

Properties of combustion waves in a model with competitive exothermic reactions

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Abstract We study the properties of travelling combustion waves in a diffusional thermal model with a two-step competitive exothermic-exothermic reaction mechanism. This investigation considers the system in one spatial dimension under adiabatic conditions. Based on the notion of the crossover temperature, the model is examined analytically using the activation energy asymptotic method to predict travelling combustion wave behaviour in the limit of large activation energies. The model is then studied numerically using a shooting-relaxation method over a wide range of parameter values, such as those describing the ratios of enthalpies, pre-exponential factors and activation energies. It is demonstrated that the flame speed as a function of these parameters is a single-valued monotonic function and there are two flame regimes identified—each region representing parameter values when one reaction dominates the other.

Keywords Combustion waves · Competitive exothermic reactions · Flame speed · Asymptotic analysis · Shooting-relaxation method

Mathematics Subject Classification 37D35 · 35K57 · 34B40

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1 Introduction

Our focus in this work is the study of a reaction scheme which is described by the model with two-stage competitive exothermic reactions, where both reactions occur simultaneously and consume the same reactants. This model has practical applications in simulating the combustion of MeCH_2 , where Me is either Titanium or Zirconium [1, 2]. Although most observed physico-chemical phenomena are a consequence of dozens, hundreds or even thousands of concurrent or consecutive endothermic and exothermic reactive processes, simple lumped models representing the elementary reactive steps can be utilized to provide useful understanding. In some cases, especially when the whole combustion process is thermally dominated by two exothermic reactive steps, the simplest useful model comprises a pair of exothermic reactions producing either metal carbo-hydrides or metal hydrides, characterized by different chemical kinetics. Since both reactions feed on the same reactant, they are referred to as competitive reactions. On the other hand, if the reactions consume different reactants, they are then referred to as parallel reactions [3]. In the competitive case the two reactions are both chemically and thermally coupled, whereas the reactions are only thermally coupled in the parallel case.

There are several studies [4–7] into the scheme describing the competitive exothermic-endothermic (exo-endo) reactions. Hmadi et al. [4] investigated the existence and stability of one-dimensional flame fronts propagating through a solid reactive slab and treated the endothermic reaction as heat loss to perturb the exothermic reaction. An analysis was given based on the limit of large activation energies and the assumption that the endothermic reaction has larger activation energy and pre-exponential factor than the exothermic reaction. Sharples et al. [5] extended the work of [4] to relax the choice of parameter values, including Lewis number, the ratios of enthalpies and pre-exponential factors. Linear stability of the combustion waves in regime where the exothermic reaction is dominating over the endothermic reaction was studied using the Evans function method. Hopf bifurcation points were found and confirmed by using a numerical method to solve the governing partial differential equations (PDES). In [6], a similar systematic stability analysis of combustion waves for the case where the endothermic reaction plays a more dominant role was carried out. It was found that the inclusion of the competitive endothermic reaction stabilized the reaction system. Gubernov et al. [7] defined a ‘crossover temperature’ to study the properties of combustion wave solutions in a diffusion-reaction model with a two-step competitive exothermic-endothermic reaction mechanism under adiabatic conditions—the heat release from the exothermic reaction is equal to the heat consumption by the endothermic reaction. Based on this definition, the regimes where exothermic and endothermic reactions dominate were identified and the properties of the combustion wave solutions, particularly the flame speed and extinction conditions, were investigated. The flame speed as a function of parameters was found to be either monotonic single-valued or double-valued C-shaped.

In contrast to the case of the competitive exo-endo reactions which have been extensively studied above, the scheme describing the competitive exothermic reactions (exo-exo reactions) has received little attention. Sidhu et al. [8] and Towers et al. [9] have investigated flame propagation in a model with two-stage competitive exo-exo

reactions and demonstrated the existence of regions of bi-stability—co-existence of two stable solutions corresponding to slow and fast branches for the same parameter values. There was a third unstable branch joining the two stable branches based on solving a system of ordinary differential equations (ODEs). They also illustrated a hysteresis type behaviour that one reaction can switch rapidly to the other by varying the activation energy of one of the reactions. In [10] we proposed an approximation theory for solid fuels under adiabatic conditions. The asymptotic results obtained for flame speed agreed well with the numerical solutions. The profiles of temperature and mass fraction were also obtained analytically using piecewise approximation method and confirmed numerically.

The work reported here presents an analysis for a two-step competitive exo-exo reaction scheme employing the definition of the crossover temperature proposed by [7]. Note that Towers et al. [9] gave a different definition of the crossover temperature by requiring that the rate constants of the first and second reactions be equal. However, here we prefer to use the definition that the heat releases by the two reactions are equal so that the crossover temperature depends on the ratio of enthalpies (an important parameter in our study). The model is analysed over a wide range of parameter values. Following [8,9], we do not consider heat loss (Newtonian or convective cooling). However, unlike the work reported in [8,9], we relax the restriction of the ratios of activation energies, pre-exponential factors and enthalpies.

2 Mathematical model

A general schematic for a two-step competitive reaction mechanism is



where A represents the reactant; B and C are chemically inert products (in other words, the reactions are irreversible); $Q_1 > 0$ and $Q_2 > 0$ are enthalpies of the first (R1) and the second (R2) reactions respectively. The reaction rate constants $k_1(T)$ and $k_2(T)$ obey Arrhenius kinetics. Following Forbes and Derrick [11], the reaction rate constants take the form

$$k_i(T) = \begin{cases} 0, & T < T_i, \\ A_i e^{-E_i/RT}, & T \geq T_i, \end{cases} \quad i = 1, 2,$$

where A_i and E_i are the pre-exponential factors and the activation energies and R is the universal gas constant. T_1 and T_2 are the threshold temperatures above which the first and second reaction occur. For simplicity, we set $T_1 = T_2 = T_a$, where T_a is the ambient temperature. With the introduction of the dimensionless variables used in [8], when $u \geq u_a$ the governing PDEs are

$$u_t = u_{xx} + v \left(e^{-1/u} + qre^{-f/u} \right), \quad (1)$$

$$v_t = Le^{-1}v_{xx} - v\beta \left(e^{-1/u} + re^{-f/u} \right), \quad (2)$$

where $q = Q_2/Q_1$, $r = A_2/A_1$ and $f = E_2/E_1$. The subscripts represent derivatives with respect to the specified independent variables.

In these equations, u and v correspond to the temperature nondimensionalized by the adiabatic flame temperature for the system with reaction R1 only and mass fraction of initial reactant A scaled over its value in the fresh mixture respectively; x and t represent dimensionless spatial and time coordinates. The parameters q , r and f are the ratios of enthalpies, the pre-exponential factors and the activation energies, respectively. The Lewis number Le is the ratio of thermal to mass diffusivities, varying from around unity for gaseous fuels to large values ($\gg 1$) for solid fuels. Finally, the parameter, β , is the ratio of the activation energy to the enthalpy of reaction R1.

Equations (1) and (2) are subject to the boundary conditions

$$u = u_a, \quad v = v_0, \quad \text{for } x \rightarrow \infty, \quad (3)$$

$$u_x = 0, \quad v_x = 0, \quad \text{for } x \rightarrow -\infty. \quad (4)$$

On the right boundary ($x \rightarrow \infty$), we have a ‘cold’ and ‘unburnt’ state (the ambient temperature is u_a and the consumption of the fuel is negligible) and no reactions occur when $u < u_a$. For definiteness and without loss of generality, the initial mass fraction v_0 is chosen to be one. Unlike [12], we do not set $u_a = 0$ but specify the value $u_a = 10^{-4}$ throughout our study (noting that this value corresponds to the ambient temperature having a value of $T_a \approx 300\text{K}$ for these types of reactions). On the left boundary ($x \rightarrow -\infty$), neither the burnt temperature denoted as u_b nor the mass fraction can be specified. We assume no reaction should occur at the left end. Consequently, the derivatives of u and v are set to zero.

We now consider a moving coordinate frame, $\xi = x - ct$. Such a consideration transforms Equations (1) and (2) to

$$u_{\xi\xi} + cu_{\xi} + v \left(e^{-1/u} + qre^{-f/u} \right) = 0, \quad (5)$$

$$Le^{-1}v_{\xi\xi} + cv_{\xi} - v\beta \left(e^{-1/u} + re^{-f/u} \right) = 0, \quad (6)$$

where the constant c represents the flame speed and the subscript represents derivative with respect to the moving front coordinate ξ .

Equations (5) and (6) are subject to the boundary conditions

$$u = u_a, \quad v = 1, \quad \text{for } \xi \rightarrow \infty, \quad (7)$$

$$u_{\xi} = 0, \quad v_{\xi} = 0, \quad \text{for } \xi \rightarrow -\infty. \quad (8)$$

3 Asymptotic analysis

To begin with, we denote the crossover temperature as u^* , at which the rate of heat release from reaction R1 is equal to the rate of heat release from reaction R2. Considering heat released by R1 and R2 in Eq. (1) and by means of simple algebraic manipulations, $u^* = (f - 1)/\ln(qr)$. Clearly, the crossover temperature depends

on the parameter values q, r and f . There are two regions when $u^* > 0$: (a) $f > 1$ and $qr > 1$, (b) $0 < f < 1$ and $0 < qr < 1$; and two regions when $u^* < 0$: (c) $f > 1$ and $0 < qr < 1$, (d) $0 < f < 1$ and $qr > 1$. One reaction always dominates the other in the parameter space where $u^* < 0$. Reaction R1 always releases much more heat than reaction R2 in region (c). We refer to this as R1 domination. On the other hand, for case (d), reaction R2 is more exothermic, and we refer to this as R2 domination. Both cases (c) and (d) are feasible in the competitive exo-exo reaction schemes but we do not present further analysis for cases (c) and (d) since these two cases do not exhibit interesting dynamic behaviour as they can be reduced to the traditional one-step scheme [12,13]. In this paper we will only focus on the investigation of the properties of the combustion waves properties for case (a) since case (b) can be mapped one-to-one to case (a) by interchanging the notations. We note that case (d) is not possible in the competitive exo-endo reaction schemes since it implies flame extinction as the rate of heat reduction by the endothermic reaction is always greater than the rate of heat release by the exothermic reaction [7].

3.1 R1 dominated regime

In the region (a) and if $f \rightarrow \infty$, reaction R1 dominates and thus the second reaction term in Eqs. (5) and (6) can be omitted. Therefore, for $f \gg 1$, we use the asymptotic results of the single step irreversible exothermic reaction model to approximate the solutions of the competitive exo-exo reaction model. To obtain asymptotic results, the large activation energy limit is exploited. This plays the same role as the large β limit, although there is not a one-to-one correspondence between them [12]. Based on this limit, the burnt temperature and flame speed using the activation energy asymptotic (AEA) method are

$$u_b = \frac{1}{\beta}, \quad c = \sqrt{\frac{2Le}{\beta}} \exp\left(-\frac{\beta}{2}\right). \tag{9}$$

Equation (9) is valid regardless of the values of the parameters q and r so long as $qr > 0$.

3.2 R2 dominated regime

For the case $f \rightarrow 1^+$ and $qr > 1$, $u^* \rightarrow 0^+$. On the other hand, reaction R2 dominates in the region $f < 1$ and $qr > 1$ (case (d) discussed earlier). Consequently, when the values of the parameters q and r ($qr > 1$) are fixed, the case $f = 1$ can be considered as a supremum (least upper bound) of region (a). When $f = 1$, the system (5) and (6) reduces to a single-step combustion model

$$u_{\xi\xi} + cu_{\xi} + v(1 + qr)e^{-1/u} = 0, \tag{10}$$

$$Le^{-1}v_{\xi\xi} + cv_{\xi} - \beta v(1 + r)e^{-1/u} = 0. \tag{11}$$

Introducing a new coordinate $\eta = \xi\sqrt{1+qr}$ and defining $\bar{c} = c/\sqrt{1+qr}$ and $\bar{\beta} = \beta(1+r)/(1+qr)$, the model can be written exactly the same as a standard single-step model. Thus once again, the expressions for the burnt temperature and flame speed written for the case when $qr > 1$ and $f = 1$ can be written in the original variables as

$$u_b = \frac{1+qr}{\beta(1+r)}, \quad c = \sqrt{\frac{2Le(1+qr)^2}{\beta(1+r)}} \exp\left(-\frac{\beta(1+r)}{2(1+qr)}\right). \quad (12)$$

In the case $qr \rightarrow \infty$ and $f > 1$, reaction R2 dominates and thus the first reaction term in Eqs. (5) and (6) can be neglected, leading to the system of ODEs

$$u_{\xi\xi} + cu_{\xi} + qrv e^{-f/u} = 0, \quad (13)$$

$$Le^{-1}v_{\xi\xi} + cv_{\xi} - \beta r v e^{-f/u} = 0. \quad (14)$$

Hence for $qr \rightarrow \infty$ and $f > 1$, the burnt temperature and the flame speed are

$$u_b = \frac{q}{\beta}, \quad c = \sqrt{\frac{2Leq^2r}{\beta f^2}} \exp\left(-\frac{\beta f}{2q}\right). \quad (15)$$

Finally, it is clear from our analysis presented in this section that the burnt temperature u_b and the flame speed c are both dependent on the type and the properties of the fuel. There is a possibility of a transition between one dominated regime to the other when these fuel properties are varied.

4 Travelling wave solutions

The two-point boundary value problem (BVP) consisting of the ODE system (5) and (6) together with boundary conditions (7) and (8) were solved numerically using a standard shooting algorithm with a Runge-Kutta integration scheme. Following the approach of [9], this solution was subsequently used in a relaxation algorithm to improve the accuracy of result. In practice, there are three types of fuels – gaseous, porous and solid fuels. Here we use $Le = 1, 2$ and 10 to represent the Lewis numbers of gaseous, porous and solid fuels respectively. Temperature and fuel profiles for different fuel types are displayed with other parameter values fixed. Typical combustion wave solution profiles are shown in a moving coordinate frame in Figs. 1 and 2. Looking from right to left, the reaction temperature is increasing monotonically until the fuel is completely consumed. The intervals of integration are scaled to range from 0 to 1 while the values of the original variable representing the integration length are approximately 1200, 900 and 600 for $Le = 1, 2$ and 10 respectively. It is readily seen in Fig. 2 that the reaction region for $Le = 10$ is much narrower than those for $Le = 1$ and $Le = 2$. The flame speed for $Le = 10$ ($c \approx 0.013$) is more than double that for $Le = 1$ ($c \approx 0.006$) and the flame speed for $Le = 2$ is in between these speeds ($c \approx 0.008$). In addition, it should be pointed out that, similar to the relationship between Le and flame speed, the larger the Lewis number the higher the value of the burnt temperature. However,

Fig. 1 Combustion wave solution profiles for dimensionless temperature $\beta u(\xi)$ and mass fraction $v(\xi)$ for $Le = 1$ (red solid lines), $Le = 2$ (blue dashed lines) and $Le = 10$ (green dot lines) with other parameter values being $\beta = 10$, $f = 1.5$, $q = 5$, $r = 5$ and $u_a = 10^{-4}$

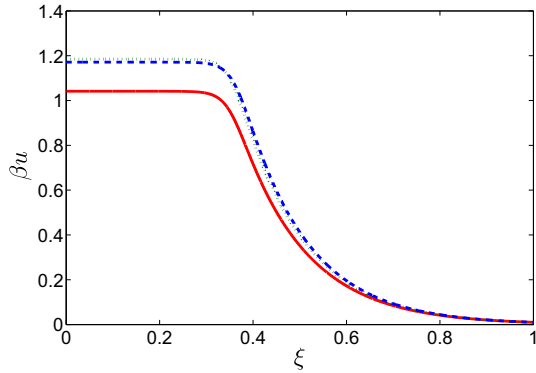
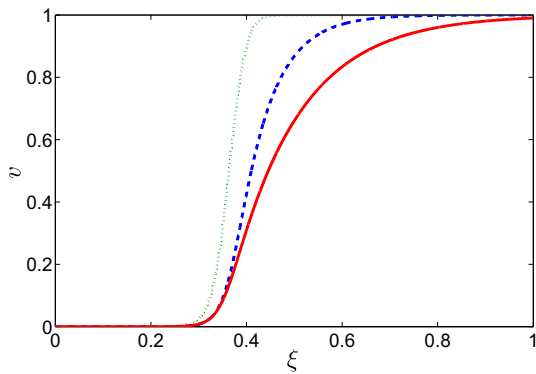


Fig. 2 Combustion wave solution profiles for mass fraction $v(\xi)$. The parameter values and notations used here are the same with those in Fig. 1



there is no simple correspondence between Lewis number and the burnt temperature as there is no clear mapping between these two parameters.

4.1 Case 1: $Le = 1$ (gaseous fuels)

To begin with, we present the numerical and asymptotic results for gaseous fuels whose Lewis number is normally set to unity (e.g. in [12]). Figure 3 shows the maximum burnt temperature as a function of f for $Le = 1$, $r = 2$ and two different values of β and q . It is readily apparent that there are two distinct regimes. When $f > 2$, reaction R2 is almost completely ‘frozen’ and the peak value of the temperature equals the adiabatic burnt temperature for the one-step model (indicated by the dashed lines). Hence, we refer to the region $f > 2$ as reaction R1 dominated regime. In this regime, the parameter q almost has no impact on the burnt temperature. However as f decreases, reaction R2 becomes more important. The burnt temperature converges to the value obtained by expression (12) as $f \rightarrow 1^+$. Varying the parameter values of q and β can result in significant changes to the value of u_b when $f = 1$ as shown in Fig. 3 (left boundary).

The dependence of the flame speed on f is illustrated in Fig. 4. The flame speed converges to the asymptotic flame speed (a constant value) for the single step model (9)

Fig. 3 Dependence of the burnt temperature u_b on f for $\beta = 5$, $q = 5$ (red curve 1), $\beta = 5$, $q = 0.45$ (blue curve 2), $\beta = 10$, $q = 5$ (green curve 3) and $\beta = 10$, $q = 0.45$ (black curve 4) with $Le = 1$, $r = 2$ and $u_a = 10^{-4}$. The dashed lines represent the asymptotic results (9) for $f \rightarrow \infty$, while diamonds correspond to the asymptotic solutions (12) for $f = 1$

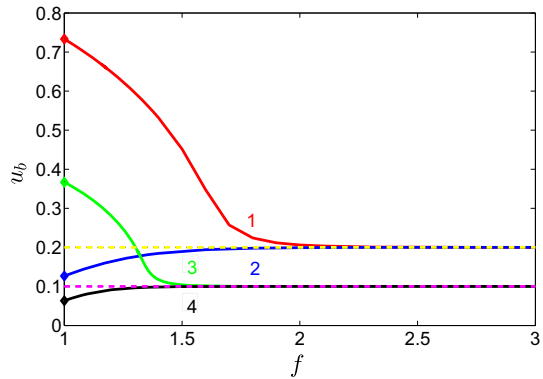
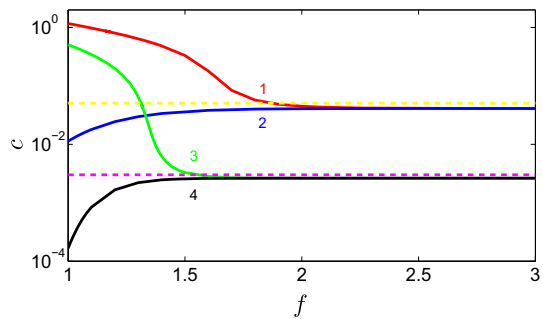


Fig. 4 Dependence of the flame speed c on f . The parameter values and the notations used here are the same as those used in Fig. 3



for large values of f ($f > 2$). The discrepancy between the numerical solutions using the shooting-relaxation method and the asymptotic results are smaller for $\beta = 10$ (curve 3, 4) than that for $\beta = 5$ (curve 1, 2). This is expected since the asymptotic results (9) are obtained in the limit of large activation energy ($\beta \gg 1$). We also note that the flame speed is almost independent of q for large values of f , while q becomes more significant as f approaches one.

The above analysis shows the effect of the ratio of the activation energies on the behaviour of combustion waves.

Next we will investigate the properties of combustion wave solutions when varying q and r . Here we choose two different values for the ratios of the activation energies: $f = 1$ and $f = 3$. The dependence of the flame speed on β is illustrated in Figs. 5 and 6. The difference between the asymptotic results and the numerical solutions reduces gradually with increasing β . Once again, it is apparent that there are two distinct regimes depending on the choice of f . For $f = 3$, the difference between the solutions corresponding to $q = 0.45$ and $q = 5$ for the flame speed is small. When $\beta = 5$, the flame speeds for both values of q are $c \approx 0.2$. However, for $f = 1$, the value of the flame speed for $q = 5$ is about 100 times larger than that for $q = 0.45$. For instance, the flame speeds for $q = 0.45$ and $q = 5$ are $c \approx 1.17$ and $c \approx 0.011$ when $\beta = 5$. Thus, the ratio of enthalpies plays a significant role in the flame speed when $f = 1$. We fix the value of β to 10 hereafter since numerical solutions agree well with asymptotic results when $\beta \geq 10$ as shown in Figs. 5 and 6.

Fig. 5 Flame speed versus β for $Le = 1$, $f = 3$, $r = 2$ and $u_a = 10^{-4}$. Numerical solutions for $q = 0.45$ and $q = 5$ are indicated by the red solid line and black diamond respectively, asymptotic results given by (9) are represented by the blue dashed line

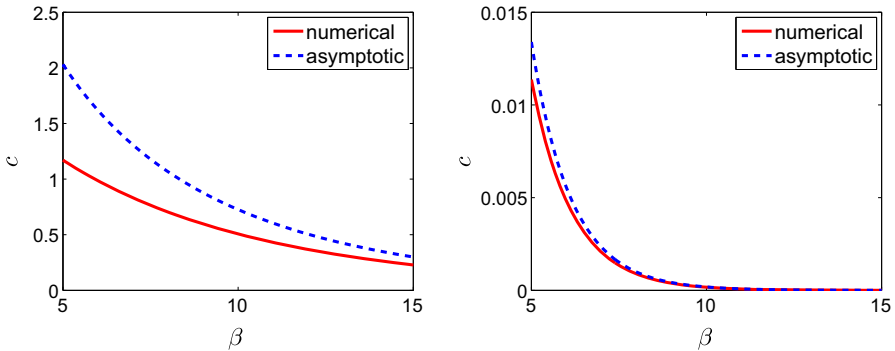
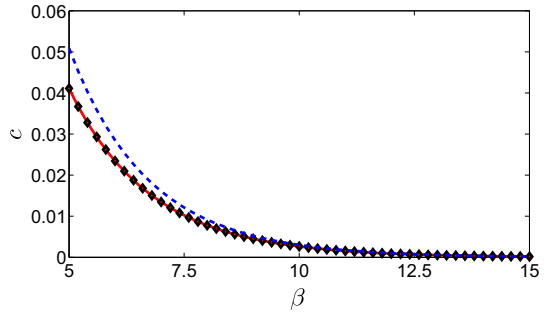


Fig. 6 Dependence of the flame speed on β for two different values of q with $Le = 1$, $f = 1$, $r = 2$ and $u_a = 10^{-4}$. The left and right graphs show the results for $q = 5$ and $q = 0.45$ respectively. The red solid line represents the numerical solutions and the blue dashed line corresponds to the asymptotic results given by (12)

Figure 7 illustrates the dependence of flame speed on q in a log-log scale. Fixing $r = 2$ and $q \geq 0.5$ (since $qr \geq 1$), the properties of the combustion waves are studied with two distinctive values of f to demonstrate two different reaction dominated regimes. In the R1 dominated regime ($f = 3$), the flame speed is almost independent of q . Furthermore, the numerical results for the flame speed are very close to the asymptotic expression (9) for the one-step model. However, in the R2 dominated regime ($f = 1$), the parameter q plays a significant role in the behaviour of combustion waves. Here, it is also shown that the flame speed behaviour shows close resemblance to the asymptotic expression (12).

Finally, the dependence of flame speed on r is plotted in Fig. 8. Similarly, in the R1 dominated regime ($f = 3$), the parameter r has almost no impact on the flame speed, while r is much more important in the R2 dominated regime ($f = 1$). We note that there is some discrepancy between the numerical and asymptotic results since the asymptotic results are only valid in the large β limit and the value of β used in this case is not very large compared with the value of qr . The difference reduces as $qr \rightarrow 1$ when $f = 1$. However, both the numerical and asymptotic results show similar generic behaviour when the parameter r is varied.

Fig. 7 Dependence of the flame speed c on q for $f = 3$ and $f = 1$ with other parameter values being $Le = 1$, $\beta = 10$, $r = 2$ and $u_a = 10^{-4}$. The green dashed line represents the asymptotic results (9) for the one-step model, while the blue dashed line represents the asymptotic results (12). Numerical solutions for $f = 1$ and $f = 3$ are indicated by red and black solid lines respectively

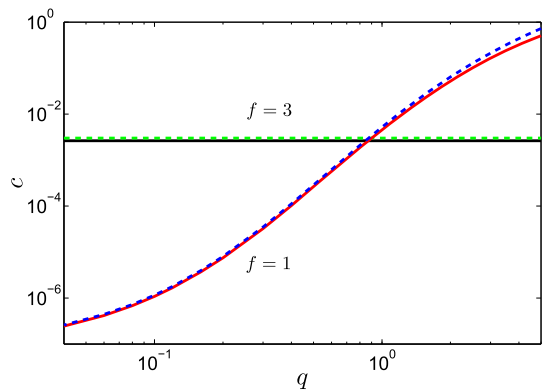
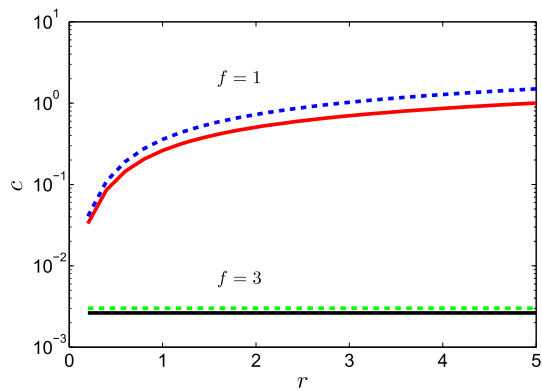


Fig. 8 Dependence of the flame speed c on r for $q = 5$. The notations and the other parameter values used here are the same with those used in Fig. 7



4.2 Case 2: $Le > 1$

In this section, we focus on the solutions corresponding to porous ($Le = 2$) and solid ($Le = 10$) fuels. The results presented in this section are relevant to cases when the fuel consists of particles of different sizes and shapes including soot powders. Figure 9 shows the dependence of burnt temperature on f for $Le = 2$ and $Le = 10$. The two curves are almost identical except that the burnt temperatures for $Le = 2$ are slightly lower than those for $Le = 10$. As can be seen from the expressions (9) and (12), the burnt temperature is independent of Lewis number. The asymptotic results for burnt temperature agree excellently with numerical solutions. Figure 10 illustrates the dependence of flame speed on f for $Le = 2$ and $Le = 10$. It is obvious that the flame speed for $Le = 10$ is greater than that for $Le = 2$. Compared with the burnt temperature (results shown in Fig. 9), Fig. 10 clearly shows that the Lewis number has a greater impact on the flame speed.

Figures 11 and 12 show the dependence of flame speed on β in the two distinct dominated regimes. It is readily seen that the two different regimes can be clearly distinguished by choosing different values of the ratio of activation energies. Figure 11 illustrates the relationship between c and β in the R1 dominated regime, whereas the

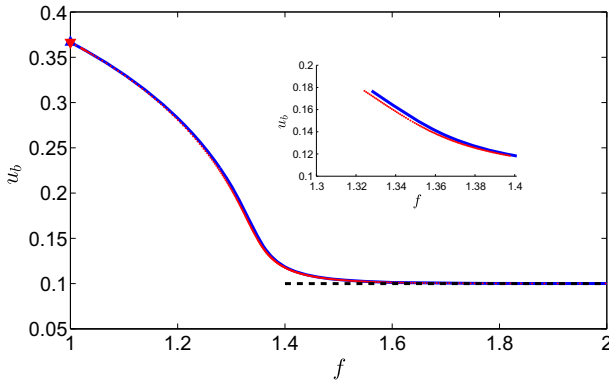


Fig. 9 Dependence of the burnt temperature u_b on f for $Le = 2$ (red dotted line) and $Le = 10$ (blue solid line) with $\beta = 10, q = 5, r = 2$ and $u_a = 10^{-4}$. The black dashed lines represent the asymptotic results (9) for $f \rightarrow \infty$, while the blue (upper) and red (inverted) triangles represent the asymptotic results (12) for $Le = 10$ and $Le = 2$ respectively for $f = 1$. The inset clearly shows that the burnt temperature for $Le = 2$ is close but always lower than the value for $Le = 10$

Fig. 10 Dependence of the flame speed c on f for $Le = 2$ (red) and $Le = 10$ (blue) with $\beta = 10, q = 5, r = 2$ and $u_a = 10^{-4}$. The dashed lines represent the asymptotic results (9) for $f \rightarrow \infty$

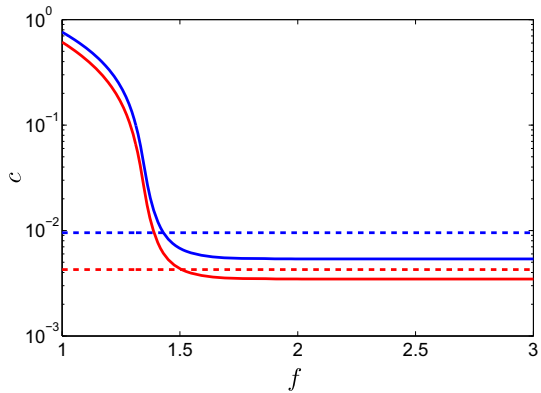


Fig. 11 Flame speed versus β for two values of Le with $f = 1, q = 5, r = 2$ and $u_a = 10^{-4}$

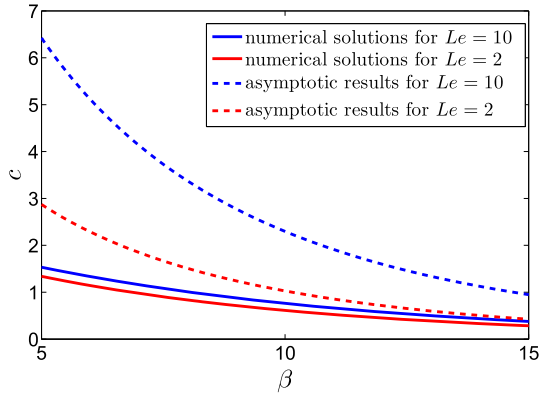


Fig. 12 Flame speed versus β for two values of Le with $f = 3$, $q = 5$, $r = 2$ and $u_a = 10^{-4}$

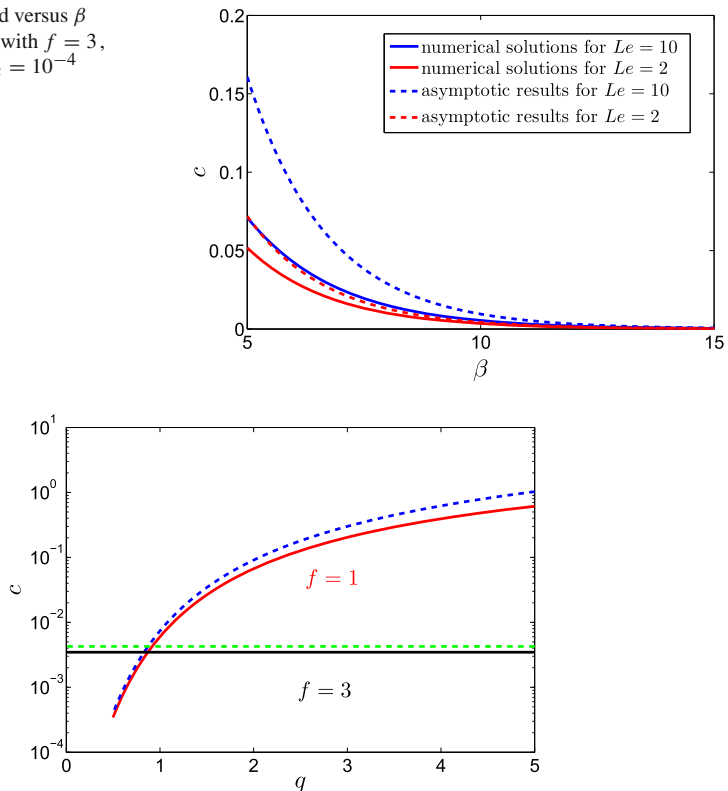


Fig. 13 Dependence of the flame speed c on q for $f = 3$ (R1 dominated regime) and $f = 1$ (R2 dominated regime) with other parameter values being $Le = 2$, $\beta = 10$, $r = 2$ and $u_a = 10^{-4}$. The green dashed line represents the asymptotic results (9) for the one-step model, while the blue dashed line represents the asymptotic results (12). Numerical solutions for $f = 1$ and $f = 3$ are indicated by red and black solid lines respectively

dependence of c on β in the R2 dominated regime is shown in Fig. 12. The asymptotic results are in qualitative agreement with the numerical solutions, although there are clear differences between them. Due to the approach taken to obtain the asymptotic results, the difference between the numerical solutions and the asymptotic results becomes greater for larger values of Lewis number.

Next the effect of the ratios of the activation energies and pre-exponential factors are presented. To be consistent with the previous section (our investigation of $Le = 1$), $f = 1$ and $f = 3$ are fixed and the effects of q and r in the R1 and R2 dominated regimes are investigated. The main results are shown in Figs. 13–16. Figures 13 and 14 illustrate the dependence of the flame speed on q for $Le = 2$ and $Le = 10$, respectively. The dependence of the flame speed on r for $Le = 2$ and $Le = 10$ are shown in Figs. 15 and 16. In the R1 dominated regime ($f = 3$), the system converges to the irreversible single exothermic reaction model and the flame speed is almost independent of the parameters q and r . Furthermore, these figures show that the difference between the numerical solutions and the asymptotic results (based on the one-step

Fig. 14 Dependence of the flame speed c on q for $Le = 10$ and $r = 2$. The notations and the other parameter values used here are the same with those used in Fig. 13

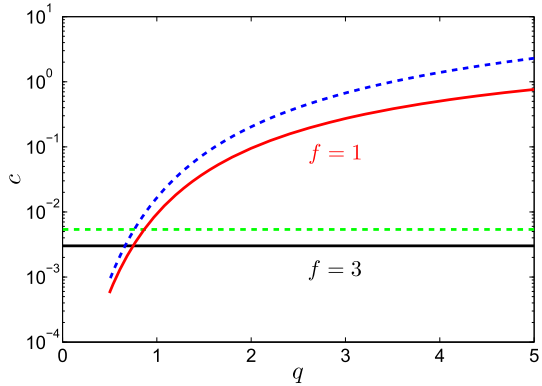


Fig. 15 Dependence of the flame speed c on r for $Le = 2$ and $q = 5$. The notations and the other parameter values used here are the same with those used in Fig. 13

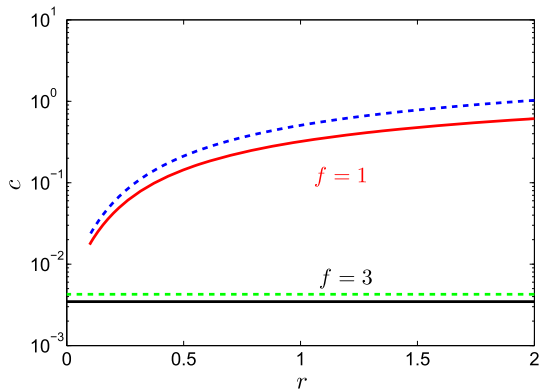
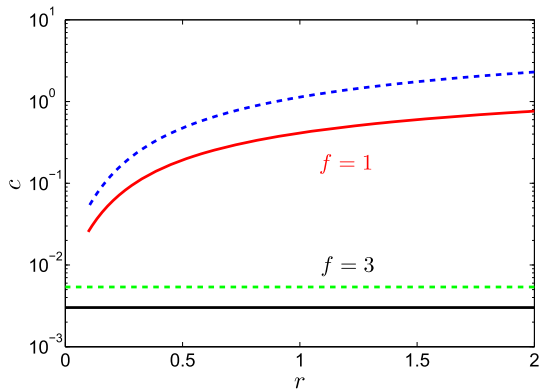


Fig. 16 Dependence of the flame speed c on r for $Le = 10$ and $q = 5$. The notations and the other parameter values are the same with those used in Fig. 13



model) is greater for higher Lewis numbers. However, in the R2 dominated regime ($f = 1$), the parameters q and r play important roles in the determination of the flame speed. It is shown that the flame speed increases monotonically as q or r increases. The asymptotic results (12) provide a good approximation for $f = 1$ especially when the product qr is of order β ($qr \ll \beta$).

5 Conclusion

We have investigated the properties of the combustion waves for a two-stage competitive exothermic reaction scheme under adiabatic conditions. The boundary value problem is studied both numerically and analytically. In particular, the asymptotic flame speed and burnt temperature for the case when the ratio of the activation energies $f = 1$ are obtained using the activation energy asymptotic method. The asymptotic results and numerical solutions are in good agreement, especially when the product qr is of the order of β . Moreover, it is found that the flame speed as a function of model parameters is a single-valued monotonic function.

When f is sufficiently large, reaction R2 is not activated and the combustion wave solutions have a similar behaviour to the irreversible one-step exothermic reaction model. This regime is referred to as the R1 dominated regime. In this regime, the flame speed is almost independent of the parameters q and r . However, when $f \rightarrow 1^+$, reaction R2 is activated and dominates reaction R1. This is accompanied by a decrease (increase) of the burnt temperature and flame speed depending on decreasing (increasing) q with other parameter values fixed. Parameter r can also make a significant impact in the R2 dominated regime. Although there is a difference between the numerical and asymptotic solutions quantitatively, the results are qualitatively in agreement.

To summarise, the combustion waves for the two-step competitive exothermic reaction model shows various dynamical behaviour depending on the choice of the parameter values. Our work clearly shows that the key parameters that governs the dynamical behaviour of the combustion waves are the ratios of the activation energies, the enthalpies and the pre-exponential factors of the two competitive exothermic steps of the reaction mechanism. In our future work, the inherent characteristic which reflects the existence of multiplicity of travelling wave solutions as reported in [8, 9] will be studied along with the linear stability of the travelling wave solutions.

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