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DETECTING BOGDANOV–TAKENS BIFURCATION OF TRAVELING WAVES IN REACTION–DIFFUSION SYSTEMS

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In this paper we investigate the onset of instabilities in a model describing the propagation of the steady planar premixed combustion wave. In particular, we are interested in determining the Bogdanov–Takens bifurcation condition, which is investigated semi-analytically. We derive an analytic condition for the existence of this type of bifurcation and based on this criterion we numerically determine the parameter values for which the Bogdanov–Takens bifurcation occurs. This numerical method is found to be more efficient than the previous methods.

Keywords: Linear stability; Evans function; Bogdanov–Takens bifurcation; traveling wave.

1. Introduction

Premixed nonadiabatic flames have been the object of numerous studies for a long time. They have been investigated both analytically using the matched asymptotic expansion method (MAE) [Joulin & Clavin, 1979; Booty *et al.*, 1987; Billingham & Mercer, 2001] and numerically by means of either direct integration of the governing Partial Differential Equations (PDEs) [Mercer *et al.*, 1998] or by investigating the corresponding system of Ordinary Differential Equations (ODEs) obtained by reducing the governing PDEs [Gubernov *et al.*, 2004]. The comparison of these methods is also discussed in the work of Gubernov *et al.* [2003].

The numerical methods and the MAE approach qualitatively agree in describing the properties and the stability of the steady nonadiabatic waves. Papers by Joulin and Clavin [1979], Booty *et al.* [1987], Billingham and Mercer [2001], and Gubernov *et al.* [2004] show that for given parameter values the solution either does not exist or there are two solutions with different values of the wave speed, which are referred to as "fast" and "slow". At the critical parameter values the "fast" and "slow" branches coincide. This event is usually called extinction (sometimes called a fold or turning point) and as shown by Gubernov *et al.* [2004] it is a saddle-node bifurcation. The linear stability problem for the traveling wave solution was solved analytically by Joulin and Clavin [1979] employing the MAE method and numerically by Gubernov *et al.* [2004] by using the Evans function approach. It was demonstrated that the "slow" branch of the solutions is unstable, whereas the "fast" branch can either be stable or unstable depending on the parameter values. In a previous paper [Gubernov *et al.*, 2004] we investigated the transition to instability in great detail. We showed that the steady traveling wave can lose stability either monotonically or in an oscillatory fashion as we approach the point of extinction along the "fast" solution branch. The switching between these two different routes of the transition to instability occurs due to the presence of the Bogdanov–Takens bifurcation [Kuznetsov, 1998].

The parameter space of the problem consists of three parameters: τ — the inverse of the Lewis number (which is the ratio of the diffusion rates for heat and fuel); β — the ratio of the activation energy to heat release; ℓ — the nondimensional heat loss (see [Gubernov *et al.*, 2004] for further details). For fixed value of τ the Bogdanov–Takens bifurcation occurs when the curve corresponding to the Hopf bifurcation intersects with the curve corresponding to the extinction (saddle-node bifurcation) on the (β, ℓ) parameter plane. So in the parameter space (τ, β, ℓ) the Bogdanov–Takens bifurcation condition corresponds to a curve. In our previous paper [Gubernov *et al.*, 2004] we undertook a preliminary investigation of the Bogdanov–Takens bifurcation condition. It is extremely difficult to calculate this bifurcation condition (i.e. the location of this curve in the parameter space) using the Evans function method which was primarily designed to locate points of the discrete spectrum of the linearized problem on the complex plane. Indeed, in order to calculate the bifurcation condition for some fixed value of τ we have to find the critical parameter values for the Hopf and saddle-node bifurcations, i.e. calculate two curves on the (β, ℓ) parameter plane and find the point where these curves intersect. The curve corresponding to the Hopf bifurcation is calculated by finding values of β and ℓ such that the discrete spectrum of the linearized problem lies on the imaginary axis apart from the origin. This is a costly procedure in terms of numerical computation. The saddle-node locus is found using the turning point condition for the speed of the combustion wave (see [Gubernov *et al.*, 2004] for further details). While applying this procedure we encounter several difficulties: (i) as we approach the point of intersection (i.e. the Bogdanov–Takens bifurcation point) the distance between the Hopf curve and extinction curve vanishes and at some stage we are not able to distinguish them. Thus we have to decrease the numerical error in the calculations which in turn increases the calculation time substantially in order to get a better resolution of the overall scheme and find the point of intersection accurately; (ii) as we increase τ the discrete spectrum shifts very close to the origin for values of β and ℓ near the Bogdanov–Takens bifurcation point. Consequently, this makes difficult the location of this bifurcation point. As a result we are not able to systematically examine the Bogdanov–Takens bifurcation condition using the Evans function method.

In this paper, we introduce an alternative method for calculating the Bogdanov–Takens bifurcation condition based on the combination of analytical and numerical approaches. This method does not rely on the solution of the linear stability problem. Instead, it relates the linear stability problem with properties of the stationary solution, namely, the search for parameter values at which the traveling wave exhibits two simultaneous singularities: a collision between the fold or turning point and an oscillatory instability. Usually, this situation (which is referred to as the Bogdanov–Takens bifurcation) is characterized by the presence of two nontrivial zeros in the spectrum of the linear stability problem and corresponds to a test function for detecting the Bogdanov–Takens bifurcation as a point with double-zero eigenvalues [Kuznetsov, 1998]. However, there is always a trivial zero eigenvalue due to the translational invariance and therefore this approach is not applicable here. In this paper we derive a new test functional which allows us to determine the Bogdanov–Takens bifurcation condition analytically by using standard bifurcation analysis. The derived condition is then used for further numerical analysis. As a result, the difficulties described above are eliminated, the calculations are substantially simplified, and the Bogdanov–Takens bifurcation condition is systematically investigated for a wide range of parameters values which were not possible using existing methods.

The rest of the paper is organized as follows. In the next section we briefly describe the model for the steady nonadiabatic flames and some of its properties which are important in our description. In Sec. 3 we derive the analytical criterion using the perturbation approach. The comparison of the numerical results obtained by Gubernov *et al.* [2004] with the analytical prediction derived in this paper is presented in Sec. 4. Finally, in the conclusion we discuss the main results obtained in this paper.

2. Model

We rewrite the nonlinear governing partial differential equations for the nonadiabatic traveling wave (which can be found in [Gubernov *et al.*, 2004]) in the form

$$\partial_t \mathbf{u} = \mathbf{D}\mathbf{u} + \mathbf{N}(\mathbf{u}), \tag{1}$$

where $\mathbf{u} = (u(\xi,t), v(\xi,t))^T$ is a vector representing the traveling solution with u being the temperature and v being the fuel concentration profiles,

$$\mathbf{D} = \begin{bmatrix} \partial_\xi^2 + c\partial_\xi & 0 \\ 0 & \tau\partial_\xi^2 + c\partial_\xi \end{bmatrix}, \tag{2}$$

is a linear differential operator, c is the speed of the traveling wave, ξ is a nondimensional coordinate in the coordinate frame moving with the wave,

$$\mathbf{N}(\mathbf{u}) = \begin{bmatrix} ve^{-1/u} - \ell u \\ -\beta ve^{-1/u} \end{bmatrix}, \tag{3}$$

is a nonlinear vector function which consists of the reaction and the heat loss terms, τ is the inverse of the Lewis number, ℓ is the nondimensional heat loss, β is the ratio of the activation energy to heat release of the reaction.

For a steady wave traveling without changing its speed and form, Eq. (1) reduces to a system of ordinary differential equations as

$$\mathbf{M}(\mathbf{u}_s) \equiv \mathbf{D}\mathbf{u}_s + \mathbf{N}(\mathbf{u}_s) = 0, \tag{4}$$

where we use subscript "s" to denote the steady traveling wave solution, which typically looks as illustrated in Fig. 1.

We can now express the linear stability problem as

$$\mathbf{L}\mathbf{u} = \lambda\mathbf{u}, \tag{5}$$

where $\mathbf{L} = \mathbf{D} + \mathbf{W}$ and

$$\mathbf{W} \equiv \frac{\partial \mathbf{N}}{\partial \mathbf{u}} = \begin{bmatrix} v_s u_s^{-2} e^{-1/u_s} - \ell & e^{-1/u_s} \\ -\beta v_s u_s^{-2} e^{-1/u_s} & -\beta e^{-1/u_s} \end{bmatrix}, \tag{6}$$

is the matrix of first derivatives of the nonlinear vector function $\mathbf{N}(\mathbf{u})$.

Gubernov *et al.* [2004] showed that for parameter values near extinction there is always at least one point of the discrete spectra in the vicinity of the origin. Below we use subscript "e" in order to denote the parameter values that correspond to extinction. As we approach the extinction limit along the "fast" solution branch either one or two

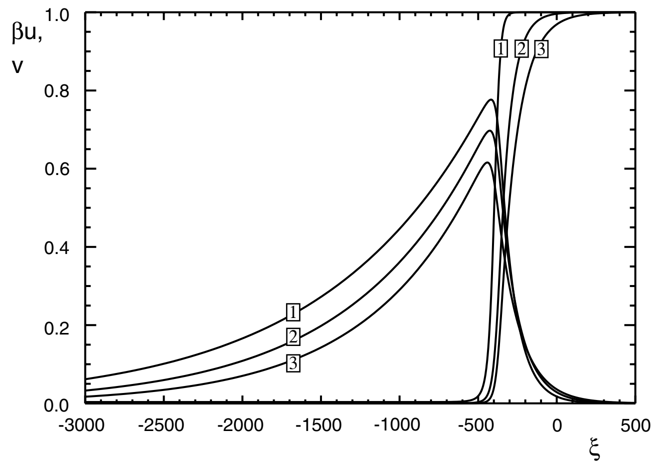

Fig. 1. Numerically determined temperature and fuel profiles of the steady traveling wave as a function of coordinate ξ for $\beta = 6$, $\ell = 10^{-5}$, and $\tau = 0.1$ (curves 1), $\tau = 0.5$ (curves 2), and $\tau = 1.0$ (curves 3). The temperature values on the graph are multiplied by β.

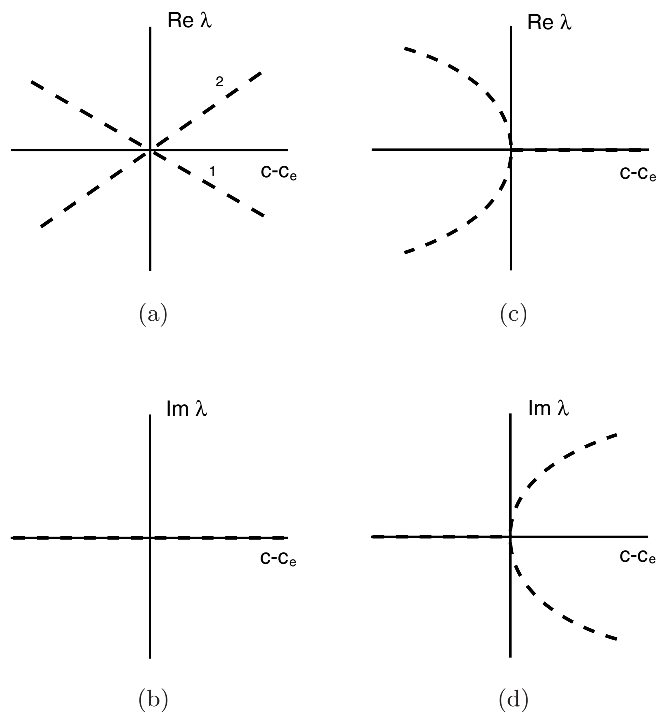

Fig. 2. Schematic diagram showing the location of the points of the discrete spectra for parameter values near the extinction limit. (a) and (b) represent the real and imaginary parts respectively of the eigenvalue moving from the left to the right half-planes (curve 1 — monotonic instability); and the eigenvalue moving from the right to the left half planes (curve 2 — oscillatory instability) respectively. (c) and (d) The real and imaginary parts respectively of a pair of eigenvalues are plotted for the case of Bogdanov–Takens bifurcation.

points of the discrete spectra coalesce with the origin and the following scenarios can occur: (i) If the instability occurs in a monotonic way, then this point moves along the real axis from the left half-plane to the right half-plane; (ii) When the transition to instability manifests itself in an oscillatory fashion, the point of the discrete spectra crosses the origin along the real axis moving from the right to the left half-planes; (iii) Finally, if the Bogdanov–Takens bifurcation occurs, then two points of the discrete spectra hit the origin along the imaginary axis giving birth to a pair of real eigenvalues after the collision. All three scenarios are plotted schematically in Fig. 2. It is convenient to consider the "slow" solution branch ($c-c_e < 0$, where c_e is the critical value of the speed that correspond to the extinction) since the eigenvalues are real in this case and in what follows we imply $\lambda \equiv \mathrm{Re}(\lambda)$. As seen from Fig. 2, the Bogdanov–Takens bifurcation is characterized by a derivative $dc/d\lambda$ being zero at the origin in contrast to the case of monotonic ($dc/d\lambda < 0$) or oscillatory ($dc/d\lambda > 0$) instabilities. Next we use this condition to obtain an analytic criteria for the existence of the Bogdanov–Takens bifurcation.

3. Perturbation Approach

In this section we solve the eigenvalue problem (5), where λ is assumed to be a small real parameter. At the point of extinction ($\mu = \mu_e$, where μ represents one of the bifurcation parameters β or ℓ; $c = c_e$) there are no solutions to (5) except for $\lambda = 0$. As we vary the system parameters slightly there appears one or two solutions with nonvanishing λ. We make a series expansion of both the solution $\mathbf{u}$ and the operator $\mathbf{L}$ near $\lambda = 0$ as

$$\begin{aligned} &\mathbf{u} = \mathbf{u}_0 + \lambda\mathbf{u}_1 + \lambda^2\mathbf{u}_2 + \cdots \quad \text{and} \\ &\mathbf{L} = \mathbf{L}_e + \lambda\mathbf{L}_{e\lambda} + \frac{1}{2}\lambda^2\mathbf{L}_{e\lambda\lambda} + \cdots, \end{aligned} \tag{7}$$

where the subscript "e" implies that the parameters are fixed at $\mu = \mu_e$ and

$$\begin{aligned} \mathbf{L}_{e\lambda} &= \frac{\partial c}{\partial\lambda}\frac{\partial\mathbf{L}}{\partial c}, \\ \mathbf{L}_{e\lambda\lambda} &= \frac{\partial^2 c}{\partial\lambda^2}\frac{\partial\mathbf{L}}{\partial c} + \frac{\partial c}{\partial\lambda}\frac{\partial^2\mathbf{L}}{\partial c^2}, \cdots \end{aligned} \tag{8}$$

For brevity we are going to use the following notation: $c_\lambda \equiv \partial c/\partial\lambda$, $c_{\lambda\lambda} \equiv \partial^2 c/\partial\lambda^2$ etc. Next, we substitute (7) into (5). In the leading order we obtain

$$\mathbf{L}_e\mathbf{u}_0 = 0. \tag{9}$$

It is easily shown that the solution to this equation is $\mathbf{u}_0 = \mathbf{u}_{s\xi}$, which sometimes is referred to as the neutral mode. Taking the derivative of (9) with respect to c and considering $\mathbf{u}_0 = \mathbf{u}_{s\xi}$ we can derive a useful expression

$$\mathbf{L}_{ec}\mathbf{u}_{s\xi} + \mathbf{L}_e\mathbf{u}_{sc\xi} = 0. \tag{10}$$

In the first order of the small parameter we obtain the equation

$$\mathbf{L}_e\mathbf{u}_1 = \mathbf{u}_{s\xi} - c_\lambda\mathbf{L}_{ec}\mathbf{u}_{s\xi}. \tag{11}$$

The solution to (11) can be found as $\mathbf{u}_1 = c_\lambda\mathbf{u}_{sc\xi} - \mathbf{u}_{sc}$, using (10) and the derivative of (4) with respect to c, namely,

$$\frac{\partial\mathbf{M}}{\partial c} = \mathbf{L}\mathbf{u}_{sc} + \frac{\partial\mu}{\partial c}\frac{\partial\mathbf{M}}{\partial\mu} + \mathbf{u}_{s\xi} = 0, \tag{12}$$

where we have taken into consideration that $\partial\mu/\partial c = 0$ for $c = c_e$. Taking a derivative of (10) with respect to c we can derive another useful expression

$$\mathbf{L}_{ecc}\mathbf{u}_{s\xi} + 2\mathbf{L}_{ec}\mathbf{u}_{sc\xi} + \mathbf{L}_e\mathbf{u}_{scc\xi} = 0. \tag{13}$$

In the second order of the small parameter expansion we obtain

$$\begin{aligned} \mathbf{L}_e\mathbf{u}_2 &= c_\lambda\mathbf{u}_{sc\xi} - \mathbf{u}_{sc} - \frac{1}{2}c_{\lambda\lambda}\mathbf{L}_{ec}\mathbf{u}_{s\xi} \\ &\quad - \frac{1}{2}c_\lambda^2\mathbf{L}_{ecc}\mathbf{u}_{s\xi} - c_\lambda^2\mathbf{L}_{ec}\mathbf{u}_{sc\xi} + c_\lambda\mathbf{L}_{ec}\mathbf{u}_{sc}. \end{aligned} \tag{14}$$

Using (10) and (13), Eq. (14) can be rewritten in the form

$$\begin{aligned} &\mathbf{L}_e\left(\mathbf{u}_2 - \frac{1}{2}c_{\lambda\lambda}\mathbf{u}_{sc\xi} - \frac{1}{2}c_\lambda^2\mathbf{u}_{sc\xi}\right) \\ &\quad = c_\lambda\mathbf{u}_{sc\xi} - \mathbf{u}_{sc} + c_\lambda\mathbf{L}_{ec}\mathbf{u}_{sc}. \end{aligned} \tag{15}$$

The solvability conditions for Eq. (15) can be written using a solution $\mathbf{v}_0$ to the problem adjoint to (9) as

$$c_\lambda(\langle\mathbf{v_0}|\mathbf{u}_{sc\xi}\rangle + \langle\mathbf{v_0}|\mathbf{L}_{ec}\mathbf{u}_{sc}\rangle) = \langle\mathbf{v_0}|\mathbf{u}_{sc}\rangle, \tag{16}$$

where we have introduced the inner product

$$\langle\mathbf{v}|\mathbf{u}\rangle = \int_{-\infty}^{+\infty}\mathbf{v}\mathbf{u}\,d\xi. \tag{17}$$

The adjoint problem is formulated as $\mathbf{L}_e^*\mathbf{v}_0 = 0$, where $\mathbf{L} = \mathbf{D}^* + \mathbf{W}^*$. Differential operator $\mathbf{D}^*$ is obtained from (2) by substituting "$-c$" instead of

"c" and $\mathbf{W}^*$ is obtained from (6) by the transposition. Differentiating (12) with respect to c and taking into account that $(\partial\mu/\partial c)_e = 0$, it can be shown that

$$\langle \mathbf{v_0} | \mathbf{u}_{sc\xi} \rangle + \langle \mathbf{v_0} | \mathbf{L}_{ec} \mathbf{u}_{sc} \rangle = -\mu_{cc} \left\langle \mathbf{v}_0 \middle| \frac{\partial \mathbf{M}}{\partial \mu} \right\rangle. \quad (18)$$

The inner product on the right-hand side of (18) does not vanish in general. Furthermore μ_{cc} does not equal zero as well since $\mu(c)$ reaches its maxima at the point of extinction. Therefore, we conclude that c_λ is equal to zero when the following condition is satisfied

$$\Psi(\mathbf{u}_s, \mathbf{v}_0) \equiv \langle \mathbf{v_0} | \mathbf{u}_{sc} \rangle = 0. \quad (19)$$

Expression (19) is the required condition for the existence of the Bogdanov–Takens bifurcation. It should be noted here that since $\mathbf{u}_s(\xi)$ is a regular function which exponentially decays on $\pm\infty$ and $\mathbf{v}_s(\xi)$ is also a regular function bounded on $\pm\infty$ (both functions depend analytically on the parameters) it is therefore expected that the functional Ψ is a bounded analytic function of the parameters. It relates the properties of the linear stability problem with certain symmetry of the stationary solution. Similar criteria were derived while investigating the linear stability of the traveling wave solutions of KdV equation [Pego *et al.*, 1993] and the nonlinear Schrödinger equation [Vakhitov & Kolokolov, 1973]. However, in both these cases it is possible to express the adjoint mode $\mathbf{v}_0$ in terms of the stationary solution $\mathbf{u}_s$ by utilizing the Hamiltonian structure of the equations. This allows rewriting the stability criteria (similar to (19)) in a simpler form. In our case the problem adjoint to (9) is more complicated than in the aforementioned examples, and to the best of our knowledge there is no clear relation between $\mathbf{v}_0$ and $\mathbf{u}_s$, which could be used to further simplify the condition (19) and hence a numerical approach is required.

4. Numerical Results

In this section we use the criteria (19) to numerically locate the Bogdanov–Takens bifurcation. It follows from this condition that we have to evaluate the functional $\Psi(\mathbf{u}_s, \mathbf{v}_0)$ and therefore it is necessary to obtain the functions $\mathbf{u}_s$ and $\mathbf{v}_0$. Using the numerical methods described by Gubernov *et al.* [2004] we calculate $\mathbf{u}_s$ for the parameter values corresponding to the extinction limit. In order to find the derivative $\mathbf{u}_{sc}$ we also determine the stationary wave solution $\mathbf{u}_s^+$ with the speed slightly greater (i.e. $c_e + \delta c$) and stationary wave solution $\mathbf{u}_s^-$ with the speed slightly less (i.e. $c_e - \delta c$) than the critical value c_e corresponding to the extinction. Then we evaluate the derivative $\mathbf{u}_{sc}$ employing the difference formula

$$\mathbf{u}_{sc} = \frac{\mathbf{u}_{sc}^+ - \mathbf{u}_{sc}^-}{2\delta c}. \quad (20)$$

We also calculate the eigenmode $\mathbf{v}_0$ of the adjoint problem by using the compound matrix method described by Gubernov *et al.* [2003] and Gubernov *et al.* [2004]. Next, the inner product of $\mathbf{u}_{sc}$ and $\mathbf{v}_0$ is determined numerically. We check the accuracy of the numerical scheme by calculating $\langle \mathbf{v}_0 | \mathbf{u}_{s\xi} \rangle$ which always has to be equal to zero since the null-space of $\mathbf{L}_e$ is automatically orthogonal to the null-space of its adjoint. In our calculations it was of the order of 10^{-6} or less. In Fig. 3 we plot the dependence of the functional $\Psi(\mathbf{u}_s, \mathbf{v}_0)$ on the heat loss for $\tau = 0.1$. The parameters of the system are varied in such a way to correspond to the limit of extinction. It is clearly seen that for some value of the heat loss ℓ, the curve crosses the axis $\Psi = 0$. This value of ℓ is the required parameter value when the Bogdanov–Takens bifurcation occurs. Next, we use the Newton–Raphson method for solving the equation $\Psi = 0$ in order to find the critical parameter values for the bifurcation. The results are presented in Figs. 4–6. We also compared the results with the parameter values for the Bogdanov–Takens bifurcation which were obtained in the paper of Gubernov *et al.* [2004] using the Evans function method. The correspondence between the predictions of the analytic method described in this paper

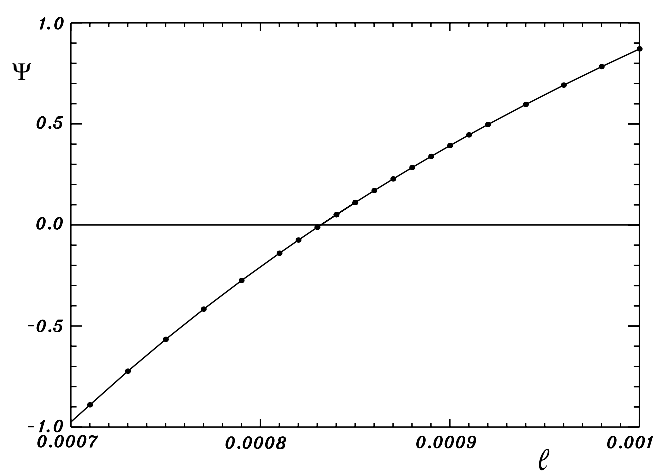

Fig. 3. Dependence of functional Ψ on heat loss parameter ℓ for $\tau = 0.1$.

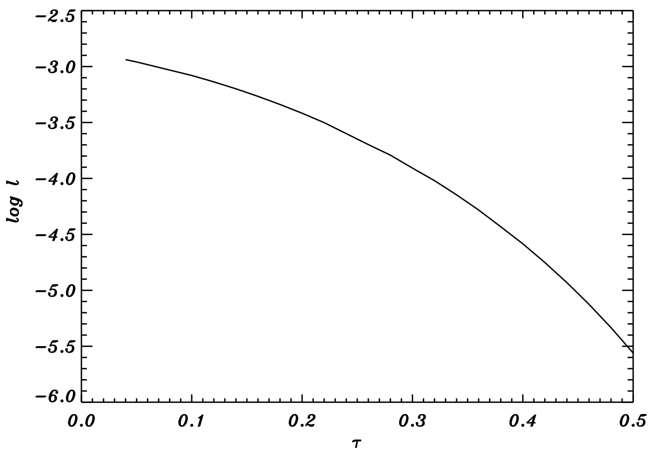

Fig. 4. The critical parameter values ℓ versus τ for the Bogdanov–Takens bifurcation.

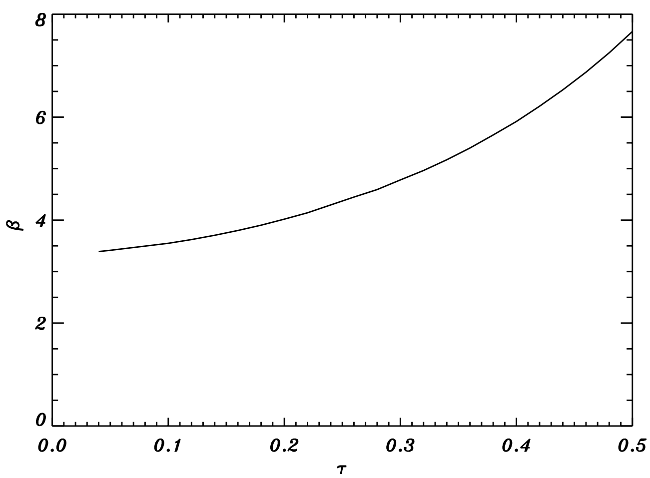

Fig. 5. The critical parameter values β versus τ for the Bogdanov–Takens bifurcation.

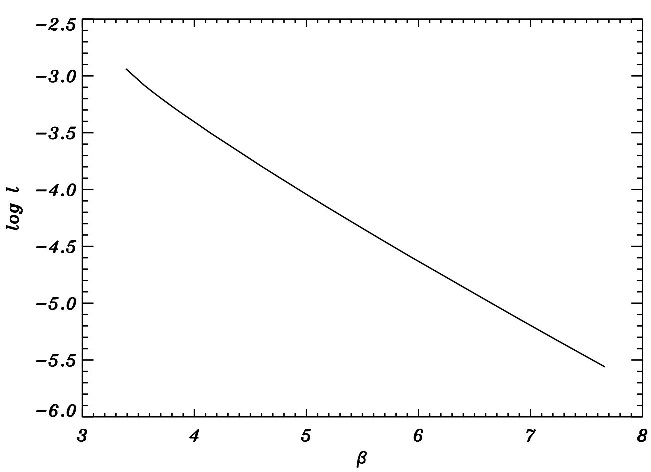

Fig. 6. The critical parameter values ℓ versus β for the Bogdanov–Takens bifurcation.

with the numerical results of Gubernov *et al.* [2004] is excellent (the difference was found in the third significant digit and hence the results from Gubernov *et al.* [2003] are not plotted). However the numerical costs involved in obtaining the results using the method described here are far less than those presented in [Gubernov *et al.*, 2003] for reasons described in the introduction. Moreover the accuracy of the results obtained in this paper is higher than the accuracy of the results which are presented in [Gubernov *et al.*, 2003], since the calculations by these authors are based upon the subjective criteria of the intersection between two curves in the parameter space, whereas in our current paper we use a strict mathematical criterion for calculating the Bogdanov–Takens bifurcation condition.

5. Conclusion

In this paper, we have investigated the Bogdanov–Takens bifurcation for the system describing the propagation of the nonadiabatic traveling premixed flames. In a previous paper [Gubernov *et al.*, 2004], we showed that in the propagation of the stationary planar combustion waves the Bogdanov–Takens bifurcation is responsible for the change in the regimes of the instability from oscillatory to monotonic. In this paper, by using the perturbation approach, we were able to derive an analytical criterion for the existence of this type of bifurcation. It relates the properties of the linear stability problem with a certain symmetry of the stationary solution. This analytical criterion was then implemented in the numerical scheme which allowed us to carry out systematic calculation of the Bogdanov–Takens bifurcation condition. We found that in terms of computational efficiency the approach presented here was far superior to that reported in [Gubernov *et al.*, 2003]. Since the perturbation analysis in Sec. 3 is applicable to any reaction–diffusion system, we believe that this approach can be easily implemented for a general class of problems leading to improved efficiency and ease of determining parameter values for which the Bogdanov–Takens bifurcation occur.

Acknowledgments

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