.

In region 1 of Figure 1 the steady-state diagram contains ignition and extinction limit points, as indicated in Figure 2(a). There are two stable branches of solution: a 'low-valued' branch on which the temperature increase is small and a 'high-valued' branch on which the dimensionless temperature increase is larger. Thus, if the biomass Semenov number is sufficiently large biological self-heating occurs. In region 2 there are no limit points, Figure 2(b), and the dimensionless temperature raise increases smoothly as the biomass Semenov number increases. Note that there is a

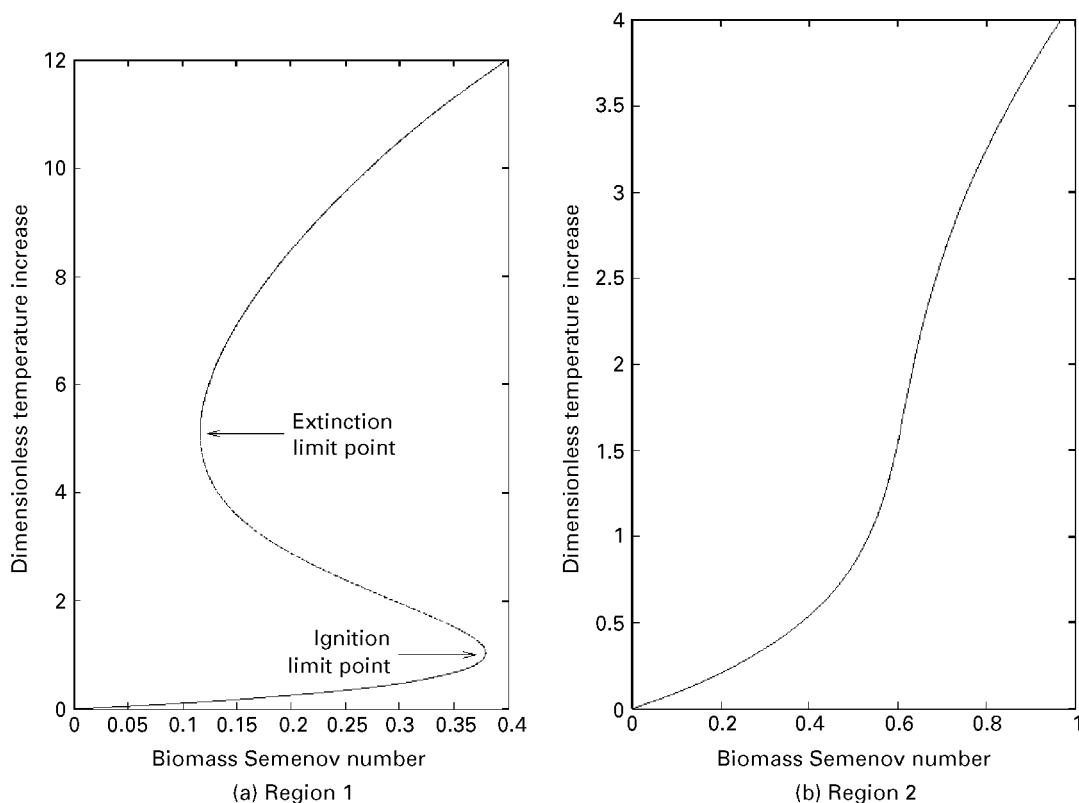


Figure 2. Generic steady-state diagrams for the biomass-only model when $\alpha > 1$. Parameter values: (a) $\psi_o = 0.01$, $\alpha_d = 1.1$; (b) $\psi_o = 0.15$, $\alpha_d = 1.1$. (a) Region 1; (b) region 2.

difference between the amount of biomass required to achieve a high degree of self-heating in Figure 2(a) and (b): the biomass Semenov number needs to be much greater than in the latter. This occurs because inhibition dominates growth in region 2.

From these figures we deduce that if you want biological self-heating to occur then the kinetic parameters for biomass deactivation (α_d , β) need to be in region 1. Thus Figure 1 allows the suitability of a micro-organism for composting to be decided once values for the two kinetic parameters have been determined.

It is possible to obtain an analytical inequality for the location of the line separating region 1 from region 2. The defining conditions for a limit point are (Golubitsky and Schaeffer, 1985):

$$G = G_\theta = 0 \quad (16)$$

$$G_{\theta\theta} \neq 0, \quad G_{\psi_b} \neq 0 \quad (17)$$

After some algebra it is found that limit points occur when

$$\beta e^{\alpha_d \theta} = \frac{\theta - 1}{1 + (\alpha_d - 1)\theta} \quad (18)$$

$$\psi_b = \theta \{1 + \beta e^{\alpha_d \theta}\} e^{-\theta} \quad (19)$$

Equation (18) is an implicit equation for the temperature at the limit point. Equation (19) then gives the critical value of the bifurcation parameter ψ_b at criticality. Let $L(\theta)$ and $R(\theta)$ be the LHS and RHS of Equation (18), respectively.

Assuming that $\alpha_d > 1$, we have

$$L(1) = \beta e^{\alpha_d} > R(1) = 0 \quad (20)$$

$$L(\infty) > R(\infty) = \frac{1}{\alpha_d - 1} \quad (21)$$

As both L and R are monotonic increasing functions of θ on the interval $[1, \infty]$, Equation (18) certainly does not have a solution, i.e. there are no limit points, if $L(1) > R(\infty)$, i.e.

$$\beta > \frac{1}{\alpha_d - 1} e^{-\alpha_d} \quad (22)$$

Self-Heating in the Presence of Cellulosic Oxidation

We start by summarizing the thermal explosion model in the absence of biological self heating [$\psi_b = 0$ in Equation (12)]. The steady-state diagram contains one limit point and for low values of θ looks similar to the steady-state diagram shown in Figure 4(a). The criticality condition in our variable is given by:

$$\psi_{o,cr} = \frac{1}{\alpha_o} \exp[-1] \quad (23)$$

For $\psi_o \leq \psi_{o,cr}$, there is a stable branch of solutions with a negligible temperature rise. For $\psi_o \geq \psi_{o,cr}$, the solution blows up in finite time (Frank-Kamenetski, 1969; Bowes, 1984).

Figure 3 shows the bifurcation diagram when heat-release due to cellulosic oxidation is present in addition to that due to biomass. Analogous to the situation in the previous section

(Figure 1), particular values for the secondary bifurcation parameters represent a specified micro-organism. Figure 3 determines the type of behaviour that can occur within the compost heap corresponding to a particular choice of micro-organism. For the value of the chemical activation energy used ($\alpha_o = 1$), the critical value of the chemical Semenov parameter is 0.368. Thus the value used, $\psi_o = 0.01$, is well below the criticality threshold for purely chemical ignition.

Comparing Figure 3 with Figure 1 we see that the inclusion of chemical reaction has extended into the feasible region. The bifurcation diagram has three regions in the feasible region, consequently there are three generic steady-state diagrams. These are shown in Figure 4(a–c) and correspond to a vertical slice through the bifurcation diagram along the line $\alpha_d = 1.2$.

Note that, whereas in Figure 2 the temperature raise is always bounded, in Figure 4 the temperature raise is unbounded for supercritical systems. In fact blow-up occurs in finite-time. This is a consequence of assuming that $\varepsilon = 0$ in Equation (11). If $\varepsilon \neq 0$ the steady-state diagram contains an additional stable branch with very high temperature raises representing ignition of the cellulosic material.

In region 1 of Figure 3 the steady-state diagram contains one limit point. For subcritical values of the biomass Semenov number there is no significant degree of self-heating, Figure 4(a). In this region self-heating due to the biomass can increase the temperature sufficiently that it

ignites the cellulosic materials, but does not create elevated stable temperatures. This is undesirable from an operational viewpoint. Thus we should not operate a compost heap with characteristics belonging to region 1.

In region 2 of Figure 3 the steady-state diagram contains three limit points. Two limit points are created at a cusp singularity as we enter region 2a from region 1 and two limit points are destroyed at a cusp singularity as enter region 1 from region 2b. Figure 4(b, c) shows that in region 2 the steady-state diagram contains two stable branches: a 'low-valued' branch on which the temperature increase is negligible and an 'elevated-temperature' branch. Assuming a typical value for the activation energy for biomass growth of $E_1 \approx 80 \times 10^3 \text{ J mol}^{-1}$, then the temperature increase on the elevated branch is of the order of 30–50°C. As mentioned previously, if we were to assume that $\varepsilon \neq 0$ there would be a third stable branch, representing ignition of the cellulosic materials. Thus, temperature rises are possible in region 2.

Observe that Figure 4(b, c) contains two ignition limit points and one extinction limit point. The distinction between region 2a and region 2b is made on the relative locations of the two ignition limit points. In region 2a the ignition limit point on the elevated temperature branch is found at a lower value of the biomass Semenov number than that on the lower stable branch ('to the left'). In region 2b the ignition limit point on the elevated temperature branch is found at a higher value of the biomass Semenov number than on the lower stable branch ('to the right'). The double-limit point curve is the set of parameter values at which two ignition limit points occur for the same value of the biomass Semenov number.

There is a practical distinction between these two regions. When the lowest branch loses stability in region 2a the solution blows-up; physically this means that the cellulosic materials are ignited. However, when the lowest branch loses stability in region 2b the system can evolve onto the elevated temperature branch. Thus if the kinetic parameters for biomass deactivation need are in region (2b) it is possible to obtain elevated temperatures within the compost heap. Figure 4(d) shows the steady-state diagram for parameter values that are in region 1, but *above* the cusp locus rather than *below* it as is the case for Figure 4(a). Both figures contain one limit-point, however the subcritical temperature increase in Figure 4(d) is considerably greater than that in Figure 4(a). Indeed the subcritical temperature increase in Figure 4(d) can become as high as that found on the elevated temperature branch in region (2). From this we conclude that elevated temperature can also be achieved if the kinetic parameters for biomass deactivation are in region (1) provided that they are located above the cusp-locus in Figure 3.

The bifurcation diagram shown in Figure 3 was obtained for a particular choice of kinetic values for the oxidation reaction. In Figure 5 we show how the bifurcation diagrams as these kinetic parameters are varied. In each of the subfigures the curve (1) is the same bifurcation diagram shown in Figure 3. Note that a distinction is not made between regions 2a and 2b in Figure 5.

In Figure 5(a) we fix the activation energy for the oxidation reaction and vary the chemical Semenov number. In Figure 5(b) we fix the chemical Semenov number and increase the activation energy. In both cases the trends are similar: the location of the quartic fold moves to the right; the area on the graph in which region 2 occurs diminishes whereas the

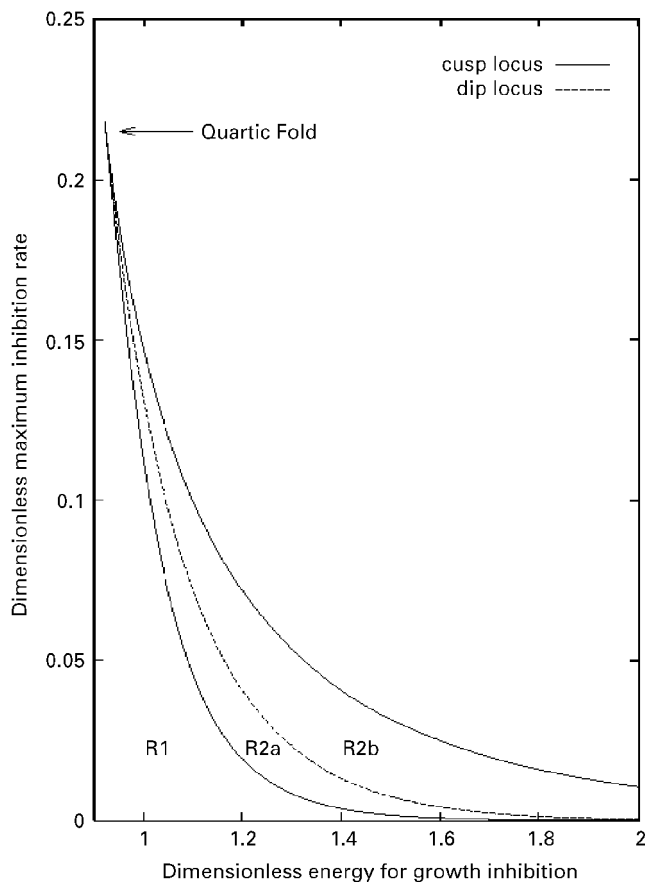


Figure 3. Bifurcation diagram for the full model. Parameter values for the oxidation reaction: dimensionless activation-energy, $\alpha_o = 1.0$; Semenov parameter, $\psi_o = 0.01$. Generic steady-state diagrams are shown in Figure 4.

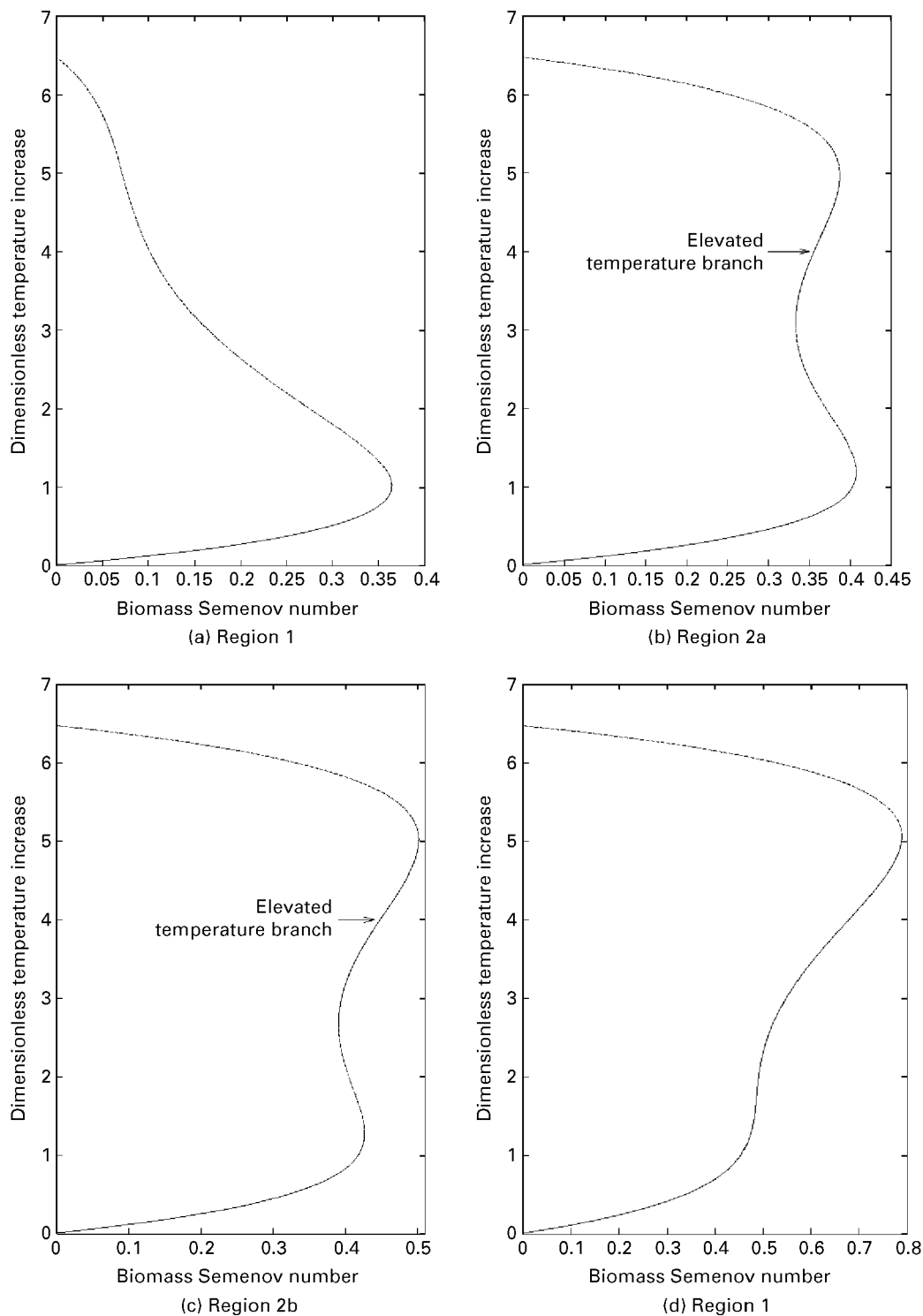


Figure 4. Generic steady-state diagrams for the full model. In each figure the dimensionless activation energy for inhibition is $\alpha_d=1.2$. The dimensionless maximum inhibition rate is: (a) $\beta=0.005$; (b) $\beta=0.028$; (c) $\beta=0.05$; (d) $\beta=0.08$. Other parameter values are as given in Figure 3. (a) Region 1; (b) region 2a; (c) region 2b; (d) region 1.

area corresponding to region 1 increases. These trends indicate that, as these parameters increase, the behaviour of the system becomes increasingly dominated by the chemical reaction and the influence of the biomass decreases. Such behaviour is undesirable. Conversely, Figure 5 shows that as the chemical activation energy is decreased the behaviour of the system becomes increasingly dominated by the biomass reaction.

The effect upon the steady-state diagram of increasing the chemical Semenov number at fixed chemical activation energy is shown in Figure 6. When the oxidation reaction is absent, curve (a), we are in region (1) of Figure 1 and elevated temperatures occur if the biomass Semenov number is sufficiently high. When the chemical Semenov number is sufficiently small the system has an elevated temperature

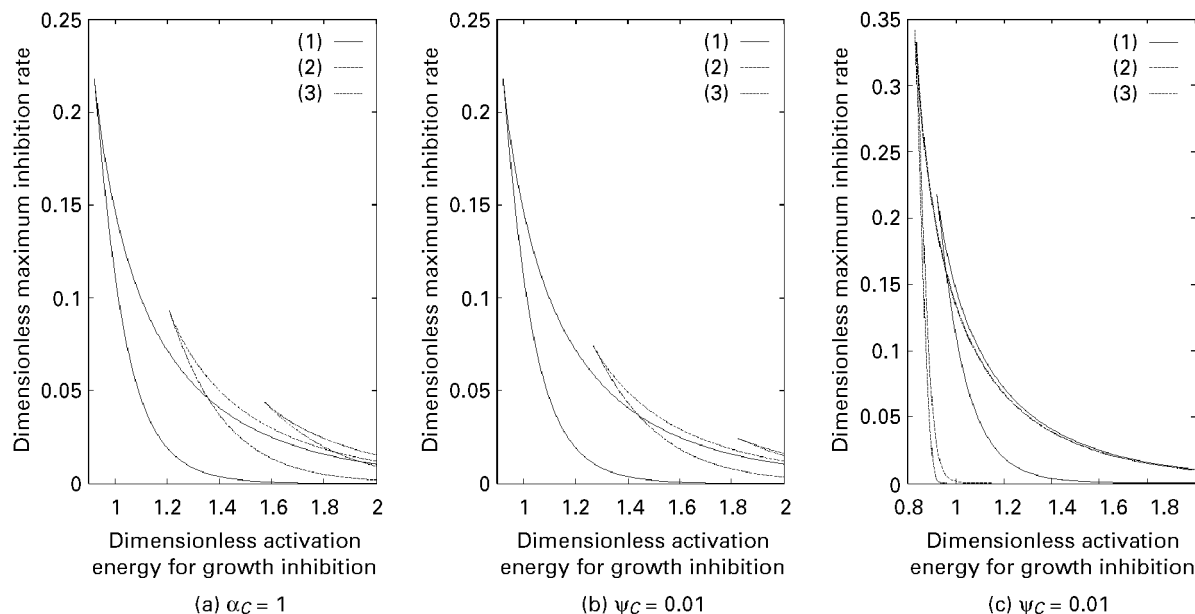


Figure 5. Bifurcation diagrams for the full model indicating the influence of the chemical parameters upon the system behaviour: (a) the effect of the chemical Semenov number with α_c constant ($\alpha_c = 1$); (b) the effect of the chemical activation energy ($\alpha_c \geq 1$) with ψ_c constant ($\psi_c = 0.01$); (c) the effect of the chemical activation energy ($\alpha_c \leq 1$) with ψ_c constant ($\psi_c = 0.01$). Parameter values: (a) (1) $\psi_c = 0.01$, (2) $\psi_c = 0.05$, (3) $\psi_c = 0.10$; (b) (1) $\alpha_c = 1$, (2) $\alpha_c = 1.5$, (3) $\alpha_c = 1.9$; (c) (1) $\alpha_c = 1$, (2) $\alpha_c = 0.5$, (3) $\alpha_c = 0.0$.

branch, curves (b, c). The range in values for the biomass Semenov number over which the elevated branch is found shrinks as the chemical Semenov number increases. When the chemical Semenov number is sufficiently large the elevated temperature branch is destroyed, curve (d). Thus if chemical activity is too high, elevated temperature cannot be obtained with the compost heap.

DISCUSSION

Self-heating in compost piles can lead to one of three types of behaviour: negligible temperature increase; an elevated temperature increase *without* ignition; and ignition of cellulosic materials. As we have made the pre-exponential approximation $\varepsilon = 0$, the model does not contain a stable solution branch representing cellulosic combustion. Instead combustion is represented by finite time blow-up. The behaviour of our system would not dramatically change if we were to take ε small and positive. However, we would then have three stable branches of solution.

Combustible systems in which there are three distinct types of behaviour are not unknown. For instance, smouldering combustion lies between the extremes of negligible decomposition and flaming combustion. It has been found that by making well-defined changes to an experimentally controllable system that smouldering states may undergo a transient evolution to either of these states (Moussa *et al.*, 1976). From a dynamical systems viewpoint it is natural to think that these physiochemical states are represented by three stable solution branches on the steady-state diagram: the lowest, middle and highest stable solution branches being identified with states of no-reaction, smouldering combustion and fully burning, respectively. The first authors to make this connection were Brindley *et al.* (1990) and Gray (1990).

It is tempting to draw an analogy between the elevated temperatures found in compost heaps with the state of

smouldering combustion. Should this be the case we can identify the former with the behaviour exhibited in region 2b of Figure 3. However, we are not aware of any experimental work showing that compost heaps in states of elevated

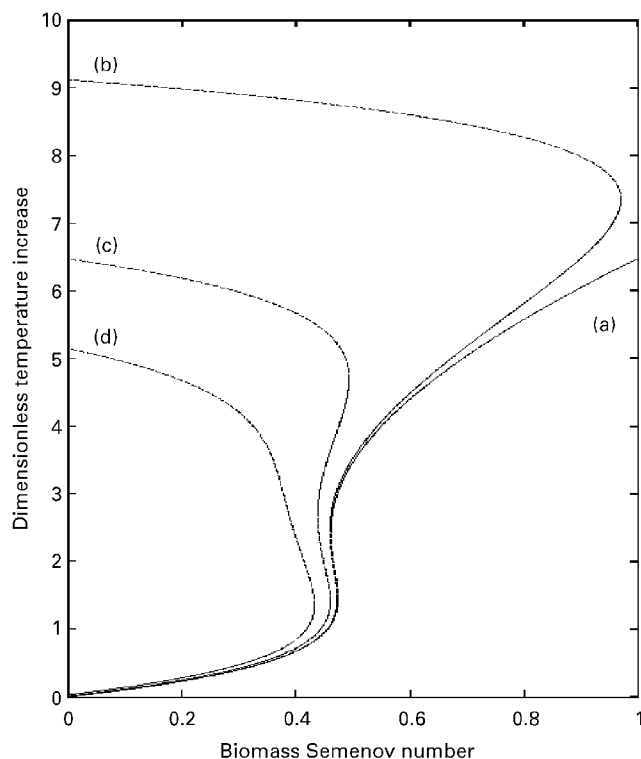


Figure 6. The effect of increasing the chemical Semenov number upon the steady-state diagram. Common parameter values: maximum dimensionless inhibition rate, $\beta = 0.01$; dimensionless activation energy for inhibition, $\alpha_d = 1.1$; chemical activation energy, $\alpha_o = 1$. Chemical Semenov number: (a) $\psi_c = 0.0$; (b) $\psi_c = 10^{-3}$; (c) $\psi_c = 10^{-2}$; (d) $\psi_c = 3 \times 10^{-2}$.

temperatures can undergo transient evolution to either states of negligible temperature increase or to flaming combustion. In the absence of experimental work along the lines of that conducted by Moussa *et al.* (1976), the phenomenon of elevated temperatures can also be equated to the steady-state solution in Figure 4(d). Thus there are two mechanisms accounting for elevated temperatures. In principle it is possible to generate elevated temperatures by either of these mechanisms by an appropriate choice of biological agent. However it is not clear what the practical advantages would be of being able to choose whether the dynamics of a compost heap were represented by a steady-state diagram such as in Figure 4(c or d)?

Although elevated temperatures due to biological self-heating are desirable, biological activity can create temperatures that sustain heat-release in bulk organic materials which, if not detected, can lead to spontaneous combustion of the heap. For instance, although the value of the chemical Semenov number (ψ_o) used in calculating the steady-state diagrams shown in Figure 4 is well below criticality, spontaneous combustion can occur if the biomass Semenov number (ψ_b) is sufficiently large.

CONCLUSION

In this paper we have investigated a simple model for self-heating in compost heaps. As the model contains few parameters it is possible to thoroughly investigate the generic behaviour generated as parameters are changed through the use of singularity theory. We have shown that elevated temperatures can be accounted for by two mechanisms. However, in the absence of experimental data it is not possible to distinguish between them. Furthermore we have shown that it is possible for the heat released by biological activity to initiate combustion of cellulosic material. Thus a situation which is judged subcritical, i.e. safe, based on classic thermal explosion theory may in fact be supercritical. This offers one explanation for the prevalence of such fires in composting facilities.

Having established a conceptual understanding for the thermal behaviour of compost heaps we plan to investigate a spatially non-uniform extension of our model including such effects as the degree of aeration and moisture content. Singularity theory will provide a useful tool in systematically studying these more complicated systems. For instance, the size of the pile is an obvious primary bifurcation parameter whilst the degree of aeration and the moisture content can be taken as secondary bifurcation parameters. From such models it will be possible to determine the critical pile size at which spontaneous combustion occurs and to investigate how the criticality condition changes as other parameters such as ambient temperature change. This is a practical consideration because, although spontaneous combustion may be the most frequent cause of fires at compost facilities, it is the hardest to detect because it is internal rather than external (Rynk, 2000). We hope to present a discussion of these points and a sample calculation using the published growth parameters as well as the heats associated with biological reactions in a subsequent paper.

NOMENCLATURE

The superscript * refers to a dimensionless quantity, P^* is a dimensionless parameter whose dimensional counterpart is P . The notation $V(t=0)$ and

$V^*(0)$ refers to the initial value of the dimensional variable V at time $t=0$ and its dimensionless counterpart at time $t^*=0$.

A_1	pre-exponential factor for biomass growth, s^{-1}
A_2	pre-exponential factor for the inhibition of biomass growth
A_3	pre-exponential factor for the oxidation of cellulose, s^{-1}
B	the concentration of biomass in the bioreactor, $kg\ m^{-3}$
B_{max}	the maximum biomass concentration, $kg\ m^{-3}$
C	the concentration of cellulose in the bioreactor, $kg\ m^{-3}$
E_1	activation energy for biomass growth, $J\ mol^{-1}$
E_2	activation energy for the inhibition of biomass growth, $J\ mol^{-1}$
E_3	activation energy for cellulose oxidation, $J\ mol^{-1}$
F_b	substrate inhibition term
Q_b	exothermicity of the biomass growth reaction, $J\ kg^{-1}$
Q_c	exothermicity of the cellulose oxidation reaction, $J\ kg^{-1}$
R	ideal gas constant, $J\ K^{-1}\ mol^{-1}$
S	the internal surface area of the bioreactor, m^2
T	the bioreactor temperature, K
T_a	the temperature of the bioreactor walls, K
V	volume of the bioreactor, m^3
c_v	heat capacity of the reaction mixture, $J\ K^{-1}\ kg^{-1}$
t	time, (s)
t^*	$t^* = t \times (cS/c_v rV)$

Greek symbols

α_d	dimensionless activation energy for the inhibition of biomass growth, $\alpha_d = E_2/E_1$
α_o	dimensionalized activation energy for cellulose oxidation, $\alpha_o = E_3/E_1$
β	maximum dimensionless rate of inhibition, $b = A_2 \exp[-E_2/RT_a]$
ε	reduced activation energy for biomass growth, $\varepsilon = RT_a/E_1$
θ	non-dimensionalized bioreactor temperature, $\theta = [E_1(T - T_a)]/RT_a$
$\theta(0)$	$\theta(0) = E_1(T(0) - T_a)/RT_a$
ρ	density of the reaction mixture, $kg\ m^{-3}$
λ	heat transfer coefficient between the reaction mixture and the bioreactor walls, $J\ s^{-1}\ m^{-2}\ K^{-1}$
ψ_b	the Semenov number for the biomass, $\psi_b = [1 - (B(0)/B_{max})]\{VB(0)Q_bF_bA_1E_1/\chi SRT_a\} \exp[-E_1/RT_a]$
ψ_o	Semenov number for the oxidation of cellulosic materials, $\psi_o = (VQ_cA_3C(0)E_1/\chi SRT_a) \exp[-E_3/RT_a]$

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