

The Semenov formulation of the biological self-heating process in compost piles

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Abstract

We formulate and investigate a uniformly distributed mathematical model (based upon Semenov's theory for thermal explosions) for the thermal response of cellulosic materials in compost piles. The model consists of a mass balance equation for oxygen, a heat balance equation, and incorporates the heat release due to biological activity within the pile. Biological heat generation is known to be present in most industrial processes handling large volumes of bulk organic materials. We utilise singularity theory to investigate the generic properties of the model, as well as to determine the locus of different singularities, namely the cusp, isola and double limit point. Singularity theory provides a useful tool to systematically analyse this system. We investigate the conditions where biological activity results in the initiation of an elevated temperature branch within the compost pile.

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1 Introduction

The phenomena of spontaneous ignition due to internal heating in bulk solids, such as coal, grain, hay, and wool wastes, can be described by thermal explosion theory as developed by Semenov and Frank–Kamenetskii [2, 4]. 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.

We consider a simple model for the thermal behaviour of compost heaps when self-heating is entirely due to the presence of micro-organisms or microbes undergoing oxidative exothermic reactions. This is a constructive first step

to understand the thermal behaviour of compost heaps when self-heating is due to a combination of low temperature heating effects, from the biomass, and higher temperature effects, from the oxidation of cellulosic material; the behaviour of the model when self-heating is entirely due to cellulosic oxidation is well known [2].

Low temperature self-heating due to the action of biomass is present in any industrial processes handling large volumes of bulk organic materials. It is due to the growth and respiration of micro-organisms such as aerobic mould fungi and bacteria. Examples of such processes include the use of large scale composting operations as a significant biorecycle process [15], the storage of industrial waste fuel, such as municipal solid waste (MSW) [6], and landfills. Although MSW does not seem an obvious source of combustible materials, in one set of experiments, approximately 85 percent of industrial waste was deemed to be combustible [6]. In these systems, temperature increases due to biological activity is an inherent consequence of the process and normally a goal, for example 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. [6].

Although it is recognised for over twenty years that “. . . biological heating may be an indispensable prelude to self ignition. . .” [2], very little information is available regarding the mechanism of fires when biological self-heating is involved. An understanding of this phenomenon is crucial as fires (most likely due to biological self-heating) are common at landfills worldwide [7]. Furthermore, spontaneous combustion may be the most frequent cause of fires at compost facilities [15].

We model the heat release rate due to biological activity as a function which exhibits two types of behaviour: over the temperature range $0 < T < a$ it is a monotonic increasing function of temperature, whereas for $T > a$ it is a monotonic decreasing function of temperature. This functionality reflects that micro-organisms die or become dormant at high temperatures. In practice, there is not a unique microbe responsible for heat generation in compost

pile, but rather many different species which thrive over a sequence of overlapping temperature intervals [9]. The temperature varying active biomass concentration is incorporated into the model through the chosen functionality for the biological heat release rate. In an earlier Semenov-type model for self-heating in compost piles it was assumed that biological heat release is independent of the oxygen concentration; that is, anaerobic conditions predominant in the pile [12]. We assume that aerobic conditions apply within the pile and model biological heat release as an oxidative process. Since we are considering a spatially uniform model, we use singularity theory to analyse the generic properties of the model. We provide a brief overview of singularity theory in the next section.

1.1 Singularity theory with a distinguished parameter

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

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

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

The parameter space 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 as a bifurcation diagram.

Golubitsky and Schaeffer [5] 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 cusp, isola and double limit point curves. Thus the bifurcation diagram is constructed by determining the locus of these three curves in physical parameter space. This divides the parameter space

into various 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 [1]. We now discuss briefly the four different types of singularities.

cusp The *cusp* variety is the set of \vec{p} satisfying the equations

$$G = G_\theta = G_{\theta\theta} = 0, \quad \text{with } G_\lambda \neq 0 \text{ and } G_{\theta\theta\theta} \neq 0. \quad (2)$$

Typically when the cusp curve is crossed a hysteresis loop appears or disappears in the steady state diagram as two limit points appear or disappear.

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

$$G = G_\theta = G_\lambda = 0, \quad \text{with } G_{\theta\theta} \neq 0 \text{ and } G_{\theta\theta}G_{\lambda\lambda} - (G_{\theta\lambda})^2 \neq 0. \quad (3)$$

When the isola curve is crossed two limit points appear or disappear. Two types of behaviour may occur. In the first, the steady state diagrams separate locally into two isolated curves (transcritical singularity). In the second, an isolated branch of connected solutions appears or disappears (isola singularity).

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

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

$$G_\theta(\theta_1, \lambda, p) = G_\theta(\theta_2, \lambda, p) = 0,$$

$$\text{with } G_{\theta\theta}(\theta_i, \lambda, p) \neq 0, \quad G_\lambda(\theta_i, \lambda, p) \neq 0, \quad \text{for } i = 1, 2. \quad (5)$$

At the double limit point variety two limit points occur at the same value of the distinguished parameter. As the double limit point variety is crossed, the relative positions of these limit points change.

quadratic fold The *quadratic fold* variety is the set of \vec{p} satisfying the equations

$$G = G_\theta = G_{\theta\theta} = G_{\theta\theta\theta} = 0. \quad (6)$$

$$G_{\text{oooo}} \neq 0, \quad G_{\lambda} \neq 0. \quad (7)$$

At a quadratic fold point, cusp singularity and double limit points singularity bifurcation curves are merged with each other. This point can be used to determine the existence of the double limit point variety.

1.2 Model

The basis of our model is similar to that developed by Semenov to explain the phenomenon of thermal explosion in well stirred systems [16]. Our model has the following features:

1. The compost pile has a uniform temperature, T , distinct from the ambient temperature, T_a ;
2. The heat transfer to the surroundings is convective and linked with the temperature difference solely by the heat transfer coefficient;
3. Consumption of the reactants is assumed to be negligible;
4. The concentration of oxygen in the pile is uniform, O_2 , and is distinct from the ambient oxygen concentration, $O_{2,a}$;
5. Oxygen transfer from the surroundings is convective and linked to the concentration difference solely by the mass transfer coefficient.

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

$$k(T) = \frac{A_1 e^{-E_1/RT}}{1 + A_2 e^{-E_2/RT}}. \quad (8)$$

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 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 (8)

to represent heat release due to biological activity it must have a global maximum on the interval $0 < T < \infty$, which leads to the requirement $E_2 > E_1$. Equation (8) has been used to model the maximum specific biomass growth rate in the aerobic biodegradation of the organic fraction of municipal solid waste [10]. It has also been used in several models for solid state fermentation processes [3, 8, 14]. More details on this formulation are provided in those articles and the references within.

2 Governing equations

2.1 Dimensionalized equations

In this investigation, we utilise the same model equations developed by Nelson et al. [13]. As mentioned earlier, we ignore depletion of cellulosic material and biomass. This model consists of a mass balance equations for oxygen and energy: Energy balance for compost pile

$$\rho c_v V \frac{dT}{dt} = Q_b V F_b \frac{A_1 e^{-E_1/RT}}{1 + A_2 e^{-E_2/RT}} B O_2 - \chi S (T - T_a); \quad (9)$$

Oxygen balance for compost pile

$$V \frac{dO_2}{dt} = -V F_b \frac{A_1 e^{-E_1/RT}}{1 + A_2 e^{-E_2/RT}} B O_2 + \chi_m S (O_{2,a} - O_2); \quad (10)$$

Initial condition

$$T(t = 0) = T(0) = T_a, \quad O_2(t = 0) = O_2(0) = O_{2,a}. \quad (11)$$

All the terms that appear in the governing equations and initial conditions (9)–(11) are defined in the nomenclature, Table 1. The first term on the right-hand side of equation (9) represents heat generation due to the biological reactions (the corresponding term appears as the first term on

the right-hand side of equation (10) representing the consumption of oxygen during the biological reaction processes), whilst the second term in equation (9) is the convective heat loss. The second term on the right-hand side of equation (10) represents the convective flow of oxygen into the compost pile.

2.2 Non-dimensionalized equations

Next we non-dimensionalized equation (9)–(10) by using the temperature, oxygen and time scales of thermal explosion theory:

$$\theta = \frac{E_1(T - T_a)}{RT_a^2}, \quad Y = \frac{O_2}{O_{2a}}, \quad t^* = t \left(\frac{\chi S}{c_v \rho V} \right), \quad \epsilon = \frac{RT_a}{E_1}.$$

The non-dimensionalization process leads to the following equations: Dimensionless energy balance

$$\frac{d\theta}{dt^*} = Y \frac{\psi_b \left[\exp\left(\frac{\theta}{1+\epsilon\theta}\right) \right]}{1 + \beta \left[\exp\left(\frac{\alpha_d \theta}{1+\epsilon\theta}\right) \right]} - \theta; \quad (12)$$

Dimensionless oxygen balance

$$\frac{dY}{dt^*} = -\psi_b \Gamma \frac{\exp\left(\frac{\theta}{1+\epsilon\theta}\right)}{1 + \beta \left[\exp\left(\frac{\alpha_d \theta}{1+\epsilon\theta}\right) \right]} Y + \sigma(1 - Y); \quad (13)$$

Dimensionless initial conditions

$$\theta(t^* = 0) = \theta(0), \quad Y(t^* = 0) = Y(0). \quad (14)$$

The parameters of the system are: ψ_b is the Semenov number for the biomass which is referred to the size of the compost pile; β is the maximum rate of inhibition of the biological activity; σ is the mass transfer number for specific compost type; and Γ is the non-dimensionalized oxygen number for the biological activity. The requirement $E_2 > E_1$ results in $\alpha_d > 1$.

2.3 Singularity function

To obtain the singularity function (G) we equate the time derivatives in equations (12) and (13) to zero and re-arrange the steady state equations to obtain the single singularity function

$$G = \psi_b(\sigma - \Gamma\theta) \exp\left(\frac{\theta}{1 + \epsilon\theta}\right) - \sigma\theta \left[1 + \beta \exp\left(\frac{\alpha_d\theta}{1 + \epsilon\theta}\right)\right] = 0. \quad (15)$$

In our investigation we use θ as the state variable parameter, ψ_b as the primary bifurcation parameter, and σ and Γ as the secondary bifurcation parameters. For our results we use the standard notation for the steady state plots: solid lines denote stable solution branch; and dashed lines represents unstable solution branch.

3 Results

The primary aim of this section is to represent the results for the isola, cusp and double limit points singularity analysis that occur for equation (15). The results overview the generic solution behaviour of this system. The analysis for both cases when $\epsilon = 0$ and $\beta = 0$ and when $\epsilon \neq 0$ and $\beta \neq 0$, have been done previously only for the isola and cusp singularities [11]. We extend the analysis by including the double limit point analysis for the case when $\epsilon = 0$ and $\beta \neq 0$. When $\beta \neq 0$, it means that biological inhibition at high temperature is now present; that is, we assume that the micro-organism and proteins are affected by the high temperature environment. The approximation for $\epsilon = 0$ is frequently made in combustion systems. Indeed it is the reason for standard choice of temperature scale. Note that for a typical activation energy of $E_1 \approx 100 \text{ kJ mol}^{-1}$ and ambient temperature $T_a = 298 \text{ K}$, $\epsilon = 0.0248$ can be considered to be small.

3.1 Isola singularity analysis

The isola singularity conditions relevant to this case are

$$G = \psi_b e^\theta (\sigma - \Gamma\theta) - \sigma\theta(1 + \beta e^{\alpha_d\theta}) = 0, \tag{16}$$

$$G_{\psi_b} = e^\theta (\sigma - \Gamma\theta) = 0. \tag{17}$$

From equation (17), we obtain $\sigma = \Gamma\theta$ (noting that e^θ is always greater than zero) and we substitute the value of σ back into equation (16). Then the G function reduces to

$$G = -\Gamma\theta^2(1 + \beta e^{\alpha_d\theta}) \neq 0. \tag{18}$$

By inspection, $\theta = 0$ is not a steady state solution from equation (16), and therefore $G \neq 0$. The values of β , α_d , θ and Γ are always greater than zero which results in the G function to be negative. Therefore the isola singularity conditions ($G = G_\theta = G_{\psi_b} = 0$) do not hold.

3.2 Cusp singularity analysis

The cusp singularity conditions relevant to this case are

$$G = \psi_b e^\theta (\sigma - \Gamma\theta) - \sigma\theta(1 + \beta e^{\alpha_d\theta}) = 0, \tag{19}$$

$$G_\theta = -\psi_b e^\theta \Gamma + \psi_b e^\theta (\sigma - \Gamma\theta) - \sigma(1 + \beta e^{\alpha_d\theta}) - \sigma\theta\beta\alpha_d e^{\alpha_d\theta} = 0, \tag{20}$$

$$G_{\theta\theta} = -2\psi_b e^\theta \Gamma + \psi_b e^\theta (\sigma - \Gamma\theta) - 2\sigma\beta\alpha_d e^{\alpha_d\theta} - \sigma\theta\beta\alpha_d^2 e^{\alpha_d\theta} = 0, \tag{21}$$

$$G_{\theta\theta\theta} = -3\psi_b e^\theta \Gamma + \psi_b e^\theta (\sigma - \Gamma\theta) - 3\sigma\beta\alpha_d^2 e^{\alpha_d\theta} - \sigma\theta\beta\alpha_d^3 e^{\alpha_d\theta} \neq 0 \tag{22}$$

By solving equations (19)–(21), we obtain

$$\psi_b = \frac{\alpha_d\theta^3}{e^\theta(\alpha_d\theta - \theta + 2)}, \tag{23}$$

$$\beta = -\frac{(\theta - 2)}{e^{\alpha_d\theta}} \frac{1}{\theta(\alpha_d - 1)^2 + 2(\alpha_d - 1)}, \tag{24}$$

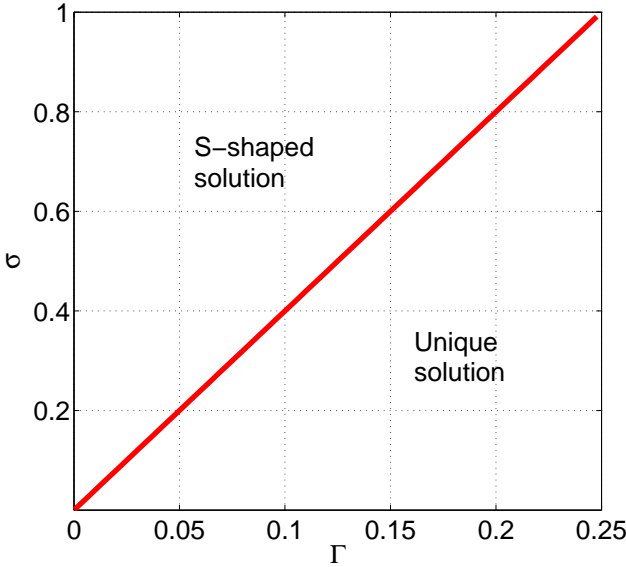


FIGURE 1: Bifurcation diagram. Parameter values are $\epsilon = 0$, $\alpha_d = 2$ and $\beta = 6 \times 10^{-5}$.

$$\Gamma = \frac{\sigma}{\theta^3(\alpha_d - 1)} [(\alpha_d - 1)\theta^2 - (\alpha_d - 2)\theta - 2]. \tag{25}$$

By substituting the values of ψ_b , β and Γ back into (22), then

$$G_{\theta\theta\theta} = \frac{[(\alpha_d - 1)\theta^2 - (2\alpha_d - 4)\theta - 6] \alpha_d \sigma}{\alpha_d \theta - \theta + 2} \neq 0. \tag{26}$$

Hence the cusp singularity conditions ($G = G_\theta = G_{\theta\theta} = 0$ and $G_{\theta\theta\theta} \neq 0$) is satisfied (the special case when $G_{\theta\theta\theta} = 0$ is investigated in the next section for a double limit point singularity). The bifurcation diagram in expression (25) depends on the values of α_d and θ . Obtain the value of θ by solving equation (24) for a given value of β .

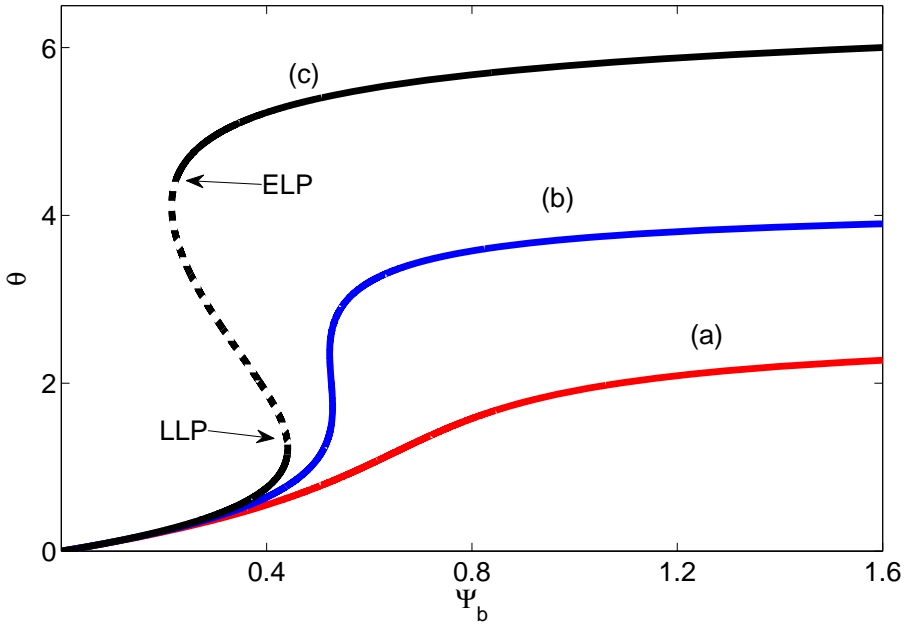


FIGURE 2: Generic steady state diagrams for oxidative self-heating model when $\Gamma = 0.15$, $\beta = 6 \times 10^{-5}$, $\epsilon = 0$ and $\alpha_a = 2$. Parameter (a) $\sigma = 0.4$, (b) $\sigma = 0.62$ and (c) $\sigma = 1$. LLP refers to the low ignition limit point and ELP denotes the extinction limit point.

Figure 1 shows the bifurcation diagram when ϵ equals to zero. Note that the value of σ and Γ are fixed for particular type of biomass, whereas, the value of Ψ_b corresponds to the size of the compost heap and the concentration of biomass which can be controlled. The values of α_a and β used here, corresponds to the same parameter values used by Sidhu et al. [17]. From Figure 1, the bifurcation diagram is separated into two regions, with each region representing different solution behaviour. When the bifurcation line is crossed, a change in the solution behaviour occurs.

Figure 2 shows the steady state curves when the value of Γ is fixed to 0.15

and the value of σ varies from the lower region across the cusp line to the upper region. Curve (a) represents the solution when $\sigma = 0.4$ in the lower region of the bifurcation diagram in Figure 1 (labelled ‘unique’). In this region, the compost heap temperature (θ) increases gradually as the size of the compost heap (ψ_b) is increased. For each value of ψ_b , there is a unique value of θ . There is no sudden ‘jump’ or ‘drop’ between solution branches. However, as the parameter values are varied to the upper region of Figure 1 (the ‘S-shaped solution’ region), the steady state solution forms the familiar S-shaped graph in thermal explosion studies as shown in curve (c). On the low temperature solution branch, the temperature increases as the compost heap size is increased. However, if the size of the compost heap is increased beyond the low ignition limit point (LLP), $\psi_b \approx 0.44$, there is a ‘jump’ from the low to high temperature solution branch. The temperature suddenly ‘jumps’ from $\theta \approx 1.2$ (306.67 K) at the LLP to $\theta \approx 5.25$ (366.76 K) on the upper stable solution branch. On the other hand, if the compost heap temperature is on the upper solution branch and the size of compost heap is decreased beyond the extinction limit point (ELP), $\psi_b \approx 0.21$, then there is a significant drop in compost heap temperature from $\theta \approx 4.15$ (328.64 K) at the ELP to $\theta \approx 0.32$ (300.36 K) on the lower stable solution branch. In the high temperature solution range, oxidation reaction of cellulosic material is well known to occur and can occur rapidly resulting in spontaneous ignition. Hence the sudden increase in temperature due to biological heating can be a prelude to spontaneous ignition. Curve (b) represents the solution behaviour on the cusp line ($\sigma \approx 0.62$ and $\Gamma \approx 0.15$). The solution behaviour is in the a transition stage from the unique solution to the S-shaped solution. In this case, the limit points (LLP and ELP) are located almost at the same value of ψ_b .

Hence Figure 2 shows the significant difference between the amount of biomass required to achieve a high degree of self-heating in curves (a) and (c), where the biomass Semenov number in the former needs to be much greater than in the latter to achieve the same level of temperature rise. From these figures we deduce that if one wants biological self-heating to occur in the compost

heap, then the parameters (Γ, σ) in Figure 1 need to be in the region with S-shaped solution.

3.3 Double limit points singularity analysis

To investigate the existence of the double limit points singularity (DLP), we simply investigate the existence of the quadratic fold singularity point. Since DLP only exists when this point does exist. Firstly, we try to find the possible location of the quadratic fold singularity point by assuming that the value of $G_{\theta\theta\theta}$ in equation (26) equal to zero in order to satisfy the quadratic fold singularity conditions.

Since the value of σ and α_d are always greater than zero, therefore from equation (26), the quadratic fold point exists only when

$$(\alpha_d - 1)\theta^2 - (2\alpha_d - 4)\theta - 6 = 0. \quad (27)$$

By rearranging the equation (27) and recalling the constrain that $\alpha_d > 1$, we obtain

$$\alpha_d = \frac{\theta^2 - 4\theta + 6}{\theta(\theta - 2)} > 1. \quad (28)$$

Solving the inequality (28), we find that there are two possible ranges of θ values that satisfy the quadratic fold singularity conditions. These are $\theta < 0$ and $2 < \theta < 3$. We analyse these two ranges separately for the occurrence of the DLP.

3.3.1 Temperature $2 < \theta < 3$

From equation (24), all values of θ in this range corresponds to negative value for β (infeasible region). Therefore the quadratic fold singularity does not exist for physically realistic parameters. Thus the model definitely contains

the DLP corresponding to negative value of β . However, we need to investigate the possibility of the DLP moving over to the positive region of β values. If the DLP is able to move to the positive region of β , then the quadratic fold singularity must occur for $\beta = 0$. Therefore we use the quadratic fold singularity conditions to find the existence of the DLP when $\beta = 0$.

The quadratic fold singularity conditions when $\beta = 0$ are

$$G = \psi_b e^\theta (\sigma - \Gamma\theta) - \sigma\theta = 0, \quad (29)$$

$$G_\theta = \psi_b e^\theta \sigma - \psi_b e^\theta \Gamma\theta - \psi_b e^\theta \Gamma - \sigma = 0, \quad (30)$$

$$G_{\theta\theta} = \psi_b e^\theta \sigma - \psi_b e^\theta \Gamma\theta - 2\psi_b e^\theta \Gamma = 0, \quad (31)$$

$$G_{\theta\theta\theta} = \psi_b e^\theta \sigma - \psi_b e^\theta \Gamma\theta - 3\psi_b e^\theta \Gamma = 0. \quad (32)$$

Solving equations (29)–(31), we obtain

$$\psi_b = 4e^{-2}, \quad \theta = 2 \quad \text{and} \quad \Gamma = \frac{\sigma}{4}.$$

Substituting the values of ψ_b , θ and Γ back into equation (32) results in

$$G_{\theta\theta\theta} = -\sigma. \quad (33)$$

Since $G_{\theta\theta\theta} \neq 0$ in equation (33) as $\sigma \neq 0$, the quadratic fold singularity conditions does not hold when $\beta = 0$ and the DLP will never occur in this case. Therefore, the DLP only occurs in this model in the negative region of β (infeasible region) and it is not able to move across to the positive β region.

3.3.2 Temperature $\theta < 0$

To complete our analysis, we consider the negative value of θ . By considering equation (25) for negative values of θ , we conclude that Γ is always negative (we only consider solutions for positive ψ_b in equation (23) as ψ_b refers to the compost pile size and must be non-negative). Therefore, the quadratic fold

point occurs in the non-feasible region of Γ . We again investigate whether the DLP is able to move over to the positive Γ region by investigating the existence of the quadratic fold point when $\Gamma = 0$. The case when $\Gamma = 0$ represents the anaerobic model (no oxygen consumption).

The quadratic fold singularity conditions when $\Gamma = 0$ are

$$G = \psi_b e^\theta \sigma - \sigma \theta (1 + \beta e^{\alpha_d \theta}) = 0, \quad (34)$$

$$G_\theta = \psi_b e^\theta \sigma - \sigma (1 + \beta e^{\alpha_d \theta}) - \sigma \theta \beta \alpha_d e^{\alpha_d \theta} = 0, \quad (35)$$

$$G_{\theta\theta} = \psi_b e^\theta \sigma - 2\sigma \beta \alpha_d e^{\alpha_d \theta} - \sigma \theta \beta \alpha_d^2 e^{\alpha_d \theta} = 0, \quad (36)$$

$$G_{\theta\theta\theta} = \psi_b e^\theta \sigma - 3\sigma \beta \alpha_d^2 e^{\alpha_d \theta} - \sigma \theta \beta \alpha_d^3 e^{\alpha_d \theta} = 0. \quad (37)$$

Solving equations (34)–(36), we obtain

$$\psi_b = \frac{\theta(\theta^2 - 2\theta + 2)}{e^\theta}, \quad \beta = \frac{\theta^2 - 2\theta + 1}{\exp\left(\frac{\theta^2 - 2\theta + 2}{\theta - 1}\right)}, \quad \text{and} \quad \alpha_d = \frac{\theta^2 - 2\theta + 2}{\theta(\theta - 1)}.$$

Substituting the values of ψ_b , β and α_d back into (37), then

$$G_{\theta\theta\theta} = \frac{(\theta^2 - 4\theta + 2)(\theta^2 - 2\theta + 2)\sigma}{(\theta - 1)\theta^2}. \quad (38)$$

The quadratic fold point singularity is satisfied only when equation (38) equals zero. By letting equation (38) equal to zero, there are two possible real values of θ which are $\theta = 2 + \sqrt{2}$ and $\theta = 2 - \sqrt{2}$. However, if we substitute these values back into the α_d equation above, we obtain $\alpha_d \approx 0.82$ and $\alpha_d \approx -4.82$ respectively which breaks our model requirement that $\alpha_d > 1$. Therefore, the DLP does not exist for $\Gamma = 0$. Hence the DLP only occurs in negative region of Γ value when θ is negative and it cannot move over to positive region of Γ .

As a result, we conclude that the quadratic fold point singularity and the DLP exist in this model for negative parameter values, and therefore do not have physical meaning. However, that they do occur may be important for future

work when we include the oxidation reaction in the model. The inclusion of the chemistry may ‘drag’ the quartic fold point into physically realistic parameter space and may have important consequences. This is an area for future investigation.

4 Conclusions

We investigated a simple model for biological oxidative self-heating in compost piles. We first non-dimensionalized both energy balance and oxygen balance equations using the Frank–Kamenetskii variables. As the model contains fewer parameters, it is possible to thoroughly investigate the generic behaviour, as the parameters are varied, through the use of singularity theory. As suspected, the cusp singularity separates the parameter plane into two regions. In the lower region, the solution behaviour is just a monotonic increasing function without any limit points. On the other hand, solution behaviour in the upper region contains limit points, and multiple solutions. If the biomass Semenov number is sufficiently large, biological self-heating can occur. By using the bifurcation diagram generated from the singularity analysis, one can deduce the parameter values required if biological self-heating is a desirable outcome. We also found that the isola singularity and double limit points singularity do not exist in this model. We also plan to investigate the possibility of the Hopf bifurcations in the future, as spontaneous combustion may occur via this type of bifurcation.

Having established a conceptual understanding for biological oxidative self-heating in compost piles, we plan to investigate a more realistic model when both oxidative biological and oxidation reactions are present with oxygen consumption. Later we also intend to investigate the effects of the flow of air into the compost heap as well as the effects of moisture content. Singularity theory will provide a useful tool in systematically analysing these more complicated systems.

TABLE 1: nomenclature.

| | |
|------------|--|
| A_1 | pre-exponential factor for biomass, s^{-1} |
| A_2 | pre-exponential factor for the inhibition of biomass, $(-)$ |
| B | the concentration of biomass in the bioreactor, $kg\ m^{-3}$ |
| C | the concentration of cellulose in the bioreactor, $kg\ m^{-3}$ |
| c_v | heat capacity of the compost heap, $J\ K^{-1}\ kg^{-1}$ |
| E_1 | activation energy for biomass growth, $J\ mol^{-1}$ |
| E_2 | activation energy for the inhibition of biomass growth, $J\ mol^{-1}$ |
| F_b | substrate inhibition term |
| O_2 | oxygen concentration within the pile, $kg\ m^{-1}$ |
| $O_{2,a}$ | ambient oxygen concentration, $kg\ m^{-1}$ |
| Q_b | exothermicity of the biomass growth reaction, $J\ kg^{-1}$ |
| R | ideal gas constant, $J\ K^{-1}\ mol^{-1}$ |
| S | the internal surface area of the bioreactor, m^{-2} |
| T | temperature within the compost pile, K |
| T_a | the ambient temperature, K |
| t | time, s |
| V | volume of the bioreactor, m^3 |
| ρ | density of the compost heap, $kg\ m^{-3}$ |
| χ | heat transfer coefficient between the compost heap and its surroundings, $J\ s^{-1}\ m^{-2}\ K^{-1}$ |
| χ_m | mass transfer coefficient between the compost heap and its surroundings, $m\ s^{-1}$ |
| α_d | dimensionless activation energy for the inhibition of biomass growth, $\alpha_d = E_2/E_1$ |
| β | maximum dimensionless rate of inhibition, $\beta = A_2 e^{-E_2/RT_a}$ |
| ϵ | reduced activation energy for biomass growth, $\epsilon = RT_a/E_1$ |
| θ | non-dimensionalized bioreactor temperature, $\theta = E_1(T - T_a)/RT_a^2$ |
| t^* | non-dimensionalized time, $t^* = t(\chi S/[c_v \rho V])$ |
| ψ_b | the Semenov number of the biomass, $\psi_b = O_{2a} B E_1 Q_b V F_b A_1 e^{-E_1/RT_a} / [\chi S R T_a^2]$ |
| σ | non-dimensionalized mass transfer number, $\sigma = c_v \rho \chi_m / \chi$ |
| Γ | non-dimensionalized oxygen number for biological reaction, $\Gamma = R T_a^2 c_v \rho / [E_1 Q_b O_{2a}]$ |

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