Bifurcation Pattern in Reaction-Diffusion Dissipative Systems

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Z. Naturforsch. **38a,** 487–492 (1983); received December 3, 1982

A detailed bifurcation analysis of the reaction-diffusion equations representing the trimolecular model of Prigogine and Lefever ("Brusselator") is performed. The model considers also the diffusion of the initial component. The homogeneous solution to the problem cannot exist and the bifurcation analysis must be performed numerically. There are two ways of possible branching, either the basic branch will be followed or branching from an isolated branch may occur. In both cases, the branching is of the type symmetric → asymmetric → symmetric, etc. For higher dimension of the system a topologically interesting isolated branch of asymmetric solutions was discovered.

1. Introduction

Interaction of diffusion and reaction processes is supposed to explain the formation of structures in living organisms. The idea of a structure emerging as a certain sequence of instabilities was proposed by Prigogine, who used a simplified model, frequently in the literature referred to as the "Brusselator" [1]. Recently different reaction rate schemes have been studied [2–5]. The model of the reaction-diffusion process has been constructed in such a way that a homogeneous steady-state may exist. Under certain circumstances the homogeneous steady state becomes unstable and a spatially non-uniform steady-state emerges.

A more realistic case of a diffusion-reaction process includes also diffusion of the initial components in the system [6, 7]. Diffusion of initial components preclude the existence of a homogeneous steady state, and only non-uniform steady states result. Mathematical analysis of this situation is much more difficult than that performed for the homogeneous steady state situation. Since the homogeneous steady state does not exist, the analysis of the process must be performed completely numerically.

In this paper we are going to analyze the effect of bifurcation on the pattern of evolving steady states. Different ways of emerging new solutions are described.

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2. Governing equations

In this paper we consider the one-dimensional reaction-diffusion equations proposed by Prigogine and Lefever [1]. The model corresponds to a single trimolecular scheme:

$$A \rightleftarrows X, \quad 2X + Y \rightleftarrows 3X,$$
$$B + X \rightleftarrows Y + D, \quad X \rightleftarrows E.$$

It is assumed that all forward kinetic constants are set to unity and the backward reaction rates are neglected. The governing equations describing the reaction and diffusion are:

$$\frac{\partial A}{\partial t} = -A + D_A \frac{\partial^2 A}{\partial z^2}, \tag{1}$$

$$\frac{\partial B}{\partial t} = -BX + D_B \frac{\partial^2 B}{\partial z^2}, \tag{2}$$

$$\frac{\partial X}{\partial t} = A + X^2 Y - (B+1)X + D_X \frac{\partial^2 X}{\partial z^2}, \tag{3}$$

$$\frac{\partial Y}{\partial t} = BX - X^2 Y + D_Y \frac{\partial^2 Y}{\partial z^2}. \tag{4}$$

Fixed boundary conditions are considered:

$$t > 0:\ z = 0, L; \quad X = X_0, \quad Y = Y_0,$$
$$A = A_0, \quad B = B_0. \tag{5}$$

3. Numerical solution

The steady state equations (1)–(5) represent a nonlinear boundary value problem for ordinary differential equations. We used the Størmer-Numerov finite-difference scheme to approximate the differential equations [8]. The set of resulting nonlinear

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finite-difference equations having band structure was solved by the Newton method. Details of the implementation of this technique to the diffusion-reaction problem may be found elsewhere [8]. The particular branches in the bifurcation diagram [cf. Fig. 11] were calculated by the continuation technique [9]. For continuation purposes, we adopted a sequential use of the Newton method. Near the limit points, where the Jacobian matrix is singular, an arc-length continuation was used [10].

An approximate location of singular points results during the continuation process; in the vicinity of such points the Newton procedure exhibits poor convergence properties. For an exact location of the singular points, a number of algorithms was developed [11–13]; apparently the Seydel algorithm [11] is superior for this type of problem.

The calculation of the bifurcation diagram reported in this paper is much more difficult than the calculation performed by Kubicek et al. [2, 3, 14]. These authors could make use of the primary bifurcation points which can be calculated analytically. For our particular problem such points do not exist and we had to continue the solution starting at very low values of the parameter L. All calculations were performed on the IBM 3033.

4. Results of continuation

Numerical computations were performed for the parameters which were used both by Herschkowitz-Kaufman [6] and by Kubicek et al. [3, 14]:

$$A = 2\,,\quad B = 4.6\,,\quad D_X = 1.6 \cdot 10^{-3},$$
$$D_Y = 8 \cdot 10^{-3},\quad D_A = 0.1\,,\quad D_B = \infty\,.$$

The results of continuation which are drawn in the bifurcation diagram "L versus $Y'(0)$" are displayed in Figures 1–10. In these figures the branches of symmetric profiles are drawn by a dashed line while the branches of asymmetric profiles are drawn by a solid line.

In Fig. 1, the branch a of symmetric profiles is shown. We can notice that this branch "corresponds" to the branch of homogeneous profiles (i.e. to the "thermodynamic branch") for the case $D_A \to \infty$. For low values of L ($L < 0.08$) the branch a is almost identical with the thermodynamic branch. We are going to call this branch the basic branch. There are four limit points and four bifurcation points (F_1, E_1, J_1, J_2) at the basic branch.

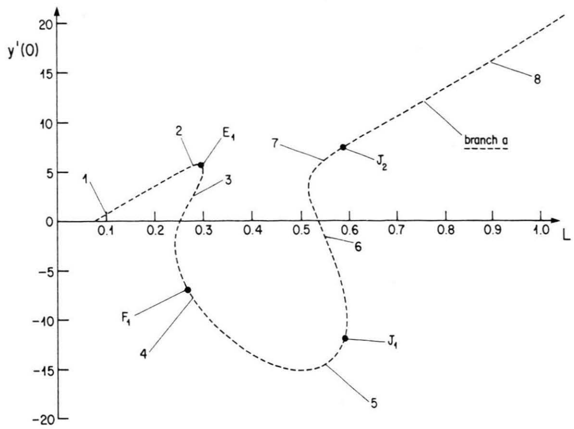

Fig. 1. Bifurcation diagram, branch a (symmetric solutions).

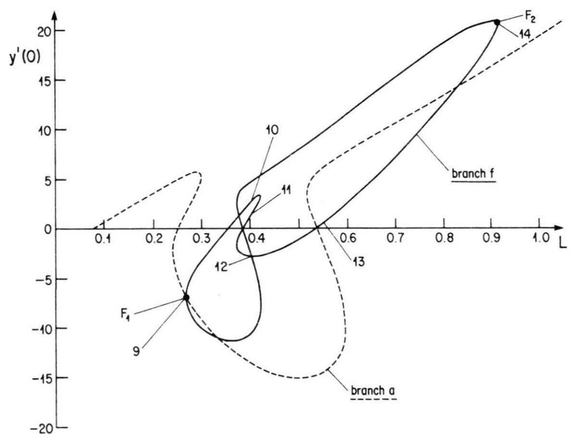

Fig. 2. Bifurcation diagram, branching of asymmetric solutions (branch f).

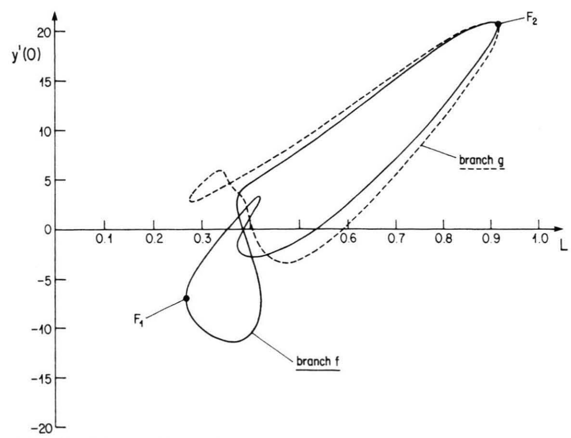

Fig. 3. Bifurcation diagram, branching of symmetric solutions (branch g).

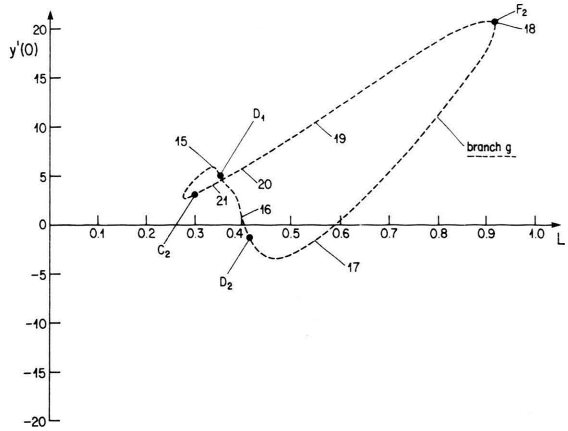

Fig. 4. Branch g of symmetric solutions having four bifurcation points C_2, D_1, D_2, F_2.

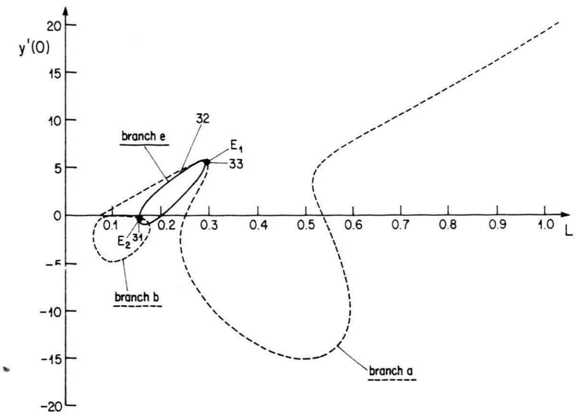

Fig. 7. Bifurcation diagram, branching of asymmetric solutions (branch e).

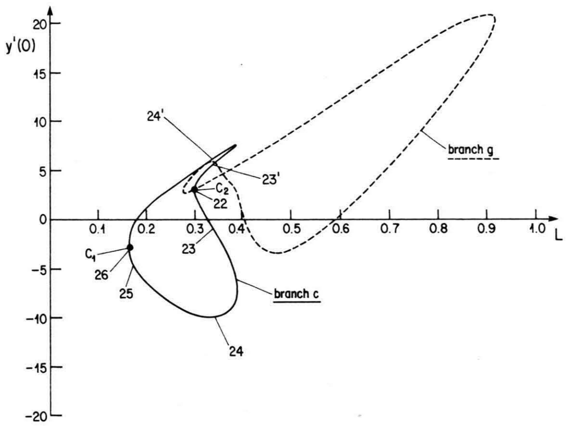

Fig. 5. Bifurcation diagram, branching of asymmetric solutions (branch c).

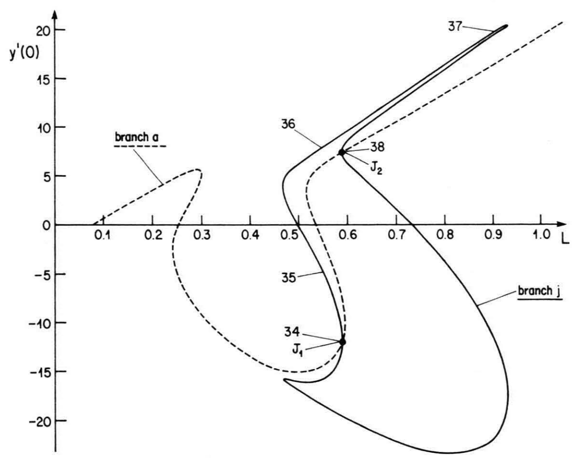

Fig. 8. Bifurcation diagram, branching of asymmetric solutions (branch j).

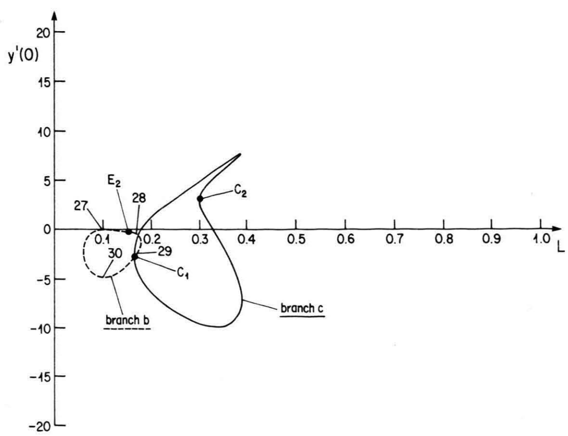

Fig. 6. Bifurcation diagram, branching of asymmetric solutions (branch b).

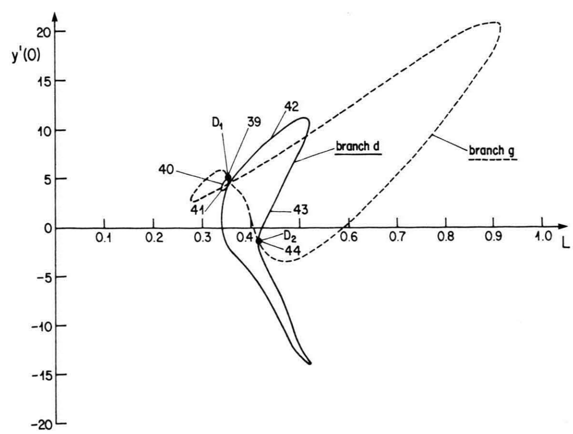

Fig. 9. Bifurcation diagram, branching of asymmetric solutions (branch d).

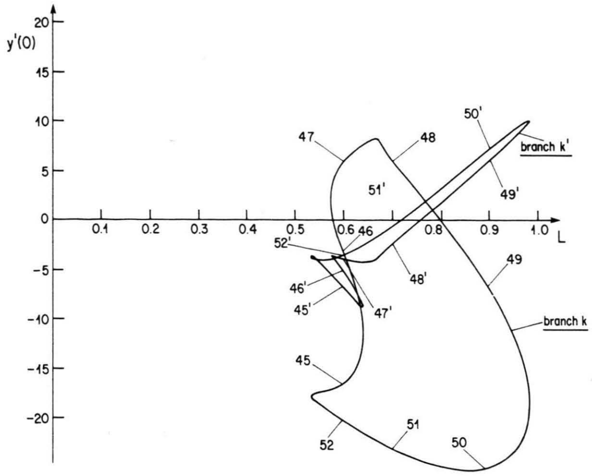

Fig. 10. Isolated branch of asymmetric solutions (branch k, k').

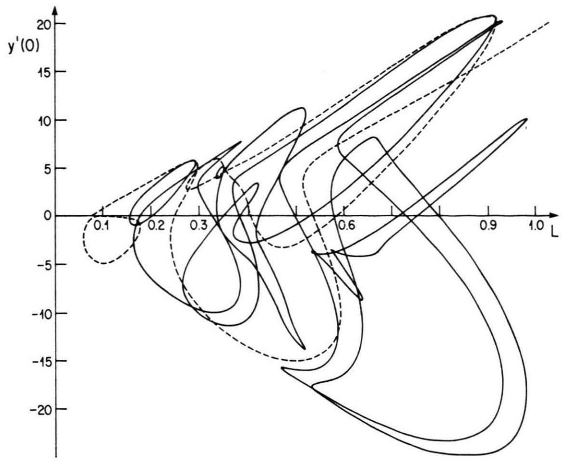

Fig. 11. The complete bifurcation diagram (··· symmetric solutions, – asymmetric solutions).

At the bifurcation point F_1 a branch of asymmetric solutions *f* emerges (see Figure 2). At the branch *f* there is a bifurcation point F_2 which gives rise to a branch g of symmetric solutions (see Figure 3). In Fig. 4 four bifurcation points, C_2, D_1, D_2, and F_2, occurring at the above mentioned branch g are depicted. At the point C_2 a bifurcation occurs and a branch c of asymmetric solutions results (see Figure 5). From the point C_1 on the asymmetric branch c a closed loop of symmetric solutions, branch b, emerges, cf. Figure 6. This isolated loop, which we have shown recently [7] to be triggered by an imperfect bifurcation mechanism, has one more bifurcation poing E_2. Bifurcation of asymmetric solutions on branch e will lead us back to the basic branch a.

Table I. Approximate coordinates of bifurcation points.

Bif. points	Value of L
F_1	0.2667
F_2	0.9151
C_1	0.1655
C_2	0.2986
E_1	0.2954
E_2	0.1565
J_1	0.5883
J_2	0.5892
D_1	0.3537
D_2	0.4158

From the bifurcation points D_1 and D_2 on the branch g of symmetric solutions a branch of asymmetric solutions d is created, see Figure 9. Bifurcation points J_1 and J_2 occurring at the basic branch a of symmetric solutions give rise to a closed branch j of asymmetric solutions, cf. Figure 8.

The branches of asymmetric solutions mentioned so far possess one typical property, namely the derivatives Y' at $z = 0$ and $z = L$ occur at the same curve. For instance the mirror symmetric profiles 23′, 24′, and 23, 24 create a different part of the same branch (cf. Figs. 5 and 12). Evidently, for this particular case after calculating a given profile we have two points on the same branch in the bifurcation diagram (e.g. 23 and 23′ in Figure 12).

Different topological properties can be observed for a branch displayed in Figure 10. Plotting derivatives $Y'(0)$ and $Y'(L)$ versus L gives rise to two isolated closed branches k and k′. The same points at to different loops k and k′ correspond to the same profile. Apparently the branches k and k′ are isolated; we have not been able to find any singular point on them.

The singular points which we have calculated in this study were (i) limit points (ii) limit-bifurcation points.

A typical limit-bifurcation point F_1 is displayed in Fig. 2 (see also 9 in Figure 12). This point is a bifurcation point of the branch a of symmetrical solutions because asymmetrical solutions may emerge. On the other hand, F_1 is a limit point at the branch f of asymmetric solutions. At this point two

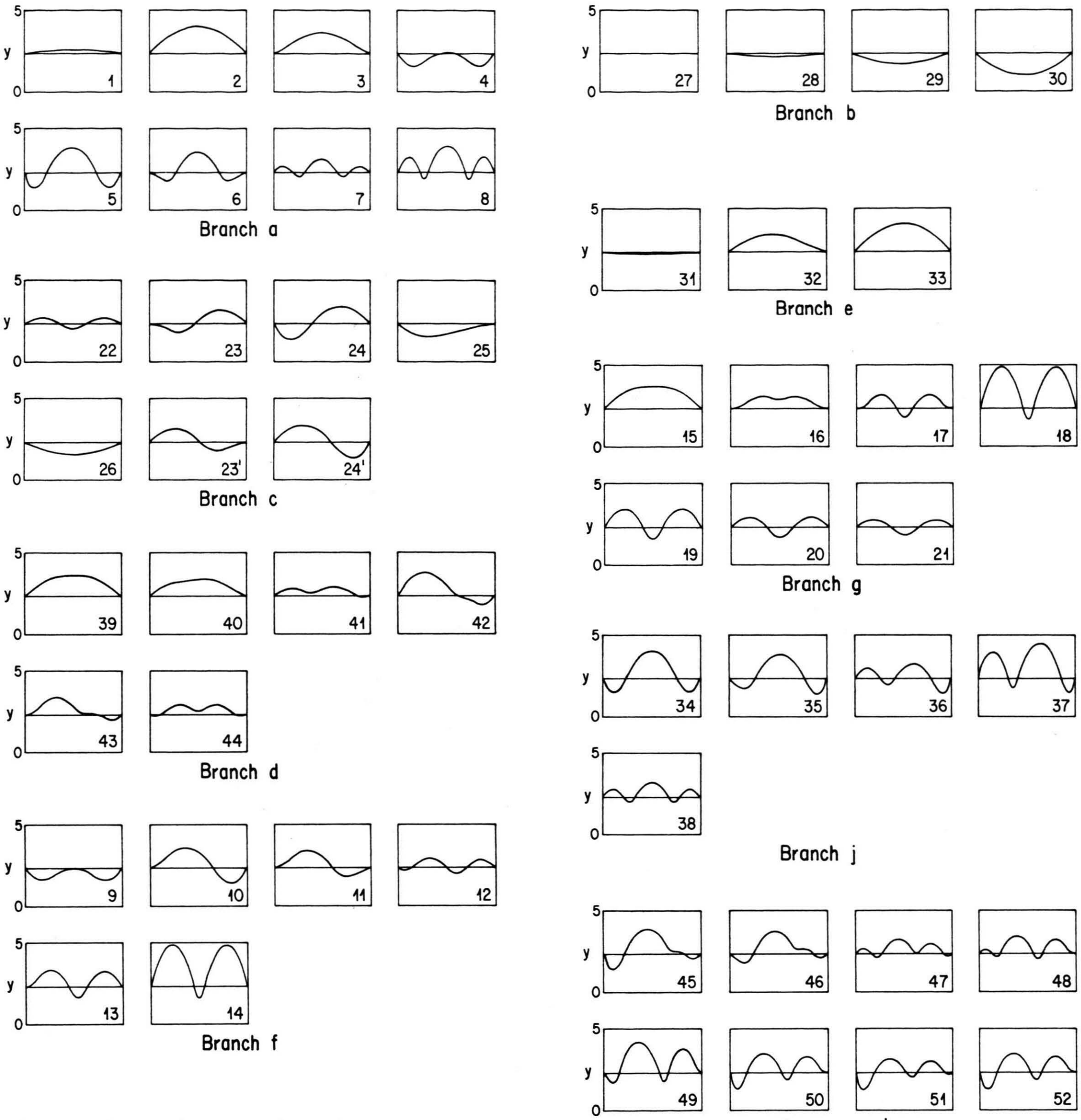

Fig.12. Typical profiles at particular branches.

asymmetric (mirror symmetric) solutions collapse in a symmetric solution.

The profiles at the bifurcation points are drawn in Fig. 12, cf. 9, 14, 18, 22, 26, 31, 33, 34, 38 and 44. The approximate coordinates of the bifurcation points are reported in Table 1.

The number of possible steady states can be found in Figure 11. It is obvious that the only possibility of calculating all admissible solutions is a careful continuation analysis. Nevertheless, we cannot be sure that we did not miss some isolated branches.

Figure 12 contains a condensed information on the properties of particular profiles. A complete information on X and Y profiles may be found in [15]. The material presented in Fig. 12 and in the bifurcation diagrams is self-explanatory. Let us notice at least the number of modes of the solution occurring at the symmetric branch a (cf. 1 − 8 in Figure 12).

V. Discussion and conclusion

This paper represents a first attempt in the literature to calculate the complete bifurcation diagram for reaction-diffusion problems where diffusion of the initial reacting component is considered. There are two possible ways of branching the solutions, either the basic branch a will be followed or branching from the isolated branch b may occur. In both cases, the branching is of the type symmetric → asymmetric → symmetric. Both ways of branching are coupled by the bifurcation point F_2.

For higher values of L a topologically interesting isolated branch of asymmetric solutions (without singular points) was discovered. We may expect some new dynamic properties of the system at this branch.

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Verantwortlich für den Inhalt: A. KLEMM
Satz und Druck: Konrad Triltsch, Würzburg