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On the structure of the spectra for a class of combustion waves

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The stability of a premixed laminar flame supported by a general combustion reaction system is considered using the Evans function method. The spectrum of the linearised second-order differential operator is investigated in detail. The special structure of the differential equations due to an Arrhenius temperature dependence is exploited. It is shown that, for certain combustion systems, the limit of the Jacobian of the reaction terms as the travelling wave coordinate approaches the front and rear of the flame is a lower triangular matrix. For this type of system a simple geometrical method is shown for the study of the essential spectrum of the linearised operator, and for determining the domain of the Evans function. The results are applied to some representative combustion reactions.

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1. Introduction

We consider the stability of a flame supported by the reactions

$$\sum_{i=1}^{n} \alpha_{ij} A_i \to \sum_{i=1}^{n} \beta_{ij} B_i \pm \text{ heat, rate } = k_j e^{-E_j/RT} \prod_{i=1}^{n} A_i^{\alpha_{ij}}, \quad (j = 1, 2, \dots, r).$$

Introducing the scaled concentrations a_i , scaled temperature b and scaled flame velocity c the equations governing our model, written in a reference frame

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moving with the flame, are [1,2]

$$L_i^{-1}a_i'' - ca_i' + \sum_{j=1}^r \Gamma_{ij}w_j(a_1, \dots, a_n, b) = 0 \quad (i = 1, 2, \dots, n),$$
(1)

$$b'' - cb' + \sum_{j=1}^{r} \Gamma_{n+1,j} w_j(a_1, \dots, a_n, b) - h(b) = 0,$$
(2)

where primes denote differentiation with respect to the travelling wave co-ordinate s, L_i (i = 1, 2, ..., n) are the Lewis numbers. The elements of the $(n + 1) \times r$ matrix Γ can be written in the form $\Gamma_{ij} = (\alpha_{ij} - \beta_{ij})\gamma_{ij}$ for $1 \le i \le n$, and $\Gamma_{n+1,j} = q_j \delta_j$, where q_j is the exothermicity of the *j*th reaction and the constants γ_{ij} , δ_j are determined by the rate constants. The nonnegative function *h* describes the heat loss in the system, h(0) = 0 is assumed. The reaction rate of the *j*th reaction is given by

$$w_j(a_1, \dots, a_n, b) = e^{\mu_j(b-1)/b} \prod_{i=1}^n a_i^{\alpha_{ij}},$$
 (3)

where μ_j is the scaled activation energy of the *j*th reaction. Equations (1) and (2) are subject to the boundary conditions

$$a_i \to a_{i,0}, \ b \to 0 \quad \text{as } s \to -\infty,$$
 (4)

$$a'_i \to 0, \ b' \to 0 \quad \text{as } s \to +\infty.$$
 (5)

Here $a_{i,0}$ denotes the initial concentration of reactant a_i in front of the wave. The boundary condition $b \to 0$ at $-\infty$ is equivalent to $T \to T_a$, where T is temperature and T_a is the ambient temperature, because the dimensionless temperature b is introduced as $b = (T - T_a)/(T_b - T_a)$ (here T_b is the burnt gas temperature). Using these notations the reaction term takes the form $\exp(\mu_j(b-1)/(b + T_a/(T_b - T_a)))$. With this reaction term we face the so-called 'cold boundary difficulty'. There are different ways to avoid that by changing the reaction term. One is introducing an ignition temperature, below which there is no reaction [3,4]. The other is introducing the reaction term given in (3), see e.g. [5,6]. There is only a negligible difference between the profiles obtained by the two methods, and the results are qualitatively the same.

Introducing the vector valued function $U = (a_1, ..., a_n, b)^T$ systems (1) and (2) can be written in the more general form

$$DU'' + BU' + F(U) = 0, (6)$$

where $U: \mathbb{R} \to \mathbb{R}^m$ is an m (= n + 1) dimensional vector-valued unknown function, D, B are $m \times m$ diagonal matrices, the diagonal elements of D are positive, and $F: \mathbb{R}^m \to \mathbb{R}^m$ is a differentiable function. We investigate the stability

of U as a travelling wave solution of the corresponding time dependent system. There are well-known methods for studying the stability of travelling waves [7–9]. Here our aim is to apply these methods, particularly the Evans function method, for combustion systems of the forms (1) and (2). The stability of combustion systems have previously been widely studied, see e.g. [4,6,10–13]. Here we apply the Evans function method, which has been applied for several models in physics [14–16], chemistry [17,18] and biology [19,20], but for only a few specialised combustion systems [17,21–23].

Our main motivating examples are the following systems.

• The first-order reaction

$$A \rightarrow P_1 + \text{heat}, \text{ rate } = ka e^{-E/RT}.$$

Here r = 1, n = 1, $\Gamma = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$. In the adiabatic case h = 0, in the case of Newtonian heat loss $h(b) = \gamma b$ with some positive constant γ . The adiabatic case has been investigated by many authors, e.g. [4,6,10,21,24]. The heat loss case was studied using asymptotic expansions in [24], theoretically in [3] and numerically in [12,23,25].

• The exothermic–endothermic system

$$A \rightarrow P_1$$
 + heat, rate $= k_1 a e^{-E_1/RT}$,
 $W \rightarrow P_2$ - heat, rate $= k_2 w e^{-E_2/RT}$.

Here r = 2, n = 2,

$$\Gamma = \begin{pmatrix} -1 & 0\\ 0 & -\beta\\ 1 & -\alpha \end{pmatrix},$$

where α , β are constants depending on the rate constants, initial concentrations and exothermicity of the reactions. Here h = 0, because the heat loss is built in the endothermic reaction. This system was investigated in [5,22,26].

The stability of U can be determined using the spectrum of the second-order differential operator

$$\mathcal{L}(V) = DV'' + BV' + F'(U)V.$$
⁽⁷⁾

The main topic of the paper is the investigation of the spectrum of \mathcal{L} , when the system has the special forms (1) and (2).

2. General properties of the spectrum

In this section we investigate the spectrum of the second-order differential operator

$$(\mathcal{L}V)(s) = DV''(s) + BV'(s) + Q(s)V(s),$$
(8)

defined in $C_0(\mathbb{R}, \mathbb{C}^m) \cap C^2(\mathbb{R}, \mathbb{C}^m)$, where

$$C_0(\mathbb{R}, \mathbb{C}^m) = \{ V : \mathbb{R} \to \mathbb{C}^m \mid V \text{ is continuous, } \lim_{\pm \infty} V = 0 \},$$

endowed with the supremum norm $||V|| = \max_{\mathbb{R}} |V(s)|$, D and B are $m \times m$ diagonal matrices with positive diagonal elements,

$$Q: \mathbb{R} \to \mathbb{R}^{m \times m}$$
 continuous there exist $Q^{\pm} = \lim_{s \to \pm \infty} Q(s)$.

Definition 1. The complex number $\lambda \in \mathbb{C}$ is called a regular value of \mathcal{L} if the operator $\mathcal{L} - \lambda I$ has bounded inverse that is defined in the whole space C_0 . That is, for any $W \in C_0$, there exists a unique solution of $\mathcal{L}V - \lambda V = W$ in C_0 , and there exists M > 0 such that, for any $W \in C_0$, $||V|| \leq M ||W||$. The spectrum of \mathcal{L} consists of non-regular values:

$$\sigma(\mathcal{L}) := \{\lambda \in \mathbb{C} \mid \lambda \text{ not regular}\}.$$

The number λ is called an eigenvalue if $\mathcal{L} - \lambda I$ has no inverse (i.e. there exists $V \in C_0$, $V \neq 0$, such that $\mathcal{L}V - \lambda V = 0$.) The essential spectrum of L is

$$\sigma_{e}(\mathcal{L}) := \{\lambda \in \sigma(\mathcal{L}) \mid \lambda \text{ is not an isolated eigenvalue}\}.$$

In order to characterise the spectrum the corresponding first-order system has to be investigated. Let $x = (V, V')^T$, $y = (0, W)^T$, then the first-order system corresponding to equation $\mathcal{L}V - \lambda V = W$ is

$$\dot{x}(s) = A_{\lambda}(s)x(s) + y(s), \tag{9}$$

where

$$A_{\lambda}(s) = \begin{pmatrix} 0 & I \\ D^{-1}(\lambda I - Q(s)) & -D^{-1}B \end{pmatrix},$$
 (10)

here we do not deal with the results concerning the first-order system, see e.g. [27,28], only their consequences concerning the operator \mathcal{L} are cited. Since function Q tends to a limit at $\pm \infty$, the limits

$$A_{\lambda}^{\pm} = \lim_{s \to \pm \infty} A_{\lambda}(s),$$

exist. The dimension of the stable, unstable and central subspaces of the matrices A_{λ}^{\pm} play an important role. Denote the number of eigenvalues (with multiplicity) of A_{λ}^{+} with positive, negative, zero real part by $n_{u}^{+}(\lambda)$, $n_{s}^{+}(\lambda)$, $n_{c}^{+}(\lambda)$, respectively. We define $n_{u}^{-}(\lambda)$, $n_{c}^{-}(\lambda)$ similarly using A_{λ}^{-} . In the case $n_{c}^{+}(\lambda) = 0 = n_{c}^{-}(\lambda)$ exponential dichotomies and perturbation theorems [27,29] can be used to show that there exists an $n_{s}^{+}(\lambda)$ dimensional subspace $E_{s}^{+}(\lambda) \subset \mathbb{C}^{2m}$ of initial conditions from which the solution of the homogeneous equation $\dot{x}(s) = A_{\lambda}(s)x(s)$ tends to zero at $+\infty$, and there exists an $n_{u}^{-}(\lambda)$ dimensional subspace $E_{u}^{-}(\lambda) \subset \mathbb{C}^{2m}$ of initial conditions from which the solution of the solution of the homogeneous equation $\dot{x}(s) = A_{\lambda}(s)x(s)$ tends to zero at $-\infty$. The following theorem is proved in [7].

Theorem 1. If $n_c^+(\lambda) > 0$ or $n_c^-(\lambda) > 0$, then $\lambda \in \sigma(\mathcal{L})$. If $n_c^+(\lambda) = 0 = n_c^-(\lambda)$, then the following two statements hold.

- 1. λ is an eigenvalue of $\mathcal{L} \Leftrightarrow \dim(E_s^+(\lambda) \cap E_u^-(\lambda)) > 0$.
- 2. λ is a regular value of $\mathcal{L} \Leftrightarrow E_s^+(\lambda) \oplus E_u^-(\lambda) = \mathbb{C}^{2m}$.

Remark 1. If $n_c^+(\lambda) = 0 = n_c^-(\lambda)$, then the operator $\mathcal{L} - \lambda I$ is Fredholm, and its Fredholm index is $\alpha(\mathcal{L} - \lambda I) = \dim E_s^+(\lambda) + \dim E_u^-(\lambda) - 2m$, see [7,28].

Using that $E_s^+(\lambda) \oplus E_u^-(\lambda) = \mathbb{C}^{2m}$ is equivalent to dim $E_s^+(\lambda) + \dim E_u^-(\lambda) = 2m$ and dim $(E_s^+(\lambda) \cap E_u^-(\lambda)) = 0$, the following statements are obvious consequences of the above theorem.

Corollary 1. Assume $n_c^+(\lambda) = 0 = n_c^-(\lambda)$.

- 1. If dim $E_s^+(\lambda)$ + dim $E_u^-(\lambda) > 2m$, then λ is an eigenvalue of \mathcal{L} .
- 2. If dim $E_s^+(\lambda)$ + dim $E_u^-(\lambda) < 2m$, then $\lambda \in \sigma(\mathcal{L})$.
- 3. If dim $E_s^+(\lambda)$ + dim $E_u^-(\lambda) = 2m$ and dim $(E_s^+(\lambda) \cap E_u^-(\lambda)) = 0$, then λ is a regular value of \mathcal{L} .
- 4. If dim $E_s^+(\lambda)$ + dim $E_u^-(\lambda) = 2m$ and dim $(E_s^+(\lambda) \cap E_u^-(\lambda)) > 0$, then λ is an eigenvalue of \mathcal{L} .

The dimension of $E_s^+(\lambda)$ and $E_u^-(\lambda)$ can be determined explicitly, because only the eigenvalues of the matrices A_{λ}^{\pm} have to be determined to obtain these dimensions. However, for dim $(E_s^+(\lambda) \cap E_u^-(\lambda))$ the full system must be solved numerically. This leads to the definition of the Evans function.

Let

$$\Omega = \{\lambda \in \mathbb{C} : n_c^+(\lambda) = 0 = n_c^-(\lambda), n_s^+(\lambda) + n_u^-(\lambda) = 2m\}.$$

For $\lambda \in \Omega$ denote the base of the subspace $E_s^+(\lambda)$ by $v_1^+, \ldots, v_{n_s^+}^+$, and the base of the subspace $E_u^-(\lambda)$ by $v_1^-, \ldots, v_{n_u^-}^-$. The assumption dim $(E_s^+(\lambda) \cap E_u^-(\lambda)) > 0$ means that the two bases together give a linearly dependent system of vectors, that is, the determinant formed by these 2m vectors is zero. Hence the eigenvalues of \mathcal{L} can be obtained using the determinant formed by the vectors of the two bases. The Evans function can be defined as this determinant.

Definition 2. The Evans function belonging to the operator \mathcal{L} is $\mathcal{D} : \Omega \to \mathbb{C}$

$$\mathcal{D}(\lambda) = \det\left(v_1^+ \dots v_{n_s^+}^+ v_1^- \dots v_{n_u^-}^-\right)$$

We have seen that the eigenvalues are the zeros of the Evans function. It can be also shown that the multiplicity of an eigenvalue is equal to the multiplicity of the zero of the Evans function, and that the Evans function is an analytic function on the domain Ω [30]. Hence the zeros of \mathcal{D} are isolated, that is in the domain where dim $E_s^+(\lambda) + \dim E_u^-(\lambda) = 2m$ there can be only isolated eigenvalues.

The bases of the stable and unstable subspaces can be determined numerically in the following way. We calculate the eigenvalues of A_{λ}^{+} with negative real part, and its corresponding eigenvectors. Denote these eigenvalues by μ_1, \ldots, μ_k , and the eigenvectors by u_1, \ldots, u_k (for short we used the notation $k = n_s^+(\lambda)$). Similarly, denote the eigenvalues of A_{λ}^{-} with positive real part by v_1, \ldots, v_l , and the corresponding eigenvectors by v_1, \ldots, v_l (for short we use the notation l = $n_{\mu}^{-}(\lambda)$). Then choosing a sufficiently large number L we solve the homogeneous equation $\dot{x}(s) = A_{\lambda}(s)x(s)$ in [0, L] starting from the right end point with initial condition $x(L) = u_i e^{\mu_i L}$ for i = 1, ..., k. Hence we get $k = n_s^+(\lambda)$ linearly independent (approximating) solutions of the differential equations, therefore their values at y = 0 give a base of $E_s^+(\lambda)$. Similarly, solving the differential equation in [-L, 0] we get a base of $E_u^-(\lambda)$, and the determinant defining the Evans function can be computed. We note that if L is very large and there is a significant difference between the real parts of the eigenvalues μ_1, \ldots, μ_k , then the solution belonging to the eigenvalue with largest real part will dominate and the solutions starting from linearly independent initial conditions will be practically linearly dependent at zero. (Similar case can occur in [-L, 0].) To overcome this difficulty the problem can be extended to a wedge product space of higher dimension [14].

We now show a method to determine the eigenvalues and eigenvectors of A_{λ}^{\pm} , which determine the dimensions of $E_s^+(\lambda)$ and $E_u^-(\lambda)$. We deal with the two cases together, therefore for short we introduce

$$A_{\lambda} = \begin{pmatrix} 0 & I \\ D^{-1}(\lambda I - Q) & -D^{-1}B \end{pmatrix},\tag{11}$$

where Q can be Q^+ or Q^- . Denote an eigenvalue of A_{λ} by μ and an eigenvector by $u = (u_1, u_2)^T$, that is

$$\begin{pmatrix} 0 & I \\ D^{-1}(\lambda I - Q) & -D^{-1}B \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \mu \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}.$$

Then $u_2 = \mu u_1$ and $D^{-1}(\lambda I - Q)u_1 - D^{-1}Bu_2 = \mu u_2$, hence

$$D^{-1}(\lambda I - Q)u_1 - D^{-1}B\mu u_1 = \mu^2 u_1,$$

yielding

$$(\mu^2 D + \mu B + Q - \lambda I)u_1 = 0.$$

Thus we have established the following proposition.

Proposition 1. The number μ is an eigenvalue and $u = (u_1, u_2)^T$ is an eigenvector of A_{λ} if and only if

$$\det(\mu^2 D + \mu B + Q - \lambda I) = 0 \text{ and } u_1 \in \ker(\mu^2 D + \mu B + Q - \lambda I), \quad u_2 = \mu u_1.$$
(12)

Thus the eigenvalues of A_{λ}^{\pm} are determined by equation (12) of degree 2m. Once these eigenvalues are found, the essential spectrum of \mathcal{L} can be given explicitly. The remaining part of the spectrum, i.e. the isolated eigenvalues, can be determined only numerically in general, a tool for which is the Evans function. However, the real part of these eigenvalues can be estimated analytically. An estimate is established in the next Proposition.

Proposition 2. Assume that the eigenfunction V corresponding to the eigenvalue λ of operator \mathcal{L} is in $L^2(\mathbb{R}, \mathbb{C}^m)$. Let

$$M_{jj} = \sup_{\mathbb{R}} Q_{jj}, \quad M_{ij} = \sup_{\mathbb{R}} |Q_{ij}|, \quad i \neq j.$$

Then we have

$$\operatorname{Re}\lambda \leqslant \sup_{|a|=1} \langle Ma, a \rangle.$$

In addition to the Evans function method the isolated eigenvalues can be found with a finite-difference discretisation of the eigenvalue problem $\mathcal{L}V = \lambda V$. This method can be faster numerically, but it gives no information on the essential spectrum. Using this method first we truncate the problem to a bounded interval [-L, L]. In [31] it is shown that the eigenvalues of the truncated problem tend to those of the original problem as $L \to \infty$. Then the truncated eigenvalue problem is discretised with finite differences on a grid of N points and the mN dimensional matrix eigenvalue problem is solved. It is known that the eigenvalues of the matrix eigenvalue problem tend to those of the truncated problem as $N \rightarrow \infty$ [32]. Finally, the values of L and N has to be increased until the required accuracy is achieved.

3. Combustion waves

In the special case when Q is an upper or lower triangular matrix the matrix in (12) is upper or lower triangular, hence its determinant is the product of its diagonal elements. Therefore the left-hand side of the equation is a product of m second degree polynomials, and the solutions can be computed explicitly. For combustion systems of the forms (1) and (2) the matrices Q^+ and Q^- are often upper or lower triangular. We will give sufficient conditions for this later in this Section. First we present a simple method for determining the dimensions of $E_s^+(\lambda)$ and $E_u^-(\lambda)$ geometrically when Q^+ and Q^- are upper or lower triangular matrices. Finally, we will illustrate the method with some examples.

We will deal with the cases $E_s^+(\lambda)$ and $E_u^-(\lambda)$ together, therefore for short we omit the \pm signs and consider the eigenvalues of A_{λ} given in (11). The number of eigenvalues (with multiplicity) with negative, zero, positive real part is denoted by $n_s(\lambda)$, $n_c(\lambda)$, $n_u(\lambda)$, respectively.

Proposition 3. If Q is an upper or lower triangular matrix, then the set $\{\lambda \in \mathbb{C} : n_c(\lambda) \ge 1\}$ consists of the following m parabolas or half lines:

$$P_j = \{\lambda_1 + i\lambda_2 \in \mathbb{C} : \lambda_1 = Q_{jj} - \frac{D_{jj}}{B_{jj}^2}\lambda_2^2\} \text{ if } B_{jj} \neq 0,$$

$$P_j = \{\lambda \in \mathbb{R} : \lambda \leq Q_{jj}\} \text{ if } B_{jj} = 0,$$

$$(j = 1, 2, \dots, m).$$

Proof. Since the matrix in (12) is upper or lower triangular, its determinant is the product of its diagonal elements. Thus μ is an eigenvalue of A_{λ} if and only if

$$\prod_{j=1}^{m} (D_{jj}\mu^2 + B_{jj}\mu + Q_{jj} - \lambda) = 0.$$

Therefore $\mu = i\omega$ (with $\omega \in \mathbb{R}$) is an eigenvalue of A_{λ} if and only if there exist an index $1 \leq j \leq m$ for which $-D_{jj}\omega^2 + iB_{jj}\omega + Q_{jj} - \lambda_1 - \lambda_2 i = 0$, that is $B_{jj}\omega = \lambda_2$ and $-D_{jj}\omega^2 + Q_{jj} = \lambda_1$. Hence eliminating ω , in the case $B_{jj} = 0$ we get $\lambda_2 = 0$, $\lambda_1 \leq Q_{jj}$; and in the case $B_{jj} \neq 0$ we get $\lambda_1 = Q_{jj} - D_{jj}\lambda_2^2/B_{jj}^2$.

To prove the next Proposition we will need the following elementary auxiliary result.

Proposition 4. Let $p \in \mathbb{R}$ and $\rho \in \mathbb{C}$ be arbitrary numbers. Then $\operatorname{Re}(\sqrt{p^2 + \rho}) > |p|$ if and only if $(\operatorname{Im} \rho)^2 > -4p^2 \operatorname{Re} \rho$.

Proposition 5. Assume that Q is an upper or lower triangular matrix the diagonal elements of which are non-positive, and let $\lambda \in \mathbb{C}$ satisfying $\lambda \notin P_j$ for all $1 \leq j \leq m$.

- 1. If $B_{jj} > 0$ for all $1 \le j \le m$, and λ is on the right-hand side of k parabolas P_j and on the left-hand side of m-k of parabolas, then $n_c(\lambda) = 0$, $n_u(\lambda) = k$, $n_s(\lambda) = 2m k$.
- 2. If $B_{jj} < 0$ for all $1 \le j \le m$, and λ is on the right-hand side of k parabolas P_j and on the left-hand side of m-k of parabolas, then $n_c(\lambda) = 0$, $n_u(\lambda) = 2m k$, $n_s(\lambda) = k$.
- 3. If $B_{jj} = 0$ for all $1 \leq j \leq m$, then $n_c(\lambda) = 0$, $n_u(\lambda) = m$, $n_s(\lambda) = m$.

Proof. We prove the case $B_{jj} > 0$, the proofs of the other cases are similar. Since the matrix in (12) is upper or lower triangular, its determinant is the product of its diagonal elements. Thus μ is an eigenvalue of A_{λ} if and only if

$$\prod_{j=1}^{m} (D_{jj}\mu^2 + B_{jj}\mu + Q_{jj} - \lambda) = 0$$

that is there exist an index $1 \leq j \leq m$ for which

$$D_{ij}\mu^2 + B_{ij}\mu + Q_{ij} - \lambda = 0.$$
(13)

We show that if λ is on the right-hand side of P_j , then (13) has one solution with positive and one solution with negative real part. On the other hand if λ is on the left-hand side of P_j , then (13) has two solutions with negative real part. Hence if λ is on the right-hand side of k parabolas, then there are k eigenvalues of A_{λ} with positive real part and 2(m-k)+k = 2m-k eigenvalues with negative real part.

The solutions of (13) are

$$\mu_{1,2} = \frac{-B_{jj} \pm \sqrt{B_{jj}^2 + 4D_{jj}(\lambda - Q_{jj})}}{2D_{jj}}$$

According to Proposition 4

$$\operatorname{Re}_{\sqrt{B_{jj}^2+4D_{jj}(\lambda-Q_{jj})}} > |B_{jj}|,$$

if and only if

$$\operatorname{Im}(4D_{jj}(\lambda - Q_{jj})) > -4B_{jj}^2\operatorname{Re}(4D_{jj}(\lambda - Q_{jj})),$$

which is equivalent to the inequality $\operatorname{Re}\lambda > Q_{jj} - D_{jj}(\operatorname{Im}\lambda/B_{jj})^2$. This inequality expresses that λ is on the right-hand side of P_j . Thus if λ is on the right hand side of P_j , then $\operatorname{Re}\mu_1 > 0 > \operatorname{Re}\mu_2$. But if λ is on the left hand side of P_j , then $\operatorname{Re}\sqrt{B_{jj}^2 + 4D_{jj}(\lambda - Q_{jj})} < |B_{jj}|$, yielding $\operatorname{Re}\mu_1 < 0$, $\operatorname{Re}\mu_2 < 0$, because $B_{jj} > 0$.

Remark 2. The values of $n_c(\lambda)$, $n_u(\lambda)$ and $n_s(\lambda)$ can be determined also in the case when the diagonal elements B_{jj} have different signs. We do not formalise the statement in this general case, because it is quite complicated and in most of the cases $B_{jj} = c$, i.e. they have the same signs.

In the case $Q = Q^+$ denote the parabolas (or half lines) by P_j^+ , and in the case $Q = Q^-$ denote the parabolas (or half lines) by P_j^- . According to Proposition 3 the parabolas (or half lines) P_j^+ , P_j^- are in the essential spectrum of \mathcal{L} . The other parts of the essential spectrum can also be given with the help of these parabolas, as the dimensions of $E_s^+(\lambda)$ and $E_u^-(\lambda)$ are given in Proposition 5. The isolated eigenvalues can be determined numerically by the Evans function, the domain of which also can be given using the above parabolas, as stated in the next Corollary of Proposition 5.

Corollary 2. Assume that the diagonal elements B_{jj} have the same sign, and Q^+ , Q^- are upper or lower triangular matrices the diagonal elements of which are non-positive. If λ is on the right hand side of all parabolas P_j^+ , P_j^- , then dim $E_s^+(\lambda) = m = \dim E_u^-(\lambda)$, hence λ is in the domain of the Evans function.

We now give sufficient conditions to ensure that Q^+ , Q^- are upper or lower triangular matrices for systems (1) and (2). The non-linear terms of systems (1) and (2) are given by the function $F : \mathbb{R}^{n+1} \to \mathbb{R}^{n+1}$ the coordinate functions are given by

$$F_i(a_1, \dots, a_n, b) = \sum_{j=1}^r \Gamma_{ij} w_j(a_1, \dots, a_n, b) - H_i(b),$$
(14)

where $H_i(b) = 0$ (i = 1, ..., n) and $H_{n+1}(b) = h(b)$. Hence from (4), (7) and (8)

$$Q^{-} = F'(a_{10}, \dots, a_{n0}, 0), \qquad Q^{+} = F'(a_{1}^{+}, \dots, a_{n}^{+}, b^{+}),$$
 (15)

where a_i^+ , b^+ are the limits of $a_i(s)$, b(s) as $s \to +\infty$ and F' denotes the Jacobian.

Proposition 6. Assume that all activation energies are non-zero, i.e. $\mu_j \neq 0$ for all j = 1, 2, ..., n. Then Q^- is a diagonal matrix with non-positive elements. If the temperature profile is pulse type, i.e. $b^+ = 0$, then Q^+ is also a diagonal matrix

with non-positive elements. (In fact, these matrices can have only one non-zero element, at the position (n + 1, n + 1).)

Proof. We show that for any a_1^*, \ldots, a_n^* the matrix $F'(a_1^*, \ldots, a_n^*, 0)$ has only one non-zero element, which is at the position (n + 1, n + 1) and is non-positive. Hence both statements follow from (15). The Jacobian matrix $F'(a_1^*, \ldots, a_n^*, 0)$ consists of the elements $\partial_k F_i(a_1^*, \ldots, a_n^*, 0)$. Since $\lim_{b\to 0} e^{\mu_j(b-1)/b} = 0$ when $\mu_j \neq 0$, from (3) we have $\partial_k w_j(a_1^*, \ldots, a_n^*, 0) = 0$ for all $j = 1, \ldots, r, k =$ $1, \ldots, n$. Similarly, $\lim_{b\to 0} \mu_j e^{\mu_j(b-1)/b}/b^2 = 0$ implies $\partial_{n+1}w_j(a_1^*, \ldots, a_n^*, 0) = 0$ for all $j = 1, \ldots, r$. Therefore using (14) we get $\partial_k F_i(a_1^*, \ldots, a_n^*, 0) = 0$ for all $k = 1, \ldots, n$. The only nonzero element of the Jacobian can be $\partial_{n+1}F_{n+1}(a_1^*, \ldots, a_n^*, 0) =$ $-h'(0) \leq 0$. The inequality follows from h(0) = 0 and $h(b) \geq 0$ for b > 0.

Proposition 7. If every species occurs in only one reaction in which it is decreasing $(\alpha_{ii} - \beta_{ii} \leq 0)$, and *h* is a non decreasing function, then Q^+ is a lower triangular matrix with non-positive elements.

Proof. It can be assumed that A_i appears only in the *i*-th reaction, and that the number of reactions is equal to the number of species, i.e. r = n. Then omitting the last row of Γ we get a diagonal matrix with non-positive elements (since $\alpha_{ii} - \beta_{ii} \leq 0$). Hence from (14)

$$F_i(a_1,...,a_n,b) = \Gamma_{ii} e^{\mu_j (b-1)/b} a_{ii}^{\alpha_{ii}}, \quad i = 1,...,n,$$

yielding $\partial_k F_i(a_1, \ldots, a_n, b) = 0$ for $1 \le k \le n$, $k \ne i$ (these equations hold for any value of a_1, \ldots, a_n, b). For k = n + 1 we have $\partial_{n+1} F_i(a_1^+, \ldots, a_n^+, b^+) = 0$, for

$$\partial_{n+1}F_i(a_1^+,\ldots,a_n^+,b^+) = \Gamma_{ii}\mu_j e^{\mu_j(b^+-1)/b^+}(b^+)^{-2}(a_i^+)^{\alpha_{ii}}$$

= $\mu_j(b^+)^{-2}F_i(a_1^+,\ldots,a_n^+,b^+) = 0,$

where the last equality follows from the differential equation (1). Thus we have shown that Q^+ is a lower triangular matrix. Now we determine the signs of the diagonal elements. For $1 \le i \le n$ we have

$$\partial_i F_i(a_1^+,\ldots,a_n^+,b^+) = \Gamma_{ii}\alpha_{ii}e^{\mu_j(b^+-1)/b^+}(a_i^+)^{\alpha_{ii}-1} \leq 0,$$

because $\Gamma_{ii} = (\alpha_{ii} - \beta_{ii})\gamma_{ii} \leq 0$ for $1 \leq i \leq n$. For the case i = n + 1

$$F_{n+1}(a_1,\ldots,a_n,b) = \sum_{i=1}^n \Gamma_{n+1,i} e^{\mu_i(b-1)/b} a_i^{\alpha_{ii}} - h(b).$$

As mentioned above $e^{\mu_i(b^+-1)/b^+}(a_i^+)^{\alpha_{ii}}=0$, hence

$$\partial_{n+1}F_{n+1}(a_1^+,\ldots,a_n^+,b^+) = \sum_{i=1}^n \Gamma_{n+1,i}\mu_i(b^+)^{-2} \mathrm{e}^{\mu_i(b^+-1)/b^+}(a_i^+)^{\alpha_{ii}} - h'(b^+) \leq 0.$$

We now apply the above results to the examples mentioned in the Introduction. In the case of the first-order reaction with Newtonian heat loss the differential equations (1) and (2) take the form

$$L_A^{-1}a'' - ca' - af(b) = 0, (16)$$

$$b'' - cb' + af(b) - \gamma b = 0, \tag{17}$$

where a is the scaled fuel concentration, b is scaled temperature, γ is the heat loss parameter and

$$f(b) = e^{\mu \frac{b-1}{b}}.$$
 (18)

The boundary conditions are

$$a \to 1, \ b \to 0 \quad \text{as } s \to -\infty, \qquad a' \to 0, \ b' \to 0 \quad \text{as } s \to +\infty.$$
 (19)

The stability of this system was investigated in detail in [23]. Now we have

$$D = \begin{pmatrix} L_A^{-1} & 0\\ 0 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} -c & 0\\ 0 & -c \end{pmatrix}, \quad Q(s) = \begin{pmatrix} -f(b(s)) & -a(s)f'(b(s))\\ f(b(s)) & a(s)f'(b(s)) - \gamma \end{pmatrix}.$$

From equation (17) follows $b \to 0$ for $y \to -\infty$ and for $y \to +\infty$, hence

$$Q^{+} = Q^{-} = \begin{pmatrix} 0 & 0 \\ 0 & -\gamma \end{pmatrix}.$$
 (20)

According to Propositions 3 and 5 the essential spectrum of the linearised operator L is determined by the parabolas

$$P_1 = \left\{ \lambda \in \mathbb{C} : \operatorname{Re}\lambda = -\frac{(\operatorname{Im}\lambda)^2}{L_A c^2} \right\}, \qquad P_2 = \left\{ \lambda \in \mathbb{C} : \operatorname{Re}\lambda = -\gamma - \frac{(\operatorname{Im}\lambda)^2}{c^2} \right\},$$
(21)

omitting the \pm indices because $P_j^+ = P_j^-$. These parabolas are shown in figure 1. They divide the complex plane into regions (in the figure the case $L_A = 1$ is shown when there are three regions) where the value of $n_s^+(\lambda)$ and $n_u^-(\lambda)$ can be easily obtained from Proposition 5. These values are also shown in figure 1. According to Theorem 1 the two parabolas belong to the essential spectrum.



Figure 1. The parabolas determining the essential spectrum of the operator obtained after linearisation of systems (16) and (17). The dimension of the subspace $E_s^+(\lambda)$ is shown in the upper part, the dimension of the subspace $E_u^-(\lambda)$ is shown in the lower part.

Since at any point λ which is not in the parabolas dim $E_s^+(\lambda) + \dim E_u^-(\lambda) = 4$ holds, Corollary 1 implies that the essential spectrum consists of the two parabolas, and the domain lying on the left-hand side of both parabolas consists of regular values of \mathcal{L} , because dim $E_s^+(\lambda) = 0$. The isolated eigenvalues can only be on the right-hand side of P_1 . In this domain the Evans function can be defined. As an illustration we determine the isolated eigenvalues of \mathcal{L} with largest real part in the case $L_A = 1$ and $\gamma < \gamma_{ext}$, where γ_{ext} is the extinction value of the heat loss parameter. For $\gamma < \gamma_{ext}$ there are two solutions of (16), (17), (19) with two different flame velocities $c_1 > c_2$. The solution with c_1 is stable, that with c_2 is unstable. This can be verified using the Evans function as follows. We compute the image of a half circle centered at the origin and lying in the right half plane under the Evans function \mathcal{D} . If the image winds around the origin, then by the argument principle there is (at least one) zero of \mathcal{D} in the half circle, that is there exists an eigenvalue of \mathcal{L} with positive real part, hence the corresponding flame is unstable. Choosing a sufficiently large half circle all the eigenvalues with positive real part are inside the half circle, because of the *a priori* estimate given in Proposition 2. If the image of this half circle does not wind around the origin, then there is no zero of the Evans function in the right half of the complex plane, i.e. the operator \mathcal{L} has no eigenvalues there, hence the corresponding flame is stable. The images of the appropriate half circles are shown in figure 2. For the flame moving with velocity c_1 the image is shown in figure 2a, where the winding number is 0, i.e. there is no eigenvalue in the right half plane, hence the flame is stable. For the flame moving with velocity c_2 the image is shown in figure 2b, where the winding number is 1, i.e. there is an eigenvalue in the right half plane, hence the flame is unstable.



Figure 2. The image of a half circle lying in the right half of the complex plane under the Evans function \mathcal{D} in the case $L_A = 1$. The value of γ is below, but close to the extinction value. (a) the velocity c_1 corresponds to the stable solution, there is no eigenvalue in the half circle, the winding number (wn) is zero. (b) the velocity c_2 corresponds to the unstable solution, there is one eigenvalue in the half circle, the winding number (wn) is one.

Now consider the case of the exothermic–endothermic system. The differential equations (1) and (2) take the form

$$L_A^{-1}a'' - c a' - af_1(b) = 0, (22)$$

$$L_W^{-1}w'' - c w' - \beta w f_2(b) = 0, \qquad (23)$$

$$b'' - cb' + af_1(b) - \alpha w f_2(b) = 0, \tag{24}$$

where a is the scaled fuel concentration, b is scaled temperature, w is the concentration of the endothermic species, and

$$f_1(b) = e^{\mu_1(b-1)/b}, \quad f_2(b) = e^{\mu_2(b-1)/b}.$$
 (25)

The boundary conditions are

$$a \to 1, \ w \to 1, \ b \to 0 \quad \text{as } s \to -\infty,$$
 (26)

$$a' \to 0, \ w' \to 0, \ b' \to 0 \quad \text{as } s \to +\infty.$$
 (27)

This system was investigated in detail in [22]. Now we have

$$D = \begin{pmatrix} L_A^{-1} & 0 & 0\\ 0 & L_W^{-1} & 0\\ 0 & 0 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} -c & 0 & 0\\ 0 & -c & 0\\ 0 & 0 & -c \end{pmatrix}$$

and

$$Q(s) = \begin{pmatrix} -f_1(b(s)) & 0 & -a(s)f'_1(b(s)) \\ 0 & -\beta f_2(b(s)) & -\beta w(s)f'_2(b(s)) \\ f_1(b(s)) & \alpha f_2(b(s)) & a(s)f'_1(b(s)) - \alpha w(s)f'_2(b(s)) \end{pmatrix}$$

From equations (22)–(24) it follows that there can be front $(\alpha > \beta)$ and pulse $(\alpha < \beta)$ type temperature profiles, see [22]. For pulses $b \to 0$ as $s \to +\infty$, and for fronts $b \to \alpha/\beta$, $a \to 0$, $w \to 0$ as $s \to +\infty$. Hence Q^- is a 3×3 zero matrix,

$$Q^{+} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \text{ for pulses, } Q^{+} = \begin{pmatrix} -q_{1} & 0 & 0 \\ 0 & -\beta q_{2} & 0 \\ q_{1} & -\alpha q_{2} & 0 \end{pmatrix} \text{ for fronts,}$$

where $q_1 = f_1(1 - \alpha/\beta)$, $q_2 = f_2(1 - \alpha/\beta)$. Since these are lower triangular matrices with non-positive diagonal elements, according to Propositions 3 and 5 the essential spectrum of the linearised operator \mathcal{L} is determined by the parabolas

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$$P_1^+ = \left\{ \lambda \in \mathbb{C} : \operatorname{Re}\lambda = -q_1 - \frac{(\operatorname{Im}\lambda)^2}{L_A c^2} \right\}, \qquad P_1^- = \left\{ \lambda \in \mathbb{C} : \operatorname{Re}\lambda = -\frac{(\operatorname{Im}\lambda)^2}{L_A c^2} \right\},$$
$$P_2^+ = \left\{ \lambda \in \mathbb{C} : \operatorname{Re}\lambda = -\beta q_2 - \frac{(\operatorname{Im}\lambda)^2}{L_W c^2} \right\}, \qquad P_2^- = \left\{ \lambda \in \mathbb{C} : \operatorname{Re}\lambda = -\frac{(\operatorname{Im}\lambda)^2}{L_W c^2} \right\},$$
$$P_3^+ = \left\{ \lambda \in \mathbb{C} : \operatorname{Re}\lambda = -\frac{(\operatorname{Im}\lambda)^2}{c^2} \right\}, \qquad P_3^- = \left\{ \lambda \in \mathbb{C} : \operatorname{Re}\lambda = -\frac{(\operatorname{Im}\lambda)^2}{c^2} \right\}.$$

(In order to treat pulses and fronts together we let $q_1 = q_2 = 0$ in the case of pulses.) These parabolas are shown in figure 3. They divide the complex plane into regions where the value of $n_s^+(\lambda)$ and $n_u^-(\lambda)$ can be easily obtained from Proposition 5. These values are also shown in figure 3. According to Theorem 1 all the parabolas belong to the essential spectrum.

In the case of a pulse solution $P_j^+ = P_j^-$, hence similarly to the previous example, the essential spectrum consists only of the three parabolas. The domain lying on the left-hand side of all parabolas contains regular values of \mathcal{L} , because dim $E_s^+(\lambda) + \dim E_u^-(\lambda) = 6$ and dim $E_s^+(\lambda) = 0$, implying dim $(E_s^+(\lambda) \cap E_u^-(\lambda)) = 0$. In the domain lying on the right-hand side of all parabolas we have dim $E_s^+(\lambda) + \dim E_u^-(\lambda) = 6$, hence the Evans function can be defined there.

In the case of a front solution the essential spectrum contains open domains as well as the three parabolas. For example in the domain between P_1^+ and P_3^+ in figure 3b we have dim $E_s^+(\lambda) + \dim E_u^-(\lambda) = 8$ (since $P_3^+ = P_3^-$), therefore Corollary 1 implies that this domain is filled with (obviously non-isolated) eigenvalues. It can be seen that, for any λ not lying on the parabolas, we have dim $E_s^+(\lambda) + \dim E_u^-(\lambda) \ge 6$, hence in the essential spectrum there are domains filled with eigenvalues. For given values of the parameters L_A , L_W , α , β these domains can be determined explicitly. The domain lying on the left-hand side of all parabolas again contains regular values of \mathcal{L} . In the domain lying on the right-hand side of all parabolas we have dim $E_s^+(\lambda) + \dim E_u^-(\lambda) = 6$, hence the Evans function can be defined there.

As an illustration we determine the isolated eigenvalues of \mathcal{L} with largest real part in the case $\alpha = 0$ for $L_A = L_W = 3$ and for $L_A = L_W = 4$. These values were chosen because there is a Hopf bifurcation between $L_A =$ 3 and $L_A = 4$. This can be verified using the Evans function similarly to the previous example. We again compute the image of a half circle centered at the origin and lying in the right half plane under the Evans function \mathcal{D} . The images of the appropriate half circles are shown in figure 4. In the case $L_A = 3$ the image is shown in figure 4a, where the winding number is 0, i.e. there is no eigenvalue in the right half plane, hence the flame is stable. In the case $L_A = 4$ the image is shown in figure 4b, where the winding number is 2, i.e. there is a pair of eigenvalues in the right half plane, hence the flame is unstable.

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Figure 3. The parabolas determining the essential spectrum of the operator obtained after linearisation of systems (22) and (23). The dimension of the subspace $E_s^+(\lambda)$ is shown in part (a) and (b). The dimension of the subspace $E_u^-(\lambda)$ is shown in part (c). (a) corresponds to pulses, (b) corresponds to fronts.



Figure 4. The image of a half circle lying in the right half of the complex plane under the Evans function \mathcal{D} in the case $\alpha = 0$ for two different values of L_A . (a) $L_A = 3$, the image does not wind around the origin, the winding number (wn) is zero, the corresponding solution is stable. (b) $L_A = 4$, the image winds twice around the origin, the winding number (wn) is two, hence there is a complex pair of eigenvalues with positive real part, the corresponding solution is unstable.

4. Conclusions

We have studied the stability of a steadily propagating planar laminar premixed flame with a general combustion reaction system using the Evans function method. The stability of the travelling wave solution of the corresponding time dependent system is determined by the spectrum of the linearised second-order differential operator. Exploiting the structure of the differential equations due to Arrhenius temperature dependence the spectrum was investigated in detail. A simple geometrical method was shown for the study of the essential spectrum, and for determining the domain of the Evans function. This method can be applied for systems when the matrices Q^+ and Q^- (which are the limits of Jacobian for $s \to \pm \infty$) are upper or lower triangular. Sufficient conditions were given for the reaction term to ensure that Q^+ and Q^- are lower triangular matrices. The results are applied to two combustion reactions: to a simple first-order reaction, and to an exothermic-endothermic system.

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