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Wavespeed analysis: Approximating Arrhenius kinetics with step-function kinetics

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Wavespeed analysis: Approximating Arrhenius kinetics with step-function kinetics

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The accuracy of using step-function approximations to the Arrhenius exponential in computing the wavespeed in combustion wave propagation is investigated. Gaseous and gasless combustion, and first- and second-order reactions are included in the study. The theoretical analysis is based on Melnikov theory from dynamical systems. The error is shown to be small in most instances. The analytical results are supported with numerical simulations.

Keywords: Arrhenius; combustion waves; Melnikov theory; step-function approximation; wavespeed

1. Introduction

Typical approaches to solving combustion wave as well as many other combustion problems are based on the fact that non-dimensional activation energies of combustion reactions are large, resulting in reaction zones that are thin compared to the preheat regions. In some works these ideas are implemented by using systematic asymptotic expansions. In other works they take the form of combustion front approximations and delta-function kinetics. There is another, related, approach to solving combustion problems that we find quite useful. It involves the use of step-functions in the reaction rate terms. This approach has a long and glorious history, beginning with works by Le Chatelier and many others who introduced the ignition temperature as a physical characteristic of the combustible material in 'pre-Arrhenius' times, and who were correctly criticized by subsequent researchers (see, e.g., [1, 2] for a more detailed discussion). By no means are we trying to revive the old theories. We do not introduce ignition temperature as a material parameter. Our use of step-functions is due to the understanding that the Arrhenius exponential and an *appropriately chosen* step-function may be close to one another in the sense of distributions and, therefore, may yield close results. We remark that in some earlier work [3, 4] step-functions were used in combustion problems to replace the entire reaction term, i.e., both the Arrhenius exponential and the kinetics function. This is different from our approach, in which only the Arrhenius temperature dependence of the reaction rate is replaced by a step-function [5–7]. (Other recent work where the accuracy of the step-function approximation is assessed by comparing analytical results with numerical solutions is [8].) The step-function is chosen

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in such a way that its maximum value is the same as that of the Arrhenius function and the integral values of the two over the entire temperature interval where the process occurs are also equal.

The step-function approach has been successfully used in both combustion and frontal polymerization problems yielding accurate and reliable results. However, there are no systematic studies that attempt to obtain analytical estimates of the accuracy of such approximations. We present such a study in this paper. The analytical tool we use is Melnikov theory [9], which has only recently been applied to combustion problems in [10], but not in the context of step-function approximations. Melnikov theory relates to determining the distance between perturbed stable and unstable manifolds in dynamical systems, and as shown in [10] can therefore be used as a criterion for the persistence of a wavefront solution to certain types of partial differential equations. We use Melnikov theory to get the error of the approximation in terms of an integral that involves the difference of the exact and approximate reaction rates, as it should be if the proximity between the two is to be understood in the distributional sense. We are thereby able to obtain theoretical wavespeed estimates for both step-function and Arrhenius reaction rates, and moreover compare these results with numerically obtained ones. We apply these methods to both gaseous and gasless combustion, and also investigate both first-order and higher-order reactions.

2. Governing equations

We consider a one-dimensional pre-mixed adiabatic combustion model, expressed non-dimensionally by

$$\left.\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2} + y^n e^{-1/u} \\ \frac{\partial y}{\partial t} &= \frac{1}{\mathrm{Le}}\frac{\partial^2 y}{\partial x^2} - \beta y^n e^{-1/u}. \end{aligned}\right\} \tag{2.1}$$

Here $u(x, t)$ is the temperature at a location x at time t, $y(x, t)$ is the concentration of the deficient reactant, β is the exothermicity parameter, Le is the Lewis number, and n is the order of the reaction. In this non-dimensionalization, the temperature u is scaled by the activation temperature E/R, where E is the activation energy and R is the universal gas constant. The parameter β is the ratio of the activation temperature E/R to the adiabatic temperature increase $T_a - T_0$, in which T_a and T_0 are the adiabatic and initial temperatures respectively.

In contrast to (2.1), consider the problem

$$\left.\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2} + y^n k(u) \\ \frac{\partial y}{\partial t} &= \frac{1}{\mathrm{Le}}\frac{\partial^2 y}{\partial x^2} - \beta y^n k(u), \end{aligned}\right\} \tag{2.2}$$

where $k(u)$ is a step-function given by

$$k(u) := e^{-\beta} H(u - u_0). \tag{2.3}$$

Here H is the Heaviside function, and u_0 is determined by setting the integral of $k(u)$ over the entire interval of temperature variation $(0, 1/\beta)$ (see below) to be the same as that for the non-dimensional Arrhenius function $\exp(-1/u)$. This results in

$$u_0 = \frac{1}{\beta} - e^{\beta} \int_0^{1/\beta} e^{-1/u} \mathrm{d}u = \frac{1}{\beta} - e^{\beta} \frac{1}{\beta} E_2(\beta) = e^{\beta} E_1(\beta), \tag{2.4}$$

where the function E_j is

$$E_j(z) := \int_1^{\infty} \frac{e^{-zt}}{t^j} \mathrm{d}t = z^{j-1} \int_z^{\infty} \frac{e^{-t}}{t^j} \mathrm{d}t$$

as defined in [11]. Equation (2.2) is meant to approximate the problem (2.1) with Arrhenius kinetics. In order to determine the error resulting from this approximation, consider the problem

$$\left.\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2} + y^n k(u) + \delta y^n [e^{-1/u} - k(u)] \\ \frac{\partial y}{\partial t} &= \frac{1}{\mathrm{Le}} \frac{\partial^2 y}{\partial x^2} - \beta y^n k(u) - \delta \beta y^n [e^{-1/u} - k(u)]. \end{aligned}\right\} \tag{2.5}$$

While (2.5) with $\delta = 1$ corresponds exactly to Arrhenius kinetics, the intention is to analyse (2.5) initially as a perturbation of (2.2), using a small δ approximation.

We are interested in uniformly propagating combustion waves which transform the initial state, with the reactant concentration $y = 1$ and the temperature $u = 0$, into the final burnt state, where the reactant is completely consumed, $y = 0$, and the temperature is increased to the burnt temperature. In particular, the focus shall be on determining the correction to the wavespeed resulting from the fact that the step-function kinetics in (2.2) is an approximation to the Arrhenius kinetics as expressed in (2.5). We will do this for several cases: (i) Le $= \infty, n = 1$; (ii) Le $= \infty, n = 2$; (iii) Le $= 1, n = 1$; (iv) Le $= 1, n = 2$, although our techniques generalize to any n.

3. Infinite Lewis number first-order reactions: Step-function problem

As a first case, we examine the step-function problem for Le $= \infty$ and $n = 1$, given in (2.2) – equivalently, $\delta = 0$ in (2.5). We introduce the wave coordinate $\xi = x - c_0 t$, where c_0 (assumed positive) is the wavespeed of the travelling wave in this $\delta = 0$ situation. Under this ansatz, (2.2) is representable as a system of two ordinary differential equations

$$\left.\begin{aligned} -c_0 u'(\xi) &= u''(\xi) + e^{-\beta} y(\xi) H(u(\xi) - u_0) \\ -c_0 y'(\xi) &= -\beta e^{-\beta} y(\xi) H(u(\xi) - u_0). \end{aligned}\right\} \tag{3.1}$$

The system has the first integral

$$\beta u' + c_0 \beta u + c_0 y = c_0,$$

which is derived by multiplying the first equation in (3.1) by β and adding to the second, then integrating the resulting equation, and finally using the boundary conditions at the cold end in order to evaluate the constant of integration. This first integral allows us to determine the burnt temperature $\bar{u}$, i.e., the temperature as $\xi \to -\infty$ as $\bar{u} = 1/\beta$ and express the reactant concentration as

$$y = 1 - \beta u - \frac{\beta}{c_0} v, \tag{3.2}$$

where $v(\xi) = u'(\xi)$. This enables the system (3.1) to be written as a two-dimensional system

$$\left.\begin{aligned} u' &= v \\ v' &= -c_0 v - e^{-\beta}\left(1 - \beta u - \frac{\beta}{c_0} v\right) H(u - u_0), \end{aligned}\right\} \tag{3.3}$$

in which a solution which progresses from the fixed point $(u, v) = (1/\beta, 0)$ (the fully burnt state) to (0, 0) (fully unburnt) is sought. We partition the (u, v) phase space into two segments: $u < u_0$ and $u \geq u_0$ (see Figure 1). In the former segment, the equations collapse to

$$\left.\begin{aligned} u' &= v \\ v' &= -c_0 v, \end{aligned}\right\} \tag{3.4}$$

in which the solution that approaches the origin as $\xi \to \infty$ is $v = -c_0 u$.

In the second region ($u \geq u_0$), the equations are

$$\left.\begin{aligned} u' &= v \\ v' &= -c_0 v - e^{-\beta}\left(1 - \beta u - \frac{\beta}{c_0} v\right), \end{aligned}\right\} \tag{3.5}$$

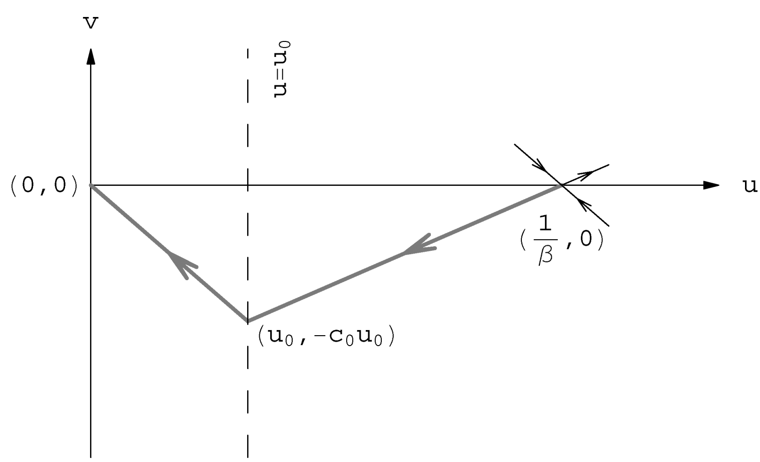

Figure 1. Heteroclinic connection in the (u, v) phase space representing a uniformly propagating wave: Le $= \infty$, $n = 1$ and $\delta = 0$.

and the solution that approaches the point $(1/\beta, 0)$ as $\xi \to -\infty$ is

$$v = \frac{\beta}{c_0} e^{-\beta} \left(u - \frac{1}{\beta} \right). \tag{3.6}$$

To achieve a continuous solution in the system (3.3), the solution (3.6) needs to connect up with the point $(u_0, -c_0 u_0)$. Imposing this condition, we get that

$$u_0 = \frac{1}{\beta + c_0^2 e^{\beta}}. \tag{3.7}$$

Combining this with (2.4) and eliminating u_0, we get the wavespeed formula

$$c_0 = e^{-\beta/2} \sqrt{\frac{e^{-\beta}}{E_1(\beta)} - \beta}. \tag{3.8}$$

A numerically computed graph of the variation of the wavespeed is given in Figure 2. The wavespeed increases from zero at $\beta = 0$ to a maximum value, and decays to zero thereafter. The non-monotonic dependence of c_0 on β is due to the non-dimensionalization; the dimensional wavespeed is $c_0(\beta)\beta^{-1/2}$, which is monotonic in β.

Taylor expansions can be used to determine approximations to c_0 in the limit of large β. Doing so, we find

$$c_0 = e^{-\beta/2} \left[1 - \frac{1}{2\beta} + \frac{11}{8\beta^2} - \frac{93}{16\beta^3} + \mathcal{O}\left(\frac{1}{\beta^4} \right) \right], \tag{3.9}$$

which agrees, to the leading order, with the well-known results in the case of Arrhenius kinetics [1, 2].

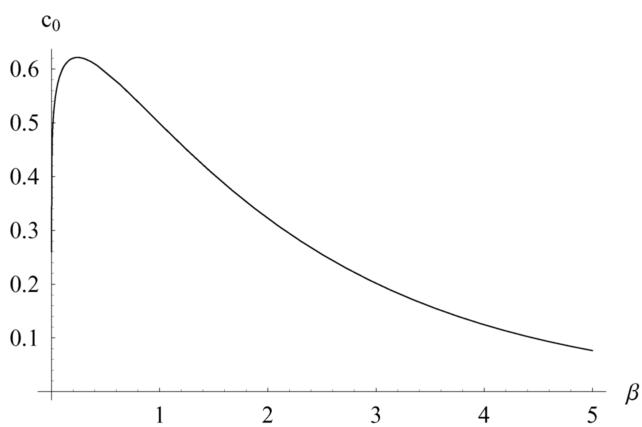

Figure 2. Wavespeed variation with β for step-function kinetics. Here $n = 1$ and Le $= \infty$.

The explicit form of $(u(\xi), v(\xi), y(\xi))$ can be determined by solving the linear systems (3.4) and (3.5), and matching them at $(u, v) = (u_0, -c_0 u_0)$. If this matching point is chosen to be $\xi = 0$, the temperature u can be written as

$$u(\xi) = \begin{cases} \dfrac{1}{\beta} - \dfrac{c_0^2 e^{\beta}}{\beta} u_0 \exp\left(\dfrac{\beta e^{-\beta}}{c_0}\xi\right) & \text{if } \xi \le 0 \\ u_0 \exp(-c_0 \xi) & \text{if } \xi > 0. \end{cases} \tag{3.10}$$

Its derivative is given by

$$v(\xi) = \begin{cases} -c_0 u_0 \exp\left(\dfrac{\beta e^{-\beta}}{c_0}\xi\right) & \text{if } \xi \le 0 \\ -c_0 u_0 \exp(-c_0 \xi) & \text{if } \xi > 0. \end{cases} \tag{3.11}$$

The fuel concentration (computed from the conservation law (3.2) in conjunction with the above solutions) is expressible by

$$y(\xi) = \begin{cases} \exp\left(\dfrac{\beta e^{-\beta}}{c_0}\xi\right) & \text{if } \xi \le 0 \\ 1 & \text{if } \xi > 0. \end{cases} \tag{3.12}$$

Figure 3 shows the temperature and fuel concentration with $\beta = 2$. In the laboratory coordinate system the wave moves to the right at a speed given by (3.8) with $\beta = 2$.

4. Infinite Lewis number first-order reactions: Wavespeed correction

In this section, the correction (due to the step-function approximation) in the wavespeed is computed. The dynamics are governed now by (2.5) with $n = 1$ rather than (2.2), and the resulting correction to the wavespeed under the condition of sufficiently small δ is obtained.

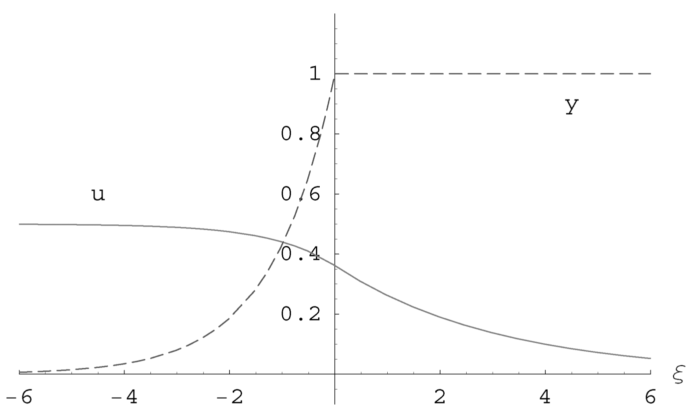

Figure 3. Wavefront at $\beta = 2$ for $n = 1$ and Le $= \infty$: temperature (solid) and fuel (dashed). The front moves to the right at a constant speed $c_0 = 0.32$.

Beginning with (2.5) with Le $=\infty$ and $n=1$, and using the ansatz $\xi = x - ct$, where c is the (positive) wavespeed, we obtain the two ordinary differential equations

$$\left.\begin{aligned} -cu'(\xi) &= u''(\xi) + y(\xi)k(u(\xi)) + \delta[e^{-1/u(\xi)} - k(u(\xi))] \\ -cy'(\xi) &= -\beta y(\xi)k(u(\xi)) - \delta\beta y(\xi)[e^{-1/u(\xi)} - k(u(\xi))]. \end{aligned}\right\} \tag{4.1}$$

Once again, the conservation law (3.2) holds (with c replacing c_0), enabling a reduction to two dimensions:

$$\left.\begin{aligned} u' &= v \\ v' &= -cv - \left(1 - \frac{\beta}{c}v - \beta u\right)k(u) - \delta\left(1 - \frac{\beta}{c}v - \beta u\right)[e^{-1/u} - k(u)]. \end{aligned}\right\} \tag{4.2}$$

We expand the wavespeed in δ in the form

$$c(\beta,\delta) = c_0(\beta) + \delta c_1(\beta) + \mathcal{O}\left(\delta^2\right); \tag{4.3}$$

the goal is to determine the leading-order correction term c_1 to the wavespeed c_0 which is shown in (3.8). Substituting in (4.2) and retaining only terms up to $\mathcal{O}(\delta)$, we obtain

$$\left.\begin{aligned} u' &= v \\ v' &= -c_0 v - \left(1 - \frac{\beta}{c_0}v - \beta u\right)k(u) \\ &\quad + \delta\left[-c_1 v\left(1 + \frac{\beta k(u)}{c_0^2}\right) - (e^{-1/u} - k(u))\left(1 - \frac{\beta}{c_0}v - \beta u\right)\right]. \end{aligned}\right\} \tag{4.4}$$

For a wavefront solution to exist, we need the system (4.4) to possess a persistent heteroclinic connection between $(1/\beta, 0)$ and $(0, 0)$ for small δ. We note that the connection exists for $\delta = 0$ (indeed, that is the system analysed in Section 3), with wavespeed given by c_0. In order to examine such a persistent heteroclinic connection, we briefly outline the Melnikov method from dynamical systems, which as shown in [10] can be used within this context (references to the more standard Melnikov approach are [9, 12, 13]; the results in [10] require some modifications of these). Consider a two-dimensional system

$$\mathbf{z}' = \mathbf{f}(\mathbf{z}) + \delta\mathbf{g}(\mathbf{z}). \tag{4.5}$$

When $\delta = 0$, suppose this system possesses a heteroclinic connection between the two saddle fixed points. (A heteroclinic connection of this sort occurs when a branch of the one-dimensional unstable manifold of one fixed point coincides with a branch of the stable manifold of the other – this certainly occurs in our system (4.4) when $\delta = 0$.) This heteroclinic trajectory can be represented as a solution $\mathbf{z} = \hat{\mathbf{z}}(\xi)$ to (4.5) with $\delta = 0$, as given in equations (3.10) and (3.11) in our case.

Now, for small $\delta > 0$ in (4.5), the fixed points retain their stable and unstable manifolds [14]. However, these need no longer coincide. Let $d(\xi, \delta)$ be the distance between these manifolds, measured along a perpendicular to the unperturbed heteroclinic drawn at $\hat{\mathbf{z}}(-\xi)$. This distance is

Taylor expandable in δ in the form

$$d(\xi, \delta) = \delta \frac{M(\xi)}{|\mathbf{f}(\hat{\mathbf{z}}(-\xi))|} + \mathcal{O}(\delta^2). \tag{4.6}$$

The quantity $M(\xi)$ is the 'Melnikov function', for which an expression is

$$M(\xi) = \int_{-\infty}^{\infty} \exp\left[-\int_{-\xi}^{r} \nabla \cdot \mathbf{f}(\hat{\mathbf{z}}(s))\mathrm{d}s\right] \mathbf{f}(\hat{\mathbf{z}}(r)) \wedge \mathbf{g}(\hat{\mathbf{z}}(r))\mathrm{d}r, \tag{4.7}$$

where the wedge product between two vectors is defined by $(a_1, a_2)^T \wedge (b_1, b_2)^T = a_1 b_2 - a_2 b_1$. Please see [10] for a detailed derivation.

The key point is that for a heteroclinic connection to persist for small δ, it is necessary that the Melnikov function (which essentially contains the leading-order information regarding the distance) be *identically* zero. That is, $M(\xi)$ should be zero for any value of ξ chosen in (4.7), and in fact any value (say, 0) that is convenient can be chosen.

By identifying the functions $\mathbf{f}$ and $\mathbf{g}$ through a comparison of Equations (4.5) and (4.4), we find that

$$\nabla \cdot \mathbf{f} = \frac{\beta k(u)}{c_0} - c_0 \tag{4.8}$$

and

$$\begin{aligned} \mathbf{f} \wedge \mathbf{g} &= v\left[-c_1 v\left(1 + \frac{\beta k(u)}{c_0^2}\right) - (e^{-1/u} - k(u))\left(1 - \frac{\beta}{c_0}v - \beta u\right)\right] \\ &= v\left[-c_1 v\left(1 + \frac{\beta k(u)}{c_0^2}\right) - y(e^{-1/u} - k(u))\right] \end{aligned} \tag{4.9}$$

by using the conservation law (3.2) for notational convenience. By substituting these values into (4.7), choosing $\xi = 0$, setting the Melnikov function equal to zero, and rearranging, we obtain

$$c_1 = \frac{\displaystyle\int_{-\infty}^{\infty} \exp\left[-\int_0^r \left(\frac{\beta k(u(s))}{c_0} - c_0\right)\mathrm{d}s\right] v(r) y(r) \left[k(u(r)) - e^{-1/u(r)}\right]\mathrm{d}r}{\displaystyle\int_{-\infty}^{\infty} \exp\left[-\int_0^r \left(\frac{\beta k(u(s))}{c_0} - c_0\right)\mathrm{d}s\right] [v(r)]^2 \left[1 + \frac{\beta k(u(r))}{c_0^2}\right]\mathrm{d}r}, \tag{4.10}$$

where each of u, v and y are the $\delta = 0$ values, expressed in Equations (3.10), (3.11) and (3.12) respectively. Using these formulas, and also the simplification afforded through the step-function nature of $k(u)$ as given in (2.3), we obtain

$$c_1 = \frac{1}{2u_0}(A + B), \tag{4.11}$$

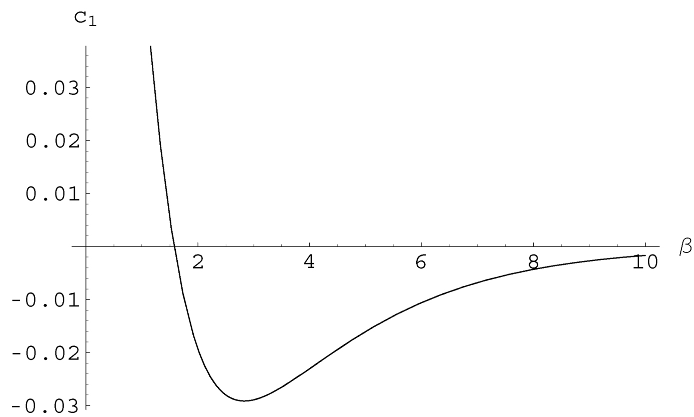

Figure 4. Leading-order wavespeed correction (c_1) with β for $n = 1$ and Le $= \infty$.

where

$$A := \int_{-\infty}^{0} \exp\left(\frac{r}{c_0 u_0 e^{\beta}}\right)\left[\exp\left(\frac{-\beta}{1 - \beta e^{\beta} u_0 c_0^2 \exp\left(\frac{\beta e^{-\beta} r}{c_0}\right)}\right) - e^{-\beta}\right] \mathrm{d}r$$

and

$$B := \int_{0}^{\infty} \exp\left(-\frac{e^{c_0 r}}{u_0}\right) \mathrm{d}r.$$

In the above expressions, c_0 is given in (3.8). The derivation of (4.11) from (4.10) is shown in Appendix A.

While B in (4.11) is positive, A is negative since the quantity in the square brackets in its integrand is negative for $r < 0$. Therefore, c_1 may be either positive or negative, depending on the combined effects of A and B. Since A is an integral over the region $r < 0$, which is behind the front, the effect of Arrhenius kinetics behind the front tries to slow it down, while its effect ahead of the front (encoded in B) tries to make its speed up. Intuitively, one would expect the front to broaden because of this process. The combination of these effects makes the front settle into a new speed, which may be either greater or less than the unperturbed (step-function kinetics) front. Figure 4 displays the numerically computed wavespeed correction, using (4.11). For small values of β, the wavespeed increases when including Arrhenius kinetics, but for larger values, the wavespeed decreases. The transition of c_1 from positive to negative occurs around $\beta = 1.6$. Moreover, as β increases, the value of $|c_1|$ appears to decrease to zero, an indication that the step-function approximation to Arrhenius kinetics is better for very large β.

Since the scale of c_1 for small β is somewhat larger than that for intermediate β values as shown in Figure 4, this small β variation is shown separately in Figure 5. Since c_1 is of the order of 0.25, this is an indication that the step-function approximation for the kinetics is unreasonable for small β (for such β, it is only for very small δ that the Taylor expansion of c would be legitimate, whereas one needs δ approaching unity to better model Arrhenius kinetics).

Our main intention is to use a perturbative method to assess the correction to the step-function solution that is needed when approaching Arrhenius kinetics ((2.5) with $\delta = 1$). The

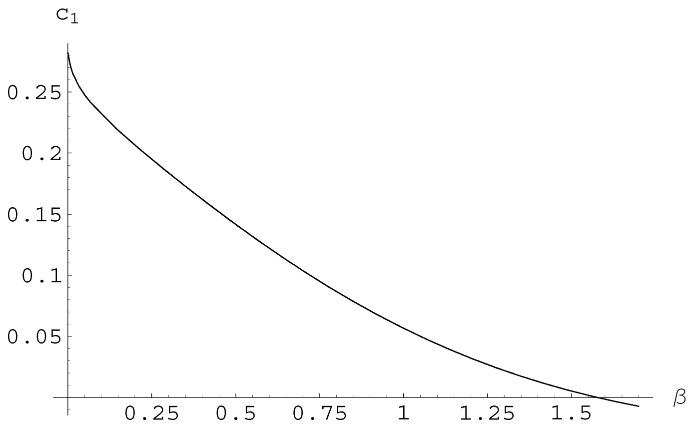

Figure 5. Leading-order wavespeed correction (c_1) with β for small β values, with $n = 1$ and Le $= \infty$.

hope is that the perturbative approach which uses $0 < \delta \ll 1$ would nevertheless provide a good approximation even when $\delta = 1$. While this may sound optimistic, a similar idea was seen to work remarkably well in [10]; a perturbative Melnikov approach for large Lewis number was seen to predict accurate wavespeeds even for Le $= 3$. With this in mind, we can think of using (4.3) for the wavespeed of (2.5) with $\delta = 1$, while neglecting $\mathcal{O}\left(\delta^2\right)$ terms. In other words, the approximation for the Arrhenius kinetics situation based on this perturbative approach would be $c_0 + 1c_1$. We show this (Arrhenius approximation) wavespeed in Figure 6 as the solid curve. The dashed curve is the wavespeed using only step-function kinetics (c_0). As we have remarked previously, using step-function kinetics to approximate Arrhenius kinetics is less accurate for small β, i.e., for smaller activation energies, but becomes better for large β, i.e., for larger activation energies. Moreover, the step-function approximation underestimates the wavespeed for small β, while it slightly overestimates the wavespeed at large β values.

5. Infinite Lewis number second-order reactions: Step function kinetics

Consider now the situation where the reaction term is second-order in the fuel concentration; that is, $n = 2$ in (2.2). Equation (3.1) then receives the simple modification of y^2 replacing y.

The conservation law (3.2) continues to hold in this situation, and we can once again reduce our emphasis to the (u, v) phase-plane. In the region $u < u_0$, the dynamics continue to be described by Equation (3.4), for which we have determined the solution in Section 3. The left part of the diagram in Figure 1 therefore continues to be valid, with the stable manifold of the origin connecting to $(u_0, -c_0 u_0)$. We need the unstable manifold emanating from $(1/\beta, 0)$ to connect up with this, but we now have a nonlinear equation

$$\left.\begin{aligned} u' &= v \\ v' &= -c_0 v - e^{-\beta}\left(1 - \beta u - \frac{\beta}{c_0} v\right)^2 . \end{aligned}\right\} \tag{5.1}$$

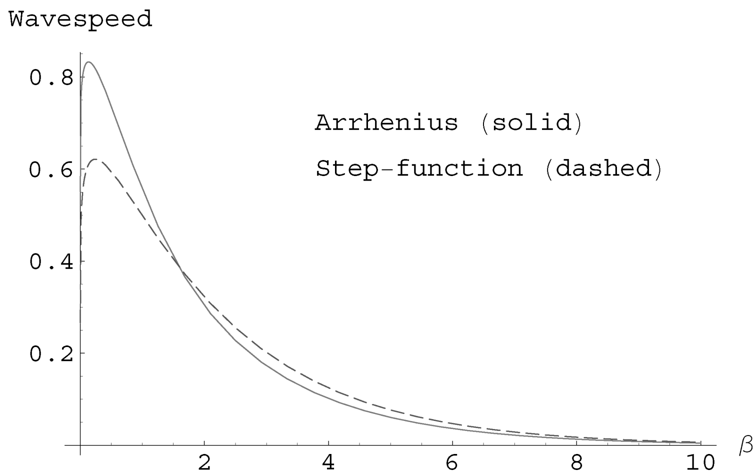

Figure 6. Wavespeed at $\delta = 1$ for $n = 1$ and Le $= \infty$, and retaining only the leading-order term in (4.3). The solid curve is this wavespeed which approximates Arrhenius kinetics ($c_0 + c_1$), while the dashed curve is that obtained from step-function kinetics (c_0).

Considering the second equation in (3.1) for $u \geq u_0$ (again, with y replaced by y^2 on the right-hand side), and imposing the condition $y(0^-) = 1$, we obtain the solution

$$y(\xi) = \frac{1}{1 - \frac{\beta e^{-\beta\xi}}{c_0}} =: y_-(\xi), \quad \xi \leq 0, \tag{5.2}$$

where the above serves to define the function $y_-(\xi)$. The corresponding u solution, subject to the condition $u(-\infty) = 1/\beta$, can be determined by using the conservation law (3.2) with the above substituted for y, replacing $v(\xi)$ with $u'(\xi)$, to get the first-order differential equation

$$u'(\xi) + c_0 u(\xi) = \frac{c_0}{\beta}\left[1 - y_-(\xi)\right].$$

Solving, we get

$$u(\xi) = \frac{c_0}{\beta} e^{-c_0\xi} \int_{-\infty}^{\xi} e^{c_0 s}\left[1 - y_-(s)\right] \mathrm{d}s. \tag{5.3}$$

This solution no longer corresponds to a straight line (as pictured in Figure 1) emanating from $(1/\beta, 0)$, but rather a curve. We picture this change in Figure 7, in which we have chosen $\beta = 0.5$. In general, the curve from the right must connect to the stable manifold of $(0, 0)$, so we need the condition $u(0) = u_0$ which yields

$$u_0 = e^{-\beta} \int_{-\infty}^{0} \frac{-s e^{c_0 s}}{1 - \frac{\beta e^{-\beta}}{c_0} s} \mathrm{d}s = \frac{1}{\beta} \int_0^{\infty} \frac{t e^{-t}}{w^2 + t} \mathrm{d}t,$$

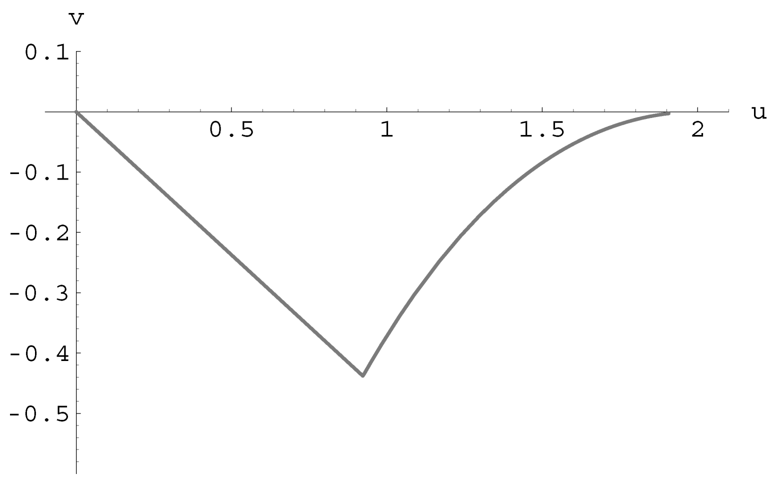

Figure 7. Heteroclinic connection in the (u, v) phase space representing a wavefront: Le $= \infty$, $n = 2$, $\delta = 0$ and $\beta = 0.5$.

where w is the scaled velocity defined by

$$w^2 := \frac{c_0^2}{\beta e^{-\beta}}. \tag{5.4}$$

Substituting $\tau = w^2 + t$ in the integral,

$$u_0\beta = 1 - w^2 e^{w^2} \int_{w^2}^{\infty} \frac{e^{-\tau}}{\tau} \mathrm{d}\tau = 1 - w^2 e^{w^2} E_1\left(w^2\right).$$

We define the invertible function

$$F(a) := a e^a E_1(a), \tag{5.5}$$

which is a monotonic function increasing from 0 at $a = 0$ and approaching 1 as a approaches ∞, for which asymptotic expressions (which will be useful later) are

$$F(a) \sim 1 - \frac{1}{a} + \frac{2}{a^2} \quad \text{for } a \gg 1 \quad \text{and} \quad F(a) \sim -a \ln a \quad \text{for } 0 < a \ll 1. \tag{5.6}$$

Using the function F, our condition is expressible as

$$F(\beta) + F(w^2) = 1, \tag{5.7}$$

and hence the wavespeed c_0 must satisfy

$$c_0 = e^{-\beta/2}\sqrt{\beta F^{-1}[1 - F(\beta)]}, \tag{5.8}$$

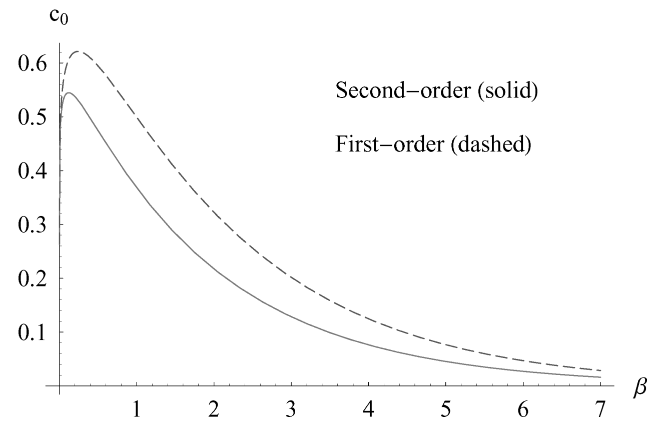

Figure 8. Wavespeed variation with β for step-function kinetics with Le $=\infty$, for second-order (solid) and first-order (dashed) reactions.

for which an easier expression is not available. A numerically computed graph of c_0 for this second-order reaction appears in Figure 8, in which a comparison to that of first-order kinetics (dashed curve) is also presented.

In the asymptotic limit $\beta \gg 1$, the condition (5.7) is approximated by $F(w^2) = 1/\beta$ (using the large a asymptotics in (5.6)). Since this means that w^2 must be small, using the small a limit in (5.6) leads to $-w^2 \ln w^2 = 1/\beta$, which gives us the asymptotic formula

$$c_0 \approx e^{-\beta/2}\sqrt{\frac{1}{\ln\beta}} \tag{5.9}$$

in the large β limit. Its comparison with the exact formula (5.8) is shown in Figure 9.

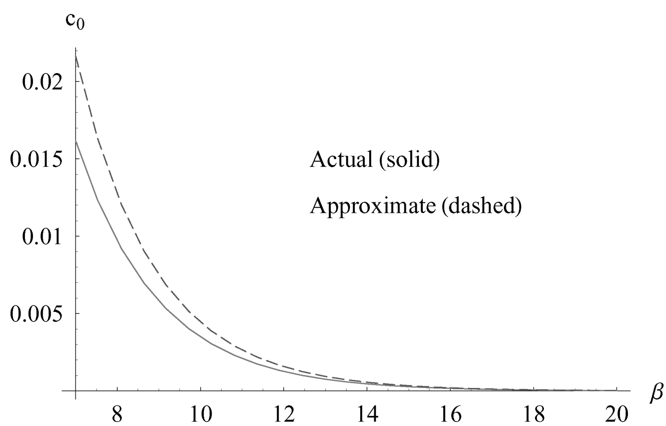

Figure 9. Comparison of actual wavespeed (5.8) with the large β approximation (5.9) for second-order reactions with Le $=\infty$.

As in Section 3, it is possible to write down the solution as a function of the spatial variable. First, the y solution is

$$y(\xi) = \begin{cases} y_-(\xi) & \text{if } \xi \leq 0 \\ 1 & \text{if } \xi > 0. \end{cases} \tag{5.10}$$

where the function y_- is defined in (5.2). The temperature satisfies

$$u(\xi) = \begin{cases} \frac{1}{\beta}\left[1 - w^2 \exp\left(\frac{w^2}{y_-(\xi)}\right) E_1\left(\frac{w^2}{y_-(\xi)}\right)\right] & \text{if } \xi \leq 0 \\ u_0 \exp\left(-c_0 \xi\right) & \text{if } \xi > 0, \end{cases} \tag{5.11}$$

as shown in Appendix 9. The v solution is most easily expressed by using the conservation law (3.2):

$$v(\xi) = \begin{cases} \dfrac{c_0}{\beta} - c_0 u_-(\xi) - \dfrac{c_0}{\beta} y_-(\xi) & \text{if } \xi \leq 0 \\ -c_0 u_0 \exp\left(-c_0 \xi\right) & \text{if } \xi > 0, \end{cases} \tag{5.12}$$

with u_- representing the u solution for $\xi < 0$. As before, solutions have been set up such that $\xi = 0$ corresponds to the matching point between the regions $u < u_0$ and $u \geq u_0$.

6. Infinite Lewis number second-order reactions: Wavespeed correction

The procedure followed in Section 4 for first-order reactions can be used to determine the wavespeed correction for second-order reactions as well. The equation corresponding to (4.2) is

$$\left.\begin{aligned} u' &= v \\ v' &= -cv - \left(1 - \frac{\beta}{c} v - \beta u\right)^2 k(u) - \delta\left(1 - \tfrac{\beta}{c} v - \beta u\right)^2 \left[e^{-1/u} - k(u)\right]. \end{aligned}\right\}$$

Expanding the wavespeed as in (4.3), and retaining only $\mathcal{O}(\delta)$ terms, we arrive at

$$\left.\begin{aligned} u' &= v \\ v' &= -c_0 v - \left(1 - \frac{\beta}{c_0} v - \beta u\right)^2 k(u) \\ &\quad + \delta\left[-c_1 v\left(1 + \frac{2\beta k(u)}{c_0^2}\left(1 - \frac{\beta}{c_0} v - \beta u\right)\right) - \left(e^{-1/u} - k(u)\right)\left(1 - \frac{\beta}{c_0} v - \beta u\right)^2\right]. \end{aligned}\right\} \tag{6.1}$$

This is in the form of (4.5) with

$$\mathbf{f} := \left(v, -c_0 v - y^2 k(u)\right)$$

and

$$\mathbf{g} := \left(0, -c_1 v\left[1 + \frac{2\beta}{c_0^2} y k(u)\right] - y^2\left(e^{-1/u} - k(u)\right)\right)$$

with $y = 1 - \frac{\beta}{c_0} v - \beta u$. Then,

$$\nabla \cdot \mathbf{f} = -c_0 + \frac{2\beta}{c_0} y k(u)$$

and

$$\mathbf{f} \wedge \mathbf{g} = v \left[-c_1 v \left(1 + \frac{2\beta}{c_0^2} y k(u) \right) - y^2 \left(e^{-1/u} - k(u) \right) \right].$$

Substituting these expressions into the Melnikov formula (4.7), taking $\xi = 0$, setting $M = 0$ and solving for c_1, we get

$$c_1 = \frac{\displaystyle\int_{-\infty}^{\infty} \exp\left[- \int_0^r \left(\frac{2\beta y(s) k\left(u(s)\right)}{c_0} - c_0 \right) \mathrm{d}s \right] v(r) \left(y(r)\right)^2 \left[k\left(u(r)\right) - e^{-1/u(r)} \right] \mathrm{d}r}{\displaystyle\int_{-\infty}^{\infty} \exp\left[- \int_0^r \left(\frac{2\beta y(s) k\left(u(s)\right)}{c_0} - c_0 \right) \mathrm{d}s \right] [v(r)]^2 \left[1 + \frac{2\beta y(r) k\left(u(r)\right)}{c_0^2} \right] \mathrm{d}r}. \tag{6.2}$$

We show in Appendix C that this is expressible as

$$c_1 = \frac{G + u_0 E_1 \left(1/u_0\right)}{\frac{c_0}{\beta^2} \left[\left(4 + \frac{2}{w^2}\right) F\left(w^2\right) - 3 - \left[F(w^2)\right]^2 \right] + u_0^2 c_0}, \tag{6.3}$$

where w and F are defined in (5.4) and (5.5), and

$$G = e^{w^2} \frac{c_0^2}{\beta^2} \int_0^1 e^{-w^2/y} \frac{1}{y} \left[F\left(w^2/y\right) - 1 \right] \left[1 - \exp \frac{-\beta F\left(w^2/y\right)}{1 - y F\left(w^2/y\right)} \right] \mathrm{d}y.$$

We use the quantity $c_0 + c_1$ as our theoretical approximation for the wavespeed in the case of Arrhenius kinetics. The relative error of the wavespeed obtained from this theoretical process (in comparison with the wavespeed obtained from a direct numerical simulation of the governing PDE (2.5) with $\delta = 1$ and $n = 2$) is given in Figure 10. The agreement is very good, with the error diminishing to 1% for the larger β values pictured.

7. Unit Lewis number first-order reactions

So far, we have considered only Le $= \infty$, i.e., the gasless combustion problem, in which the mass diffusion can be neglected in comparison to that of heat. We now focus on gaseous combustion, in which the diffusivities are comparable, and we take Le $= 1$. As an initial step, we will examine the first-order reaction ($n = 1$). The travelling wave solution problem has the form

$$u''(\xi) + c_0 u'(\xi) + y(\xi) e^{-\beta} H\left(u(\xi) - u_0\right) = 0,$$
$$y''(\xi) + c_0 y'(\xi) - \beta y(\xi) e^{-\beta} H\left(u(\xi) - u_0\right) = 0.$$

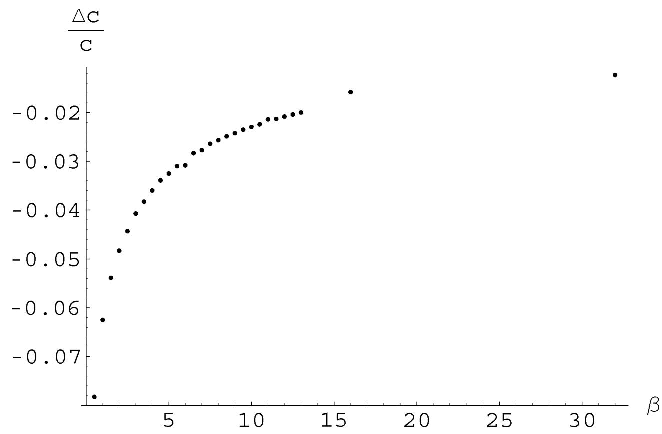

Figure 10. Relative error in using $c_0 + c_1$ to estimate the wavespeed for Arrhenius kinetics with second-order reaction and infinite Lewis number.

While this is a four-dimensional system, a reduction is possible by adding β times the first equation to the second and integrating, resulting in

$$(y + \beta u)' + c_0 (y + \beta u) = \text{constant}.$$

Since $u = 0$ and $y = 1$ at $\xi = \infty$, the constant is c_0. As before, the limiting value of u as $\xi \to -\infty$, where $y = 0$, is $1/\beta$. Solving the first-order differential equation, we obtain the conservation law

$$y(\xi) = 1 - \beta u(\xi). \tag{7.1}$$

Thus, the dynamics can be represented purely with the u differential equation. Letting $v(\xi) = u'(\xi)$ as in previous sections, we obtain

$$\left.\begin{aligned} u' &= v \\ v' &= -c_0 v - e^{-\beta} (1 - \beta u) H (u - u_0) . \end{aligned}\right\} \tag{7.2}$$

For $u < u_0$, the solution is exactly as in Section 4, and consists of a straight line connecting $(u_0, -c_0 u_0)$ (at $\xi = 0$) to $(0, 0)$ (at $\xi = \infty$). The equations in $u \geq u_0$ are also linear, and have the solution

$$u(\xi) = \begin{cases} \dfrac{1}{\beta} - \left(\dfrac{1}{\beta} - u_0\right) \exp(\mu\xi) & \text{if } \xi \leq 0 \\ u_0 \exp(-c_0 \xi) & \text{if } \xi > 0. \end{cases} \tag{7.3}$$

where

$$\mu = \frac{1}{2}\left[-c_0 + \sqrt{c_0^2 + 4\beta e^{-\beta}}\right].$$

Since this solution must reach $(u_0, -c_0 u_0)$ as $\xi \to 0^-$,

$$-u_0 c_0 = -\left(\frac{1}{\beta} - u_0\right)\mu = -\frac{1}{\beta}\left(1 - F(\beta)\right)\mu,$$

by using (2.4) and the definition of F given in (5.5). Substituting for μ and simplifying,

$$c_0 = e^{-\beta/2}\left[1 - F(\beta)\right]\sqrt{\frac{\beta}{F(\beta)}}. \tag{7.4}$$

In the limit of large β, Taylor expansions tell us that

$$c_0 = e^{-\beta/2}\sqrt{\frac{1}{\beta}}\left[1 - \frac{3}{2\beta} + \frac{35}{8\beta^2} + \frac{287}{16\beta^3} + \frac{11907}{128\beta^4} + \mathcal{O}\left(\frac{1}{\beta^5}\right)\right]. \tag{7.5}$$

The (exact) expression for c_0 permits us to write

$$\mu = e^{-\beta/2}\sqrt{\beta F(\beta)}. \tag{7.6}$$

We note that for large β, $(c_0/\mu) \sim (1/\beta) \ll 1$, and therefore for $\xi < 0$ (i.e., in the reaction zone), $|c_0 u'| \ll |u''|$. Thus, for large β, the term $c_0 v$ can be neglected in (7.2) in the region $\xi < 0$; this is further analysed in Section 8.

Now we consider the problem of determining the wavespeed correction in the presence of non-zero δ. Following the approach of Section 4, our equations in this instance are

$$\left.\begin{aligned} u' &= v \\ v' &= -cv - (1 - \beta u)\,k(u) - \delta\,(1 - \beta u)\left[e^{-1/u} - k(u)\right]. \end{aligned}\right\}$$

Expanding the wavespeed in δ as in (4.3), we obtain

$$\left.\begin{aligned} u' &= v \\ v' &= -c_0 v - (1 - \beta u)\,e^{-\beta} H(u - u_0) \\ &\qquad + \delta\left[-c_1 v + (1 - \beta u)\left(e^{-\beta} H(u - u_0) - e^{-1/u}\right)\right]. \end{aligned}\right\} \tag{7.7}$$

This is once again in the form (4.5), with

$$\nabla \cdot \mathbf{f} = -c_0$$

and

$$\mathbf{f} \wedge \mathbf{g} = v\left[-c_1 v + y\left(e^{-\beta} H(u - u_0) - e^{-1/u}\right)\right]$$

where we have used y for convenience based on (7.1). Once again, computing the Melnikov function from (4.7) and setting it equal to zero, we obtain

$$c_1 = \frac{\int_{-\infty}^{\infty} e^{c_0 r} v(r) y(r) \left[k\left(u(r)\right) - e^{-1/u(r)}\right] \mathrm{d}r}{\int_{-\infty}^{\infty} e^{c_0 r} \left[v(r)\right]^2 \mathrm{d}r}. \tag{7.8}$$

In Appendix D we show that

$$c_1 = \frac{\beta^2 (1+F)}{2 c_0 F^2} \left[N_- + N_+\right], \tag{7.9}$$

where

$$N_- = \frac{e^{-\beta}}{\beta} \left[-\frac{F(1-F)^2}{1+F} + \left(\frac{1}{1-F}\right)^{\frac{1-F}{F}} \int_0^{1-F} s^{1/F} \exp\left(-\beta \frac{s}{1-s}\right) \mathrm{d}s \right],$$
$$N_+ = \beta u_0^2 e^{-1/u_0} \left[\frac{\beta+1}{\beta} F\left(1/u_0\right) - 1 \right]$$

and F when presented with no argument means $F(\beta)$.

We can now compare the theoretical approximation we get from this process with a direct numerical simulation of the PDEs, and show this in Figure 11. Within the range $0.5 \leq \beta \leq 50$ in which we performed computations, the quantity $c_0 + c_1$ is at worst 7% off from the wavespeed obtained using a direct numerical simulation.

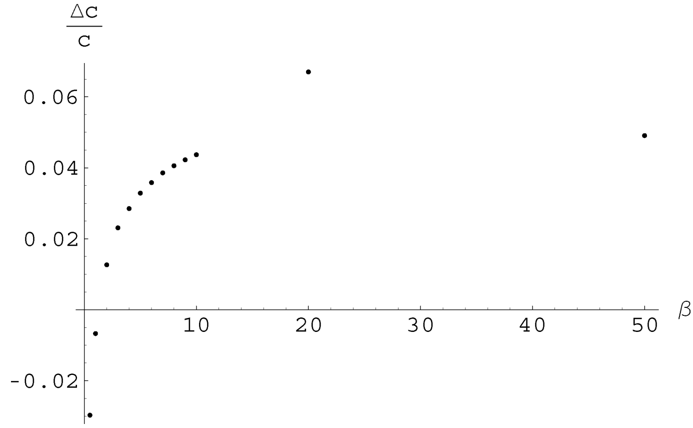

Figure 11. Relative error in using $c_0 + c_1$ to estimate the wavespeed for Arrhenius kinetics with first-order reaction and unit Lewis number.

In the large β limit, the behaviour of c_1/c_0 turns out to approach a constant. This is since

$$\frac{c_1}{c_0} = \frac{-\frac{F(1-F)^2}{1+F} + \left(\frac{1}{1-F}\right)^{\frac{1-F}{F}} \int_0^{1-F} s^{1/F} e^{-\beta s/(1-s)} \mathrm{d}s + e^{\beta(1-1/F)} F^2 \left[\frac{\beta+1}{\beta} F\left(\frac{\beta}{F}\right) - 1\right]}{\frac{2}{1+F}(1-F)^2}$$

(with $F = F(\beta)$, except for the one term with an explicit argument), and using the asymptotics (5.6), we obtain

$$\frac{c_1}{c_0} \sim \frac{-\frac{1}{2\beta^2} + \frac{1}{\beta^2}\int_0^1 t e^{-t} \mathrm{d}t + e^{-1}\frac{2}{\beta^2}}{\frac{1}{\beta^2}} = \frac{1}{2}.$$

Thus, for large β, the wavespeed has the structure

$$c = c_0 \left[1 + \frac{1}{2}\delta + \mathcal{O}(\delta^2)\right].$$

8. Unit Lewis number *n*th-order reactions

We will briefly outline the arguments associated with computing the wavespeed in this instance; our brevity is since the computations are very similar to those presented in detail in previous sections. When Le $= 1$, but for general reaction order $n > 1$, we have the $\delta = 0$ equations

$$u''(\xi) + c_0 u'(\xi) + (1 - \beta u(\xi))^n e^{-\beta} H(u(\xi) - u_0) = 0,$$

in which $u(-\infty) = 1/\beta$, $u(0) = u_0$ and $u(\infty) = 0$, exactly as in the previous section. While this is easily solvable in $\xi > 0$, the nonlinearities in $\xi \leq 0$ make this a difficult problem to continue. We therefore concentrate on the large β limit only, in this section. In this limit, we have remarked in Section 7 that the convective term (involving the first derivative of u) can be neglected. We can therefore write this modified equation as

$$u''(\xi) + c_0 u'(\xi) H(u_0 - u(\xi)) + (1 - \beta u(\xi))^n e^{-\beta} H(u(\xi) - u_0) = 0.$$

This has the solution

$$u(\xi) \approx \begin{cases} u_0 e^{-c_0 \xi} & \text{if } \xi > 0 \\ \dfrac{1}{\beta} - \dfrac{1}{\beta}\dfrac{1 - \beta u_0}{[1 - \xi K_n]^{2/(n-1)}} & \text{if } \xi \leq 0, \end{cases} \tag{8.1}$$

in which

$$K_n := \frac{n-1}{2}(1 - \beta u_0)^{\frac{n-1}{2}} \sqrt{\frac{2\beta e^{-\beta}}{n+1}}.$$

Imposing the condition that $v(0^-) = -c_0 u_0$, we get the wavespeed to be

$$c_0 \approx \frac{[1 - F(\beta)]^{\frac{n+1}{2}}}{F(\beta)} \sqrt{\frac{2\beta e^{-\beta}}{n+1}}, \tag{8.2}$$

which is only valid for large β. Taylor expansions (as before) show us that

$$c_0 = e^{-\beta/2} \left(\frac{1}{\beta}\right)^{n/2} \frac{1}{\sqrt{1+n}} \left[\sqrt{2} - \sqrt{2}n\left(\frac{1}{\beta}\right) + \frac{1+4n+n^2}{\sqrt{2}}\left(\frac{1}{\beta}\right)^2 + \mathcal{O}\left(\frac{1}{\beta^3}\right)\right], \tag{8.3}$$

for reaction orders $n > 1$.

We now turn our attention to $\delta \neq 0$, i.e., to the equation

$$\begin{aligned} u'' + cu'H(u_0 - u) + (1-\beta u)^n e^{-\beta} H(u - u_0) \\ -\delta cu' [H(u_0 - u) - 1] - \delta (1 - \beta u)^n \left[e^{-\beta} H(u - u_0) - e^{-1/u}\right] = 0. \end{aligned} \tag{8.4}$$

Expanding c as $c_0 + \delta c_1$, and following the standard process, we are able to derive that

$$c_1 = \frac{1}{u_0^2 c_0} [N_- + N_+], \tag{8.5}$$

in which

$$N_- = -\frac{e^{-\beta}(1 - F(\beta))^{n+1}}{(n+1)(n+3)\beta F(\beta)} [(n-1)F(\beta) + 4] + \int_{u_0}^{1/\beta} (1 - \beta u)^n e^{-1/u} \mathrm{d}u,$$

and

$$N_+ = u_0 \int_0^{u_0} \frac{(1-\beta u)^n}{u} e^{-1/u} \mathrm{d}u.$$

We refer the reader to Appendix E for these derivations.

Henceforth, we focus explicitly on the case $n = 2$. This is since when n is large, features of wide reaction zones become important, and therefore the errors in our calculations increase. For details on why increasing n reduces the accuracy, the reader is referred to [15]. Numerical calculations of the relative departure of $c_0 + c_1$ from the wavespeed obtained by direct numerical simulation are presented in Figure 12. While some data points differ from numerical simulations only by 4%, others differ by fully 39%. Our results in this Le $= 1$ and $n > 1$ situation are therefore significantly worse than for our previously examined cases. The necessity to perform an approximation (in which the convective term was discarded in the reaction zone) in order to obtain the $\delta = 0$ solution explicitly, may be to blame. If we do not do this approximation, we are able to derive an explicit expression for c_1 in terms of the $\delta = 0$ solution, but will not be able to obtain an *analytical* expression such as is given in (8.5). Consequently, a purely numerical evaluation of c_1 would itself be necessary, undermining our theoretical approach.

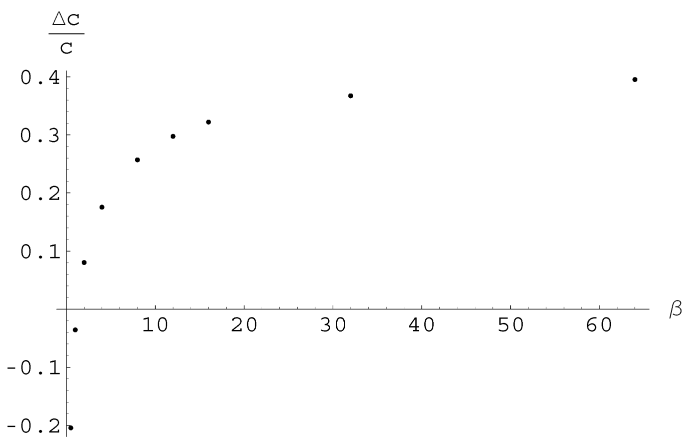

Figure 12. Relative error in using $c_0 + c_1$ to estimate the wavespeed for Arrhenius kinetics with second-order reaction and unit Lewis number.

9. Conclusions

In this paper we discuss how combustion problems can be solved approximately by replacing the Arrhenius temperature dependence of the reaction rate by an appropriately chosen step-function of the temperature. We illustrate our approach by considering both gasless and gaseous combustion, with reactions of various orders. We demonstrate that the accuracy of such approximations is quite satisfactory not only when the non-dimensional activation energy (which is related to the Zeldovich number) is large, but also when it is an order one quantity. This method is particularly useful, as an alternative to systematic asymptotic expansions, in complex problems that involve more than one reaction with high activation energies so that there are more than one large (or small) parameters in the problem. The asymptotic treatment then typically requires considering distinguished limits because uniform results are usually impossible to obtain. These distinguished limits, even when seeming physically relevant, do not give a complete picture of the process. Using step-function approximations may provide a more complete set of results. We remark that the step-function approach has been justified in stability studies [8].

Appendix

A Derivation of (4.11) from (4.10)

Since

$$k\left(u(s)\right) = e^{-\beta} H\left(u(s) - u_0\right),$$

and $u(\xi)$ has the monotonic structure as given in Figure 3 such that $u(0) = u_0$, we have

$$k\left(u(s)\right) = e^{-\beta}\left[1 - H(s)\right].$$

Consider now the interior integral appearing in both the numerator and the denominator of (4.10):

$$\exp\left[-\int_0^r \left(\frac{\beta k\left(u(s)\right)}{c_0} - c_0\right) \mathrm{d}s\right] = \exp\left[-\int_0^r \left(\frac{\beta e^{-\beta}\left(1 - H(s)\right)}{c_0} - c_0\right) \mathrm{d}s\right]$$

$$= \exp\left[\left(-\frac{\beta e^{-\beta}}{c_0}(1 - H(r)) + c_0\right) r\right],$$

since if $r > 0$, $1 - H(s) = 0$ in the domain $(0, r)$, whereas if $r < 0$, $1 - H(s) = 1$ in $(r, 0)$. Now, work on the denominator (D) of (4.10):

$$\begin{aligned}
D &= \int_{-\infty}^{\infty} \exp\left[\left(-\frac{\beta e^{-\beta}}{c_0}(1 - H(r)) + c_0\right) r\right] [v(r)]^2 \left[1 + \frac{\beta(1 - H(r))\, e^{-\beta}}{c_0^2}\right] \mathrm{d}r \\
&= \int_{-\infty}^{0} \exp\left[\left(c_0 - \frac{\beta e^{-\beta}}{c_0}\right) r\right] \left(\frac{-c_0}{\beta + c_0^2 e^{\beta}}\right)^2 \exp\left[\frac{2\beta e^{-\beta}}{c_0} r\right] \left(1 + \frac{\beta e^{-\beta}}{c_0^2}\right) \mathrm{d}r \\
&\quad + \int_{0}^{\infty} \exp\left[c_0 r\right] \left(\frac{-c_0}{\beta + c_0^2 e^{\beta}}\right)^2 \exp\left[-2c_0 r\right] \mathrm{d}r \\
&= \frac{2c_0}{\left(\beta + c_0^2 e^{\beta}\right)^2} = 2c_0 u_0^2.
\end{aligned}$$

In the above calculation, the expression for $v(r)$ from (3.11) was used, and ultimately the relationship between u_0 and c_0 as given in (3.7). We similarly split the numerator (N) of (4.10) into the domains $(-\infty, 0)$ and $(0, \infty)$ to obtain

$$\begin{aligned}
N &= \int_{-\infty}^{0} \exp\left[\left(c_0 - \frac{\beta e^{-\beta}}{c_0}\right) r\right] \left(\frac{-c_0}{\beta + c_0^2 e^{\beta}}\right) \exp\left[\frac{\beta e^{-\beta} r}{c_0}\right] \exp\left[\frac{\beta e^{-\beta} r}{c_0}\right] \left(e^{-\beta} - \exp\left[\frac{-1}{u(r)}\right]\right) \mathrm{d}r \\
&\quad + \int_{0}^{\infty} \exp\left[c_0 r\right] \left(\frac{-c_0}{\beta + c_0^2 e^{\beta}}\right) \exp\left[-c_0 r\right] (1) \left(-\exp\left[\frac{-1}{u(r)}\right]\right) \mathrm{d}r \\
&= \frac{-c_0}{\beta + c_0^2 e^{\beta}} \int_{-\infty}^{0} \exp\left[\frac{c_0^2 + \beta e^{-\beta}}{c_0} r\right] \left\{ e^{-\beta} - \exp\left[\frac{-\left(\beta + c_0^2 e^{\beta}\right)\beta}{\beta + c_0^2 e^{\beta} - \beta e^{\beta} c_0^2 \exp\left(\frac{\beta e^{-\beta} r}{c_0}\right)}\right]\right\} \mathrm{d}r \\
&\quad + \frac{c_0}{\beta + c_0^2 e^{\beta}} \int_{0}^{\infty} \exp\left[-\left(\beta + c_0^2 e^{\beta}\right) e^{c_0 r}\right] \mathrm{d}r \\
&= c_0 u_0 \int_{-\infty}^{0} \exp \frac{r}{u_0 c_0 e^{\beta}} \left\{ \exp\left[-\frac{\beta / u_0}{(1/u_0) - \beta e^{\beta} c_0^2 \exp\left(\frac{\beta e^{-\beta} r}{c_0}\right)}\right] - e^{-\beta} \right\} \mathrm{d}r \\
&\quad + c_0 u_0 \int_{0}^{\infty} \exp\left[-\frac{e^{c_0 r}}{u_0}\right] \mathrm{d}r \\
&= c_0 u_0 A + c_0 u_0 B
\end{aligned}$$

as defined in (4.11). Now, since $c_1 = N/D$, Equation (4.11) results.

B Derivation of (5.11)

Using Equation (5.3) for $\xi < 0$,

$$
\begin{aligned}
u(\xi) &= \frac{c_0}{\beta} e^{-c_0\xi} \left\{ \frac{e^{c_0 s}}{c_0}\Big|_{-\infty}^{\xi} - \int_{-\infty}^{\xi} \frac{e^{c_0 s}}{1 - \frac{\beta e^{-\beta}}{c_0} s} \mathrm{d}s \right\} \\
&= \frac{c_0}{\beta} e^{-c_0\xi} \left\{ \frac{e^{c_0\xi}}{c_0} - \int_{\infty}^{1/y_-(\xi)} \frac{\exp\left[\frac{(1-t)c_0^2}{\beta e^{-\beta}}\right]}{t} \left(-\frac{c_0}{\beta e^{-\beta}}\right) \mathrm{d}t \right\} \\
&= \frac{1}{\beta} + \frac{1}{\beta} w^2 e^{w^2} e^{-c_0\xi} \int_{\infty}^{1/y_-(\xi)} \frac{e^{-w^2 t}}{t} \mathrm{d}t \\
&= \frac{1}{\beta}\left[1 + w^2 \exp\left(w^2 - c_0\xi\right) \int_{\infty}^{w^2/y_-(\xi)} \frac{e^{-t}}{t} \mathrm{d}t \right] \\
&= \frac{1}{\beta}\left[1 - w^2 \exp \frac{w^2}{y_-(\xi)} E_1\left(\frac{w^2}{y_-(\xi)}\right)\right].
\end{aligned}
$$

C Derivation of (6.3) from (6.2)

Consider first the interior integral appearing in both the numerator and denominator of (6.2). If $r < 0$,

$$
\exp\left[-\int_0^r \left(\frac{2\beta}{c_0} y(s) k\left(u(s)\right) - c_0\right) \mathrm{d}s\right] = e^{c_0 r} \exp\left[-\frac{2\beta}{c_0 e^{\beta}} \int_0^r y(s)\mathrm{d}s\right].
$$

However,

$$
y' = \frac{\beta e^{-\beta}}{c_0} y^2
$$

and hence

$$
\frac{y'}{y} = \frac{\beta e^{-\beta}}{c_0} y.
$$

Integrating from 0 to r, and with the observation that $y(0) = 1$,

$$
\ln y(r) = \frac{\beta e^{-\beta}}{c_0} \int_0^r y(s)\mathrm{d}s.
$$

Thus, for $r < 0$,

$$
\exp\left[-\int_0^r \left(\frac{2\beta}{c_0} y(s) k\left(u(s)\right) - c_0\right) \mathrm{d}s\right] = e^{c_0 r} \exp\left[-2 \ln y(r)\right] = \frac{e^{c_0 r}}{[y(r)]^2}.
$$

When $r > 0$, on the other hand, $k(u) = 0$, and this quantity becomes simply $e^{c_0 r}$.

Consider now the numerator of (6.2). Split the integral into $(-\infty, 0)$ (call this G) and $(0, \infty)$ (call this H). Then

$$G = \int_{-\infty}^{0} e^{c_0 r} v(r) \left[e^{-\beta} - e^{-1/u} \right] \mathrm{d}r.$$

We will convert this to an integral over y with the help of the expressions (5.11) and (5.12), valid in the domain $\xi \le 0$. Thus, for $r \le 0$,

$$\begin{aligned} v(r) &= \frac{c_0}{\beta} \left[1 - \left(1 - w^2 \exp \frac{w^2}{y_-(r)} E_1 \left(\frac{w^2}{y_-(r)} \right) \right) - y_-(r) \right] \\ &= \frac{c_0}{\beta} y_-(r) \left[F \left(\frac{w^2}{y_-(r)} \right) - 1 \right], \end{aligned}$$

with the help of the definitions (5.4) and (5.5). Moreover, from (5.11),

$$e^{-1/u(r)} = \exp \frac{-\beta y_-(r) F \left(\frac{w^2}{y(r)} \right)}{1 - y_-(r) F \left(\frac{w^2}{y_-(r)} \right)}.$$

Applying now the change of variable $y = 1/(1 - c_0 r / w^2)$,

$$G = e^{w^2} \frac{c_0^2}{\beta^2} \int_0^1 e^{-w^2/y} \frac{1}{y} \left[F \left(\frac{w^2}{y} \right) - 1 \right] \left[1 - \exp \frac{-\beta F \left(w^2/y \right)}{1 - y F \left(w^2/y \right)} \right] \mathrm{d}y,$$

as required. The second integral, on $(0, \infty)$, becomes

$$\begin{aligned} H &= - \int_0^{\infty} e^{c_0 r} v(r) \left[y(r) \right]^2 e^{-1/u(r)} \mathrm{d}r \\ &= - \int_0^{\infty} \frac{u_0}{u(r)} u'(r) e^{-1/u(r)} \mathrm{d}r = \int_0^{u_0} \frac{u_0}{u} e^{-1/u} \mathrm{d}u \\ &= u_0 \int_1^{\infty} \frac{1}{t} e^{-t/u_0} \mathrm{d}t = u_0 E_1 \left(\frac{1}{u_0} \right), \end{aligned}$$

which completes the expression for the numerator in (6.3). Now, split the denominator also into the regions $(-\infty, 0)$ and $(0, \infty)$. The first of these, J_1, becomes

$$\begin{aligned} J_1 &= \int_{-\infty}^{0} e^{c_0 r} \left(\frac{v(r)}{y(r)} \right)^2 \left[1 + \frac{2 \beta e^{-\beta}}{c_0^2} y(r) \right] \mathrm{d}r \\ &= \int_{\infty}^{0} e^{c_0 r} \frac{c_0^2}{\beta^2} \left[F \left(\frac{w^2}{y} \right) - 1 \right]^2 \left[1 + \frac{2}{w^2} y(r) \right] \mathrm{d}r \\ &= \frac{c_0^2}{\beta^2} \frac{c_0}{\beta e^{-\beta}} \int_0^1 \exp \left[w^2 \left(1 - \frac{1}{y} \right) \right] \left[F \left(\frac{w^2}{y} \right) - 1 \right]^2 \left[1 + \frac{2}{w^2} y \right] \frac{1}{y^2} \mathrm{d}y \end{aligned}$$

$$= \frac{c_0}{\beta^2} e^{w^2} \int_{w^2}^{\infty} e^{-t} \left[F(t) - 1\right]^2 \left(1 + \frac{2}{t}\right) \mathrm{d}t$$

$$= \frac{c_0}{\beta} e^{w^2} e^{-t} \left[(F(t))^2 - \left(4 + \frac{2}{t}\right) F(t) + 3\right]_{t=w^2}^{t=\infty}$$

$$= -\frac{c_0}{\beta^2} \left[\left(F(w^2)\right)^2 - \left(4 + \frac{2}{w^2}\right) F(w^2) + 3\right].$$

The second integral is easier:

$$J_2 = \int_0^{\infty} e^{c_0 r} \left[v(r)\right]^2 \mathrm{d}r = \int_0^{\infty} e^{c_0 r} u_0^2 c_0^2 e^{-2c_0 r} \mathrm{d}r = u_0^2 c_0.$$

This completes the derivation of Equation (6.3).

D Derivation of (7.9)

The numerator of (7.8) will be split into two in the usual way. The first of these, upon conversion of the integration from r to u, is

$$N_- := \int_{-\infty}^{0} e^{c_0 r} v(r) y(r) \left[k\left(u(r)\right) - e^{-1/u(r)}\right] \mathrm{d}r$$

$$= \int_{1/\beta}^{u_0} \exp\left[\frac{c_0}{\mu} \ln\left(\frac{u - 1/\beta}{u_0 - 1/\beta}\right)\right] \left[1 - \beta u\right] \left(e^{-\beta} - e^{-1/u}\right) \mathrm{d}u$$

$$= \frac{-1}{\beta \left[1 - F(\beta)\right]^{\frac{c_0}{\mu}}} \int_0^{1-F(\beta)} s^{\frac{c_0}{\mu}+1} \left[e^{-\beta} - \exp\left(-\frac{\beta}{1-s}\right)\right] \mathrm{d}s$$

$$= -\frac{e^{-\beta}}{\beta \left[1 - F(\beta)\right]^{\frac{1-F(\beta)}{F(\beta)}}} \frac{1}{\frac{1+F(\beta)}{F(\beta)}} s^{\frac{1+F(\beta)}{F(\beta)}} \Big|_0^{1-F(\beta)}$$

$$+ \frac{e^{-\beta}}{\beta \left(1 - F(\beta)\right)^{\frac{c_0}{\mu}}} \int_0^{1-F(\beta)} s^{1/F(\beta)} \exp\left[-\beta \frac{s}{1-s}\right] \mathrm{d}s$$

$$= \frac{e^{-\beta}}{\beta} \left[-\frac{F\left(1 - F\right)^2}{1 + F} + \left(\frac{1}{1 - F}\right)^{\frac{1-F}{F}} \int_0^{1-F} s^{1/F} \exp\left(-\beta \frac{s}{1-s}\right) \mathrm{d}s\right]$$

where (7.3) has been used to connect u with r, $1 - \beta u_0 = F(\beta)$ (based on (2.4) and (5.5)), and $c_0/\mu = [1 - F(\beta)]/F(\beta)$, based on (7.6). For brevity, F presented with no argument means $F(\beta)$. The second part of the numerator is

$$N_+ := -\int_0^{\infty} e^{c_0 r} v(r) y(r) \left[k\left(u(r)\right) - e^{-1/u(r)}\right] \mathrm{d}r$$

$$= \int_0^{u_0} \frac{u_0}{u} \left(1 - \beta u\right) e^{-1/u} \mathrm{d}u$$

$$= u_0 E_1\left(\frac{1}{u_0}\right) - \beta u_0^2 e^{-1/u_0} + \beta u_0 E_1\left(\frac{1}{u_0}\right)$$
$$= \beta u_0^2 e^{-1/u_0}\left[\frac{\beta+1}{\beta} F\left(\frac{1}{u_0}\right) - 1\right].$$

The denominator is given by

$$D = \int_{-\infty}^{0} e^{c_0 r}\left(\frac{1}{\beta} - u_0\right)^2 \mu^2 e^{2\mu r}\,\mathrm{d}r + \int_0^\infty e^{c_0 r} u_0^2 c_0^2 e^{-2c_0 r}\,\mathrm{d}r$$
$$= \left(\frac{1}{\beta} - u_0\right)^2 \mu^2 \frac{1}{2\mu + c_0} + u_0^2 c_0 = \frac{2c_0 F^2}{\beta^2\left[1+F\right]}.$$

Putting these together gives us (7.9).

E Derivation of (8.5)

In (8.4), we set $v = u'$ as usual, to obtain a system for (u, v) in the form (4.5) in which

$$\mathbf{f} = \left(v, -c_0 v H(u_0 - u) - (1-\beta u)^n e^{-\beta} H(u - u_0)\right)$$

and

$$\mathbf{g} = (0, -c_1 v H(u_0 - u) + c_0 v[H(u_0 - u) - 1] + (1-\beta u)^n [e^{-\beta} H(u - u_0) - e^{-1/u}]).$$

Therefore,

$$\nabla \cdot \mathbf{f} = -c_0 H\left(u_0 - u\right)$$

and

$$\mathbf{f} \wedge \mathbf{g} = v\{-c_1 v H(u_0 - u) + c_0 v[H(u_0 - u) - 1] + (1-\beta u)^n [e^{-\beta} H(u - u_0) - e^{-1/u}]\}.$$

Substituting into the Melnikov formula (4.7), setting it equal to zero, and solving for c_1 as usual, we are able to write

$$c_1 = \frac{N_- + N_+}{D_- + D_+}$$

where the subscript indicates whether the integral is over the negative or positive half line, and N and D stand for numerator and denominator respectively, each term of which we will compute momentarily. First, we note that the interior integral within the Melnikov formula takes the value

$$\exp\left[-\int_0^r \nabla \cdot \mathbf{f}\left(\hat{\mathbf{z}}(s)\right) \mathrm{d}s\right] = \begin{cases} 1 & \text{if } \xi \leq 0 \\ e^{c_0 r} & \text{if } \xi > 0. \end{cases}$$

Now, since $v(r)\mathrm{d}r = u'(r)\mathrm{d}r = \mathrm{d}u$ as before,

$$
\begin{aligned}
N_- &= \int_{-\infty}^{0} v[-c_0 v + (1-\beta u)^n \left(e^{-\beta} - e^{-1/u}\right)]\mathrm{d}r \\
&= -\int_{u_0}^{1/\beta} \left[c_0^2 u_0 \left(\frac{1-\beta u}{1-\beta u_0} \right)^{\frac{n+1}{2}} + (1-\beta u)^n \left(e^{-\beta} - e^{-1/u}\right) \right] \mathrm{d}u \\
&= -\frac{e^{-\beta}\left(1-F(\beta)\right)^{n+1}}{(n+1)(n+3)\beta F(\beta)} \left[(n-1)F(\beta)+4\right] + \int_{u_0}^{1/\beta} (1-\beta u)^n \, e^{-1/u}\mathrm{d}u,
\end{aligned}
$$

by performing calculations similar to those in Appendix 9. Also,

$$
\begin{aligned}
N_+ &= \int_0^{\infty} e^{c_0 r} v (1-\beta u)^n \left(-e^{-1/u}\right) \mathrm{d}r \\
&= u_u \int_0^{u_0} \frac{(1-\beta u)^n}{u} e^{-1/u} \mathrm{d}u.
\end{aligned}
$$

In the denominator, $D_- = 0$ since the convective term which multiplies c_1 in $\mathbf{f} \wedge \mathbf{g}$ is zero in $\xi \leq 0$. On the other hand,

$$
D_+ = \int_0^{\infty} e^{c_0 r} \left[v(r)\right]^2 \mathrm{d}r = \int_0^{\infty} e^{c_0 r} \left(-c_0 u_0\right)^2 e^{-2c_0 r} \mathrm{d}r = u_0^2 c_0.
$$

Putting these together give us (8.5).

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