Criticality in Reactors under Domain or External Temperature Perturbations

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Criticality in reactors under domain or external temperature perturbations

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The conditions for the onset of thermal runaway in reactors with small non-uniformities is investigated. The reaction is modelled by an Arrhenius heat generation term with a finite activation energy and the dimensionless temperature, u_0, is taken to satisfy a nonlinear equation of the form

$$\Delta u_0 + \lambda_0 F(u_0) = 0, \quad x \in D; \quad \partial_\nu u_0 + b u_0 = 0, \quad x \in \partial D.$$

We investigate three classes of perturbations of this problem. First, we treat a small temperature variation maintained on the boundary of the domain. Secondly, we consider a small distortion of the boundary of a circular cylindrical domain, and thirdly, we analyse the effect of a small hole in the domain. In each case we derive asymptotic expansions for the critical Frank–Kamenetskii parameter, $\lambda_c(\epsilon)$, where ϵ is a measure of the size of the perturbation. A numerical scheme is then used to determine numerical values for the coefficients in the asymptotic expansion of λ_c. Finally, some of the asymptotic results are compared with corresponding numerical results obtained from a full numerical solution of the perturbed problem.

1. Introduction

In steady-state thermal explosion theory the dimensionless temperature distribution, u_0, in an exothermically active material, is usually taken to satisfy a nonlinear equation of the form

$$\left.\begin{aligned} \Delta u_0 + \lambda_0 F(u_0) = 0, \quad x \in D, \\ \partial_\nu u_0 + b u_0 = 0, \quad x \in \partial D. \end{aligned}\right\} \tag{1.1}$$

Here, $b > 0$ is the dimensionless Biot number, λ_0 is the Frank–Kamenetskii parameter, and D is the two- or three-dimensional domain. In addition, $\partial_\nu u_0$ is the derivative of u with respect to the outer normal to D. To model the reaction in D, an Arrhenius heat generation term of the form $F(u) = \exp(u/(1+\beta u))$ is usually specified. Here, $\beta \geqslant 0$ is a dimensionless activation energy parameter with $\beta = 0$ corresponding to an infinite activation energy.

With $F(u)$ as given above, it is well known that for some range of λ_0 multiple solutions to (1.1) can occur. The conditions on b and β for the occurrence of these multiple solutions in slab, circular cylindrical and spherical domains is also well established (see Boddington *et al.* 1983). We assume that when multiple solutions to (1.1) occur, they can be parametrized in terms of a parameter $\alpha > 0$ as $u_0(x, \alpha)$, $\lambda_0(\alpha)$. The graph of α against λ_0 is then multiple valued with a simple fold point at $\lambda_c =$

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$\lambda_0(\alpha_0)$ where $\lambda_0'(\alpha_0) = 0$. The determination of these critical values of the Frank–Kamenetskii parameter is important in reactor design in that as λ passes through λ_c a dramatic increase in the maximum temperature of the reactor can occur (i.e. a thermal explosion).

Our goal is to determine the effect upon λ_c of three classes of perturbations of (1.1). First, we treat a small temperature variation maintained on the boundary of D. Secondly, we consider a small distortion of the boundary of a circular cylindrical domain, and thirdly, we analyse the effect of a small hole in the domain. In each case λ_c is expanded in terms of a small parameter, ϵ, which is a measure of the size of the perturbation. In the analysis we will emphasize the similarities in the methods used to treat these classes of perturbations. An outline of this paper and a brief description of some previous work in this area will now be given.

In §2 we determine the critical conditions for a reactor in which there is a small temperature variation maintained on its boundary. The theory developed in §2 is then applied in §3 to a circular cylindrical reactor. The method used to determine λ_c uses a combination of asymptotic and numerical techniques. Therefore we can allow for a small but arbitrary temperature variation and are not restricted to the case of infinite activation energies in which an exact solution to (1.1) can be found. The asymptotic results for λ_c derived in §§3.1 and 3.2 for the reactive circular cylinder are compared in §3.3 with corresponding numerical results obtained from a full two-dimensional finite difference solution of the perturbed problem.

In §4 we determine the critical conditions for a nearly circular cylindrical reactor whose cross-section, in terms of the polar coordinates (r, θ), is given by $r = 1 + \epsilon h(\theta)$. This problem was recently considered by Adler (1987) who determined λ_c in the limit $\epsilon \to 0$ for the case $\beta = 0$ and $h(\theta) = \cos\theta$. In §4 we extend this previous work to treat the more general case of a finite activation energy ($\beta > 0$) and a small, but otherwise arbitrary, distortion of the nearly circular cylindrical domain.

In §5 we consider a different class of domain perturbation. Here we determine λ_c when a small subdomain D_ϵ of 'radius' ϵ is removed from D and a boundary condition imposed on the resulting hole. The theory to determine λ_c in this case was initiated in Ward & Keller (1991) and was extended and validated numerically in Ward & Van de Velde (1991). In §5 we further extend the theory by deriving a two term expansion for λ_c in the limit of small-hole radius. For some special geometries, we then describe a scheme to determine numerical values for the coefficients in the asymptotic expansion of λ_c.

In §6 we give a new method for determining the maximum value of the activation energy parameter β for which multiple solutions to (1.1) occur in slab, circular cylindrical and spherical domains (the class A geometries). These transitional values of β were first computed for the class A geometries by Kordylewski (1979) who formulated and solved numerically a time dependent system of partial differential equations. Minor modifications of this time dependent formulation have been made by several investigators (see Boddington *et al.* (1983) and the references therein) to compute the transitional parameters more accurately. Our method differs from these previous methods in that we determine the transitional value of β by solving a set of boundary-value problems for ordinary differential equations. Therefore, more accurate solutions for the transitional quantities can be obtained by our method for the class A geometries. Our results are found to agree to many significant digits with those of Gustafson & Eaton (1982) where an alternative approach, also based on the solution of a set of ordinary differential equations, was used.

Finally, in §7 we give a qualitative discussion on the effect of the three classes of perturbations on the critical Frank–Kamenetskii parameter.

2. Small temperature variation on the reactor boundary

The perturbed problem in $m = 2, 3$ dimensions is taken to be

$$\Delta u + \lambda F(u) = 0, \quad x \in D, \tag{2.1a}$$

$$\partial_\nu u + b(u - \epsilon h(s)) = 0, \quad x \in \partial D, \tag{2.1b}$$

where D is a bounded domain in $\mathbb{R}^m$. Here s parametrizes ∂D and $\epsilon h(s)$ is the small external temperature variation. We now determine the critical value of λ, labelled by $\lambda_c(\epsilon)$, for $\epsilon \ll 1$.

We seek the solution to (2.1) in the parametric form $u(x, \alpha, \epsilon)$, $\lambda(\alpha, \epsilon)$ and we expand

$$u = u_0(x, \alpha) + \epsilon u_1(x, \alpha) + \epsilon^2 u_2(x, \alpha) + \ldots, \quad \lambda = \lambda_0(\alpha) + \epsilon\lambda_1(\alpha) + \epsilon^2\lambda_2(\alpha) \ldots. \tag{2.2}$$

Substituting this expansion into (2.1) and equating powers of ϵ given

$$\Delta u_1 + \lambda_0 F^0_u u_1 = -\lambda_1 F^0, \quad x \in D \tag{2.3a}$$

$$\partial_\nu u_1 + b u_1 = b h(s), \quad x \in \partial D \tag{2.3b}$$

$$\Delta u_2 + \lambda_0 F^0_u u_2 = -\lambda_2 F^0 - \lambda_1 u_1 F^0_u - \tfrac{1}{2}\lambda_0 u_1^2 F^0_{uu}, \quad x \in D \tag{2.4a}$$

$$\partial_\nu u_2 + b u_2 = 0, \quad x \in \partial D. \tag{2.4b}$$

Here, $F^0 \equiv F(u_0(x, \alpha))$ and F^0_u, F^0_{uu} denote derivatives of F with respect to u evaluated at the unperturbed solutions u_0.

To determine the location of the fold point we expand $\alpha = \alpha(\epsilon) = \alpha_0 + \epsilon\alpha_1 + \epsilon^2\alpha_2 + \ldots$. To the order of terms retained, α_0, α_1 and α_2 are determined by the condition that $\mathrm{d}\lambda/\mathrm{d}\alpha = 0$ shall be independent of ϵ. Then defining $\lambda_c(\epsilon) \equiv \lambda(\alpha(\epsilon), \epsilon)$, we obtain

$$\lambda_c = \lambda_0(\alpha_0) + \epsilon\lambda_1(\alpha_0) + \epsilon^2[\lambda_2(\alpha_0) - (\lambda_1'(\alpha_0))^2/2\lambda_0''(\alpha_0)] + \ldots. \tag{2.5}$$

We now determine $\lambda_0''(\alpha_0)$, $\lambda_2(\alpha_0)$, $\lambda_1(\alpha_0)$ and $\lambda_1'(\alpha_0)$ from (1.1), (2.3) and (2.4).

To determine these quantities, we differentiate (1.1) with respect to α to obtain

$$\left.\begin{aligned} \Delta u_{0\alpha} + \lambda_0 F^0_u u_{0\alpha} &= -\lambda_0' F^0, \quad x \in D, \\ \partial_\nu u_{0\alpha} + b u_{0\alpha} &= 0, \qquad\quad x \in \partial D. \end{aligned}\right\} \tag{2.6}$$

At the fold point $\alpha = \alpha_0$ we have $\lambda_0'(\alpha_0) = 0$ by assumption, so (2.6) is the homogeneous form of both (2.3) and (2.4). Since the operator in (2.3) and (2.4) has a one-dimensional nullspace at α_0, then the inhomogeneous terms in each of these equations must satisfy one solvability condition. To derive the solvability condition for (2.3) we apply Green's theorem to $u_{0\alpha}$ and u_1 in D to obtain

$$\lambda_1(\alpha_0)\,(u_{0\alpha}, F^0) = \int_{\partial D} h(s)\,\partial_\nu u_{0\alpha}\,\mathrm{d}s, \quad \text{at} \quad \alpha = \alpha_0. \tag{2.7}$$

Here, the inner product (v, w) is defined by $(v, w) = \int_D vw\,\mathrm{d}x$. By a similar procedure we obtain the following solvability condition for (2.4):

$$\lambda_2(\alpha_0)\,(u_{0\alpha}, F^0) = -\lambda_1(u_{0\alpha}, u_1 F^0_u) - \tfrac{1}{2}\lambda_0(u_{0\alpha}, u_1^2 F^0_{uu}), \quad \text{at} \quad \alpha = \alpha_0. \tag{2.8}$$

To determine $\lambda_1'(\alpha_0)$ we differentiate (2.3a, b) with respect to α so that

$$\left.\begin{aligned} \Delta u_{1\alpha}+\lambda_0 F_u^0 u_{1\alpha} &= -\lambda_0' F_u^0 u_{0\alpha}-\lambda_0 F_{uu}^0 u_1 u_{0\alpha}-\lambda_1' F^0-\lambda_1 F_u^0 u_{0\alpha}, && x\in D,\\ \partial_\nu u_{1\alpha}+b u_{1\alpha} &= 0, && x\in\partial D. \end{aligned}\right\} \tag{2.9}$$

Applying Green's theorem to $u_{0\alpha}$ and $u_{1\alpha}$ in D we find that

$$\lambda_1'(\alpha_0)\,(u_{0\alpha}, F^0) = -\lambda_0(u_{0\alpha}^2, F_{uu}^0 u_1)-\lambda_1(u_{0\alpha}^2, F_u^0). \tag{2.10}$$

Finally, to determine $\lambda_0''(\alpha_0)$ we differentiate (2.6) with respect to α to obtain

$$\left.\begin{aligned} \Delta u_{0\alpha\alpha}+\lambda_0 F_u^0 u_{0\alpha\alpha} &= -\lambda_0 F_{uu}^0 u_{0\alpha}^2-2\lambda_0' F_u^0 u_{0\alpha}-\lambda_0'' F^0, && x\in D,\\ \partial_\nu u_{0\alpha\alpha}+b u_{0\alpha\alpha} &= 0, && x\in\partial D. \end{aligned}\right\} \tag{2.11}$$

Then applying Green's theorem to $u_{0\alpha}$ and $u_{0\alpha\alpha}$ in D we find that

$$\lambda_0''(\alpha_0)\,(u_{0\alpha}, F^0) = -\lambda_0(u_{0\alpha}^3, F_{uu}^0). \tag{2.12}$$

Using (2.7), (2.8), (2.10), and (2.12) in (2.5) we have a two-term expansion for λ_c when $\epsilon \ll 1$. We emphasize that all the quantities appearing in these equations are to be evaluated at $\alpha = \alpha_0$.

3. A circular cylindrical reactor: small temperature variation

Let D be a circular cylindrical reactor of radius one and assume that the nonlinear heating term is $F(u) = \exp(u/(1+\beta u))$. We now briefly outline some well-known results on the qualitative behaviour of solutions to the unperturbed problem (1.1) with the Arrhenius heating term specified above (see Bebernes & Eberly (1989) and the references therein for details).

All positive solutions to (1.1) in circular cylindrical domains are radially symmetric and are monotone decreasing functions of r for $r > 0$. If $\beta = 0$ and $0 < b \leqslant \infty$ then there exists a $\lambda_c < \infty$ such that there is no solution to (1.1) for all $\lambda > \lambda_c$. In this case if $\lambda < \lambda_c$ there are two solutions to (1.1). Now if $\beta > 0$ and $0 < b \leqslant \infty$ then solutions to (1.1) exist for all $\lambda > 0$ and furthermore, if $\beta \geqslant \beta_{tr}(b)$, the solutions to (1.1) are unique for all $\lambda \geqslant 0$. However, when $\beta < \beta_{tr}(b)$, multiple solutions to (1.1) occur for some range of λ. This transitional value of β, labelled by $\beta_{tr}(b)$, has been computed numerically in Fenaughty *et al.* (1982) and Boddington *et al.* (1983) for various values of b. Finally, we mention that explicit formulas for the solutions to (1.1) in circular cylindrical domains can only be found when $\beta = 0$.

We now present a method to obtain numerical values for the coefficients of order ϵ and ϵ^2 in the expansion of λ_c given in (2.5) for the case $0 \leqslant \beta < \beta_{tr}(b)$. In (2.1$b$) we take $s = \theta$ and we assume that $h(\theta)$ is a smooth 2π periodic function. Then we look for a solution to (2.3a, b) in the form

$$u_1(r,\theta) = \tfrac{1}{2}w_0(r)+\sum_{n=1}^{\infty}(w_n(r)\cos n\theta + v_n(r)\sin n\theta). \tag{3.1}$$

Substituting (3.1) in (2.3a, b) we obtain, in $0 \leqslant r \leqslant 1$,

$$L_n w_n+\lambda_0 F_u^0 w_n = -2\lambda_1 F^0\delta_{n0},\quad w_n'(1)+b w_n(1) = b c_n,\quad n\geqslant 0, \tag{3.2a}$$

$$L_n v_n+\lambda_0 F_u^0 v_n = 0,\quad v_n'(1)+b v_n(1) = b d_n,\quad n\geqslant 1. \tag{3.2b}$$

Here δ_{n0} is the Kronecker delta, $L_n v \equiv r^{-1}(rv_r)_r - r^{-2}n^2 v$, and the numbers c_n and d_n are the Fourier coefficients of $h(\theta)$:

$$c_n = \frac{1}{\pi}\int_0^{2\pi} h(\theta)\cos n\theta\,\mathrm{d}\theta, \quad d_n = \frac{1}{\pi}\int_0^{2\pi} h(\theta)\sin n\theta\,\mathrm{d}\theta. \tag{3.3}$$

At criticality, where $\alpha = \alpha_0$, it follows from (2.7) that there is no solution to (3.2a) when $n = 0$ unless

$$\lambda_1(\alpha_0) = u_{0\alpha r}(1)\,c_0/(2\langle u_{0\alpha}, F^0\rangle), \quad \text{at} \quad \alpha = \alpha_0. \tag{3.4}$$

Here we have defined the angle brackets by $\langle u, v\rangle = \int_0^1 uvr\,\mathrm{d}r$. At criticality, the solution to (3.2a), with $n = 0$ and $\lambda_1(\alpha_0)$ as given above, can be made unique by specifying $\langle u_{0\alpha}, w_0\rangle = 0$ at $\alpha = \alpha_0$.

By using (3.1) in (2.8) and (2.10) we obtain at $\alpha = \alpha_0$,

$$\lambda_1'(\alpha_0)\langle u_{0\alpha}, F^0\rangle = -\tfrac{1}{2}\lambda_0\langle u_{0\alpha}, F^0_{uu}\,u_{0\alpha}\,w_0\rangle - \lambda_1\langle u_{0\alpha}, F^0_u\,u_{0\alpha}\rangle, \tag{3.5}$$

$$\lambda_2(\alpha_0)\langle u_{0\alpha}, F^0\rangle = -\tfrac{1}{2}\lambda_1\langle u_{0\alpha}, w_0 F^0_u\rangle - \tfrac{1}{8}\lambda_0\langle u_{0\alpha}, w_0^2 F^0_{uu}\rangle - \tfrac{1}{4}\lambda_0\sum_{n=1}^{\infty}\langle u_{0\alpha}F^0_{uu}, w_n^2 + v_n^2\rangle. \tag{3.6}$$

Thus using (2.12), (3.4), (3.5) and (3.6) in (2.5) gives a two term expansion for λ_c when D is a circular cylindrical domain.

A special case of the above result occurs when the average temperature variation on the boundary is zero so that $c_0 = 0$. Then from (3.4) we have that $\lambda_1(\alpha_0) = 0$ and from (3.2a), upon recalling $\langle u_{0\alpha}, w_0\rangle = 0$, it follows that $w_0 \equiv 0$ at $\alpha = \alpha_0$. Now from (3.5) we find that $\lambda_1'(\alpha_0) = 0$ and so from (3.6) and (2.5) the correction to the fold point becomes

$$\lambda_c = \lambda_0(\alpha_0) + \epsilon^2\lambda_2(\alpha_0) + \ldots, \quad \lambda_2(\alpha_0) = -\frac{\lambda_0}{4\langle u_{0\alpha}, F^0\rangle}\sum_{n=1}^{\infty}\langle u_{0\alpha}F^0_{uu}, w_n^2 + v_n^2\rangle. \tag{3.7}$$

To compute the various quantities in (2.12), (3.4), (3.5), (3.6) and (3.7) we first consider the extended system obtained from (1.1) and (2.6) which is written, in $0 \leqslant r < 1$, as

$$Lu_0 + \lambda_0 F(u_0) = 0, \quad F(u) = \exp(u/(1+\beta u)), \tag{3.8a}$$

$$Lu_{0\alpha} + \lambda_0 F_u(u_0)\,u_{0\alpha} = -\lambda_0' F(u_0), \tag{3.8b}$$

$$u_0' + bu_0 = 0, \quad u_{0\alpha}' + bu_{0\alpha} = 0 \quad \text{on} \quad r = 1, \tag{3.8c}$$

$$u_0'(0) = 0, \quad u_{0\alpha}'(0) = 0, \quad u_0(0) = \alpha, \quad u_{0\alpha}(0) = 1. \tag{3.8d}$$

Here α is chosen to be the maximum temperature for the unperturbed problem and the operator L is defined by $Lv = r^{-1}(rv_r)_r$.

To determine the location of the 'first' fold point for the unperturbed problem with β fixed, we solve (3.8) subject to the side condition $\lambda_0'(\alpha_0) = 0$ and $\lambda_0'(\alpha) > 0$ for $0 < \alpha < \alpha_0$. For fixed α and β the boundary value problem (3.8) is solved for u_0, $u_{0\alpha}$, λ_0, and λ_0' using the collocation package COLSYS developed by Ascher *et al.* (1979). A continuation in α is used to detect the first sign change of λ_0' and then a Newton iteration scheme is used to locate the first fold point $(\lambda_0(\alpha_0), \alpha_0)$ accurately. Once this fold point is located accurately the quantities $u_0(r)$, $u_{0\alpha}(r)$ at $\alpha = \alpha_0$, which are needed

in (2.12) and (3.4), are known. The integrals appearing in these expressions are evaluated numerically using Simpson's rule. In addition, with $u_0(r)$ known at $\alpha = \alpha_0$ we solve (3.2a, b) numerically for w_n and v_n. Then a numerical quadrature in (3.5) and (3.6) gives $\lambda_1'(\alpha_0)$ and $\lambda_2(\alpha_0)$, from which we determine λ_c from (2.5). Finally, a continuation scheme in β is used to locate the first fold point and to determine the fold point correction λ_c as a function of β. We now give some examples.

3.1. *A circular cylindrical reactor*: $c_0 = 0$

Now we consider the special case $c_0 = 0$ (e.g. the mean temperature variation vanishes) and for positive integers n we take $h(\theta) = c_n \cos n\theta$. Then from (3.7) we find that, at $\alpha = \alpha_0$,

$$\lambda_c = \lambda_0(\alpha_0) + \epsilon^2 \lambda_2(\alpha_0) + \ldots, \quad \lambda_2(\alpha_0) = -\frac{\lambda_0}{4\langle u_{0\alpha}, F^0\rangle}\langle u_{0\alpha} F^0_{uu}, w_n^2\rangle. \tag{3.9}$$

Here, w_n for $n \geqslant 1$ is found from (3.2a) and F is given in (3.8a).

Infinite activation energy: $\beta = 0$

With $\beta = 0$ and $F = e^u$ then $\lambda_0(\alpha_0)$ can be found analytically and the fold correction, $\lambda_2(\alpha_0)$, can be determined up to a quadrature. When $\beta = 0$ the solution to the unperturbed problem (1.1) is well known (see Gray & Lee 1967). It is given by

$$u_0(r, \alpha) = 2\ln\left(\frac{1+\alpha}{1+\alpha r^2}\right) + \frac{4\alpha}{b(1+\alpha)}, \quad \lambda_0(\alpha) = \frac{8\alpha}{(1+\alpha)^2}\exp\left[-\frac{4\alpha}{b(1+\alpha)}\right], \tag{3.10}$$

where $\alpha \geqslant 0$. Criticality occurs when $\lambda_0'(\alpha_0) = 0$, which yields $\alpha_0^2 - 1 + 4\alpha_0/b = 0$. The positive root of this expression is

$$\alpha_0 = -2/b + (1 + 4/b^2)^{\frac{1}{2}}. \tag{3.11}$$

Note that the definition of α taken here differs slightly from the one used in (3.8), where α was the maximum temperature.

At $\alpha = \alpha_0$ the solution to (3.2a), which is regular at $r = 0$, is found to be

$$w_n(r) = \frac{4\alpha_0 c_n}{n(1+\alpha_0)}[(1+\alpha_0) + n(1-\alpha_0)]^{-1} r^n \left(\frac{1-\alpha_0 r^2}{1+\alpha_0 r^2} + n\right). \tag{3.12}$$

In addition, by using (3.10) a simple calculation shows that

$$u_{0\alpha}(r, \alpha_0) = \frac{(1-\alpha_0 r^2)}{\alpha_0(1+\alpha_0 r^2)}, \quad \langle u_{0\alpha}, e^{u_0}\rangle = -\frac{u_{0\alpha r}(1, \alpha_0)}{\lambda_0(\alpha_0)} = \frac{4(1+\alpha_0)^{-2}}{\lambda_0(\alpha_0)}, \tag{3.13}$$

at $\alpha = \alpha_0$. Substituting (3.10), (3.12), and (3.13) in (3.9) we obtain

$$\lambda_2(\alpha_0) = -\frac{4c_n^2 \lambda_0(\alpha_0)}{n^2}\alpha_0^2[(1+\alpha_0) + n(1-\alpha_0)]^{-2}\int_0^1 G_n(s, \alpha_0)\, e^{n \ln s}\, ds, \tag{3.14}$$

where $G_n(s, \alpha_0)$ is defined by

$$G_n(s, \alpha_0) = (1+\alpha_0 s)^{-5}(1-\alpha_0 s)[n(1+\alpha_0 s) + (1-\alpha_0 s)]^2. \tag{3.15}$$

Although it does not appear possible to evaluate the integral appearing in (3.14) analytically for arbitrary n, we can easily determine $\lambda_2(\alpha_0)$ for $n = 1$ and for $n \gg 1$.

Table 1. $\lambda_2(\alpha_0)$ *with* $\beta = 0$ *and for various* b, *from* (3.14)

n	$b = \infty$	$b = 5$	$b = 3$	$b = 1$
1	-0.2500	-0.1616	-0.1177	-0.2749×10^{-1}
2	-0.6250×10^{-1}	-0.3806×10^{-1}	-0.2629×10^{-1}	-0.5298×10^{-2}
3	-0.2778×10^{-1}	-0.1582×10^{-1}	-0.1045×10^{-1}	-0.1909×10^{-2}
4	-0.1563×10^{-1}	-0.8307×10^{-2}	-0.5288×10^{-2}	-0.9017×10^{-3}
5	-0.1000×10^{-1}	-0.4971×10^{-2}	-0.3069×10^{-2}	-0.4971×10^{-3}
6	-0.6944×10^{-2}	-0.3235×10^{-2}	-0.1947×10^{-2}	-0.3031×10^{-3}
7	-0.5102×10^{-2}	-0.2233×10^{-2}	-0.1316×10^{-2}	-0.1985×10^{-3}
8	-0.3906×10^{-2}	-0.1611×10^{-2}	-0.9322×10^{-3}	-0.1370×10^{-3}
9	-0.3086×10^{-2}	-0.1203×10^{-2}	-0.6851×10^{-3}	-0.9857×10^{-4}
10	-0.2500×10^{-2}	-0.9229×10^{-3}	-0.5186×10^{-3}	-0.7328×10^{-4}

For $n = 1$, upon evaluating the integral in (3.14), (3.9) becomes

$$\lambda_c = \lambda_0(\alpha_0) + \epsilon^2 \lambda_2(\alpha_0) + \ldots, \quad \lambda_2(\alpha_0) = -2\lambda_0(\alpha_0)\alpha_0^2 c_n^2/(1+\alpha_0)^4, \tag{3.16}$$

where α_0 is given in (3.11). If in addition $b \to \infty$, then $\lambda_0 \to 2$ and $\alpha_0 \to 1$, so that (3.16) reduces to $\lambda_c = 2(1 - \frac{1}{8}\epsilon^2 c_n^2 + \ldots)$. This result is in agreement with Adler (1978) who, for the case with $c_n = 1$, estimated that $\lambda_c = 2(1 + k\epsilon^2)^{-1}$ where $\frac{1}{12} \leqslant k \leqslant \frac{1}{6}$. Thus we predict that the correct value of k is $\frac{1}{8}$, which is the mean of $\frac{1}{12}$ and $\frac{1}{6}$.

For the case $n \to \infty$, $\lambda_2(\alpha_0)$ can be evaluated asymptotically using Laplace's method (see Bleistein & Handelsman 1975). A routine application of this method provides

$$\int_0^1 G_n(s, \alpha_0)\, \mathrm{e}^{n \ln s}\, \mathrm{d}s \sim \frac{G_n(1, \alpha_0)}{n} - \frac{(G_n(1, \alpha_0) + \partial_s G_n(1, \alpha_0))}{n^2} + \ldots \quad \text{as} \quad n \to \infty.$$

Then from (3.15) we obtain

$$\int_0^1 G_n(s, \alpha_0)\, \mathrm{e}^{n \ln s}\, \mathrm{d}s = n(1+\alpha_0)^{-3}(1-\alpha_0) + (1+\alpha_0)^{-4}(1+\alpha_0^2) + O(n^{-1}) \quad \text{as} \quad n \to \infty. \tag{3.17}$$

Finally, using (3.17) in (3.14), the asymptotic behaviour of $\lambda_2(\alpha_0)$ is

$$\lambda_2(\alpha_0) \sim -\frac{4\lambda_0(\alpha_0)\alpha_0^2 c_n^2}{n^2(1+\alpha_0)^4} \frac{n(1-\alpha_0^2) + (1+\alpha_0^2)}{[n(1-\alpha_0) + (1+\alpha_0)]^2} \quad \text{as} \quad n \to \infty. \tag{3.18}$$

From (3.18) we note that $\lambda_2(\alpha_0) = O(n^{-2})$ when $\alpha_0 = 1$ ($b = \infty$) and $\lambda_2(\alpha_0) = O(n^{-3})$ when $\alpha_0 \neq 1$ ($b < \infty$). Specifically, the leading order term as $n \to \infty$ in each case is

$$\lambda_2(\alpha_0) \sim -\frac{4\lambda_0(\alpha_0)\alpha_0^2 c_n^2}{n^3(1+\alpha_0)^3(1-\alpha_0)} \quad \alpha_0 \neq 1, \quad \lambda_2(\alpha_0) \sim -\frac{c_n^2}{4n^2} \quad \alpha_0 = 1. \tag{3.19}$$

Now setting $c_n = 1$ we compare the expression for $\lambda_2(\alpha_0)$ given in (3.14) with the asymptotic result (3.18) valid for $n \gg 1$. To evaluate the integral appearing in (3.14) accurately we used Romberg's method with a high-order extrapolation. Amazingly, we find that for all $n \geqslant 1$ and $\alpha_0 > 0$, the asymptotic result (3.18) approximates the exact result (3.14) to within four significant digits. In table 1 we give numerical values for $\lambda_2(\alpha_0)$ obtained from (3.14) for various n and b values. We note from this table that $\lambda_2(\alpha_0) < 0$ and that $\lambda_2(\alpha_0)$ increases monotonically with n. Thus we

conclude that small temperature variations on the boundary of mean zero make the reactor less stable. However, the onset of thermal runaway is only marginally hastened by a small but rapidly varying temperature profile on the reactor boundary.

Finite activation energy: $0 < \beta < \beta_{tr}(b)$

For the case of finite activation energies in which $\beta > 0$ it is not possible to solve (3.2a) explicitly for arbitrary n. However, in two special cases we can determine $\lambda_2(\alpha_0)$ without having to solve (3.2a) numerically. These special cases provided a partial check on the numerical computations that follow.

If $n = 1$ then, for any $\alpha \geqslant 0$, the solution to (3.2a) is given by

$$w_1(r) = Ac_1 u_{0r}(r), \quad \text{where} \quad A = b/(u_{0rr}(1) + bu_{0r}(1)). \tag{3.20}$$

Evaluating w_1 at $\alpha = \alpha_0$ and substituting (3.20) in (3.9) we see that

$$\lambda_2(\alpha_0) = -\frac{\lambda_0 A^2 c_1^2}{4\langle u_{0\alpha}, F^0\rangle}\langle u_{0\alpha} F^0_{uu}, u_{0r}^2\rangle \quad \text{at} \quad \alpha = \alpha_0, \quad \text{when} \quad n = 1. \tag{3.21}$$

The remaining quantities in (3.21) must be determined using the numerical solution to (3.8) at $\alpha = \alpha_0$.

In the case where $n \to \infty$ the solution to (3.2a) can be constructed asymptotically using the method of matched asymptotic expansions (see, for example, Kervorkian & Cole 1981). For large n the solution to (3.2a) is of boundary layer type with a boundary layer occurring near $r = 1$. Upon replacing w_n in (3.9) by its leading order composite expansion, the inner product $\langle u_{0\alpha} F^0_{uu}, w_n^2\rangle$ can be evaluated asymptotically using Laplace's method.

By using the method of matched asymptotic expansions to solve (3.2a) for $n \gg 1$, the leading order composite expansion for w_n is found to be

$$w_n \sim (bc_n/n)\,\mathrm{e}^{n(r-1)}, \quad b < \infty; \quad w_n \sim c_n\,\mathrm{e}^{n(r-1)}, \quad b = \infty. \tag{3.22}$$

Asymptotically, as $n \to \infty$, the inner product $\langle u_{0\alpha} F^0_{uu}, w_n^2\rangle$ at $\alpha = \alpha_0$ is given by

$$\langle u_{0\alpha} F^0_{uu}, w_n^2\rangle \sim -(bu_{0\alpha r}(1,\alpha_0)\, c_n^2/2n^3) F_{uu}(u_0(1,\alpha_0)), \quad b < \infty, \tag{3.23a}$$

$$\langle u_{0\alpha} F^0_{uu}, w_n^2\rangle \sim -(u_{0\alpha r}(1,\alpha_0)\, c_n^2/4n^2) F_{uu}(u_0(1,\alpha_0)), \quad b = \infty. \tag{3.23b}$$

Substituting (3.23) in the expression for $\lambda_2(\alpha_0)$ given in (3.9) we find that

$$\lambda_2(\alpha_0) \sim \frac{b\lambda_0(\alpha_0)\, u_{0\alpha r}(1,\alpha_0)\, c_n^2}{8n^3\langle u_{0\alpha}, F^0\rangle} F_{uu}(u_0(1,\alpha_0)), \quad b < \infty, \tag{3.24a}$$

$$\lambda_2(\alpha_0) \sim \frac{\lambda_0(\alpha_0)\, u_{0\alpha r}(1,\alpha_0)\, c_n^2}{16n^2\langle u_{0\alpha}, F^0\rangle} F_{uu}(u_0(1,\alpha_0)), \quad b = \infty. \tag{3.24b}$$

By using (3.24) in (3.9) then determines λ_c for $\epsilon \ll 1$ and $n \gg 1$ in terms of the unperturbed solution at the fold point. As a remark, if $\beta = 0$ then substituting (3.10) in (3.24) we can recover (3.19). In addition we also note that (3.24) is not uniform in b when b becomes large. To obtain a uniform expansion in the Biot number for $\lambda_2(\alpha_0)$ as $n \to \infty$ one would have to separately analyse the case $b = b_0 n$ with b_0 fixed. We do not pursue this here.

In table 2 we give numerical values for $\lambda_2(\alpha_0)$ for various β and n when $b = \infty$ and $c_n = 1$. From this table we observe that reactors with smaller activation energies are

Table 2. $\lambda_2(\alpha_0)$ *with* $b = \infty$ *and for various* $\beta > 0$, *from* (3.9)

n	$\beta = 0.0444$	$\beta = 0.1111$	$\beta = 0.1556$	$\beta = 0.1778$
1	-0.2077	-0.1447	-0.1030	-0.8200×10^{-1}
2	-0.5337×10^{-1}	-0.3929×10^{-1}	-0.2953×10^{-1}	-0.2445×10^{-1}
3	-0.2411×10^{-1}	-0.1835×10^{-1}	-0.1425×10^{-1}	-0.1206×10^{-1}
4	-0.1371×10^{-1}	-0.1066×10^{-1}	-0.8450×10^{-2}	-0.7260×10^{-2}
5	-0.8839×10^{-2}	-0.6975×10^{-2}	-0.5611×10^{-2}	-0.4869×10^{-2}
6	-0.6171×10^{-2}	-0.4922×10^{-2}	-0.4002×10^{-2}	-0.3499×10^{-2}
7	-0.4552×10^{-2}	-0.3661×10^{-2}	-0.3001×10^{-2}	-0.2638×10^{-2}
8	-0.3496×10^{-2}	-0.2829×10^{-2}	-0.2334×10^{-2}	-0.2061×10^{-2}
9	-0.2769×10^{-2}	-0.2253×10^{-2}	-0.1868×10^{-2}	-0.1655×10^{-2}
10	-0.2247×10^{-2}	-0.1836×10^{-2}	-0.1529×10^{-2}	-0.1359×10^{-2}

less sensitive to temperature variations than reactors with larger activation energies. For all β we also note that the onset of thermal runaway is only marginally hastened by a rapidly varying temperature profile. In table 3 we give numerical values for $\lambda_2(\alpha_0)$ for different Biot numbers but with $\beta > 0$ fixed. If $c_n \neq 1$ then the entries in tables 2 and 3 should be multiplied by c_n^2. In determining $\lambda_2(\alpha_0)$ we solved both (3.8) and (3.2a) numerically and then used a numerical quadrature to evaluate the integrals appearing in (3.9). We claim that the results for $\lambda_2(\alpha_0)$ are correct to at least three significant digits. We also mention that the asymptotic result for $\lambda_2(\alpha_0)$ as $n \to \infty$ given in (3.24a, b) is typically within 10% of the values shown in tables 2 and 3 when $n \geqslant 7$.

In figure 1 we let $n = 1$ and $c_1 = 1$ and we plot $\lambda_2(\alpha_0)$ against β for different Biot numbers. From this plot we observe that the dependence of $\lambda_2(\alpha_0)$ on β is roughly linear with a slope depending on the Biot number.

3.2. *A circular cylindrical reactor*: $c_0 \neq 0$

We first consider the case with infinite activation energy ($\beta = 0$) and we take $h(\theta) = \frac{1}{2}c_0 + c_n \cos n\theta$ for positive integers n. By using $(u_{0\alpha}, F^0) = -2\pi u_{0\alpha r}(1)/\lambda_0$ at criticality, then (3.4) yields $\lambda_1(\alpha_0) = -\frac{1}{2}c_0\lambda_0(\alpha_0)$. Now noting that $F = F_u = F_{uu}$, the solution to (3.2a) with $n = 0$ can be chosen as $w_0(r) = c_0$ at $\alpha = \alpha_0$. Substituting $w_0 = c_0$ in (3.5) and (3.6) we find $\lambda_1'(\alpha_0) = 0$ and

$$\lambda_2(\alpha_0) = \tfrac{1}{8}c_0^2\lambda_0 - \tfrac{1}{4}\lambda_0\langle u_{0\alpha}F^0_{uu}, w_n^2\rangle/\langle u_{0\alpha}, F^0\rangle. \tag{3.25}$$

Thus the two-term expansion to the location of the fold point, given in (2.5), becomes

$$\lambda_c = \lambda_0(\alpha_0) - \tfrac{1}{2}c_0\lambda_0(\alpha_0)\epsilon + \epsilon^2\lambda_2(\alpha_0) + \ldots, \quad \text{when} \quad \beta = 0. \tag{3.26}$$

Here u_0, λ_0 are given in (3.10), w_n is specified in (3.12), and α_0 is given in (3.11). In addition, the term in (3.25) involving the ratio of two inner products is written explicitly in (3.14) and is tabulated for various n and b in table 1. In particular, when $n = 1$, this term was written explicitly in (3.16) and so (3.25) and (3.26) provide

$$\lambda_c = \lambda_0(\alpha_0)\left[1 - \tfrac{1}{2}c_0\epsilon + \left(\tfrac{1}{8}c_0^2 - \frac{2\alpha_0^2 c_n^2}{(1+\alpha_0)^4}\right)\epsilon^2 + \ldots\right] \quad \text{when} \quad \beta = 0, n = 1. \tag{3.27}$$

To determine $\lambda_2(\alpha_0)$ in (3.25) for arbitrary n we can replace the term involving the ratio of two inner products by the highly accurate approximation (3.18).

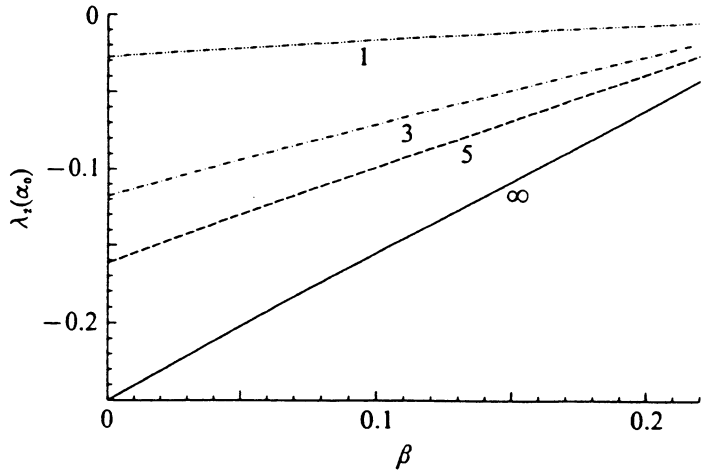

Figure 1. Small temperature variation of mean zero: $\lambda_2(\alpha_0)$ against β for $n = 1$ and different Biot numbers (values as indicated).

Table 3. $\lambda_2(\alpha_0)$ *with* $\beta = 0.1111$ *and for various* b, *from* (3.9)

n	$b = 5$	$b = 3$	$b = 1$	$b = 0.25$
1	-0.9181×10^{-1}	-0.6542×10^{-1}	-0.1425×10^{-1}	-0.5227×10^{-3}
2	-0.2301×10^{-1}	-0.1533×10^{-1}	-0.2802×10^{-2}	-0.9123×10^{-4}
3	-0.9902×10^{-2}	-0.6255×10^{-1}	-0.1022×10^{-2}	-0.3115×10^{-4}
4	-0.5315×10^{-2}	-0.3220×10^{-2}	-0.4863×10^{-3}	-0.1423×10^{-4}
5	-0.3227×10^{-2}	-0.1890×10^{-2}	-0.2696×10^{-3}	-0.7663×10^{-5}
6	-0.2121×10^{-2}	-0.1209×10^{-2}	-0.1650×10^{-3}	-0.4594×10^{-5}
7	-0.1476×10^{-2}	-0.8220×10^{-3}	-0.1084×10^{-3}	-0.2969×10^{-5}
8	-0.1071×10^{-2}	-0.5851×10^{-3}	-0.7500×10^{-4}	-0.2029×10^{-5}
9	-0.8031×10^{-2}	-0.4316×10^{-3}	-0.5406×10^{-4}	-0.1448×10^{-5}
10	-0.6185×10^{-2}	-0.3277×10^{-3}	-0.4026×10^{-4}	-0.1069×10^{-5}

We also note that (3.26) can be derived in a simpler way by using the change of variables: $\tilde{u} = u - \frac{1}{2}\epsilon c_0$ and $\tilde{\lambda} = \lambda e^{\epsilon c_0/2}$. Then $\tilde{u}, \tilde{\lambda}$ satisfy (2.1) and the average temperature variation on the boundary vanishes. Thus (3.9) is applicable for $\tilde{\lambda}$. Finally, relating $\tilde{\lambda}$ to λ and expanding for $\epsilon \ll 1$ we obtain (3.26).

For the case of finite activation energies $\beta > 0$ we must use our numerical scheme, described following (3.8), to compute the coefficients needed for the two term expansion given in (2.5). The temperature variation is again taken to be $h(\theta) = \frac{1}{2}c_0 + c_n \cos n\theta$ for positive integers n. To display our results it is convenient to decompose $\lambda_2(\alpha_0)$, given in (3.6), in terms of a component that depends on n and a component that is independent of n. Thus we write $\lambda_2(\alpha_0) = \lambda_{20}(\alpha_0) + \lambda_{2n}(\alpha_0)$, where

$$\lambda_{20}(\alpha_0) = -\frac{1}{\langle u_{0x}, F^0\rangle}[\tfrac{1}{2}\lambda_1\langle u_{0x}, w_0 F^0_u\rangle + \tfrac{1}{8}\lambda_0\langle u_{0x}, w_0^2 F^0_{uu}\rangle], \tag{3.28a}$$

$$\lambda_{2n}(\alpha_0) = -\lambda_0\langle u_{0x}, F^0_{uu} w_n^2\rangle / 4\langle u_{0x}, F^0\rangle. \tag{3.28b}$$

Then (2.5) can be written as

$$\lambda_c = \lambda_0(\alpha_0) + \epsilon\lambda_1(\alpha_0) + \epsilon^2[\lambda_{2n}(\alpha_0) + \hat{\lambda}_{20}(\alpha_0)] + \ldots, \quad \hat{\lambda}_{20}(\alpha_0) \equiv \lambda_{20}(\alpha_0) - (\lambda_1'(\alpha_0))^2/2\lambda_0''(\alpha_0). \tag{3.29}$$

Table 4. *Coefficients in the expansion of* $\lambda_c(\epsilon)$ *for a temperature fluctuation with non-zero mean and with* $b = \infty$

β	$\lambda_0(\alpha_0)$	$\lambda_0''(\alpha_0)$	$\lambda_1(\alpha_0)$	$\hat{\lambda}_{20}(\alpha_0)$
0	2.0000	−1.0000	−1.0000	0.2500
0.0222	2.0502	−0.8831	−0.9790	0.2449
0.0444	2.1044	−0.7707	−0.9562	0.2396
0.0667	2.1630	−0.6632	−0.9312	0.2341
0.0889	2.2270	−0.5606	−0.9036	0.2285
0.1111	2.2973	−0.4632	−0.8729	0.2228
0.1333	2.3753	−0.3712	−0.8380	0.2170
0.1556	2.4630	−0.2849	−0.7975	0.2113
0.1778	2.5634	−0.2046	−0.7491	0.2063
0.2000	2.6814	−0.1306	−0.6881	0.2037

where $\lambda_1'(\alpha_0)$ and $\lambda_0''(\alpha_0)$ are given in (3.5) and (2.12) respectively. With this decomposition $\hat{\lambda}_{20}(\alpha_0)$ is independent of n. In addition, it is easily verified that $\hat{\lambda}_{20}(\alpha_0)$ does not depend upon how the solution, w_0, to (3.2*a*) is normalized at $\alpha = \alpha_0$.

For different β and with $c_0 = 1$ and $b = \infty$, in table 4 we give numerical values for $\lambda_0(\alpha_0)$, $\lambda_0''(\alpha_0)$, $\lambda_1(\alpha_0)$, and $\hat{\lambda}_{20}(\alpha_0)$ found from (3.8), (2.12), (3.4) and (3.29) respectively. If $c_0 \neq 1$ then the entries in columns four and five should be multiplied by c_0 and c_0^2 respectively. In addition, we note that $\lambda_{2n}(\alpha_0)$ in (3.28*b*) is precisely that quantity which was tabulated, when $c_n = 1$, in table 2. If $c_n \neq 1$ and $n \geqslant 1$, then the entries in table 2 should be multiplied by c_n^2. Thus, using the numerical values for the coefficients from these tables, a two term expansion for $\lambda_c(\epsilon)$ from (3.29) is known.

As a partial check on the results we note that the first row of table 4 reproduces the analytical results derived above when $\beta = 0$. As a remark, our numerical procedure is also capable of obtaining numerical values for the coefficients in the expansion of λ_c when $\beta > 0$ and for arbitrary Biot numbers. However, we do not display these results.

3.3. *A circular cylindrical reactor: numerical solution to* (2.1)

In this section, we solve the two-dimensional problem (2.1) numerically and we compare numerical and asymptotic predictions for the location of the fold point when $\epsilon \ll 1$. We limit the discussion to the case $b = \infty$, i.e. pure Dirichlet boundary conditions. The general case, $0 < b \leqslant \infty$, could be included easily, however. The numerical procedure is defined by two main elements: the discretization of the problem for fixed parameters λ, ϵ and β, and the continuation procedure. We describe the discretization in the next paragraph. To compute solution paths of (2.1) with varying parameters we used a concurrent implementation of Keller's pseudo-arclength continuation procedure. We refer to Keller (1987) for details on pseudo-arclength continuation and to Van de Velde & Lorenz (1990) for a description of the concurrent implementation. Our computations were carried out on Caltech's Symult S2010, a multicomputer with up to 192 processors; see Seitz *et al.* (1988) for more details on the computer architecture.

We transform the original problem (2.1) with $b = \infty$ from the unit disc D to a rectangular domain. The most obvious method to accomplish this is by a polar coordinate transformation, which maps the unit disc into $[0, 2\pi] \times [0, 1]$. However, some numerical difficulties are associated with the singularity of the polar coordinate

Table 5. *Comparison of asymptotic and numerical predictions for* λ_c *when* $\epsilon = 0.1$ *with* $h(\theta) = \cos^2(\theta)$ *and* $h(\theta) = \cos(2\theta)$

β	$\lambda_c(3.26)$ asy.	$\lambda_c(2.1)$ num.	$\lambda_c(3.9)$ asy.	$\lambda_c(2.1)$ num.
0	1.9019	1.9020	1.9994	1.9990
0.0444	2.0110	2.0106	2.1039	2.1035
0.0889	2.1388	2.1384	2.2265	2.2266
0.1111	2.2121	2.2117	2.2969	2.2965
0.1333	2.2936	2.2933	2.3749	2.3746
0.1556	2.3853	2.3848	2.4627	2.4623
0.1778	2.4905	2.4920	2.5632	2.5627

transformation at the origin of the disc. Hence, we opted for another coordinate transformation, one that is regular in the interior of D. The coordinate transformation given by

$$x = \sin p, \quad y = \sin q, \tag{3.30}$$

transforms the problem (2.1), with $b = \infty$, to

$$\left.\begin{aligned} \sec p \frac{\partial}{\partial p}\left(\sec p \frac{\partial u}{\partial p}\right) + \sec q \frac{\partial}{\partial q}\left(\sec q \frac{\partial u}{\partial q}\right) + \lambda F(u) = 0, \quad (p,q) \in D', \\ u = \epsilon h(\theta), \quad (p,q) \in \partial D'. \end{aligned}\right\} \tag{3.31}$$

Here, D' is the image of D under the transformation. It is easily verified that the domain D' is the square with vertices $(\frac{1}{2}\pi, 0)$, $(0, \frac{1}{2}\pi)$, $(-\frac{1}{2}\pi, 0)$, and $(0, -\frac{1}{2}\pi)$, (i.e. the edges of the square make 45° angles with the coordinate axes). The vertices of this square are images of $(1,0)$, $(0,1)$, $(-1,0)$ and $(0,-1)$ respectively. The edges are images of the corresponding unit circle arcs.

We introduce a square grid on D' with grid lines parallel to the coordinate axes and grid spacing $h = 1/N$. The partial differential operator on this grid is discretized using a five-point central differencing scheme. With $p_i = ih$ and $-N < i < N$, the part of the partial differential operator along the p-direction is approximated at p_i by

$$h^{-2} \sec p_i (\sec p_{i+0.5}(u_{i+1} - u_i) - \sec p_{i-0.5}(u_i - u_{i-1})).$$

The other term in the partial differential operator is discretized in an analogous fashion. The nonlinear heating term $F(u) = \exp(u/(1+\beta u))$ is linearized, and the solution to the full nonlinear problem is found by Newton iterations (in the pseudo-archlength continuation method the Newton iteration must be adapted (see Keller 1987; Van de Velde & Lorenz 1989)).

Since $b = \infty$, all boundary conditions are of Dirichlet-type, and thus are easily imposed. For simplicity, the temperature profiles $h(\theta)$ considered here are such that the solution to (2.1) has a symmetry with respect to both the x and y axis. This symmetry is exploited to reduce the number of unknowns by a factor of four.

To compare the asymptotic and numerical predictions for λ_c we have taken $h(\theta) = \cos(2\theta)$ and $h(\theta) = \cos^2(\theta)$, and thus the second profile has a non-zero mean. In table 5, we compare λ_c predicted by our asymptotic analysis with the corresponding value of λ_c obtained from a full numerical solution to (2.1). The comparisons are made at a fixed $\epsilon = 0.1$ but for various activation energy parameters

Table 6. *Comparison of asymptotic and numerical predictions for* λ_c *when* $\beta = 0$ *with* $h(\theta) = \cos(2\theta)$ *and for different* ϵ

ϵ	$\lambda_c(3.9)$ asy.	$\lambda_c(2.1)$ num.
0.10	1.9994	1.9990
0.15	1.9986	1.9983
0.20	1.9975	1.9972
0.25	1.9961	1.9958

β. The second and third columns of this table are the results for $h(\theta) = \cos^2(\theta)$ while the fourth and fifth columns are the results for $h(\theta) = \cos(2\theta)$. The numerical computations were done using $h = 1/64$. We note that for most of the β values given in table 5 the asymptotic predictions for $\lambda_c(\epsilon)$ through terms of $O(\epsilon^2)$ are easily obtained from the data in tables 1, 2 and 4. As seen from table 5 the asymptotic and numerical predictions for $\lambda_c(\epsilon)$ agree to about four significant figures.

In table 6 we give the asymptotic and numerical predictions for λ_c when $\beta = 0$ and $h(\theta) = \cos(2\theta)$ but for various ϵ values. From this table we anticipate that the asymptotic prediction for λ_c will be close to the corresponding numerical values even for moderate values of ϵ.

4. A nearly circular cylindrical reactor

The perturbed problem in the nearly circular domain D_ϵ is

$$\Delta u + \lambda F(u) = 0, \quad x \in D_\epsilon, \tag{4.1a}$$

$$\partial_\nu u + bu = 0, \quad x \in \partial D_\epsilon. \tag{4.1b}$$

The boundary of the domain is written as $\partial D_\epsilon : r = 1 + \epsilon h(\theta)$, where $h(\theta)$ is a smooth 2π periodic function. In terms of polar coordinates (4.1*b*) becomes

$$\left(u_r - \frac{\epsilon h'}{(1+\epsilon h)^2} u_\theta\right) + b\left(1 + \frac{\epsilon^2 (h')^2}{(1+\epsilon h)^2}\right)^{\frac{1}{2}} u = 0 \quad \text{on} \quad r = 1 + \epsilon h(\theta). \tag{4.2}$$

We now determine a two term expansion for $\lambda_c(\epsilon)$ when $\epsilon \ll 1$.

We seek the solution to (4.1) in the form (2.2). Substituting this expansion into (4.1*a*) and (4.2) and equating powers of ϵ gives

$$\Delta u_1 + \lambda_0 F^0_u u_1 = -\lambda_1 F^0, \quad r < 1, \tag{4.3a}$$

$$u_{1r} + b u_1 = -bhu_{0r} - hu_{0rr}, \quad \text{on} \quad r = 1, \tag{4.3b}$$

$$\Delta u_2 + \lambda_0 F^0_u u_2 = -\lambda_2 F^0 - \lambda_1 u_1 F^0_u - \tfrac{1}{2}\lambda_0 u_1^2 F^0_{uu}, \quad r < 1, \tag{4.4a}$$

$$u_{2r} + b u_2 = -hu_{1rr} - \tfrac{1}{2}h^2 u_{0rrr} + h' u_{1\theta} + \tfrac{1}{2}(h')^2 u_{0r} - bhu_{1r} - \tfrac{1}{2}bh^2 u_{0rr}, \quad \text{on} \quad r = 1. \tag{4.4b}$$

To evaluate the coefficients in the expansion of $\lambda_c(\epsilon)$ in (2.5) we now proceed as in §2 to derive the solvability conditions for (4.3) and (4.4). These conditions will determine $\lambda_1(\alpha_0)$, $\lambda_1'(\alpha_0)$ and $\lambda_2(\alpha_0)$, which are needed in (2.5). Numerical values for $\lambda_0(\alpha_0)$ and $\lambda_0''(\alpha_0)$, determined from the unperturbed problem, are given in table 4 when $b = \infty$. We note that the extended system for $u_0(r, \alpha)$ and $u_{0\alpha}(r, \alpha)$ is again given in (3.8).

At $\alpha = \alpha_0$ the solvability condition for (4.3) provides

$$\lambda_1(\alpha_0) = (\bar{h}u_{0x}(1)/2\pi\langle u_{0x}, F^0\rangle)\,(bu_{0r}(1)+u_{0rr}(1)), \quad \text{at} \quad \alpha = \alpha_0. \tag{4.5a}$$

Here we have defined

$$\langle u, v\rangle = \int_0^1 uvr\,\mathrm{d}r \quad \text{and} \quad \bar{h} = \int_0^{2\pi} h(\theta)\,\mathrm{d}\theta.$$

Now using (3.8a), then (4.5a) can be alternatively written at criticality as

$$\lambda_1(\alpha_0) = -(\bar{h}/2\pi\langle u_{0x}, F^0\rangle)\,[u_{0r}(1)\,(u_{0xr}(1)+u_{0x}(1))+\lambda_0 u_{0x}(1)F(u_0(1))]. \tag{4.5b}$$

A similar procedure is used to compute $\lambda_2(\alpha_0)$ from (4.4). Writing $u_1 = u_1(r,\theta)$ and invoking a solvability condition on (4.4) we find

$$\begin{aligned}\lambda_2(\alpha_0)\,(u_{0x}, F^0) = &-\lambda_1(u_{0x}, F^0_u\,u_1)-\tfrac{1}{2}\lambda_0(u_{0x}, F^0_{uu}\,u_1^2)+u_{0x}(1)\,\overline{hu_{1rr}(1,\theta)}\\ &+\tfrac{1}{2}\overline{h^2}u_{0x}(1)\,[u_{0rrr}(1)+bu_{0rr}(1)]-u_{0x}(1)\,\overline{h'u_{1\theta}(1,\theta)}\\ &-\tfrac{1}{2}\overline{(h')^2}u_{0x}(1)\,u_{0r}(1)+bu_{0x}(1)\,\overline{hu_{1r}(1,\theta)}.\end{aligned} \tag{4.6}$$

Here $(u, v) = \int_{D_0} uv\,\mathrm{d}x$.

Now to determine $\lambda_1'(\alpha_0)$ we differentiate (4.3a, b) with respect to α so that

$$\left.\begin{aligned}\Delta u_{1x}+\lambda_0 F^0_u\,u_{1x} &= -\lambda_0' F^0_u\,u_{0x}-\lambda_0 F^0_{uu}\,u_1\,u_{0x}-\lambda_1' F^0-\lambda_1 F^0_u\,u_{0x}, \quad r<1,\\ u_{1xr}+bu_{1x} &= -bhu_{0xr}-hu_{0xrr} \quad \text{on} \quad r=1.\end{aligned}\right\} \tag{4.7}$$

Then invoking a solvability condition on (4.7), and using (3.8b), we derive

$$\begin{aligned}\lambda_1'(\alpha_0)\,(u_{0x}, F^0) = &-\lambda_0(u_{0x}, F^0_{uu}\,u_{0x}\,u_1)-\lambda_1(u_{0x}, F^0_u\,u_{0x})\\ &-\bar{h}[u_{0xr}(1)\,(u_{0xr}(1)+u_{0x}(1))+\lambda_0 u_{0x}^2(1)\,F^0_u(u_0(1))],\end{aligned} \tag{4.8}$$

at criticality. Finally, the remaining quantity $\lambda_0''(\alpha_0)$ needed in (2.5) is given in (2.12). Again we emphasize that all quantities appearing in (4.5), (4.6) and (4.8) are to be evaluated at $\alpha = \alpha_0$.

We now look for a solution to (4.3) in the form (3.1). Substituting (3.1) in (4.3) we obtain

$$L_n w_n+\lambda_0 F^0_u\,w_n = -2\lambda_1 F^0\delta_{n0}, \quad w_n'(1)+bw_n(1) = -[bu_{0r}(1)+u_{0rr}(1)]\,c_n, \tag{4.9a}$$

$$L_n v_n+\lambda_0 F^0_u\,v_n = 0, \quad v_n'(1)+bv_n(1) = -[bu_{0r}(1)+u_{0rr}(1)]\,d_n. \tag{4.9b}$$

Here δ_{n0}, L_n were defined following (3.2) and c_n and d_n are the Fourier coefficients of $h(\theta)$ given in (3.3).

From (4.5) we see that there is no solution to (4.9a) at criticality with $n = 0$ unless

$$\lambda_1(\alpha_0) = (c_0\,u_{0x}(1)/2\langle u_{0x}, F^0\rangle)\,(bu_{0r}(1)+u_{0rr}(1)), \quad \text{at} \quad \alpha = \alpha_0. \tag{4.10}$$

At $\alpha = \alpha_0$ and with $n = 0$ the solution to (4.9a) is made unique by specifying $\langle u_{0x}, w_0\rangle = 0$.

Now substituting (3.2) into the inner product terms appearing in (4.6) and (4.8) we derive

$$(u_{0x}, F^0_u\,u_1) = \pi\langle u_{0x}, F^0_u\,w_0\rangle, \tag{4.11a}$$

$$(u_{0x}, F^0_{uu}\,u_{0x}\,u_1) = \pi\langle u_{0x}, F^0_{uu}\,u_{0x}\,w_0\rangle, \tag{4.11b}$$

$$(u_{0x}, F^0_{uu}\,u_1^2) = \tfrac{1}{2}\pi\langle u_{0x}, F^0_{uu}\,w_0^2\rangle+\pi\sum_{n=1}^{\infty}\langle u_{0x}F^0_{uu}, w_n^2+v_n^2\rangle. \tag{4.11c}$$

In addition, the boundary terms appearing in (4.6) are evaluated, at $\alpha = \alpha_0$, as follows:

$$\overline{hu_{1rr}(1,\theta)} = \tfrac{1}{2}\pi c_0 w_0''(1) + \pi \sum_{n=1}^{\infty} [c_n w_n''(1) + d_n v_n''(1)], \tag{4.12a}$$

$$\overline{h^2} = \tfrac{1}{2}\pi c_0^2 + \pi \sum_{n=1}^{\infty} (c_n^2 + d_n^2), \quad \overline{(h')^2} = \pi \sum_{n=1}^{\infty} n^2 (c_n^2 + d_n^2), \tag{4.12b}$$

$$\overline{hu_{1r}(1,\theta)} = \tfrac{1}{2}\pi c_0 w_0'(1) + \pi \sum_{n=1}^{\infty} [c_n w_n'(1) + d_n v_n'(1)], \tag{4.12c}$$

$$\overline{h' u_{1\theta}(1,\theta)} = \pi \sum_{n=1}^{\infty} n^2 [c_n w_n(1) + d_n v_n(1)]. \tag{4.12d}$$

Therefore with u_0, $u_{0\alpha}$, w_n and v_n known from the numerical solution to (3.8) and (4.9) at $\alpha = \alpha_0$, we can determine the quantities appearing in (4.11) and (4.12). The inner product terms in (4.11) are evaluated by a numerical quadrature. Then using (4.11) and (4.12) in (4.5), (4.6) and (4.8), a two term expansion for $\lambda_c(\epsilon)$ can be found from (2.5). We now consider in detail the special case where the mean radius is unchanged so that $c_0 = 0$.

4.1. *A nearly circular cylindrical reactor*: $c_0 = 0$

We now assume that $\bar{h} = c_0 = 0$ and for positive integers n we take $h(\theta) = c_n \cos n\theta$. Then from (4.5) we find that $\lambda_1(\alpha_0) = 0$. Now from (4.9a) and $\langle u_{0\alpha}, w_0 \rangle = 0$ we have $w_0 \equiv 0$ and so (4.8) yields $\lambda_1'(\alpha_0) = 0$. Thus (2.5) becomes

$$\lambda_c = \lambda_0(\alpha_0) + \epsilon^2 \lambda_2(\alpha_0) + \ldots . \tag{4.13a}$$

Now setting $h(\theta) = c_n \cos n\theta$ in (4.11), (4.12) and substituting in (4.6) we derive, with the aid of (3.8) and (4.9a),

$$\begin{aligned}\lambda_2(\alpha_0)\langle u_{0\alpha}, F^0 \rangle = &-\tfrac{1}{4}\lambda_0 \langle u_{0\alpha}, F^0_{uu} w_n^2 \rangle - \tfrac{1}{2} u_{0\alpha}(1) c_n [w_n'(1) + \lambda_0 F_u(u_0(1)) w_n(1)] \\ &+ \tfrac{1}{4} u_{0\alpha}(1) c_n^2 [u_{0rrr}(1) + b u_{0rr}(1) - n^2 u_{0r}(1)] - \tfrac{1}{2} u_{0\alpha r}(1) c_n w_n'(1),\end{aligned} \tag{4.13b}$$

at $\alpha = \alpha_0$. Here w_n is to be found from (4.9a). We now consider the case $b = \infty$ for which (4.13b) simplifies considerably.

Infinite Biot number: $b = \infty$

Assuming that $b = \infty$ then (4.13b), with $u_{0\alpha}(1) = 0$ and $u_{0\alpha r}(1) = -b u_{0\alpha}(1)$, reduces to

$$\lambda_2(\alpha_0)\langle u_{0\alpha}, F^0 \rangle = -\tfrac{1}{4}\lambda_0 \langle u_{0\alpha}, F^0_{uu} w_n^2 \rangle - \tfrac{1}{2} c_n u_{0\alpha r}(1) w_n'(1) - \tfrac{1}{4} c_n^2 u_{0\alpha r}(1) u_{0rr}(1), \tag{4.14}$$

at $\alpha = \alpha_0$. To determine numerical values for $\lambda_2(\alpha_0)$ for arbitrary β and n we first solve (3.8) numerically with $b = \infty$ and locate the first fold point α_0. Then solving (4.9a) with $b = \infty$ numerically at $\alpha = \alpha_0$, we find w_n and finally a numerical quadrature of the inner product integral in (4.14) determines $\lambda_2(\alpha_0)$. As a partial check on the calculations we now note that when $\beta = 0$, $\lambda_2(\alpha_0)$ can be found almost explicitly.

For the case $\beta = 0$ and $b = \infty$ the solution to the unperturbed problem from (3.10) can be written as

$$u_0(r,\alpha) = 2 \ln\left(\frac{1+\alpha}{1+\alpha r^2}\right), \quad \lambda_0(\alpha) = 8\alpha/(1+\alpha)^2. \tag{4.15}$$

With this definition of α, criticality occurs at $\alpha = \alpha_0 = 1$. Now at criticality the solution to (4.9a), with $w_n(1) = -c_n u_{0r}(1) = 2c_n$, is

$$w_n(r) = \frac{2c_n}{n} r^n \left[\frac{1-r^2}{1+r^2} + n\right]. \tag{4.16}$$

This special solution was derived in Adler (1987). Then with $\langle u_{0\alpha}, F^0\rangle = \frac{1}{2}$, $u_{0rr}(1) = 0$, $u_{0\alpha r}(1) = -1$, and $\lambda_0(\alpha_0) = 2$, (4.14) becomes

$$\lambda_2(\alpha_0) = -\frac{16c_n^2}{n^2}\int_0^1 \frac{(1-r^2)}{(1+r^2)^3}\left[\frac{1-r^2}{1+r^2}+n\right]^2 r^{2n+1}\,\mathrm{d}r + 2c_n^2\left(n-\frac{1}{n}\right). \tag{4.17}$$

If $n = 1$ then upon integrating (4.17) explicitly, (4.13a) reduces to

$$\lambda_c = 2-\epsilon^2 c_n^2 + \ldots, \quad \beta = 0, b = \infty, n = 1. \tag{4.18a}$$

In this limiting case we recover the result of Adler (1987). For $n > 1$ we evaluate the integral in (4.17) numerically, upon setting $c_n = 1$, to obtain

$$\left.\begin{aligned} &\lambda_2(\alpha_0) = -1.0, \quad n = 1; \quad \lambda_2(\alpha_0) = 2.75, \quad n = 2; \quad \lambda_2(\alpha_0) = 5.22, \quad n = 3;\\ &\lambda_2(\alpha_0) = 7.44, \quad n = 4; \quad \lambda_2(\alpha_0) = 9.56, \quad n = 5; \quad \lambda_2(\alpha_0) = 11.64, \quad n = 6. \end{aligned}\right\} \tag{4.18b}$$

In particular we note that for $n \geqslant 2$ ($n < 2$) the reactor is more (less) stable than a circular cylindrical reactor of the same radius. Another limiting case is when n tends to infinity. In this limit the integral appearing in (4.17) is $O(n^{-2})$ and so $\lambda_2(\alpha_0) = 2c_n^2(n-1/n) + O(n^{-2})$ for $n \gg 1$. Thus we notice that our expansion breaks down when $e^2 n = O(1)$.

For arbitrary $\beta \geqslant 0$ and $n \geqslant 1$ it is not possible to solve (4.9a) analytically. However, for the two special cases $n = 1$ and $n \gg 1$ we can avoid having to solve (4.9a) numerically. These special cases again provide a check on the numerical computations that follow. If $n = 1$ the solution to (4.9a) with $b = \infty$ is $w_1(r) = -c_1 u_{0r}(r)$. Then from (4.14) we obtain

$$\lambda_2(\alpha_0)\langle u_{0\alpha}, F^0\rangle = -\tfrac{1}{4}\lambda_0 c_1^2 \langle u_{0\alpha} F^0_{uu}, u_{0r}^2\rangle + \tfrac{1}{4}c_1^2 u_{0\alpha r}(1)\, u_{0rr}(1).$$

This expression can be simplified by noticing that $\langle u_{0\alpha} F^0_{uu}, u_{0r}^2\rangle = -u_{0\alpha r}(1) F^0(u_0(1))$. Then, upon using (3.8$a$), the previous expression becomes

$$\lambda_2(\alpha_0) = -c_1^2 u_{0r}(1)\, u_{0\alpha r}(1)/4\langle u_{0\alpha}, F^0\rangle. \tag{4.19}$$

Thus when $n = 1$, $\lambda_2(\alpha_0)$ can be found only from the numerical solution to (3.8).

Now for $\beta \geqslant 0$ and $n \geqslant 1$ we first solve (4.9a) with $b = \infty$ by the method of matched asymptotic expansions. A simple application of this method provides

$$w_n(r) = -c_n u_{0r}(1)\, \mathrm{e}^{n(r-1)}[1-\tfrac{1}{2}n(r-1)^2 + \ldots]. \tag{4.20}$$

With w_n given asymptotically in (4.20) we use Laplace's method on the inner product integral appearing in (4.14) to estimate $\langle u_{0\alpha} F^0_{uu}, w_n^2\rangle = O(n^{-2})$. Then from (4.14) we find

$$\lambda_2(\alpha_0)\langle u_{0\alpha}, F^0\rangle \sim \frac{nc_n^2 u_{0r}(1)\, u_{0\alpha r}(1)}{2\langle u_{0\alpha}, F^0\rangle} - \frac{c_n^2 u_{0\alpha r}(1)\, u_{0rr}(1)}{4\langle u_{0\alpha}, F^0\rangle} + o(1), \quad \text{as} \quad n \to \infty. \tag{4.21}$$

Again we note that our expansions break down when $\epsilon^2 n = O(1)$.

In figure 2 we take $c_n = 1$ and we plot $\lambda_2(\alpha_0)$ against β for different n values.

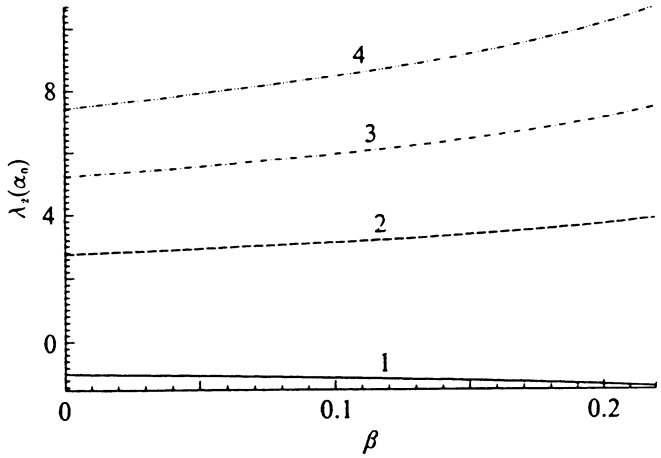

Figure 2. Nearly circular cylindrical reactor: $\lambda_2(\alpha_0)$ against β for $b = \infty$ and different n (values as indicated).

obtained from the numerical solution to (3.8) and (4.9a). Some of these results are tabulated in table 7. Note that the second column of this table reproduces the results obtained in (4.18a, b) for $\beta = 0$. These results indicate that, except for the $n = 1$ mode, $\lambda_2(\alpha_0) > 0$ and is an increasing function of β. Although $\lambda_2(\alpha_0) < 0$ when $n = 1$, a simple calculation shows that the data in the first row of table 7 does not contradict the well known qualitative result (see Adler 1987) that for cylinders of the same cross-sectional area the circular cylinder is the least stable. Finally, we remark that the asymptotic result (4.21) for $\lambda_2(\alpha_0)$ is found to be within 5% of the tabulated values when $n \geqslant 5$.

Finite Biot number: $b < \infty$

For the case of a finite Biot number and with $\beta = 0$, we can solve (4.9a) explicitly. By using (3.10) in (4.9a) we solve the resulting equation at criticality to obtain

$$w_n(r) = \frac{4\alpha_0 c_n}{n(1+\alpha_0)+n^2(1-\alpha_0)} r^n \left[\frac{1-\alpha_0 r^2}{1+\alpha_0 r^2}+n\right]. \tag{4.22}$$

Here α_0 is given in (3.11). Then using (4.22), (3.10) and (3.13) a lengthy but straightforward calculation gives the following expressions for the various terms in (4.13b) at $\alpha = \alpha_0$:

$$\left.\begin{aligned}
[u_{0rrr}(1)+bu_{0rr}(1)-n^2u_{0r}(1)]\frac{u_{0\alpha}(1)}{4\langle u_0, e^{u_0}\rangle} &= \frac{\lambda_0(1-\alpha_0)}{4(1+\alpha_0)^2}\gamma_1,\\
-\frac{\lambda_0\langle u_{0\alpha}, e^{u_0}w_n^2\rangle}{4\langle u_{0\alpha}, e^{u_0}\rangle} &= -\frac{4\lambda_0\alpha_0^2c_n^2}{n^2\gamma_-^2}(1+\alpha_0)^2\int_0^1 G_n(s,\alpha_0)\,e^{s\ln n}\,ds,\\
-\frac{(u_{0\alpha}(1)+u_{0\alpha r}(1))\,w_n'(1)}{2\langle u_{0\alpha}, e^{u_0}\rangle} &= \frac{\lambda_0 c_n(\alpha_0^2+4\alpha_0-1)}{2n\gamma_-(1+\alpha_0)^2}[n(1+\alpha_0)\gamma_+-4\alpha_0],\\
-\frac{u_{0\alpha}(1)\,\lambda_0\,e^{u_0}w_n(1)}{2\langle u_{0\alpha}, e^{u_0}\rangle} &= -\frac{4\lambda_0 c_n\,\alpha_0(1-\alpha_0)\gamma_+}{n(1+\alpha_0)^2\gamma_-}.
\end{aligned}\right\} \tag{4.23}$$

Here $G_n(s,\alpha_0)$ is defined in (3.15) and we have labelled $\gamma_1 = n^2(1+\alpha_0)^2+2\alpha_0-2\alpha_0^2$, and

$$\gamma_+ = n(1+\alpha_0)+(1-\alpha_0), \quad \gamma_- = n(1-\alpha_0)+(1+\alpha_0). \tag{4.24}$$

Table 7. $\lambda_2(\alpha_0)$ *with* $b = \infty$ *and for various* $\beta > 0$, *from* (4.14)

n	$\beta = 0$	$\beta = 0.0444$	$\beta = 0.1111$	$\beta = 0.1556$	$\beta = 0.1778$
1	−1.000	−1.052	−1.149	−1.232	−1.282
2	2.750	2.894	3.160	3.390	3.530
3	5.222	5.506	6.035	6.494	6.775
4	7.438	7.845	8.603	9.262	9.666
5	9.560	10.083	11.057	11.903	12.421
6	11.639	12.274	13.456	14.483	15.111
7	13.694	14.439	15.825	17.028	17.763
8	15.734	16.588	18.175	19.551	20.392
9	17.765	18.726	20.513	22.061	23.006
10	19.790	20.858	22.842	24.561	25.609

Table 8. $\lambda_2(\alpha_0)$ *with* $\beta = 0.1111$ *and for various* b, *from* (4.14)

n	$b = 5$	$b = 3$	$b = 1$	$b = 0.25$
1	−0.6681	−0.4988	−0.2018	−0.0527
2	1.2954	0.8734	0.3417	0.0983
3	2.6944	2.0236	1.0275	0.3324
4	4.1077	3.3311	1.9370	0.6564
5	5.6556	4.8743	3.0861	1.0716
6	7.3853	6.6828	4.4802	1.5784
7	9.3215	8.7710	6.1218	2.1770
8	11.479	11.147	8.0120	2.8674
9	13.867	13.817	10.152	3.6497
10	16.492	16.782	12.541	4.5239

By using a numerical quadrature to evaluate the integral in (4.23), $\lambda_2(\alpha_0)$ can easily be found for $b < \infty$ and for positive integers n. We notice from this result that $\lambda_2(\alpha_0) \sim \frac{1}{4}\lambda_0(1-\alpha_0)n^2c_n^2$ as $n \to \infty$. Thus our expansion breaks down when $\epsilon^2 n^2 = O(1)$.

In the case $n = 1$, $c_n = 1$ and $\beta = 0$ then we can recover the result of Adler (1987). Setting $n = 1$ and $c_n = 1$ in (4.23) and (4.24) and using

$$\int_0^1 G_1(s, \alpha_0)\, s\, \mathrm{d}s = 2(1+\alpha_0)^{-4},$$

we find from (4.13*b*) that

$$\lambda_2(\alpha_0) = [\lambda_0(\alpha_0)(1-\alpha_0)/4(1+\alpha_0)^2](\alpha_0^2 - 4\alpha_0 - 1) - 2\lambda_0\alpha_0^2/(1+\alpha_0)^2.$$

Finally, using $\alpha_0^2 - 1 + 4\alpha_0/b = 0$, we can rewrite this expression as

$$\lambda_2(\alpha_0) = -\lambda_0(\alpha_0)\left(\frac{\alpha_0^2}{(1+\alpha_0)} + \frac{\alpha_0(1+3\alpha_0)}{b(1+\alpha_0)^2}\right), \tag{4.25}$$

which is Adler's result.

In the case of finite activation energies ($\beta > 0$) and $n = 1$ we again note that $w_1(r)$ is proportional to u_{0r} so that $\lambda_2(\alpha_0)$ can be written explicitly in terms of the unperturbed solution. However, for $n > 1$ we must use our full numerical scheme to determine $\lambda_2(\alpha_0)$. By using this scheme in table 8 we fix β and we give numerical values for $\lambda_2(\alpha_0)$ for various n and b. From this table we observe that for $n > 1$, $\lambda_2(\alpha_0)$ is an increasing function of b. In figure 3 we have taken $n = 1$ and we plot $\lambda_2(\alpha_0)$ as

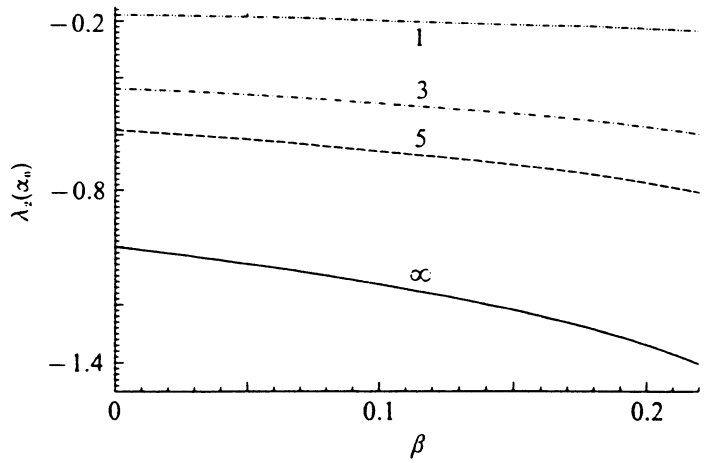

Figure 3. Nearly circular cylindrical reactor: $\lambda_2(\alpha_0)$ against β for $n = 1$ and different Biot numbers (values as indicated).

a function of β for different Biot numbers. When $n = 1$ we note that $\lambda_2(\alpha_0) < 0$ and is a decreasing function of β. Thus when $n = 1$ the reactor is more unstable than one with an equivalent mean radius.

5. Strong localized perturbations: higher order theory

In this section we consider a different class of domain perturbation than that considered in §4. The perturbed problem is now taken to be

$$\Delta u + \lambda F(u) = 0, \quad x \in D \backslash D_\epsilon, \tag{5.1a}$$

$$\partial_\nu u + bu = 0, \quad x \in \partial D, \tag{5.1b}$$

$$\epsilon \partial_\nu u + \kappa u = 0, \quad x \in \partial D_\epsilon, \tag{5.1c}$$

where $F(u)$ is given in (3.8a) and κ is a positive constant. Here D_ϵ is a domain of 'radius' ϵ containing a point, x_0, in the interior of D and $\partial_\nu u$ is the derivative of u with respect to the outer normal to $D \backslash D_\epsilon$. In three (two) dimensions, D_ϵ can be interpreted as a small cooling pellet (rod) located inside a reactive solid.

An asymptotic theory to determine $\lambda_c(\epsilon)$ for (5.1), and for more general strong localized perturbations, was initiated in Ward & Keller (1991) and was extended and validated numerically in Ward & Van de Velde (1991). The asymptotic theory presented there typically provided only the first correction to the location of the unperturbed fold point. We now show how, in principle, a two term expansion for λ_c when $\epsilon \ll 1$ can be obtained for (5.1) by using a method similar to that used in §2. We first consider the three-dimensional case.

The three-dimensional case

The solution to (5.1) is constructed using the method of matched asymptotic expansions. In the outer region away from D_ϵ we look for a solution to (5.1) in the form (2.2). Substituting this expansion into (5.1a) and (5.1b) and, collecting powers of ϵ, we derive (2.3a,b) and (2.4a,b) with homogeneous boundary data ($h = 0$ in (2.3b)).

We now construct the inner expansion near the cooling pellet D_ϵ, which is centred at some x_0 in D. For clarity, in the notation below we have suppressed the

dependence of the inner and outer solution on α. In the inner region we define the stretched variables $y = \epsilon^{-1}(x - x_0)$ and $v(y, \epsilon) = u(x_0 + \epsilon y, \epsilon)$ and we expand $v = v_0 + \epsilon v_1 + \epsilon^2 v_2 + \ldots$. Substituting this expansion into (5.1 a) and (5.1 c), and collecting powers of ϵ, we obtain

$$\Delta_y v_j = 0, \quad y \notin D_1; \quad \partial_\nu v_j + \kappa v_j = 0, \quad y \in \partial D_1, \tag{5.2}$$

for $j = 0, 1$. Here Δ_y and ∂_ν denote derivatives with respect to y and D_1 is the domain D_ϵ in the y variable. By expanding the outer solution as we approach x_0, the far field behaviour as $y \to \infty$ for (5.2), expressed in summation notation, is

$$v_0(y) \sim u_0(x_0) \quad \text{as} \quad y \to \infty, \quad v_1(y) \sim y_i \partial_{x_i} u_0(x_0) \quad \text{as} \quad y \to \infty. \tag{5.3}$$

In three dimensions the solution to (5.2), with far field behaviour (5.3), has the asymptotic form

$$v_0(y) = u_0(x_0)\left[1 - \frac{C}{|y|} + \frac{C_i y_i}{|y|^3} + \ldots\right] \quad \text{as} \quad y \to \infty, \tag{5.4a}$$

$$v_1(y) = \partial_{x_i} u_0(x_0)\left[y_i + \frac{P_i}{|y|} + \frac{P_{ij} y_j}{|y|^3} + \ldots\right] \quad \text{as} \quad y \to \infty. \tag{5.4b}$$

Here C, C_i, P_i, P_{ij} are constants which depend on both κ and the domain D_1. When $\kappa = \infty$, then C is the capacitance of D_1. Now writing the far field expansion of $v = v_0 + \epsilon v_1 + \ldots$ in the x variable we have

$$v \sim u_0(x_0) + \partial_{x_i} u_0(x_0)\,(x_i - x_{0i}) - \frac{C u_0(x_0)\,\epsilon}{|x - x_0|} + \epsilon^2\left(\frac{\partial_{x_i} u_0(x_0)\, P_i}{|x - x_0|} + \frac{u_0(x_0)\, C_i (x_i - x_{0i})}{|x - x_0|^3}\right). \tag{5.5}$$

Then matching (5.5) to the outer solution, whose form is given in (2.2), we require

$$u_1 \sim -C u_0(x_0)/|x - x_0| \quad \text{as} \quad x \to x_0, \tag{5.6a}$$

$$u_2 \sim \frac{\partial_{x_i} u_0(x_0)\, P_i}{|x - x_0|} + \frac{u_0(x_0)\, C_i (x_i - x_{0i})}{|x - x_0|^3} \quad \text{as} \quad x \to x_0. \tag{5.6b}$$

To determine u_1 and u_2 we now must solve (2.3) and (2.4) (with $h = 0$) subject to the required singular behaviour (5.6 a, b).

With the effective boundary condition for u_1 and u_2 given in (5.6 a, b) we now derive solvability conditions for (2.3) and (2.4), applicable at $\alpha = \alpha_0$, to obtain expressions for the coefficients in the asymptotic expansion of λ_c given in (2.5). To incorporate the required singular behaviour of u_1 and u_2 as $x \to x_0$ it is convenient to write (2.3 a) and (2.4 a), in terms of the Dirac delta function $\delta(x - x_0)$ as

$$\Delta u_1 + \lambda_0 F^0_u u_1 = -\lambda_1 F^0 + 4\pi C u_0(x_0)\,\delta(x - x_0), \tag{5.7a}$$

$$\begin{aligned}\Delta u_2 + \lambda_0 F^0_u u_2 = {} & -\lambda_2 F^0 - \lambda_1 u_1 F^0_u - \tfrac{1}{2}\lambda_0 u_1^2 F^0_{uu} \\ & + 4\pi(u_0(x_0)\, C_i \partial_{x_i}\delta(x - x_0) - \partial_{x_i} u_0(x_0)\, P_i\, \delta(x - x_0)).\end{aligned} \tag{5.7b}$$

Furthermore, by differentiating (5.7 a) with respect to α we obtain

$$\Delta u_{1\alpha} + \lambda_0 F^0_u u_{1\alpha} = -\lambda_0' F^0_u u_{0\alpha} - \lambda_0 F^0_{uu} u_1 u_{0\alpha} - \lambda_1' F^0 - \lambda_1 F^0_u u_{0\alpha} + 4\pi C u_{0\alpha}(x_0)\,\delta(x - x_0). \tag{5.7c}$$

We now simply quote the results for $\lambda_1(\alpha_0)$, $\lambda_2(\alpha_0)$ and $\lambda_1'(\alpha_0)$ obtained from applying a solvability condition to each of (5.7*a–c*). The solvability conditions provide

$$\lambda_1(\alpha_0)\,(u_{0\alpha}, F^0) = 4\pi C u_0(x_0)\,u_{0\alpha}(x_0), \tag{5.8a}$$

$$\lambda_1'(\alpha_0)\,(u_{0\alpha}, F^0) = -\lambda_0(u_{0\alpha}, F^0_{uu}\,u_{0\alpha}\,u_1) - \lambda_1(u_{0\alpha}, F^0_u\,u_{0\alpha}) + 4\pi C(u_{0\alpha}(x_0))^2, \tag{5.8b}$$

$$\lambda_2(\alpha_0)\,(u_{0\alpha}, F^0) = -\lambda_1(u_{0\alpha}, u_1 F^0_u) - \tfrac{1}{2}\lambda_0(u_{0\alpha}, u_1^2 F^0_{uu}) - 4\pi(u_0(x_0)\,C_i\,\partial_{x_i} u_{0\alpha}(x_0) + \partial_{x_i} u_0(x_0)\,P_i\,u_{0\alpha}(x_0)), \tag{5.8c}$$

where all quantities appearing above are to be evaluated at $\alpha = \alpha_0$. Thus using (5.8*a–c*) and (2.12) in (2.5) we have a two term expansion for $\lambda_c(\epsilon)$ for this class of domain perturbation.

A spherical reactor

We now apply the theory presented above to determine the effect on λ_c of a small cooling pellet located at the centre of a spherical reactor of radius one. Defining $r = |x|$ then the extended system obtained from (1.1) and (2.6) satisfies (3.8) where the operator L is now defined by $Lv = r^{-2}(r^2 v_r)_r$. We then solve (3.8) numerically, by the method described following (3.8), to locate the first fold point $(\lambda_0(\alpha_0), \alpha_0)$, and thus determine both $u_0(r, \alpha_0)$ and $u_{0\alpha}(r, \alpha_0)$.

With u_0 and $u_{0\alpha}$ known at criticality, we now determine $u_1 = u_1(r)$ from (5.7*a*) with $u_1' + bu_1 = 0$ on $r = 1$. Noting from (3.8*d*) that $u_0(0) = \alpha_0$, the problem for u_1, at $\alpha = \alpha_0$, is

$$\left.\begin{aligned} Lu_1 + \lambda_0 F^0_u\,u_1 &= -\lambda_1 F^0, \quad \text{in} \quad r < 1, \\ u_1'(1) + bu_1(1) &= 0, \quad u_1 \sim -C\alpha_0/r + o(1) \quad \text{as} \quad r \to 0. \end{aligned}\right\} \tag{5.9}$$

Here, $\lambda_1(\alpha_0)$ is found from (5.8*a*) and (3.8*d*)

$$\lambda_1(\alpha_0) = C\alpha_0/\langle u_{0\alpha}, F^0\rangle. \tag{5.10}$$

The angle brackets appearing in (5.10) are defined by $\langle u, v\rangle = \int_0^1 uvr^2\,\mathrm{d}r$.

To facilitate the numerical solution of (5.9) with $\lambda_1(\alpha_0)$ given in (5.10), we define $v_1(r) = ru_1(r)$. Then from (5.9), v_1 satisfies

$$\left.\begin{aligned} v_1'' + \lambda_0 F^0_u\,v_1 &= -\lambda_1 rF^0, \quad \text{in} \quad r < 1, \\ v_1'(1) + (b-1)\,v_1(1) &= 0, \quad v_1(0) = -\alpha_0 C, \quad v_1'(0) = 0. \end{aligned}\right\} \tag{5.11}$$

The condition $v_1'(0) = 0$ ensures that the solution to (5.11) is unique at $\alpha = \alpha_0$ and that $u_1 \sim -\alpha_0 C/r + O(r)$ as $r \to 0$.

With $u_1 = v_1/r$ known from the numerical solution to (5.11) at criticality, we now compute $\lambda_1'(\alpha_0)$ and $\lambda_2(\alpha_0)$ from (5.8*b*) and (5.8*c*). By using (3.8*d*) these expressions become,

$$\lambda_1'(\alpha_0)\langle u_{0\alpha}, F^0\rangle = -\lambda_0\langle u_{0\alpha}, F^0_{uu}\,u_{0\alpha}\,u_1\rangle - \lambda_1\langle u_{0\alpha}, F^0_u\,u_{0\alpha}\rangle + C, \tag{5.12a}$$

$$\lambda_2(\alpha_0)\langle u_{0\alpha}, F^0\rangle = -\lambda_1\langle u_{0\alpha}, u_1 F^0_u\rangle - \tfrac{1}{2}\lambda_0\langle u_{0\alpha}, u_1^2 F^0_{uu}\rangle, \tag{5.12b}$$

at criticality. A numerical quadrature in (5.12*a*, *b*) is then used to determine $\lambda_1'(\alpha_0)$ and $\lambda_2(\alpha_0)$.

To display our results we write (2.5) as

$$\lambda_c = \lambda_0(\alpha_0) + \epsilon C\lambda_1(\alpha_0) + \epsilon^2 C^2 \hat{\lambda}_2(\alpha_0) + \ldots, \tag{5.13}$$

where $\hat{\lambda}_2(\alpha_0) \equiv \lambda_2(\alpha_0) - (\lambda_1'(\alpha_0))^2/2\lambda_0''(\alpha_0)$.

Here $\lambda_1(\alpha_0)$, $\lambda_1'(\alpha_0)$ and $\lambda_2(\alpha_0)$ are found from (5.10), (5.12*a*) and (5.12*b*) respectively,

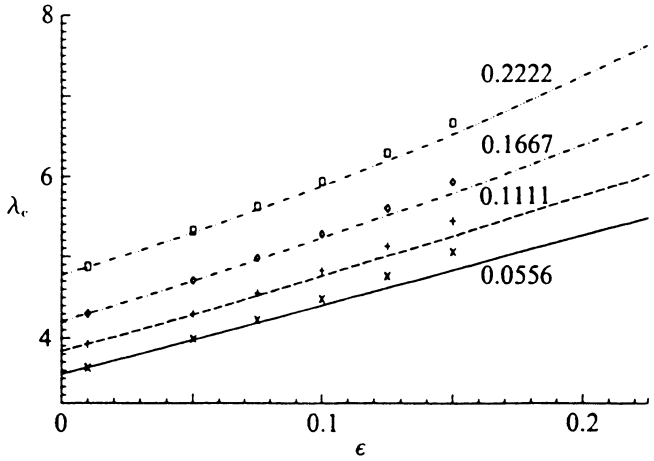

Figure 4. Hole in three dimensions: $\lambda_c(\epsilon)$ against ϵ for different β (values as indicated). $b = \infty$, $\kappa = \infty$.

Table 9. *Coefficients in the expansion of* $\lambda_c(\epsilon)$ *from* (5.13) *for a pellet located at the centre of a spherical reactor with* $b = \infty$

β	$\lambda_0(\alpha_0)$	$\lambda_0''(\alpha_0)$	$\lambda_1(\alpha_0)$	$\lambda_2(\alpha_0)$
0	3.3220	−1.0979	8.0787	−2.0749
0.0278	3.4313	−0.9363	8.2564	−0.7710
0.0556	3.5519	−0.7830	8.4492	0.6252
0.0833	3.6860	−0.6382	8.6595	2.1338
0.1111	3.8370	−0.5025	8.8908	3.7828
0.1389	4.0097	−0.3763	9.1475	5.6154
0.1667	4.2117	−0.2599	9.4355	7.7034
0.1944	4.4563	−0.1545	9.7618	10.190
0.2222	4.7733	−0.0603	10.124	13.505

upon setting $C = 1$ and $\lambda_0''(\alpha_0)$ is found from (2.12). Numerical values for these quantities for different activation energies, β, but with $C = 1$ and $b = \infty$ are given in table 9.

In the case where $\kappa = \infty$, so that $u = 0$ on ∂D_ϵ, then C is the capacitance of the stretched domain D_1. If in addition D_ϵ is a sphere of radius ϵ, then $C = 1$. In this special case, and with $b = \infty$, Ward & Van de Velde (1991) computed the numerical solution to the perturbed problem given in (5.1) and located the first fold point for various ϵ and β. This computation was done by solving a stiff boundary-value problem for ordinary differential equations. The also compared their numerical results with the asymptotic expansion of λ_c through terms of order ϵ.

By using the coefficients in table 9, in figure 4 we plot the two term expansion for $\lambda_c(\epsilon)$ given in (5.13) for different β. In this figure we also show the results obtained from the numerical solution to the full problem (5.1) for different ϵ and β. The solid lines in this figure are the asymptotic results and the labelled points are the numerical results of Ward & Van de Velde (1991). The agreement between the two term asymptotic expansion and the numerical results is seen to be rather good for $\epsilon \leqslant 0.15$.

The two-dimensional case

We now derive expressions for the coefficients in the asymptotic expansion of λ_c in the two-dimensional case. The analysis is similar to that used in the three-dimensional case except that here the expansion of λ_c and the outer solution proceed

in powers of $-1/\ln\epsilon$ rather than powers of ϵ. Thus in (2.2) we replace ϵ by $-1/\ln\epsilon$ and we again derive (2.3) and (2.4) for the temperature corrections, u_1 and u_2 in the outer region. The expansion of the fold point, λ_c, is again given in (2.5) upon replacing ϵ by $-1/\ln\epsilon$.

We now construct the inner expansion near the cooling rod. In the inner region we let $y=\epsilon^{-1}(x-x_0)$ and we expand $v=(-1/\ln\epsilon)[v_0(y)+\epsilon^2 v_1(y)+\ldots]$, so that $v_0(y)$ satisfies (5.2). A solution to (5.2), which matches to the unperturbed solution, u_0, has the asymptotic form

$$v_0(y)\sim u_0(x_0)[\ln|y|+d(\kappa)] \quad \text{as} \quad y\to\infty. \tag{5.14}$$

Here, $d(\kappa)$ is related to the logarithmic capacitance of D_1. Matching (5.14) to the outer solution, we require

$$u_1\sim u_0(x_0)[\ln|x-x_0|+d(\kappa)] \quad \text{as} \quad x\to x_0, \tag{5.15}$$

and that $u_2\to 0$ as $x\to x_0$.

With the effective boundary conditions for u_1 and u_2 given above, we now invoke solvability conditions on (2.3) and (2.4), which are applicable at $\alpha=\alpha_0$. These conditions will provide expressions for $\lambda_1(\alpha_0)$ and $\lambda_2(\alpha_0)$. In addition, $\lambda_1'(\alpha_0)$ is determined by differentiating (2.3) and (5.15) with respect to α and then invoking a solvability condition on the resulting equation. Omitting the details of the calculation we find

$$\lambda_1(\alpha_0)(u_{0\alpha},F^0)=2\pi u_0(x_0)\,u_{0\alpha}(x_0), \tag{5.16a}$$

$$\lambda_2(\alpha_0)(u_{0\alpha},F^0)=-\lambda_1(u_{0\alpha},u_1F^0_u)-\tfrac{1}{2}\lambda_0(u_{0\alpha},u_1^2F^0_{uu}), \tag{5.16b}$$

$$\lambda_1'(\alpha_0)(u_{0\alpha},F^0)=-\lambda_1(u_{0\alpha},F^0_u\,u_{0\alpha})-\lambda_0(u_{0\alpha},F^0_{uu}\,u_{0\alpha}\,u_1)+2\pi(u_{0\alpha}(x_0))^2, \tag{5.16c}$$

at criticality. From (5.16*a*) we note that $\lambda_1(\alpha_0)$ is independent of $d(\kappa)$. However, since u_1 depends on $d(\kappa)$ then so do both $\lambda_2(\alpha_0)$ and $\lambda_1'(\alpha_0)$.

A circular cylindrical reactor

We now determine a two term expansion for λ_c, corresponding to the first fold point, when a small cooling rod is placed at the centre of a circular cylindrical reactor of radius one. Defining $r=|x|$, the extended system obtained from (1.1) and (2.6) satisfies (3.8) where the operator, L, is given by $Lv=r^{-1}(rv_r)_r$. By using the numerical procedure described following (3.8) we can locate the first fold point $(\lambda_0(\alpha_0),\alpha_0)$ and determine both $u_0(r)$ and $u_{0\alpha}(r)$. Then, in terms of $u_1(r)$, (5.16) can be written as

$$\lambda_1(\alpha_0)\langle u_{0\alpha},F^0\rangle=\alpha_0, \tag{5.17a}$$

$$\lambda_2(\alpha_0)\langle u_{0\alpha},F^0\rangle=-\lambda_1\langle u_{0\alpha},u_1F^0_u\rangle-\tfrac{1}{2}\lambda_0\langle u_{0\alpha},u_1^2F^0_{uu}\rangle, \tag{5.17b}$$

$$\lambda_1'(\alpha_0)\langle u_{0\alpha},F^0\rangle=-\lambda_1\langle u_{0\alpha},F^0_u\,u_{0\alpha}\rangle-\lambda_0\langle u_{0\alpha},F^0_{uu}\,u_{0\alpha}\,u_1\rangle+1. \tag{5.17c}$$

Here, the angle brackets are defined by $\langle u,v\rangle=\int_0^1 uvr\,dr$.

To determine $u_1(r)$ at criticality we must solve (2.3) (with $h=0$), at $\alpha=\alpha_0$, subject to the singular behaviour (5.15) as $r\to 0$. To clearly exhibit the dependence of λ_c on $d(\kappa)$, it is convenient to decompose u_1 by

$$u_1=\alpha_0\ln r+d(\kappa)\,\alpha_0\,u_{0\alpha}(r)+w_1(r). \tag{5.18}$$

Then from (2.3) and (5.15) the bounded function w_1 satisfies

$$\left.\begin{aligned} Lw_1+\lambda_0F^0_u\,w_1&=-\lambda_1F^0-\lambda_0\alpha_0F^0_u\ln r, \quad 0<r<1,\\ w_1(0)&=0, \quad w_1'(1)+bw_1(1)=-\alpha_0. \end{aligned}\right\} \tag{5.19}$$

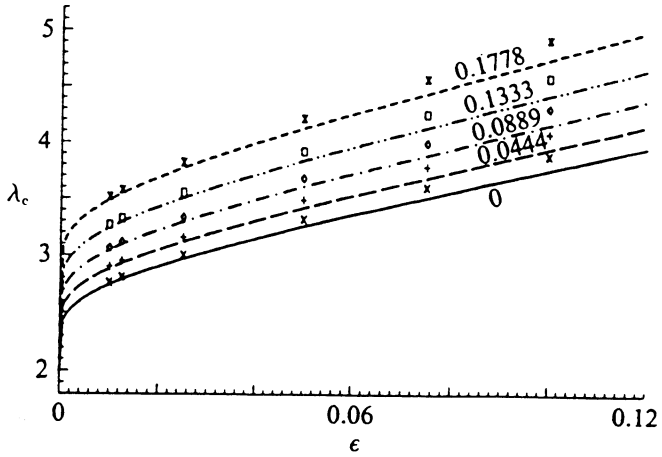

Figure 5. Hole in two dimensions: $\lambda_c(\epsilon)$ against ϵ for different β (values as indicated). $b = \infty$, $\kappa = \infty$.

Table 10. *Coefficients in the expansion of* $\lambda_c(\epsilon)$ *from* (5.21) *for a cooling rod located at the centre of a circular cylindrical reactor with* $b = \infty$

β	$\lambda_0(\alpha_0)$	$\lambda_1(\alpha_0)$	a_0
0	2.0000	2.7726	2.9610
.0222	2.0502	2.8334	3.0335
0.0444	2.1044	2.8986	3.1113
0.0889	2.2270	3.0451	3.2856
0.1111	2.2973	3.1283	3.3844
0.1333	2.3753	3.2198	3.4931
0.1778	2.5634	3.4366	3.7503
0.2000	2.6814	3.5689	3.9076

With w_1 known from the numerical solution of (5.19) at $\alpha = \alpha_0$, we now determine the form of the two-term expansion for λ_c. By using (5.18) in (5.17*b*) and (5.17*c*) and upon recalling (2.12) it can be shown that

$$\lambda_2(\alpha_0) - (\lambda_1'(\alpha_0))^2/2\lambda_0''(\alpha_0) = a_0 - \lambda_1(\alpha_0)\, d(\kappa). \tag{5.20}$$

Here, a_0 depends on w_1 and the unperturbed solution but is independent of $d(\kappa)$. The explicit formula for a_0 is lengthy and so we omit writing it. Thus using (5.20) and (5.17*a*) in (2.5), a two term expansion for λ_c is given by

$$\lambda_c = \lambda_0(\alpha_0) + (-1/\ln\epsilon)\,\lambda_1(\alpha_0) + (-1/\ln\epsilon)^2\,[a_0 - \lambda_1(\alpha_0)\, d(\kappa)] + \ldots, \tag{5.21}$$

where $\lambda_1(\alpha_0)$ is written in (5.17*a*). Numerical values for these quantities for different activation energies and with $b = \infty$ are given in table 10.

In the special case when $\beta = 0$, Ward & Keller (1991) found $u_1(r)$ analytically and thus obtained a two-term expansion for λ_c without recourse to numerical methods. The numerical values for the coefficients obtained there agree with those shown in the first row of table 10.

In the special case when $\kappa = \infty$ and D_ϵ is a circle of radius ϵ centred at the origin, then $d(\infty) = 0$. For this geometry, we can compare the two term asymptotic result for λ_c with the corresponding numerical results obtained from the numerical solution to the full problem (5.1). The procedure used to determine $\lambda_c(\epsilon)$ from the full problem (5.1) is described in Ward & Van de Velde (1991). The asymptotic and numerical

results, assuming $b = \infty$, are compared in figure 5 where good agreement is obtained for $\epsilon \leqslant 0.10$. In this figure the solid lines are the asymptotic results and the labelled points are the numerical results. We remark that the one term expansion for λ_c agrees rather poorly unless ϵ is very small.

6. Transitional values for the activation energy

In this section we again take $F(u) = \exp(u/(1+\beta u))$ and we describe a simple procedure to determine the transitional value, $\beta_{tr}(b)$, of the activation energy parameter for a slab, circular cylindrical or spherical domain (the class A geometries). As mentioned in §3, this transitional value is characterized by the fact that for $\beta > \beta_{tr}(b)$ the solutions to (1.1) are unique. In terms of the maximum temperature $\alpha = u(0)$, the transitional value β_{tr} is found from the conditions $\lambda_{0\alpha}(\alpha) = 0$ and $\lambda_{0\alpha\alpha}(\alpha) = 0$.

There have been many studies devoted to computing $\beta_{tr}(\infty)$ for the class A geometries. A detailed summary and comparison of some previous work, as well as an extensive list of references, is given in Boddington *et al.* (1983). In addition, the dependence of β_{tr} on the Biot number has been determined in Fenaughty *et al.* (1982) and Boddington *et al.* (1983) for the class A geometries. In most of these studies the procedure used to determine β_{tr} has been based on the numerical solution of a time dependent system of partial differential equations originally formulated by Kordylewski (1979) (see Kordylewski 1979; Boddington *et al.* 1983 for details). A notable exception is the work of Gustafson & Eaton (1982) who determined β_{tr} by a shooting method.

We now give a simple procedure, which uses readily available software, to determine β_{tr} for class A geometries. In contrast to Kordylewski (1979) and Boddington *et al.* (1983), our procedure is based on the numerical solution of a system of boundary-value problems. Thus our method is much less computer intensive and can also be used to generate highly accurate results. For illustration purposes we consider only the case $b = \infty$.

We begin by writing, on $0 < r < 1$, the augmented system formed from (1.1), (2.6) and (2.11) in m dimensions:

$$\left.\begin{aligned} Lu_0 + \lambda_0 F(u_0) &= 0, \\ Lu_{0\alpha} + \lambda_0 F_u(u_0)\, u_{0\alpha} &= -\lambda_{0\alpha} F(u_0), \\ Lu_{0\alpha\alpha} + \lambda_0 F_u(u_0)\, u_{0\alpha\alpha} &= -\lambda_0 F^0_{uu}(u_{0\alpha})^2 - 2\lambda_{0\alpha} F^0_u\, u_{0\alpha} - \lambda_{0\alpha\alpha} F^0. \end{aligned}\right\} \tag{6.1}$$

Here, Lu is defined by $Lu = r^{1-m}(r^{m-1}u')'$ and the primes denote derivatives with respect to r. The boundary conditions for (6.1) are taken to be

$$\left.\begin{aligned} &u_0(1) = 0, \quad u_{0\alpha}(1) = 0, \quad u_{0\alpha\alpha}(1) = 0, \quad u_0(0) = \alpha, \\ &u_{0\alpha}(0) = 1, \quad u_{0\alpha\alpha}(0) = 0, \quad u_0'(0) = u_{0\alpha}'(0) = u_{0\alpha\alpha}'(0) = 0. \end{aligned}\right\} \tag{6.2}$$

The numerical solution of this system is accomplished using the readily available collocation package COLSYS developed by Ascher *et al.* (1979). To fit (6.1) and (6.2) into the format of the package we must write the trivial additional equations $\lambda_0' = 0$, $\lambda_{0\alpha}' = 0$, and $\lambda_{0\alpha\alpha}' = 0$. Then (6.1) can be written as a first-order system of nine equations with the nine boundary conditions (6.2). Since the system is parametrized by α, rather than λ_0, no sophisticated continuation procedure to compute past fold points is necessary.

Table 11. *Transitional values of β, $\alpha = u(0)$, and λ_0 for the slab, circular cylinder and sphere*

m	α_0	$\lambda_0(\alpha_0)$	$\beta_{tr}(\infty)$
1	4.896548	1.307374	0.2457804
2	5.943243	3.006301	0.2421062
3	7.184944	5.041112	0.2387971

To determine the transitional value of β we solve (6.1) and (6.2) subject to the side conditions $\lambda_{0\alpha}(\alpha_0) = 0$ and $\lambda_{0\alpha\alpha}(\alpha_0) = 0$. A Newton iteration scheme, using a numerically computed jacobian, is then used to determine α_0 and β_{tr}. The results of the computations are shown in table 11 for the slab, circular cylindrical and spherical geometries. The tolerances in COLSYS and in our Newton iteration scheme were adjusted to ensure that the results for the transitional parameters are correct to the number of significant digits shown. These results agree with those of Gustafson & Eaton (1982) for all the Class A geometries. However, our results tend to disagree in the fourth decimal place with the computations of Boddington *et al.* (1983) who used the time-dependent formulation of Kordylewski (1979). Similar computations, using this method, can be done for the case of finite Biot number or for other nonlinear heating terms $F(u)$.

7. Discussion

We conclude by giving some possible directions for additional work in this area. The analysis presented here to treat the three classes of perturbations is not restricted to the Arrhenius heat generation term. Similar computations can be done to determine the change in λ_c under these classes of perturbations when the reaction is modelled by the 'bimolecular' law $F(u) = (1+\beta u)^{\frac{1}{2}}\exp(u/(1+\beta u))$.

A more significant extension would be to treat the three classes of perturbations considered here for more general domains. In this case the extended system obtained from (1.1) and (2.6) forms a coupled system of partial differential equations and a continuation scheme in λ_0 would then be needed. In addition, the theory presented here can probably be modified to determine the changes in the transitional value of β under various classes of perturbations and for different nonlinear heating terms. Finally, it should also be possible to determine the corrections to the fold points for systems of nonlinear elliptic equations under various classes of perturbations. In the combustion context, such a system arises when modelling chemical reactors while allowing for the effect of reactant consumption.

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