Self-heating in compost piles due to biological effects

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Abstract

The increase in temperature in compost piles/landfill sites due to micro-organisms undergoing exothermic reactions is modelled. A simplified model is considered in which only biological self-heating is present. The heat release rate due to biological activity is modelled by a function which is a monotonic increasing function of temperature over the range $0 \leqslant T \leqslant a$, whilst for $T \geqslant a$ it is a monotone decreasing function of temperature. This functional dependence represents the fact that micro-organisms die or become dormant at high temperatures. The bifurcation behaviour is investigated for 1-d slab and 2-d rectangular slab geometries. In both cases 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 elevated temperature raises due to jumps in the steady temperature.

This problem is used to test a recently developed semi-analytical technique. For the 2-d problem a four-term expansion is found to give highly accurate results—the error of the semi-analytical solution is much smaller than the error due to uncertainty in parameter values. We conclude that the semi-analytical technique is a very promising method for the investigation of bifurcations in spatially distributed systems.
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1. Introduction

The phenomenon of spontaneous ignition due to internal heating in bulk solids such as coal, grain, hay, wool wastes, and other materials, can be described by thermal explosion theory (Bowes, 1984; Frank-Kamenetskii, 1969). In such models heat release is usually represented by a *single* Arrhenius reaction. However, in industrial processes involving large volumes of bulk organic materials there are *two* sources of heat-generation: a low-temperature process involving the growth and respiration of micro-organisms, such as aerobic mould-fungi and bacteria, and a high-temperature process due to oxidation of cellulosic materials. Examples of processes where biological heating is important include large-scale composting operations (Rynk, 2000), the storage of industrial waste fuel, such as municipal solid waste, and landfills. In these, for example in composting

(Brinton et al., 1995), self-heating due to biological activity is a desired outcome. Elevated temperatures of the order 70–90 °C may be found within a few months or even a few days (Hogland et al., 1996). Although it has been recognised for over 20 years that "biological heating may be an indispensable prelude to self-ignition" (Bowes 1984, p. 373), little information is available regarding the mechanism of fires when biological self-heating is involved—despite fires at landfills being common worldwide (Hudak, 2001).

The case when self-heating is entirely due to cellulosic oxidation is well known (Bowes, 1984; Frank-Kamenetskii, 1969). Here we consider a scenario when self-heating is entirely due to the biomass. This is a constructive step towards the analysis of a model containing heat-release due to both biological and chemical activity as it establishes regions in parameter space in which biological self-heating leads to elevated temperature raises—the main feature of interest in landfill sites. Furthermore, a model without chemical self-heating applies to environments under which anaerobic biodegradation

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predominates; anaerobic oxidation being a known technology to treat the organic component of municipal solid wastes. The resulting mathematical model also serves as a useful testing ground for a new method of carrying out bifurcational analysis of spatially distributed systems that has been developed by one of the authors. This is discussed in Section 4.2. An advantage of this method, over direct numerical integration, is that all solution branches are found, not just the stable branches.

Comprehensive mathematical models for the combustion of biomass have been published in recent years (Jand and Foscolo, 2005; Radmanesh et al., 2006; Wurzenberger et al., 2002). These models have been developed to optimise the thermal conversion of biomass in furnaces and to predict the composition of the product gas. Such models may include detailed consideration of the physics of the furnace (including hydrodynamics), chemical kinetics (pyrolysis chemistry and heterogeneous/homogeneous gas-phase reactions) and knowledge of physical data such as fuel density, thermodynamic, and transport properties. Thus knowledge of a large number of physical and kinetic parameters is required. Such detail is not warranted in the present case, where we extend classical thermal explosion theory to cover the case of biological self-heating. Our aim is to comprehensively identify the generic behaviour exhibited by a simple model, in particular identifying parameter regions where significant self-heating occurs, rather than to present detailed simulations showing the evolution of a compost pile in such regions.

1.1. Bifurcation theory for spatially distributed reactor models

In this paper we use a Galerkin method to obtain a semi-analytical approximation to the solution of a spatially distributed reactor model. This techniques yields a system of coupled non-linear ordinary differential equations, which can be analysed using standard methods. In this section we outline some alternative approaches that can be used to investigate the behaviour of spatially structured reactor models.

A naive approach to dealing with a distributed reactor model is to discretise it to produce a set of ordinary differential equations and to then use standard numerical bifurcation algorithms. For 1-d models good results can be obtained for discretisations using of the order of 10^2 points. However, for 2-d and 3-d models the growth in nodal points makes it impractical to compute the Jacobian matrix and eigenvectors using such a direct approach (Balakotaiah and Khinast, 2000). For problems in one spatial dimension an efficient, and powerful technique, is to combine Liapunov–Schmidt reduction with shooting methods (Balakotaiah and Khinast, 2000; Subramanian and Balakotaiah, 1996). However, this method does not generalise to problems in two, or more, spatial dimensions. For problems in higher dimensions, Subramanian and Balakotaiah (1996) suggest that the model equations be averaged in the spatial directions in which the variables do not change rapidly.

An alternatively averaging method uses the Liapunov–Schmidt technique to perform spatial homogenization over small scales. Averaging is done over the local (transverse) dimensions. This leads to a series solution in a small parameter which is the ratio of local diffusion time to convection time of the system. This method has been applied to convection–diffusion–reaction (CDR) equations to obtain low-dimensional models. The first-order term in the series expansion parameter is sufficient to retain all the qualitative features of the CDR model (Chakraborty and Balakotaiah, 2002a). In the low-dimensional models the concentration of a chemical species is not given by a single equation but by a system of differential–algebraic equations. The differential equation describes the variation of the "cup-mixing" concentration with the residence time whilst the algebraic equation(s) captures mixing on local scales. Typically, one algebraic equation is used to model micromixing. (For non-isothermal systems there are multiple temperature equations).

This method has been applied to thermal and solutal dispersion (Balakotaiah and Chang, 2003), laminar flow in isothermal tubular reactors with homogeneous reactions (Chakraborty and Balakotaiah, 2002a, b, 2003), to a variety of isothermal wall-catalyzed and coupled homogeneous–heterogeneous reacting flows (Balakotaiah and Chakraborty, 2003) and to non-isothermal reactor systems (Chakraborty and Balakotaiah, 2004). The methodology developed in these papers is limited to CDR models with Neumann (zero flux), Robin or periodic boundary conditions. Furthermore, the averaged models exist only when the local diffusion time is much smaller than the convective and characteristic reaction times.

2. Model equations

2.1. Temperature dependence of the reaction rate

The basis of our model is that developed by Frank-Kamenetskii (FK) to explain the phenomenon of thermal explosions in spatially distributed systems (Bowes, 1984; Frank-Kamenetskii, 1969). However, the temperature dependence of the reaction rate is not given by an Arrhenius expression but is instead parameterised in the form:

$$k(T) = \frac{A_1 \exp\left[\frac{-E_1}{RT}\right]}{1 + A_2 \exp\left[\frac{-E_2}{RT}\right]}, \quad E_2 > E_1. \tag{1}$$

The formulation of Eq. (1) encapsulates that activation and inactivation processes occur over different temperature ranges. At low temperatures the metabolic activity of the biomass grows with increasing temperature as enzyme activity raises. These processes are governed by the parameters A_1 and E_1.

Eq. (1) can be derived theoretically by assuming that the biomass growth rate is determined by a rate limiting step in which there is an equilibrium between "activated" and "unactivated" forms of the biomass (Roels, 1983, Chapters 7.5.2 and 9.5). From this, thermodynamic, perspective the term $A_2 \exp[-E_2/RT]$ represents the temperature dependence of the equilibrium constant whilst the expression $A_1 \exp[-E_1/RT]$ is the maximum forward rate of reaction in the rate limiting step. Roels (1983, p. 253) notes that

"Although this model is based on a highly simplified image of the complexity of the growth process, it can be considered an efficient tool to model the temperature dependence of the maximum rate of growth".

Eq. (1) has been used to model the maximum specific biomass growth rate in the aerobic biodegradation of the organic fraction of municipal solid waste (Liwarska-Bizukojc et al., 2001). It has also been used in a number of models for solid-state fermentation processes (Khanahmadi et al., 2004; Mitchell and von Meien, 2000; von Meien and Mitchell, 2002; von Meien et al., 2004).

2.2. Dimensional equations

Ignoring depletion of biomass our model equation is derived by considering an energy balance. The geometry of the compost pile is a slab on the domain $-L \leqslant x \leqslant L$. We invoke symmetry considerations to reduce the domain to $0 \leqslant x \leqslant L$. The governing equation, initial and boundary conditions are

$$\rho c \frac{\partial T}{\partial x} = k \frac{\partial^2 T}{\partial x^2} + Q_b \frac{A_1 \exp\left[\frac{-E_1}{RT}\right]}{1 + A_2 \exp\left[\frac{-E_2}{RT}\right]} B \left(1 - \frac{B}{B_{\max}}\right), \quad (2)$$

$$\left.\frac{\partial T}{\partial x}\right|_{x=0} = 0, \quad T(x = L) = T_a, \quad T(x, 0) = T_a. \quad (3)$$

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 in Eq. (2) we let the biomass density, B, take a representative constant value (B_b). Further information regarding the formulation of Eq. (2) can be found elsewhere (Chen and Mitchell, 1996).

2.3. Dimensionless equations

Eq. (2) is made dimensionless using the standard length, temperature, and time scales of spatially distributed thermal explosion theory, see Notation for details. This leads to the dimensionless equations

$$\frac{\partial \theta}{\partial t^*} = \frac{\partial^2 \theta}{\partial x^{*2}} + \frac{\delta \exp\left[\frac{\theta}{1+\varepsilon\theta}\right]}{1 + \beta \exp\left[\frac{\alpha\theta}{1+\varepsilon\theta}\right]}, \quad 0 \leqslant x^* \leqslant 1, \quad (4)$$

$$\left.\frac{\partial \theta}{\partial x^*}\right|_{x^*=0} = 0, \quad \theta(x^* = 1) = 0, \quad \theta(x^*, 0) = 0. \quad (5)$$

In Eq. (4) the conditions $\alpha = 0$ or $\beta = 0$ reduces the model to the FK model for thermal explosion (Bowes, 1984; Frank-Kamenetskii, 1969). Note that the requirement $E_2 > E_1$ implies that $\alpha > 1$.

The 2-d slab is described by a straightforward generalisation of the 1-d equations

$$\frac{\partial \theta}{\partial t^*} = \frac{\partial^2 \theta}{\partial x^{*2}} + \frac{\partial^2 \theta}{\partial y^{*2}} + \frac{\delta \exp\left[\frac{\theta}{1+\varepsilon\theta}\right]}{1 + \beta \exp\left[\frac{\alpha\theta}{1+\varepsilon\theta}\right]},$$

$$\frac{\partial \theta}{\partial x^*} = 0 \text{ at } x^* = 0, \quad \frac{\partial \theta}{\partial y^*} = 0 \text{ at } y^* = 0,$$

$$\theta^* = 0 \text{ at } x^*, y^* = 1, \quad \theta^*(x^*, y^*, t^* = 0) = 0. \quad (6)$$

In analysing the 1-d and 2-d systems we make the standard simplifying assumption, the pre-exponential approximation, that $\varepsilon = 0$.

3. Semi-analytical theory

The Galerkin method is used to obtain semi-analytical solutions for the compost problem in the 1- and 2d-dimensional slab geometries. This involves approximating the spatial structure of the temperature profile in the compost heap using trial functions that satisfy the boundary conditions. The semi-analytical model is then obtained by averaging the governing energy equation. As the expression for biological self-heating cannot be integrated explicitly, the semi-analytical model is given by a system of integrodifferential equations. Steady-state diagrams may be obtained from these as the solutions to a set of transcendental equations (the integrals are evaluated using quadrature rules). Singularity theory (Golubitsky and Schaeffer, 1985) is applied to evaluate all qualitatively distinct behaviour in the model. This semi-analytic method was previously applied to the catalytic pellet problem (Marchant and Nelson, 2004), where a comparison with results in the literature showed that highly accurate results could be obtained with two- (1-d) and four-term (2-d) expansions.

In this section we describe the application of the semi-analytical method to the 2-d slab, problem (6). The application to the 1-d slab is not described, as it is similar to the 2-d theory; see also Marchant and Nelson (2004). The temperature profile is approximated by a series of orthogonal basis functions. The expansion

$$\theta(x^*, y^*, t^*) = \theta_1(t^*) \cos\left(\frac{\pi x^*}{2}\right) \cos\left(\frac{\pi y^*}{2}\right)$$
$$+ \theta_2(t^*) \cos\left(\frac{3\pi x^*}{2}\right) \cos\left(\frac{\pi y^*}{2}\right)$$
$$+ \theta_2(t^*) \cos\left(\frac{\pi x^*}{2}\right) \cos\left(\frac{3\pi y^*}{2}\right)$$
$$+ \theta_3(t^*) \cos\left(\frac{3\pi x^*}{2}\right) \cos\left(\frac{3\pi y^*}{2}\right), \quad (7)$$

is used, which satisfies the boundary conditions in (6), but not the governing pde. The expansion has four terms, but symmetry implies that two of the terms have the same coefficient. In Section 4.2, the leading-order approximation, when $\theta_2 = \theta_3 = 0$, and Richardson extrapolation, is used to estimate the accuracy of the expansion (7).

The expansion (7) is substituted into (6) with the equation weighted by the first basis function, $\cos(\pi x^*/2)\cos(\pi y^*/2)$. Averaging then gives an ode for θ_1. Repeating the averaging procedure for the other basis functions gives the system of three odes

$$\frac{d\theta_1}{dt^*} = f_1 = -\theta_1 \frac{\pi^2}{2} + \delta I_1,$$
$$\frac{d\theta_2}{dt^*} = f_2 = -\theta_2 \frac{5\pi^2}{2} + \delta I_2,$$
$$\frac{d\theta_3}{dt^*} = f_3 = -\theta_3 \frac{9\pi^2}{2} + \delta I_3, \tag{8}$$

where the integrals are given by

$$I_1 = 4 \int_0^1 \int_0^1 \cos\left(\frac{\pi x^*}{2}\right) \cos\left(\frac{\pi y^*}{2}\right) \frac{e^\theta}{1 + \beta e^{\alpha\theta}} dx^* dy^*,$$
$$I_2 = 4 \int_0^1 \int_0^1 \cos\left(\frac{\pi x^*}{2}\right) \cos\left(\frac{3\pi y^*}{2}\right) \frac{e^\theta}{1 + \beta e^{\alpha\theta}} dx^* dy^*,$$
$$I_3 = 4 \int_0^1 \int_0^1 \cos\left(\frac{3\pi x^*}{2}\right) \cos\left(\frac{3\pi y^*}{2}\right) \frac{e^\theta}{1 + \beta e^{\alpha\theta}} dx^* dy^*, \tag{9}$$

with θ given by (7).

Singularity theory is now applied to the semi-analytical model (8) and (9) to determine the singular points of the system. In particular we wish to determine the degenerate hysteresis points which allow the parameter region(s) in which multiple steady-state solutions occur, to be found. The steady-state equations have the general form

$$f_i(\theta_1, \theta_2, \theta_3, \alpha, \beta, \delta) = 0, \quad i = 1, 2, 3, \tag{10}$$

where δ is taken as the primary bifurcation parameter. The conditions

$$\frac{d\delta}{d\theta_1} = \frac{d^2\delta}{d\theta_1^2} = 0, \tag{11}$$

correspond to the creation or loss of a hysteresis loop in a θ versus δ, steady-state response curve. It is not possible to rearrange the steady-state equations (10) to give an explicit relationship for δ. Instead, the total derivative of (10), with respect to θ_1 is taken,

$$\frac{df_i}{d\theta_1}(\theta_1, \theta_2, \theta_3) = f_{i\theta_1} + f_{i\theta_2}\frac{d\theta_2}{d\theta_1} + f_{i\theta_3}\frac{d\theta_3}{d\theta_1} = 0, \quad i = 1, 2, 3 \tag{12}$$

and the conditions (11) are applied implicitly. Here the three equations in Eq. (10) are regarded as defining implicitly δ, θ_2, and θ_3 as functions of just the one independent variable θ_1. In (12) the f_i are written as functions of the θ_i and not the other variables α, β and δ. This is because α and β are constant for a given steady-state diagram and the first of (11) states $d\delta/d\theta_1 = 0$.

As the second of (11) involves a second derivative, the second total derivative of (10) must be taken to apply this condition

implicitly. This gives

$$\frac{d^2 f_i}{d\theta_1^2}(\theta_1, \theta_2, \theta_3) = f_{i\theta_1\theta_1}$$
$$+ 2f_{i\theta_1\theta_2}\frac{d\theta_1}{d\theta_2} + 2f_{i\theta_1\theta_2}\frac{d\theta_1}{d\theta_3} + \frac{d^2 f_i}{d\theta_2^2}\left(\frac{d\theta_2}{d\theta_1}\right)^2$$
$$+ \frac{d^2 f_i}{d\theta_3^2}\left(\frac{d\theta_3}{d\theta_1}\right)^2 + 2\frac{d^2 f_i}{d\theta_2\,d\theta_3}\frac{d\theta_2}{d\theta_1}\frac{d\theta_3}{d\theta_1}$$
$$+ f_{i\theta_2}\frac{d^2\theta_2}{d\theta_1^2} + f_{i\theta_3}\frac{d^2\theta_3}{d\theta_1^2} = 0,$$
$$i = 1, 2, 3, \tag{13}$$

where again the f_i are only functions of the θ_i. The steady-state equations and the first and second total derivatives (10), (11) and (13) represent nine equations in the 10 variables $\theta_1, \theta_2, \theta_3, \alpha, \beta, \delta, d\theta_2/d\theta_1, d\theta_3/d\theta_1, d^2\theta_2/d\theta_1^2$, and $d^2\theta_3/d\theta_1^2$. The last four variables have been introduced into the system as a consequence of the implicit differentiation.

Hence, the degenerate hysteresis bifurcation points for the semi-analytical model are a line in the (α, β) parameter plane, see Figs. 2 and 4. Also note that, even though α and β are constant for a given steady-state diagram, the total parameter space, in which they vary, must be considered to calculate the degenerate hysteresis points.

The system of equations (10), (11), and (13) contain the integrals I_i, plus various derivatives of these integrals. They are evaluated using a quadrature formula (Abramowitz and Stegun 1965, p. 892). For the examples considered in Section 4, the integrals I_i, and their derivatives, have converged when $20 \times 20 = 400$ subintervals are used. The resulting set of transcendental equations for the degenerate hysteresis points, are solved numerically, using the root-finding routine from the IMSL library.

4. Results

As stated above we make the standard simplifying assumption, the pre-exponential approximation, that $\varepsilon = 0$. The biomass FK parameter (δ) includes the size of the compost heap and is a controllable parameter; it is taken as the primary bifurcation parameter. For a particular type of biomass the reduced inhibition activation energy (α) and the reduced deactivation rate (β) are fixed and these are therefore viewed as unfolding parameters.

In Section 4.1 we use the continuation and bifurcation software Auto 97 (Doedel et al., 1998) to determine the steady-state solutions of problem (4)–(5)—note that Auto does not determine stability for boundary value problems. In Section 4.2 we determine the multiplicity regions of problem (4)–(5), and problem 6, using a semi-analytic method.

4.1. Auto results

Fig. 1 shows the two generic steady-state diagrams that are found when $\alpha > 1$. Fig. 1(a) shows a classic "S"-shaped
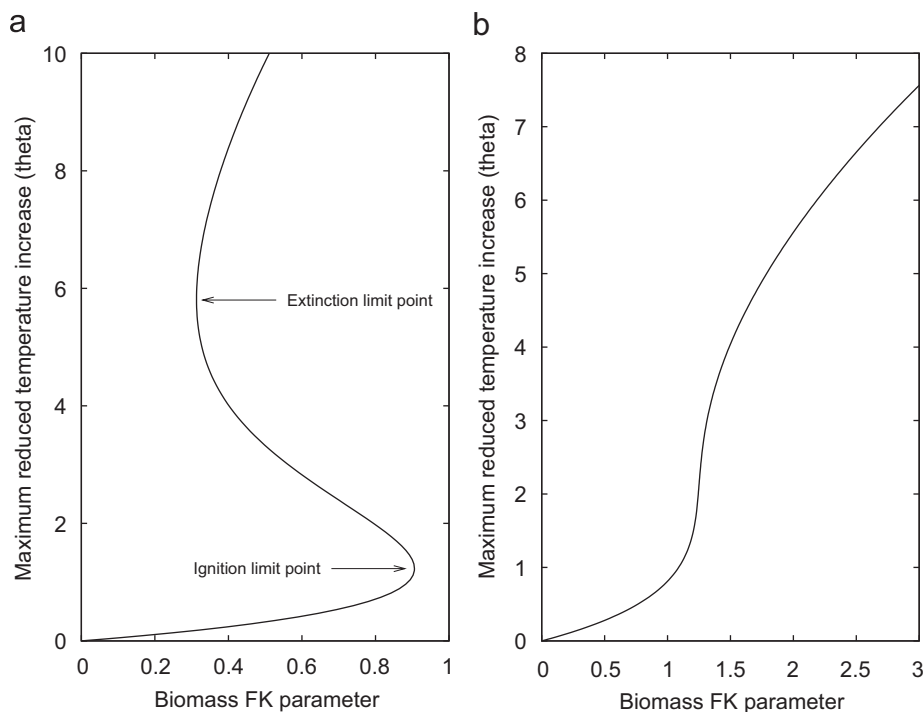
Fig. 1. Generic steady-state diagrams when $\alpha > 1$ showing variation of the maximum temperature increase (θ) with the biomass Frank-Kamenetskii parameter (δ). Parameter value: $\alpha = 1.1$.

steady-steady diagram containing two limit points and three solution branches: a 'low-valued' solution branch, representing negligible reaction, on which the temperature increase is small; an "intermediate" solution branch and a "high-valued" solution branch. Biological self-heating occurs if the biomass FK parameter is sufficiently large. In this figure the critical value of the FK parameter is very near the classical value $\delta_{cr} \approx 0.88$, that is when $\beta = 0$. In Fig. 1(b) the maximum temperature is a smooth function of the biomass FK parameter and there is always a unique steady-state solution. The value of the biomass FK parameter required to achieve a given temperature increase is much greater for the system represented by Fig. 1(b) than that represented by Fig. 1(a).

Fig. 2 is a bifurcation diagram for biological self-heating. In the feasible region ($\alpha > 1$) the cusp locus divides the secondary bifurcation plane into two regions. Thus there are two generic steady-state diagrams. In one of these there are multiple steady-states, whereas in the other there is a unique steady-state solution. These steady-state diagrams are quantitatively the same as those shown in Fig. 1. Note that the behaviour of the bifurcation diagram is not continuous as the value of the reduced inhibition activation energy is reduced below the value $\alpha = 1$. There is a quartic fold singularity at the point $(\alpha, \beta) = (0.8351, 0.3052)$. The quartic fold point is not of physical interest because it is not in the feasible region. When chemical heat-release is included in the model the quartic fold point can be unfolded with the kinetic parameters of the oxidation reaction (Nelson et al., 2003).

This figure contains an analytical bound for critical-ity that is obtained by applying a result from Aris (1975,
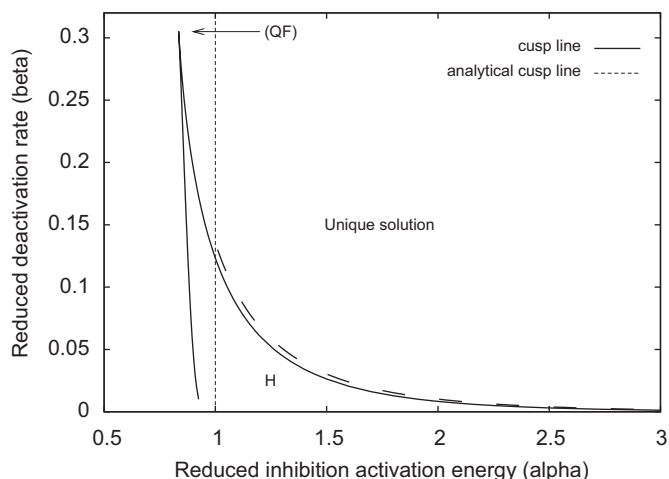

Fig. 2. Bifurcation diagram for biological self-heating. The feasible region is $\alpha > 1$. Shown is the Auto result (solid line) and the analytical result (15) (dashed curve). Below and above the cusp line in the feasible region the steady-state diagram is given by Fig. 1(a) and (b), respectively. Notation: (H) = hysteresis, (QF) = quartic fold.

Section 6.3) regarding the uniqueness of solutions to the general reaction–diffusion problem

$$\nabla^2 u + \lambda f(u) = 0, \quad x \in \Omega \subseteq \mathbb{R}^n, \quad |\Omega| < \infty,$$
$$\frac{\partial u}{\partial n} + B_i \cdot u = 0, \quad x \in \partial\Omega, \tag{14}$$

where B_i, and λ are parameters and $f(u) \geqslant 0$. This result states that if the function $f(u)/u$ is monotonic-decreasing in u, $u > 0$,
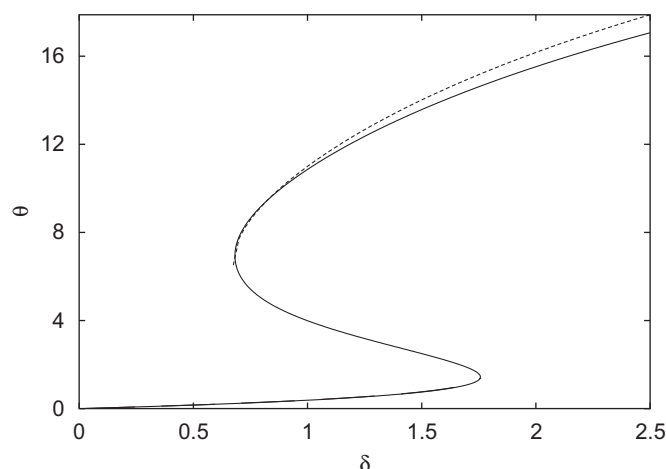
Fig. 3. Steady-state diagram for a 2-d slab showing the variation of the maximum temperature increase (θ) with the biomass Frank-Kamenetskii parameter (δ). Shown are semi-analytical results (solid curve) and numerical results (dashed curve). Parameter values: $\alpha = 1.1$, $\beta = 0.01$.

Fig. 4. Bifurcation diagram for biological self-heating showing the cusp line in the α–β plane. The feasible region is $\alpha > 1$. Shown is the semi-analytical solution for the 1-d (solid line) and 2-d (dashes) slabs.

then the system defined by Eq. (14) has a unique solution. Calculation for problem (4)–(5) shows that there is a unique solution when $\alpha \geqslant 1$ and $\beta > \beta_{cr}$ where

$$\beta_{cr} = \frac{w-1}{1+(\alpha-1)w} \exp(-\alpha w),$$
$$w = \frac{(\alpha-2)+\sqrt{\alpha^2+4\alpha-4}}{2(\alpha-1)}. \qquad (15)$$

The relationship (15) is plotted in Fig. 2. There is an excellent comparison between this curve and the AUTO results. The value of β_{cr} in the limit that $\alpha \to 1^+$ is e^{-2}, which is within 10% of the numerical result ($\beta_{cr} \approx 0.123282$). The absolute error in the analytical β_{cr} decreases as the value for α increases. The difference between the analytical and numerical curves arises because the restriction on the function $f(u)/u$ provides a sufficient, but not necessary, condition for uniqueness.

Biological self-heating in compost piles can lead to significant temperature increases over ambient temperature. From Figs. 1 and 2 we deduce that for practical degrees of biological self-heating to occur the kinetic parameters for biomass deactivation (α, β) need to be in the feasible part of the hysteresis region of Fig. 2.

4.2. Semi-analytic results

Fig. 3 shows the maximum temperature increase versus the biomass FK parameter for the 2-d compost pile. Shown are the semi-analytical solution (7) at the centre of the pile ($x = y = 0$) and a numerical solution obtained using a finite-difference scheme. No numerical solution is shown on the middle branch, as it is unstable. The figure shows an excellent comparison between the two solutions. At large temperatures on the upper branch there is a slight variation (5% at $\beta = 2.5$) due to the quenching of the profile at large temperatures. The series solution (7) breaks down in the limit of very flat temperature profiles. A semi-analytical solution was also obtained for a
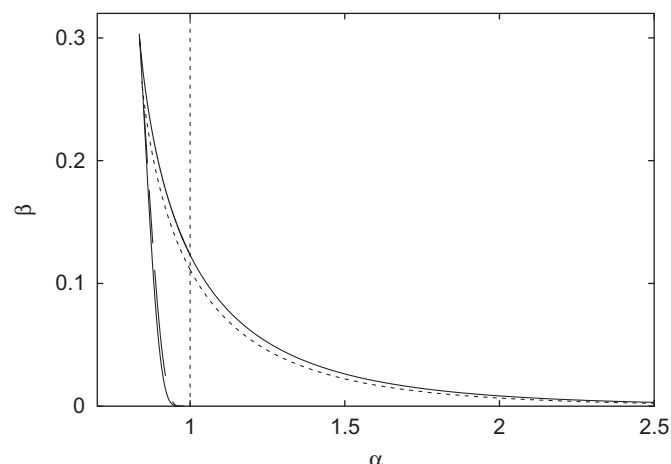
1-d compost pile, corresponding to the parameter values used in Fig. 1(a). This is not shown in Fig. 1(a) as, to within graphical accuracy, it is the same as the Auto result.

Fig. 4 shows the hysteresis curves in the α–β plane for the 1-d and 2-d configurations. This curve divides the parameter space into regions in which multiple steady-state and unique steady-state responses occur (for large α multiple solutions occur only for small values of β). The two hysteresis curves are located very close to each other in parameter space. The main variation is the location of the quartic fold point. For the 1-d slab it is at $(\alpha, \beta) = (0.8356, 0.3034)$, while for the 2-d slab it is at $(\alpha, \beta) = (0.8432, 0.2673)$. Using Auto the location of this point in the 1-d slab is estimated to be $(\alpha, \beta) = (0.8351, 0.3052)$.

For the 1-d slab the point $(\alpha, \beta) = (1, 0.123279)$ lies on the semi-analytical curve of degenerate hysteresis points. The corresponding point obtained via Auto is $(\alpha, \beta) = (1, 0.123282)$, hence the semi-analytical estimate is accurate to five decimal places. Accepting the Auto results as being correct, the error in the semi-analytical answer for the three points of comparison are: 0.06%, 0.6% and 0.002%, respectively. The values of physical and chemical constants are, of course, not known precisely, with uncertainties of 10% being common in many combustion problems. Thus the error associated with a four-term Galerkin approximation is two or three orders of magnitude lower than the uncertainty in parameter values. We therefore conclude that solutions obtained using a four-term expansion are accurate for practical purposes.

For the 2-d slab the solution to (10), (12), and (13) and a cruder approximation, where $\theta_2 = \theta_3 = 0$ in (7), were compared. These two approximations were compared by tracing the cusp singularity in the (α–β) plane. The two approximations were found to be same to graphical accuracy, indicating the high accuracy of the semi-analytical method. The accuracy of the four-term approximation was further tested by considering a particular point on the cusp curve for the 2-d slab: namely $(\alpha, \beta) = (1, 0.11123)$. The accuracy of this semi-analytical solution was estimated using a Richardson extrapolation series

convergence technique. It was found that the results are accurate to at least four decimal places.

5. Discussion

When heat-release due to cellulosic oxidation is incorporated into the model the energy balance Eq. (1) becomes

$$\frac{\partial \theta}{\partial t^*} = \frac{\partial^2 \theta}{\partial x^{*2}} + \frac{\delta \exp\left[\frac{\theta}{1+\varepsilon\theta}\right]}{1 + \beta \exp\left[\frac{\alpha\theta}{1+\varepsilon\theta}\right]} + \delta_0 \exp\left[\frac{\alpha_0\theta}{1 + \varepsilon\theta}\right], \qquad (16)$$

in which δ_0 is a FK parameter for chemical heating and α_0 is a reduced activation energy for chemical heating. The dimensionless grouping δ_0 contains the relevant kinetic parameters for chemical heating. It is defined in an analogous way to the standard approach (Bowes, 1984; Frank-Kamenetskii, 1969) except that the reference activation energy is that for the growth of biomass (E_1) rather than that for chemical heat-release (E_3).

We anticipate that self-heating now leads to one of three types of behaviour: negligible temperature increase; an elevated temperature increases *without ignition*; and ignition of cellulosic materials. If the pre-exponential approximation $\varepsilon = 0$ is made, the model will not contain a stable solution branch representing cellulosic combustion. This state is instead represented by finite time blow-up. If ε is small and positive the behaviour of the system is not dramatically changed except that there is now a stable high-temperature branch representing ignition of cellulosic materials.

The spatial structure of solutions to Eq. (16), i.e., temperature as a function of spatial distance within the compost pile, are of interest. Is there a pronounced "hot spot" at the centre of the pile or is the temperature distribution "flatter"? The identification of a possible "hot spot" may have important practical considerations and will therefore be of interest.

When either $\beta = 0$ or $\alpha = 0$ the biological heating term in Eq. (16) reduces to an Arrhenius expression. Eq. (16) now models self-heating due to two parallel exothermic reactions. The theory of such systems in one-dimension was investigated by Boddington et al. (1984). Thus self-heating due to a combination of biological and chemical mechanisms is a generalisation of self-heating due to two chemical reactions.

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 increases the temperature sufficiently to trigger significant oxidation of cellulosic materials (Bowes, 1984, Chapter 9.2). So far, however, only the influence of oxidative processes has been considered. The present model provides a firm foundation from which to investigate such effects.

6. Conclusions

In this paper we have investigated a model for biological self-heating in spatially distributed compost heaps. After making the pre-exponential approximation the model only contains three parameters. Consequently it is possible to thoroughly investigate the generic behaviour of the model and to identify parameter regions in which biological self-heating can give rise to elevated temperatures, which is the feature of practical interest. A novel semi-analytical method was used to generate highly accurate solutions using a very low number of terms. This method has the potential to be used for improved analysis of chemical engineering processes, particularly for more practical 2-d and 3-d geometries.

The model used in this paper provides qualitative insights into the generic behaviours that can be exhibited by a compost pile and their dependence upon kinetic values. In order to provide more detailed information relevant to the operation of "real" compost piles additional factors need to be included in the model. These include phenomena such as convection within the pile, ambient conditions such as wind, boundary conditions that more closely represent whether the pile is open or closed and moisture effects. The semi-analytical method will be an important tool to investigate how the incorporation of these effects changes the location of the regions where substantial self-heating are found in parameter space.

A particularly important factor to include in future work is the incorporation of heat-release due to the oxidation of cellulosic materials. Although elevated temperatures due to biological self-heating are desirable, biological activity can create temperatures that initiate heat-release in bulk organic materials which, if not detected, can lead to spontaneous combustion of the heap. Thus landfill sites that are judged subcritical, and safe, based purely on chemical heat-release considerations may, in fact, be supercritical, and unsafe.

Notation

A_1	pre-exponential factor for biomass growth, s^{-1}
A_2	pre-exponential factor for deactivation of biomass, dimensionless
B	the biomass density, $kg\,m^{-3}$
B_b	Representative value for the biomass density, $kg\,m^{-3}$
B_{max}	the maximum biomass density, $kg\,m^{-3}$
c	specific heat of the compost pile, $J\,K^{-1}\,kg^{-1}$
E_1	activation energy for biomass growth, $J\,mol^{-1}$
E_2	activation energy for the deactivation of biomass, $J\,mol^{-1}$
E_3	activation energy for cellulose oxidation, $J\,mol^{-1}$
k	thermal conductivity, $J\,s^{-1}\,m^{-1}\,K^{-1}$
L	the half length of the compost heap, m
Q_b	exothermicity of the biomass growth reaction, $J\,kg^{-1}$
R	idea gas constant, $J\,K^{-1}\,mol^{-1}$
t	time, s
t^*	dimensionless time, $t^* = \frac{k}{\rho c L^2} \cdot t$, dimensionless
T	temperature, K
T_a	ambient temperature, K
x	position within the compost pile, m
x^*	dimensionless position within the compostpile, $\frac{x}{L}$, dimensionless

Greek letters

α reduced biomass deactivation activation energy, $\alpha = \frac{E_2}{E_1}$, dimensionless

α_0 reduced activation energy for cellulose oxidation, $\alpha_0 = \frac{E_3}{E_1}$, dimensionless

β reduced deactivation rate, $\beta = A_2 \exp\left[\frac{-E_2}{RT_a}\right]$, dimensionless

δ biomass FK (Frank-Kamenetskii) parameter,
$$\delta = \frac{A_1 B_b \left(1 - \frac{B_b}{B_{\max}}\right) E_1 F_b L^2 Q_b}{RT_a^2 k} \cdot \exp\left[-\frac{E_1}{RT_a}\right], \text{dimensionless}$$

ε reduced activation energy for biomass growth, $\varepsilon = \frac{RT_a}{E_1}$, dimensionless

θ reduced temperature increase, $\theta = \frac{E_1(T - T_a)}{RT_a^2}$, dimensionless

ρ density of the compost pile, kg m^{-3}

ρ_s density of biomass substrate, kg m^{-3}

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References

Abramowitz, M., Stegun, L., 1965. Handbook of Mathematical Functions. Dover, New York.

Aris, R., 1975. The Mathematical Theory of Diffusion and Reaction in Permeable Catalysts II Questions of Uniqueness, Stability, and Transient Behaviour. Clarendon Press, Oxford.

Balakotaiah, V., Chakraborty, S., 2003. Averaging theory and low-dimensional models for chemical reactors. Chemical Engineering Science 58, 4769–4786.

Balakotaiah, V., Chang, H.-C., 2003. Hyperbolic homogenized models for thermal and solutal dispersion. SIAM Journal on Applied Mathematics 63, 1231–1258.

Balakotaiah, V., Khinast, J., 2000. Numerical bifurcation techniques for chemical reactor problems. In: Doedel, E., Tuckerman, L.S. (Eds.), Numerical Methods for Bifurcation Problems and Large-scale Dynamical Systems. The IMA Volumes in Mathematics and Its Applications, vol. 119. Springer, Berlin, pp. 1–36.

Boddington, T., Gray, P., Wake, G.C., 1984. Theory of thermal explosions with simultaneous parallel reactions I. Foundations and the one-dimensional case. Proceedings of the Royal Society of London A 393, 85–100.

Bowes, P.C., 1984. Self-heating: Evaluating and Controlling the Hazards. Elsevier, Amsterdam.

Brinton Jr., W.F., Evans, E., Droffner, M.L., Brinton, R.B., 1995. Standardized test for evaluation of compost self-heating. BioCycle 36, 65–69.

Chakraborty, S., Balakotaiah, V., 2002a. Low-dimensional models for describing mixing effects in laminar flow tubular reactors. Chemical Engineering Science 57, 2545–2564.

Chakraborty, S., Balakotaiah, V., 2002b. Two-mode models for describing mixing effects in homogeneous reactors. American Institute of Chemical Engineers Journal 48, 2571–2586.

Chakraborty, S., Balakotaiah, V., 2003. A novel approach for describing mixing effects in homogeneous reactors. Chemical Engineering Science 58, 1053–1061.

Chakraborty, S., Balakotaiah, V., 2004. Multi-mode low-dimensional models for non-isothermal homogeneous and catalytic reactors. Chemical Engineering Science 59, 3695–3724.

Chen, X.D., Mitchell, D.A., 1996. Start-up strategies for self-heating and efficient growth in stirred bioreactors for solid state fermentation. In: Weiss, G. (Ed.), CHEMECA '96, 24th Australian and New Zealand Chemical Engineering Conference, vol. 4. The Institute of Engineers, pp. 111–116. ISBN 0-85825-658-4.

Doedel, E.J., Fairgrieve, T.F., Sandstede, B., Champneys, A.R., Kuznetsov, Y.A., Wang, X., 1998. AUTO 97: continuation and bifurcation software for ordinary differential equations (with Homcont). Available by anonymous ftp from ⟨ftp.cs.concordia.ca/pub/doedel/auto⟩.

Frank-Kamenetskii D.A., 1969. Diffusion and Heat Transfer in Chemical Kinetics, second ed. Plenum Press, New York.

Golubitsky, M., Schaeffer, D., 1985. Singularities and Groups in Bifurcation Theory. Applied Mathematical Sciences 51, vol. 1. Springer, New York.

Hogland, W., Bramryd, T., Persson, I., 1996. Physical, biological and chemical effects of unsorted fractions of industrial solid waste in waste fuel storage. Waste Management and Research 14, 197–210.

Hudak, P.F., 2001. Spontaneous combustion of shale spoils at a sanitary landfill. Waste Management 22, 687–688.

Jand, N., Foscolo, P.U., 2005. Decomposition of wood particles in fluidized beds. Industrial & Engineering Chemistry Research 44, 5079–5089.

Khanahmadi, M., Roostaazad, R., Safekordi, A., Bozorgmehri, R., Mitchell, D.A., 2004. Investigating the use of cooling surfaces in solid-state fermentation tray bioreactors: modelling and experimentation. Journal of Chemical Technology and Biotechnology 79, 1228–1242.

Kubler, H., 1987. Heat generating processes as cause of spontaneous ignition in forest products. Forest Products Abstracts 10, 299–327.

Liwarska-Bizukojc, E., Bizukojc, M., Ledakowicz, S., 2001. Kinetic model for the process of aerobic biodegradation of organic fraction of municipal solid waste. Bioprocess and Biosystems Engineering 24, 195–202.

Marchant, T., Nelson, M.I., 2004. Semi-analytical solutions for one and two-dimensional pellet problems. Proceedings of the Royal Society of London A 460, 2381–2394.

Mitchell, D.A., von Meien, O.F., 2000. Mathematical modeling as a tool to investigate the design and operation of the Zymotis packed-bed bioreactor for solid state fermentation. Biotechnology and Bioengineering 68, 127–135.

Nelson, M.I., Balakrishnan, E., Chen, X.D., 2003. A Semenov model of self-heating in compost piles. Transactions of the Institution of Chemical Engineers, Part B 81, 375–383.

Radmanesh, R., Chaouki, J., Guy, C., 2006. Biomass gasification in a bubbling fluidized bed reactor: experiments and modeling. American Institute of Chemical Engineers Journal 52, 4258–4272.

Roels, J.A., 1983. Energetics and Kinetics in Biotechnology. Elsevier Biomedical Press, Amsterdam.

Rynk, R., 2000. Fires at composting facilities: causes and conditions. BioCycle Magazine 41, 54–58.

Subramanian, S., Balakotaiah, V., 1996. Classification of steady-state and dynamic behaviour of distributed reactor models. Chemical Engineering Science 51(3), 401–421.

von Meien, O.F., Mitchell, D.A., 2002. A two-phase model for water and heat transfer within an intermittently-mixed solid-state fermentation bioreactor with forced aeration. Biotechnology and Bioengineering 79, 416–428.

von Meien, O.F., Luz Jr., L.F.L., Mitchell, D.A., Pérez-Correa, J.R., Agosin, E., Fernández-Fernández, M., Arcas, J.A., 2004. Control strategies for intermittently mixed, forcefully aerated solid-state fermentation bioreactors based on the analysis of a distributed parameter model. Chemical Engineering Science 59, 4493–4504.

Wurzenberger, J.C., Wallner, S., Raupenstrauch, H., Khinast, J.G., 2002. Thermal conversion of biomass: comprehensive reactor and particle modeling. American Institute of Chemical Engineers 48, 2398–2411.