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Characteristic Phenomena in Combustion

DIRK MEINKÖHN

DLR-German Aerospace Research Establishment, D-74239 Hardthausen, Germany

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For the case of a reaction–diffusion system, the stationary states may be represented by means of a state surface in a finite-dimensional state space. In the simplest example of a single semi-linear model equation given in terms of a Fredholm operator, and under the assumption of a centre of symmetry, the state space is spanned by a single state variable and a number of independent control parameters, whereby the singularities in the set of stationary solutions are necessarily of the cuspoid type. Certain singularities among them represent critical states in that they form the boundaries of sheets of regular stable stationary solutions. Critical solutions provide ignition and extinction criteria, and thus are of particular physical interest. It is shown how a surface may be derived which is below the state surface at any location in state space. Its contours comprise singularities which correspond to similar singularities in the contours of the state surface, i.e., which are of the same singularity order. The relationship between corresponding singularities is in terms of lower bounds with respect to a certain distinguished control parameter associated with the name of Frank-Kamenetzkii.

Keywords: Semi-linear elliptic differential equations, Bifurcation, Criticality, Ignition, Extinction

1 INTRODUCTION

Apparently, literature offers little help in providing a comprehensive definition of combustion [1], a process which is nevertheless of considerable importance for our present-day industrial civilization. It has therefore been suggested that combustion is perhaps best described by means of a working definition, e.g., combustion is the science of exothermic reactions in flows with heat and mass transfer. Such definition, as has already been observed [1], is too narrow because there are combustion phenomena which are not encompassed by it. On the other hand, the above definition is too loose in that it comprises many processes which do not qualify as combustive ones. The conversion of iron into its oxide, for example, constitutes an exothermic reaction which one would hesitate to designate as combustive if it is a slow corrosion process. There are some qualifications lacking in the above definition, and they are precisely those which make the combustion processes interesting from the point of view of a physicist or applied mathematician: for an exothermic reaction accompanied by heat and mass transfer to qualify as combustive, it needs to evolve far away from thermodynamic equilibrium such that the nonlinearities in the process mechanism cause the appearance of certain characteristic phenomena. These could be in the form of self-similar combustion waves which are for instance connected with the concept of flame propagation as an inherent characteristic of the system, or ignition and extinction phenomena which are related to the characteristic singularities in the solution set and to the branching of solutions. Therefore, supplementing the above working definition, combustion processes comprise exothermic reactions accompanied by heat and mass transfer, for which the nonlinearities of the process mechanism are essential.

2 COMBUSTION AND REACTION–DIFFUSION SYSTEMS

Although there are many combustion processes for which convection is of major importance, reaction–diffusion processes exist which are capable of combustion also. For such systems, convective transport does not occur but due to catalytic or thermal feed-back, the process can reach critical states and is capable of self-acceleration, two properties which are regarded as hallmarks of combustion [2]. Thus, in reaction–diffusion systems, the phenomena of ignition and extinction and of combustion wave propagation are observed.

Generally, in the investigation of the characteristic phenomena of a process, the asymptotic states of the system (e.g., the steady states) are found to be of primary importance. Due to the essential role of diffusive transport in combustion, its mathematical representation – excepting some rare cases of high symmetry – is given in terms of partial differential equations. Therefore, the characteristic features of combustion should be obtained by means of an investigation of the asymptotic states of a model system of partial differential equations.

Due to the essential role of nonlinearity in combustion, the modelling equations are highly nonlinear and thus present tremendous mathematical difficulties, as there are as yet no generally applicable solution methods available. A special case may arise depending on whether a certain solution strategy is applicable which is based on what has been termed "nontrival local behaviour". Here, the system is viewed as a collection of identical local homogeneous elements ("particles", so to speak), and local behaviour thus is equivalent to the temporal evolution of the local element which is modelled by a system of ordinary differential equations on account of the assumption of local homogeneity. The overall behaviour of the system then results from diffusively coupling the local elements. The case of autocatalytic feed-back for isothermal systems lends itself particularly to this treatment [3], but typically, combustion processes are accompanied by heat release and therefore are strongly susceptible to thermal feed-back due to the strongly nonlinear temperature dependence of the Arrhenius expression for the reaction rates. These are given in terms of the exponential function and thus no nontrivial local behaviour arises and the strategy of perceiving the system as a collection of identical local elements cannot be pursued. In order to derive the asymptotic states of the system and the characteristics of its spatio-temporal evolution, a straight-forward solution of the nonlinear partial differential equations of the model is required.

It is the objective of this paper to show how to determine the critical stationary states which are intimately connected with ignition and extinction, and the appearance of combustion waves of small amplitude. This is achieved by deriving necessary conditions in the form of lower bounds for the bifurcation set and the bifurcation diagrams associated with the set of stationary solutions of the model system.

3 THE MODEL PROBLEM

A simple example which allows for the discussion of the characteristic features of combustion is provided by the following single equation:

$$\frac{\partial y}{\partial t} = L[y] + \lambda w(y;\xi) \quad \text{in } D, \qquad y = 0 \quad \text{on } \partial D. \tag{1}$$

Eq. (1) typically results for a reaction–diffusion system for which the Lewis-number Le is equal to 1, with L designating a uniformly elliptic differential operator, y the temperature, t the time, λ, ξ some control parameters, and w a nonlinear function of y and ξ. Thus, Eq. (1) represents the initial/boundary value problem of a semi-linear parabolic differential equation for a region D with boundary ∂D. The function $w(y;\xi)$ incorporates the combined effects of heat release and reactant consumption in a thermodynamic system which is open according to the boundary condition for Eq. (1). The control parameter λ is distinguished in that its changes have no influence on the convexity with respect to y of the function $w(y;\xi)$, this convexity being of primary importance for the occurrence of characteristic phenomena in the solution set of Eq. (1). λ represents the well-known "Frank-Kamenetzkii parameter".

For Eq. (1) to treat homogeneous and quasi-homogeneous chemical reactions [6–8], a general rate law for w is assumed:

$$w(y;\xi,\beta,n) = (1-\xi y)^n \exp(y/(1+\beta y)). \tag{2}$$

Here, ξ, β, n designate control parameters which influence the convexity of w with respect to y, with ranges according to:

$$\beta \geqq 0, \quad n \gtreqless 0, \quad \xi \gtreqless 0. \tag{3}$$

The physical and mathematical characteristics of the system modelled by Eq. (1) are to a large extent due to the properties of the function w. An important one among these is the requirement of $w(0)>0$ due to which solutions of Eq. (1) exist which are strictly positive in D. For these solutions to be smooth in D, the following restrictions have to be imposed:

$$y < 1/\xi \quad (\text{in case } \xi > 0), \quad \lambda \geqq 0. \tag{4}$$

Inspection of Eq. (1) reveals that under the conditions of Eqs. (2)–(4), $y \equiv 0$ results for $\lambda = 0$, representing the only stable homogeneous state of the system.

4 THE STEADY STATE MANIFOLD

The stationary states are given as solutions of the semi-linear elliptic boundary value problem associated with Eq. (1), which results from imposing the condition of stationarity:

$$\frac{\partial y}{\partial t} = 0. \tag{5}$$

The set of stationary solutions of Eq. (1) is to be investigated for the class of reaction rates w with a shape given by Eq. (2), with stability and bifurcation depending on the values of the control parameters λ, ξ, β, n. In order to facilitate this investigation, only a relatively simple geometry is admitted: the region D is supposed to be entirely convex, with a centre of symmetry at $x_0 \in D$. Under this condition, a stationary solution y of Eq. (1) possesses a unique maximum y_m which is located at x_0:

$$y_m = y(x_0), \quad x_0 \in D. \tag{6}$$

As has been shown in [4,5], y_m may be used as an independent parameter, such that the set of stationary solutions of Eq. (1) results in the following parametric representation:

$$(\lambda(y_m;\xi,\beta,n),\ y(y_m;\xi,\beta,n)). \tag{7}$$

By means of Eq. (7), the stationary solutions of Eq. (1) are represented by a state surface:

$$\lambda = \lambda(y_m;\xi,\beta,n). \tag{8}$$

In a finite-dimensional state space spanned by y_m, ξ, β, n. The cross section $\lambda(y_m)$ of the state surface obtained by keeping ξ, β, n constant is termed "bifurcation diagram", whereas the projection of the surface along the y_m-axis into the subspace of control parameters λ, ξ, β, n is called "bifurcation set" [7].

5 AN APPROXIMATION OF THE STATE SURFACE

In order to determine those sheets of the surface given by Eq. (8) which represent stable stationary solutions of Eq. (1), the bifurcation points have to be determined. A numerical search for these in a multi-dimensional parameter space is a "hopeless task without an intelligent strategy for locating the likely places to start the search" [9]. Such information, e.g. as to sheets of stable stationary solutions and as to the geometry of their boundaries, may be gained with the help of lower bounds of the state surface given by Eq. (8). For ease of application, the lower bounds are derived from linear boundary value problems associated with Eq. (1).

For a given value of y_m, let $M(y; y_m) = ay + b$ be a linear majorant of $w(y)$ for $0 \leqq y \leqq y_m$:

$$0 < w(y) \leqq M(y; y_m). \tag{9}$$

Here, the coefficients a, b are appropriate functions of y_m (for an example, cf. Eq. (22)). Then a parameter λ_M may be determined from the following linear elliptic boundary value problem obtained from the stationary version of Eq. (1) by replacing $w(y;\xi)$ by $M(y; y_m)$:

$$\begin{aligned} &L[u] + \lambda_M M(u; y_m) = 0 \quad \text{in } D, \\ &u = 0 \quad \text{on } \partial D, \qquad u(x_0) = y_m. \end{aligned} \tag{10}$$

It is important to note that the properties of the nonlinear function $w(y;\xi)$ persist in having an influence on the linear problem of Eq. (10) via the coefficients a, b of M.

In parametric representation, the solution of Eq. (10) is of the following form:

$$(\lambda_M(y_m),\ u(y_m)). \tag{11}$$

Subtracting Eq. (10) from Eq. (1) for the case of stationary solutions furnishes:

$$\begin{aligned} &L[y-u] + \lambda w(y) - \lambda_M(au+b) = 0 \quad \text{in } D, \\ &y - u = 0 \ \text{ on } \partial D, \quad (y-u)|_{x_0} = 0. \end{aligned} \tag{12}$$

A rearrangement of Eq. (12) leads to

$$L[y-u] + \lambda_M a(y-u) + \lambda w(y) - \lambda_M(ay+b) = 0. \tag{13}$$

Assuming for a moment: $\lambda_M > \lambda$, Eq. (13) furnishes on account of Eq. (9):

$$\begin{aligned} &L[y-u] + \lambda_M a(y-u) > 0 \quad \text{in } D, \\ &B[y-u] = y - u = 0 \quad \text{on } \partial D, \qquad (y-u)|_{x_0} = 0. \end{aligned} \tag{14}$$

For the solutions of Eq. (10) to be useful in the context of an investigation of the stationary solutions of Eq. (1), they have to be strictly positive in D (cf. the discussion which led to the restrictions embodied in Eq. (4)). Therefore, it is required that

$$\lambda_M a < \mu_1. \tag{15}$$

Here, μ_1 designates the principal eigenvalue of the operator (L, B). Under the condition of Eq. (15), there exists an inverse of the operator $((L + \lambda_M a)[y-u], B[y-u])$ which is in the form of an integral operator with strictly negative kernel in D [10]. Therefore, a solution $(y-u)$ of Eq. (14) is strictly negative in D and the condition $(y-u) = 0$ at the interior point $x_0 \in D$ cannot be satisfied. Consequently,

$$\lambda_M(y_m) \leqq \lambda(y_m). \tag{16}$$

The solution set of Eq. (10) therefore furnishes a surface $\lambda_M(y_m;\xi,\beta,n)$ in the state space defined for Eq. (1) which bounds the state surface $\lambda(y_m;\xi,\beta,n)$ (cf. Eq. (8)) from below:

$$\lambda_M(y_m;\xi,\beta,n) \leqq \lambda(y_m;\xi,\beta,n). \tag{17}$$

For any combination of the independent control parameters ξ,β,n, the parameter λ_M may be obtained for the chosen value of y_m with the help of a characteristic curve $\tilde{\lambda}_M(\tilde{y}_m)$ which is derived from the solution of the following reduced problem associated with Eq. (10):

$$\begin{aligned} &L[\tilde{u}] + \tilde{\lambda}_M(\varepsilon\tilde{u}+1) = 0 \quad \text{in } D,\\ &\tilde{u} = 0 \quad \text{on } \partial D, \qquad \tilde{u}(x_0) = \tilde{y}_m. \end{aligned} \tag{18}$$

Here, $\varepsilon = +1$ for linear majorants $M(y;y_m)$ with positive slopes and $\varepsilon = -1$ for negative slopes. The usefulness of linear majorants and the corresponding linear problem of Eq. (10) which is associated with Eq. (1) stems from the fact [11] that the solutions of Eq. (10) represent so-called upper solutions from which the stationary solutions of Eq. (1) may be obtained by monotonously decreasing iteration. This is a consequence of Eq. (9), from which it is deduced that the expression $(\varepsilon\tilde{u}+1)$ in Eq. (18) must be positive in D. Thus, the following conditions are obtained:

$$\begin{aligned} &\varepsilon = +1 \rightarrow \tilde{\lambda}_M < \mu_1,\\ &\varepsilon = -1 \rightarrow 0 < \tilde{u} < 1 \quad \text{in } D. \end{aligned} \tag{19}$$

Here, as in Eq. (15), μ_1 designates the principal eigenvalue of the elliptic differential operator L, under the condition of the eigenfunction vanishing on the boundary ∂D.

The two cases $\varepsilon = \pm 1$ give rise to two separate branches of the characteristic curve $\tilde{\lambda}_M(\tilde{y}_m)$, one of which is the extension of the other, because the case of $\varepsilon = -1$ results from the case of $\varepsilon = +1$ by formally allowing negative values for $\tilde{\lambda}_M$ and for $\tilde{u}$ in Eq. (18):

$$\begin{aligned} &L[\tilde{u}] + \tilde{\lambda}_M(-\tilde{u}+1) = 0 \quad \text{in } D,\\ &\tilde{u} = 0 \quad \text{on } \partial D, \qquad \tilde{u}(x_0) = \tilde{y}_m;\\ &\text{and with } \tilde{\lambda}_M \rightarrow -\tilde{\lambda}_M, \quad \tilde{u} \rightarrow -\tilde{u}\\ &L[\tilde{u}] + \tilde{\lambda}_M(\tilde{u}+1) = 0 \quad \text{in } D,\\ &\tilde{u} = 0 \quad \text{on } \partial D, \qquad \tilde{u}(x_0) = -\tilde{y}_m. \end{aligned} \tag{20}$$

The general shape of the characteristic curve $\tilde{\lambda}_M(\tilde{y}_m)$ is displayed in Fig. 1. Inspection of Fig. 1 reveals that the two stipulations of Eq. (19) are indeed satisfied. With the help of the maximum principle [10], it is easily derived that the characteristic curve $\tilde{\lambda}_M(\tilde{y}_m)$ is strictly increasing whereby the inverse function $\tilde{y}_m = \tilde{y}_m(\tilde{\lambda}_M)$ exists also.

A general linear majorant M will be of the following form:

$$M(y;y_m) = ay + b. \tag{21}$$

Here, the coefficients a, b are functions of y_m. For the example displayed in Fig. 2, $M(y;y_m)$ represents a secant with

$$a = (w(y_m) - w(0))/y_m, \quad b = w(0). \tag{22}$$

According to Eq. (10), the corresponding lower bound $\lambda_M(y_m)$ of $\lambda(y_m)$ derives from the solution of the following problem:

$$\begin{aligned} &L[u] + \lambda_M(au+b) = 0 \quad \text{in } D\\ &u = 0 \quad \text{on } \partial D, \qquad u(x_0) = y_m. \end{aligned} \tag{23}$$

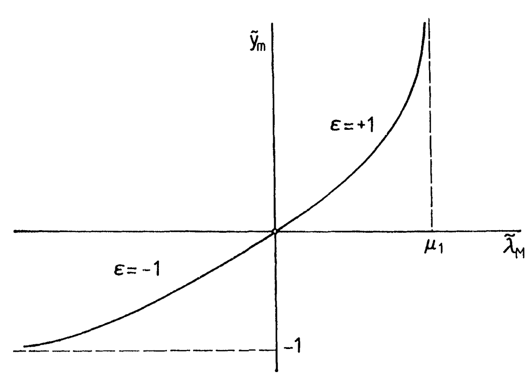

FIGURE 1 The characteristic curve for the reduced problem given by Eq. (18).

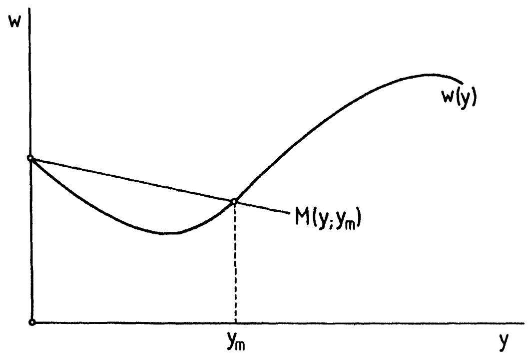

FIGURE 2 An example of a majorant $M(y; y_m)$ of the function $w(y)$ for $0 \leqq y \leqq y_m$.

Under the condition of $\lambda_M a < \mu_1$, Eq. (23) possesses a unique solution. Due to the operator L being homogeneous, Eq. (23) may be reduced to Eq. (18) by a simple stretching transformation, provided a, $b \neq 0$:

$$\begin{aligned} &L\left[\frac{a}{b}u\right] + a\lambda_M\left(\frac{a}{b}u + 1\right) = 0 \quad \text{in } D, \\ &\frac{a}{b}u = 0 \quad \text{on } \partial D, \quad \frac{a}{b}u(x_0) = \frac{a}{b}y_m. \end{aligned} \tag{24}$$

Comparison of Eq. (24) with Eq. (23) reveals their being equal. Therefore, the solution $(\lambda_M(y_m), u(y_m))$ of Eq. (23) may be obtained from the reduced problem (Eq. (18)) by the stretching transformation:

$$\tilde{u} = \frac{a}{b}u, \quad \tilde{\lambda}_M = a\lambda_M. \tag{25}$$

$\lambda_M(y_m)$ in particular may be determined from the characteristic curve $\tilde{\lambda}_M(\tilde{y}_m)$ as follows:

$$\lambda_M(y_m) = \frac{1}{a}\tilde{\lambda}_M\left(\frac{a}{b}y_m\right). \tag{26}$$

For a given geometry, the characteristic curve $\tilde{\lambda}_M(\tilde{y}_m)$ associated with the stationary system may be derived analytically or numerically from Eq. (18) once and for all. For a given combination of parameters y_m, ξ, β, n, a suitable linear majorant $M(y; y_m)$ (cf. Eqs. (9),(21)) furnishes a lower bound $\lambda_M(y_m)$ of $\lambda(y_m)$ by means of Eq. (26).

6 AN EXAMPLE FOR A SURFACE OF LOWER BOUNDS

In order to provide an example, functions $w(y)$ are investigated which are strictly increasing at least for an initial part of the positive y-axis (i.e., for $0 \leqq y \leqq y_0$) so that there exists a unique inverse function of w on this interval. In addition to that, if $w(y)$ is convex or convex–concave for $0 \leqq y_m \leqq y_0$, then there exists a subinterval $0 \leqq y \leqq y_1 \leqq y_0$, where secants may serve as linear majorants according to Eq. (9) (cf. Fig. 3). With the help of Eq. (22), a secant-majorant is obtained for $0 \leqq y_m \leqq y_1$, for which:

$$M(y; y_m) = ay + b = y(w(y_m) - w(0))/y_m + w(0). \tag{27}$$

By choosing an appropriate scale for the w-axis, $w(0) = 1$ may be obtained, so that:

$$a = (w(y_m) - 1)/y_m, \quad b = 1. \tag{28}$$

Under the conditions of Eq. (19), a unique solution exists for Eq. (18), where $\varepsilon = +1$ for the present case, as $w(y)$ is strictly increasing. The inverse of the operator

$$K[\tilde{u}] \equiv L[\tilde{u}] + \tilde{\lambda}_M\tilde{u} \tag{29}$$

may be represented by an integral operator with negative kernel G which depends on $\tilde{\lambda}_M$, so that the solution of Eq. (18) is obtained in the

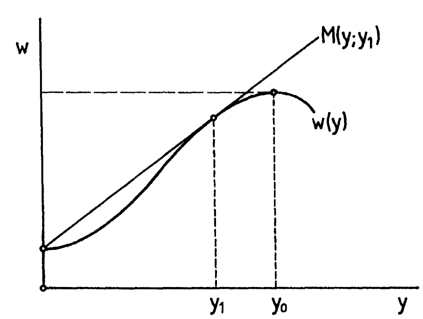

FIGURE 3 A strictly increasing function $w(y)$ which is convex–concave for $0 \leqq y \leqq y_0$.

following form:

$$\tilde{u} = -\tilde{\lambda}_M \int_D G(x, x'|\tilde{\lambda}_M)\mathrm{d}x'. \tag{30}$$

Due to the existence of the centre of symmetry at $x_0 \in D$, the location of the maximum $\tilde{y}_\mathrm{m}$ of $\tilde{u}$ is fixed, so that Eq. (30) furnishes

$$\tilde{y}_\mathrm{m} = -\tilde{\lambda}_M \int_D G(x_0, x' \,|\, \tilde{\lambda}_M)\mathrm{d}x'. \tag{31}$$

Abbreviating

$$F(\tilde{\lambda}_M) = -\int_D G(x_0, x' \,|\, \tilde{\lambda}_M)\mathrm{d}x' \tag{32}$$

the characteristic curve $\tilde{\lambda}_M(\tilde{y}_\mathrm{m})$ is given implicitly due to Eq. (31) as

$$\tilde{y}_\mathrm{m} = \tilde{\lambda}_M F(\tilde{\lambda}_M). \tag{33}$$

For an arbitrary value of y_m with $0 \leqq y_\mathrm{m} \leqq y_1$, the lower bound $\lambda_M(y_\mathrm{m})$ (cf. Eq. (23)) is found from Eq. (33) according to Eq. (26) as

$$\frac{a}{b} y_\mathrm{m} = a\lambda_M F(a\lambda_M). \tag{34}$$

For secant-majorants, the coefficients a and b are given by Eq. (28) whereby Eq. (34) reduces to the following form:

$$w(y_\mathrm{m}) = 1 + \zeta F(\zeta). \tag{35}$$

Here, a parameter ζ is introduced with

$$\zeta = a\lambda_M = (w(y_\mathrm{m}) - 1)\lambda_M / y_\mathrm{m}. \tag{36}$$

For strictly increasing functions $w(y)$, an inverse function exists, so that Eq. (35) may be solved for $y_\mathrm{m} = y_\mathrm{m}(\zeta)$. Inserting $y_\mathrm{m}(\zeta)$ in Eq. (36) furnishes $\lambda_M(\zeta)$ as

$$\lambda_M(\zeta) = y_\mathrm{m}\zeta / (w(y_\mathrm{m}) - 1). \tag{37}$$

By means of $y_\mathrm{m}(\zeta)$ from Eq. (35) and $\lambda_M(\zeta)$ from Eq. (37), the lower bounds $\lambda_M(y_\mathrm{m})$ are given in parametric representation

$$(y_\mathrm{m}(\zeta), \lambda_M(\zeta)). \tag{38}$$

With the help of Eq. (38), a surface $\lambda_M(y_\mathrm{m}; \xi, \beta, n)$ is thus obtained which is below the state surface $\lambda(y_\mathrm{m}; \xi, \beta, n)$ for any combination of the parameters $y_\mathrm{m}, \xi, \beta, n$.

7 THE GEOMETRY OF THE STATE SURFACE

According to Eq. (17), $\lambda_M(y_\mathrm{m}; \xi, \beta, n)$ represents a surface in the state space associated with the stationary solutions of Eq. (1) which is below the surface $\lambda(y_\mathrm{m}; \xi, \beta, n)$ at any point $(y_\mathrm{m}, \xi, \beta, n)$. Employing the concepts of singularity theory [7], the geometry of the surface $\lambda_M(y_\mathrm{m}; \xi, \beta, n)$ may be investigated with the help of its bifurcation diagrams, i.e., the cross sections $\lambda_M(y_\mathrm{m})$ which result for constant combinations of the parameters ξ, β, n. The bifurcation set is another useful concept which allows for a geometrical interpretation: it designates the contours of the surface $\lambda_M(y_\mathrm{m}; \xi, \beta, n)$ which by definition represent those locations in state space where

$$\frac{\partial \lambda_M}{\partial y_\mathrm{m}} = 0. \tag{39}$$

Geometrically speaking, the contours become visible by viewing (i.e., by projecting) the surface $\lambda_M(y_\mathrm{m}; \xi, \beta, n)$ along the y_m-axis from the subspace of control parameters λ, ξ, β, n.

The geometry of the state surface $\lambda(y_\mathrm{m}; \xi, \beta, n)$ may be investigated also by employing the above concepts: its bifurcation set, therefore, designates those locations in state space where

$$\frac{\partial \lambda}{\partial y_\mathrm{m}} = 0. \tag{40}$$

On account of Eq. (40), the bifurcation set of the state surface comprises those combinations of the control parameters λ, ξ, β, n, for which Eq. (1)

possesses singular stationary solutions. In the set of all stationary solutions of Eq. (1), the singular solutions represent the branching points which separate adjoining sheets of regular stationary solutions. Due to the quasi-regularity of Eq. (1) at the singularities characterized by Eq. (40), the contours represent smooth curves in the state surface.

According to Eq. (8), the stationary solutions of Eq. (1) may be represented by a state surface in a finite-dimensional state space. Therefore, the concepts of singularity theory [12] apply due to which there is a hierarchical order in the set of all singularities. Accordingly, a singular stationary solution of Eq. (1) is said to be of order k, if:

$$\frac{\partial \lambda}{\partial y_{\mathrm{m}}}=\frac{\partial^2 \lambda}{\partial y_{\mathrm{m}}^2}=\cdots=\frac{\partial^k \lambda}{\partial y_{\mathrm{m}}^k}=0, \quad \frac{\partial^{k+1} \lambda}{\partial y_{\mathrm{m}}^{k+1}} \neq 0. \tag{41}$$

Geometrically speaking, the order of singularity is equivalent to the order of tangency of the projection (the line of sighting, so to speak) of the state surface $\lambda(y_{\mathrm{m}}; \xi, \beta, n)$ into the subspace of control parameters λ, ξ, β, n. Consequently, a given order of singularity corresponds to a certain type of singularity in the bifurcation set. According to singularity theory (Whitney's thoerem, cf. discussion in [13]), there is only one generic singularity in the bifurcation set associated with the state surface given by Eq. (8), and, similarly, in the bifurcation set associated with the surface of lower bounds given by Eq. (17). This is in the form of a cusp which corresponds to a singular stationary solution of Eq. (1) of second order (i.e., $k=2$). For $k=1$, the singularity of Eq. (1) is of the fold-type, which corresponds to a regular point of a smooth arc of the bifurcation set, while singularities of order $k>2$ are of cuspoid type, which is to say that they correspond to nongeneric singularities of the bifurcation set (i.e., nongeneric folds, nongeneric cusps) resulting from a superposition of cusps and smooth arcs.

For the construction of the state surface and, similarly, the surface of lower bounds, only a single state variable y_{m} is employed, whereas the remaining variables λ, ξ, β, n are of the control parameter type. Therefore, only singularities of co-rank 1 occur which is the mathematical reason for their cuspoid character [12].

In order to give an example of nongeneric singularities, singularity order $k=3$ and $k=4$ are discussed, with $k=3$ designating a swallow-tail-type singularity, $k=4$ a butterfly (for the terminology, cf. [12]).

A swallow-tail corresponds to a singularity P^+ of the bifurcation set representing a nongeneric fold. Therefore, P^+ is found to be a regular point of a smooth arc of the bifurcation set, such that at P^+ a cusp doublet is generated (cf. Fig. 4).

A butterfly corresponds to a singularity Q^+ of the bifurcation set representing a nongeneric cusp. At Q^+, a cusp triplet is generated (cf.Fig. 5). It thus appears that the singularities of higher order may be classified as to whether they are associated with a nongeneric fold or a nongeneric cusp. This corresponds to the observation that for the bifurcation diagram $\lambda(y_{\mathrm{m}})$ associated with a singular stationary solution of Eq. (1), only two cases arise: either the singularity is of the turning point type (generic or nongeneric fold, cf. point P in Fig. 6) or of the inflection point type (generic or nongeneric cusp in the bifurcation set, cf. point Q in Fig. 7). The order

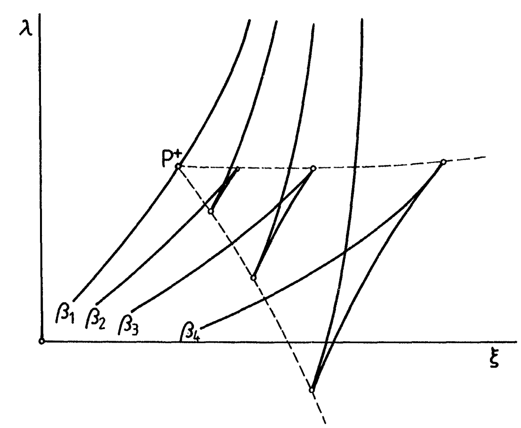

FIGURE 4 A swallow tail singularity P^+ with a selection of contours of the state surface for varied values of β displaying the creation of a cusp doublet (dashed lines).

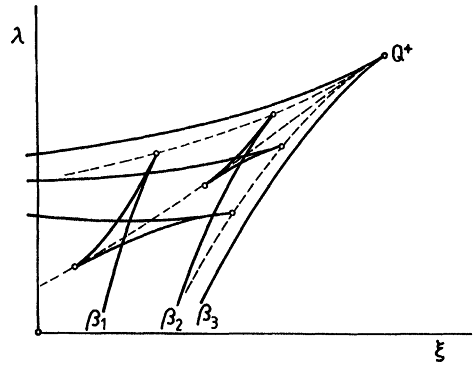

FIGURE 5 A butterfly singularity Q^+ with a selection of contours displaying the creation of a cusp triplet (dashed lines).

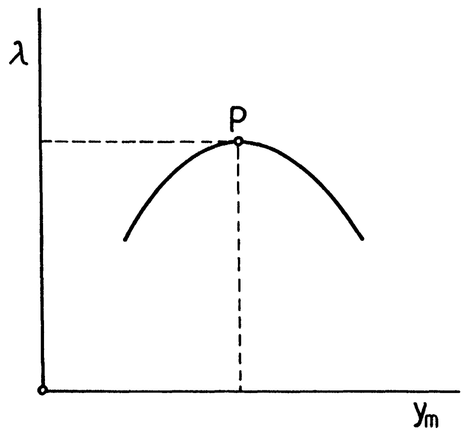

FIGURE 6 A bifurcation diagram with turning point P.

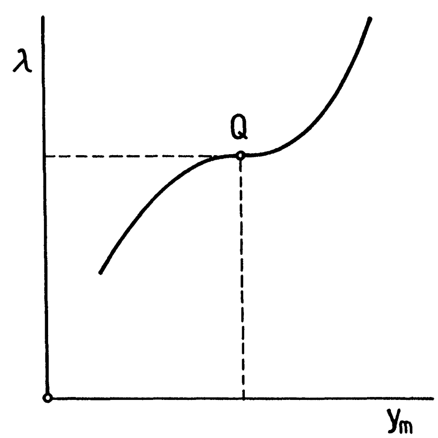

FIGURE 7 A bifurcation diagram with point of inflection Q.

k of singularity (cf. Eq. (41)) corresponds to the order of tangency at P or Q, while a necessary condition for the contours to appear consists in the tangent being horizontal, i.e., parallel to the y_m-axis which is the direction of projection (cf. Figs. 6, 7).

8 THE STATE SURFACE GEOMETRY AND THE GEOMETRY OF THE SURFACE OF LOWER BOUNDS

A function $w(y)$ is termed "concave in the generalized sense", if it is either concave in the usual sense or only weakly convex. The condition for generalized concavity is as follows:

$$w(y) - yw'(y) \geqq 0. \qquad (42)$$

It has been shown in [14] that no singular stationary solutions of Eq. (1) exist with $0 \leqq y_m \leqq y_c$, if the function $w(y)$ in Eq. (1) is concave in the generalized sense for $0 \leqq y \leqq y_c$. For any smooth function $w(y)$ with $w(0) > 0$ a value $y_c > 0$ exists such that $w(y)$ is concave in the generalized sense for $0 \leqq y \leqq y_c$. The value of y_c therefore may serve as a convexity index, in that it provides a necessary condition (in the form of a lower bound for y_m) for the occurrence of singular stationary solutions. Recalling that the shape of the function $w(y)$ is influenced by the control parameters ξ, β, n (cf. the expression for $w(y)$ given by Eq. (2)), continuous changes of the control parameters ξ, β, n may be envisaged which lead to a deformation of $w(y)$ such that the convexity index y_c changes to lower values in a continuous or discontinuous fashion. A discontinuous change of y_c to a lower value y_{cc}. (cf. Fig. 8) therefore constitutes a precondition for the appearance of a newly formed pair of singular stationary solutions of Eq. (1)."Newly formed" is to indicate a creation "out of the blue", as opposed to the shifting of a previously existing maximum/minimum pair in the bifurcation diagram $\lambda(y_m)$. Consequently, such a discontinuous

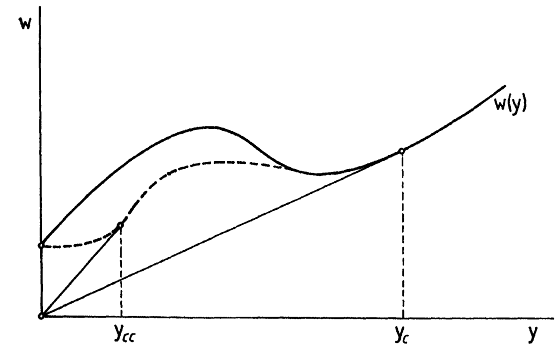

FIGURE 8 A discontinuous change of the convexity index from y_c to y_{cc} due to a deformation (dashed) of $w(y)$.

change of the convexity index due to a smooth change in the control parameters is associated with a deformation process in the corresponding bifurcation diagram where the appearance of y_{cc} corresponds to the appearance of a point of inflection Q with a horizontal tangent (cf. Fig. 7) at an interior point of a regular branch of $\lambda(y_m)$. The singularity order of the stationary solution of Eq. (1) associated with Q is $k=2q(q=1,2,\ldots)$, with the lowest order $k=2$ designating a generic cusp in the bifurcation set which is indicative of the creation of a single maximum/minimum pair in the bifurcation diagram $\lambda(y_m)$. For higher order singularities $k=2q>2$, additional maximum/minimum pairs originate from the point of inflection Q. In the example of $k=4$ (singularity of butterfly type), the counter image Q^+ of Q on the state surface $\lambda(y_m;\xi,\beta,n)$ is the source of three contours which represent three lines of cusps (cf. the dashed lines in Fig. 5).

Generally, functions $w(y)$ of the set defined by Eqs. (2)–(4) may be classified as to their asymptotic behaviour for $y\to\infty$ (in case $\xi<0$) or $y\to 1/\xi$ (in case $\xi>0$). For functions $w(y)$ which are asymptotically strongly convex and increasing, there exists a finite least upper limit $\bar{\lambda}$ for the values of the distinguished control parameter λ:

$$\lambda(y_m) \leqq \bar{\lambda} = \sup \lambda. \tag{43}$$

If for some value $\bar{y}_m$ of y_m, $\lambda(y_m)$ reaches the supremum $\bar{\lambda}$ (i.e., $\bar{\lambda}=\lambda(\bar{y}_m)$), then $\bar{\lambda}$ of necessity corresponds to a maximum of the bifurcation diagram $\lambda(y_m)$ (e.g., Fig. 9(a)). For all other functions $w(y)$ which thus fail to be strongly enough convex and increasing, there either is no finite supremum or there is no maximum $\bar{\lambda}$ of $\lambda(y_m)$ (cf. Fig. 9(b)). This classification may be derived with the help of monotonous iteration based on upper and lower solutions, with the upper solutions resulting from appropriate linear majorants. A maximum $\bar{\lambda}$ which constitutes the supremum of $\lambda(y_m)$ represents a fold-type singular stationary solution of Eq. (1) which thus is of singularity order $k=2q+1$, $(q=0,1,2,\ldots)$. For a generic fold singularity: $k=1$, whereas for nongeneric folds $k>1$. In the example of

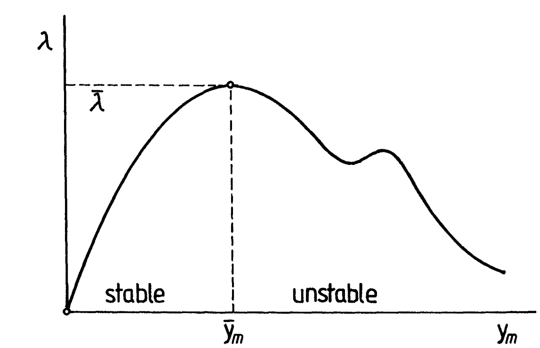

FIGURE 9(a) The bifurcation diagram for entirely convex functions $w(y)$, with the stable branch of $\lambda(y_m)$ bounded by a supremum–maximum $\bar{\lambda}$.

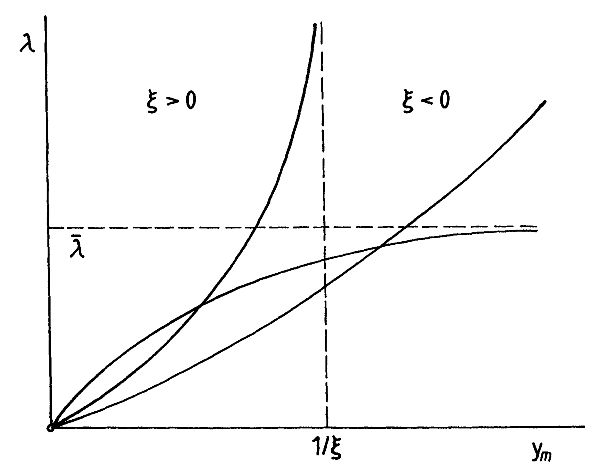

FIGURE 9(b) The bifurcation diagram for functions $w(y)$ which are entirely concave in the generalized sense.

$k=3$ (swallow tail), the nongeneric fold singularity is associated with an interior point P^+ of a regular arc of the bifurcation set such that P^+ is the source of two curves, the points of which designate cusp singularities (cf. the dashed lines in Fig. 4).

For certain critical stationary solutions of Eq. (1), it is possible to establish a relationship between the structure of the state surface and that of the surface of lower bounds. Here, a particular singular stationary solution of Eq. (1), is "critical" [14], if it separates a sheet of regular stable stationary solutions of Eq. (1) from a sheet of unstable ones. Thus, critical solutions are associated by means of Eq. (40) with some parts of the contours, i.e., with some part of the bifurcation set. From the point of view of physics, the critical solutions are obviously of foremost interest because they bound stable, i.e., physically attainable, stationary states of the system. Singular stationary solutions which are noncritical separate sheets of regular unstable stationary solutions which cannot be established for a physical system.

For a function $w(y)$ which is entirely convex, only a single critical solution of Eq. (1) can occur which of necessity corresponds to a supremum–maximum $\bar{\lambda} = \lambda(\bar{y}_\mathrm{m})$ [14]. Thus, there is a branch of $\lambda(y_\mathrm{m})$ issuing from the origin and terminating in $(\bar{\lambda}, \bar{y}_\mathrm{m})$. This branch represents the regular stable stationary solutions of Eq. (1) (cf. Fig. 9(a)), whereas for $y_\mathrm{m} > \bar{y}_\mathrm{m}$ only unstable stationary solutions exist. Consequently, no critical minima and no further critical maxima beyond the first one exist. Therefore

$$\bar{\lambda} = \sup \lambda(y_\mathrm{m}). \tag{44}$$

According to Eq. (16), a lower bound $\lambda_M(y_\mathrm{m}) \leqq \lambda(y_\mathrm{m})$ exists. If a supremum $\bar{\lambda}$ of $\lambda(y_\mathrm{m})$ occurs, then there exists a supremum λ_M of $\bar{\lambda}_M(y_\mathrm{m})$ also, for which of necessity.

$$\bar{\lambda}_M \leqq \bar{\lambda}. \tag{45}$$

Projecting the state surface into the subspace of control parameters λ, ξ, β, n, the supremum $\bar{\lambda}$ results as part of the contours. Because the direction of projection is along the y_m-axis, Eq. (45) holds for the bifurcation set also. Consequently, the contours corresponding to $\bar{\lambda}$ are bounded from below by the contours corresponding to $\bar{\lambda}_M$.

For smooth changes of the shape-relevant control parameters ξ, β, n, two bifurcation phenomena may occur:

(a) An interior point of a sheet of regular stable stationary solutions turns into a critical solution. This corresponds to the appearance of a point of inflection with horizontal tangent for $\lambda(y_\mathrm{m})$ (e.g., in Fig. 9(a) for y_m with $0 < y_\mathrm{m} < \bar{y}_\mathrm{m}$). According to the above discussion, such a critical solution is of singularity order $k = 2q$ $(q = 1, 2, \ldots)$, with the lowest possible order $k=2$ representing a generic cusp and any higher order $k = 2q > 2$ a nongeneric one.

(b) The supremum $\bar{\lambda}$ of $\lambda(y_\mathrm{m})$ changes from representing a generic fold into representing a nongeneric one (cf. at $\bar{y}_\mathrm{m}$ in Fig. 9(a)). According to the above discussion, a fold corresponds to a singularity order $k = 2q+1$ $(q = 0, 1, 2, \ldots)$, with the lowest possible order $k=1$ representing the generic fold and the higher order $k = 2q+1 > 1$ the nongeneric ones.

Therefore, smooth changes in the shape relevant control parameters lead to the appearance of maximum/minimum pairs in the bifurcation diagram, with these pairs either emerging from an interior point of a stable branch of $\lambda(y_\mathrm{m})$ (at y_m with $0 < y_\mathrm{m} < \bar{y}_\mathrm{m}$, cf. Fig. 9(a)) or from the supremum $\bar{\lambda}$ at $\bar{y}_\mathrm{m}$ where $\bar{y}_\mathrm{m}$ designates the boundary of the branch. It has been shown in [11], that for a maximum/minimum pair λ^*/λ^{**} appearing at an interior point or at the boundary point of that particular stable branch of $\lambda(y_\mathrm{m})$ which emerges from the origin $(\lambda = 0, y_\mathrm{m} = 0)$, a corresponding maximum/minimum pair $\lambda_M^*/\lambda_M^{**}$ exists for $\lambda_M(y_\mathrm{m})$, so that:

$$\lambda_M^* \leqq \lambda^*, \quad \lambda_M^{**} \leqq \lambda^{**}. \tag{46}$$

Maxima, minima, and points of inflection with horizontal tangents give rise to visible contours according to Eq. (40). Due to the projection being in the direction of the y_m-axis, Eq. (46) holds for the corresponding points of the bifurcation sets also. This can be illustrated for the case of a swallow tail singularity, for which two maximum/minimum pairs emerge from a supremum–maximum $\bar{\lambda}$. Thus, $\bar{\lambda}$ represents the boundary point of the stable branch of the bifurcation diagram $\lambda(y_m)$, which issues from the origin $(\lambda=0, y_m=0)$. For a fixed value of $n=2.0$ and parametrically varied values of β, with region D in the shape of a unit sphere (radius $R=1$), Fig. 10 displays the contours (i.e., the bifurcation set) of the surface of lower bounds $\lambda_M(\xi, \beta, n)$ which are found to comprise two lines of cusps. Each cusp corresponds to the creation of a maximum/minimum pair of $\lambda_M(y_m)$ for appropriate changes of the control parameter ξ. $\lambda_M(y_m)$ is given in terms of the parametric representation of Eq. (38), with the location of the swallow tail derived from the condition for a singularity order $k=3$:

$$\frac{\partial \lambda_M}{\partial y_m}=0, \quad \frac{\partial^2 \lambda_M}{\partial y_m^2}=0, \quad \frac{\partial^3 \lambda_M}{\partial y_m^3}=0. \tag{47}$$

For the unit sphere

$$F=\frac{1}{\zeta}\left(\frac{\sqrt{\zeta}}{\sin\sqrt{\zeta}}-1\right) \tag{48}$$

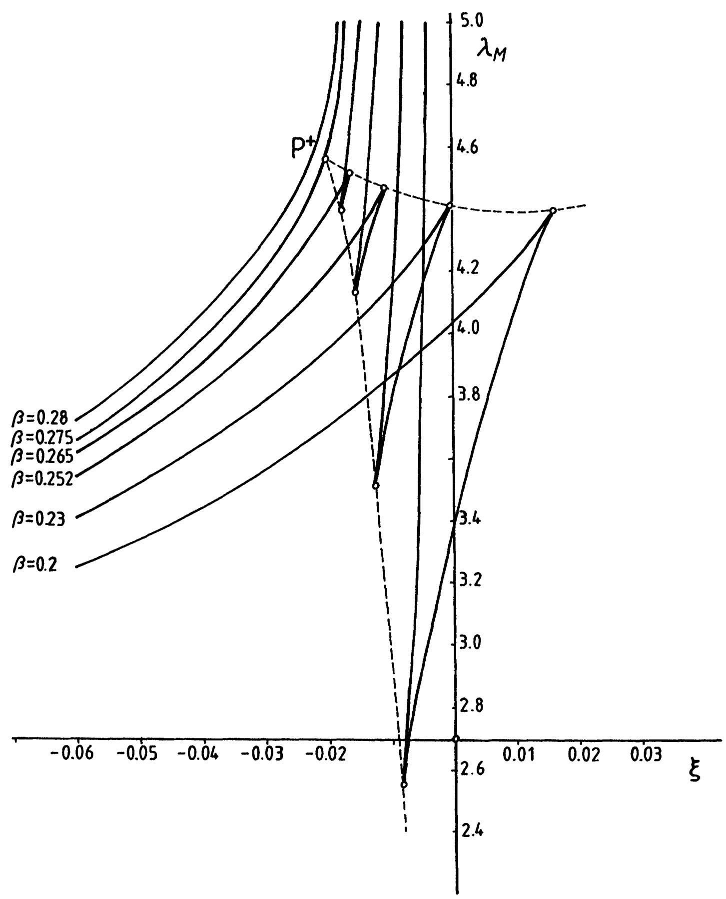

FIGURE 10 The bifurcation set for D in the shape of a unit sphere: swallow tail singularity P^+ in terms of lower bounds λ_M.

with $0 < \zeta < \pi^2$. F is derived according to Eq. (32) and the parameter ζ defined according to Eq. (36).

The solid curves (Fig. (10)) represent the location of the generic and nongeneric folds. For $n = 2.0$, they are thus the solution of the following system of equations:

$$\begin{aligned} w(y_m) &= (1 - \xi y_m)^2 \exp(y_m/(1 + \beta y_m)), \\ w(y_m) &= 1 + \zeta F(\zeta), \\ \lambda_M &= \xi y_m/(w(y_m) - 1), \\ \frac{\partial \lambda_M}{\partial y_m} &= 0. \end{aligned} \tag{49}$$

From Eq. (49), an individual solid curve of Fig. 10 results for a fixed setting of the parameter β in the following parametic representation:

$$(\lambda_M(\zeta), \xi(\zeta)). \tag{50}$$

Along such a curve of the bifurcation set, y_m increases monotonically because $y_m(\zeta)$ is implicitly given by

$$w(y_m) = 1 + \zeta F(\zeta). \tag{51}$$

Investigations are restricted to those ranges of the control parameters ξ, β where the function $w(y; \xi, \beta, n)$ is strictly increasing, so that the inverse function exists and is strictly increasing also.

9 CONCLUSION

It has been shown that for a reaction–diffusion system modelled by Eq. (1), the singularities in the set of stationary solutions are of the cuspoid type and thus are associated with generic or nongeneric cusp- or fold-type singularities in the appropriate bifurcation set. In the case of critical singularities, corresponding singularities exist for a surface of lower bounds which is dervied by linear methods and which is everywhere below the state surface of the system. It has been thus demonstrated that linear methods provide information on properties of the system which are essentially caused by its nonlinearity. In particular, the value of the distinguished parameter λ_M at a singularity in the bifurcation set of the surface of lower bounds provides by itself a lower bound for the value of λ at the corresponding singularity of the state surface. In the case of slab geometry, this correspondence is illustrated by Figs. 4 and 7 in [4]. In the present paper, lower bounds are derived for the example of a spherical region D, with a swallow tail singularity appearing in the bifurcation set for $n = 2.0$ at $\beta = 0.275$ (cf. Fig. 10).

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