Three Coupled Cells with Brusselator Reaction

exa1

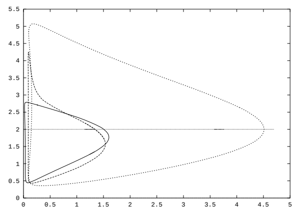
Variables and parameters:

y_1, y_2: substances in the first cell
y_3, y_4: substances in the second cell
y_5, y_6: substances in the third cell
λ: coupling coefficient (bifurcation parameter)

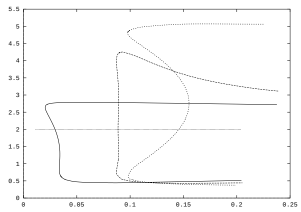
System of equations:

$$\begin{aligned}
2 - 7y_1 + y_1^2 y_2 + \lambda(y_3 - y_1) &= 0 \\
6y_1 - y_1^2 y_2 + 10\lambda(y_4 - y_2) &= 0 \\
2 - 7y_3 + y_3^2 y_4 + \lambda(y_1 + y_5 - 2y_3) &= 0 \\
6y_3 - y_3^2 y_4 + 10\lambda(y_2 + y_6 - 2y_4) &= 0 \\
2 - 7y_5 + y_5^2 y_6 + \lambda(y_3 - y_5) &= 0 \\
6y_5 - y_5^2 y_6 + 10\lambda(y_4 - y_6) &= 0
\end{aligned}$$

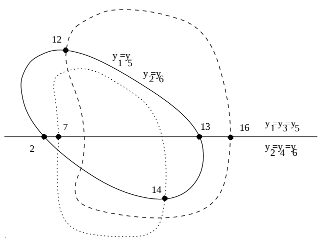
Figures:

1 

Bifurcation diagram y_1 versus λ.

2 

y_1 versus λ, detail of Figure 1.

3 

Schematic bifurcation; for numbers of bifurcations see Table.

Comments and explanations:

The trimolecular reaction

$$A \rightleftharpoons X$$

$$2X + Y \rightleftharpoons 3X$$
$$B + X \rightleftharpoons Y + D$$
$$X \rightleftharpoons E$$

was introduced in P. Glansdorff, I. Prigogine: Thermodynamic Theory of Structure, Stability and Fluctuations. Wiley-Interscience, London 1971.
The concentrations of the chemicals A, B, D, E are assumed to remain at a constant level. Taking all direct kinetic constants equal to one, and neglecting the reverse processes, the reaction is described by the differential equations

$$\frac{\partial X}{\partial t} = A + X^2 Y - BX - X + D_1 \frac{\partial^2 X}{\partial x^2}$$
$$\frac{\partial Y}{\partial t} = BX - X^2 Y + D_2 \frac{\partial^2 Y}{\partial x^2}$$

The variable x measures the length of the reactor. In what follows, we shall concentrate on the kinetic equations—that is, we neglect the diffusion terms ($D_1 = D_2 = 0$). Here we consider the steady-state situation ($\dot{X} = \dot{Y} = 0$) in three connected reaction cells with coefficients $A = 2$, $B = 6$. y_1 and y_2 stand for X and Y in the first cell, and so on.

An inspection of the equations reveals that an exchange

$$y_1 \leftrightarrow y_5, \quad y_2 \leftrightarrow y_6$$

yields the same equations. After a permutation of the order of equations, we arrive back at the original equation. This process of exchanging is described by the transformation

$$\mathbf{Sy} := \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \end{pmatrix}.$$

We realize that this transformation and the equation written as $\mathbf{f}(\mathbf{y}, \lambda) = \mathbf{0}$ satisfy the equivariance condition

$$\mathbf{f}(\mathbf{Sy}, \lambda) = \mathbf{Sf}(\mathbf{y}, \lambda),$$

and $\mathbf{S}^2 = \mathbf{I}$ holds. That is, the equation is $\mathbf{Z}_2$ symmetric. Hence, in this example, we expect pitchfork bifurcations with symmetry breaking.

As an inspection of the equations shows, there is a stationary solution for all λ,

$$X = A, \quad Y = \frac{B}{A}.$$

For our choice of parameters this solution is given by

$$\mathbf{y} = (2, 3, 2, 3, 2, 3)^{tr}.$$

TABLE: stationary bifurcations.

No.	λ_0	$y_1(\lambda_0)$	Type of branch point
1	0.0203067	2.64153	Turning point (TP)
2	0.0295552	2.00000	Transcritical bif. pt.
3	0.0335279	0.838479	TP
4	0.0341459	1.265004	TP
5	0.0872084	0.764918	TP
6	0.0872084	3.98597	TP
7	0.0886656	2.00000	Pitchfork bif. pt.
8	0.0893470	1.35524	TP
9	0.0893470	2.87172	TP
10	0.0976019	4.80000	TP
11	0.0976019	0.653982	TP
12	0.155218	2.75475	Pitchfork bif. pt.
13	1.50378	2.00000	Transcritical bif. pt.
14	1.53561	1.57162	Pitchfork bif. pt.
15	1.60171	1.76993	TP
16	4.51133	2.00000	Pitchfork bif. pt.

We restrict a numerical analysis to the parameter range $0 < \lambda < 5$. The resulting branching diagram is depicted in Figure 1, and a detail for small values of λ is shown in Figure 2. As these figures show, there are a great number of turning points, pitchfork bifurcations, and transcritical bifurcations. The branch points are listed in the Table (rounded to six digits). In addition, Hopf bifurcations exist.

Figure 3 condenses the bifurcation behavior in a qualitative way. The nontrivial branches are connected with the trivial branch via bifurcation points 2, 7, 13, 16. Because only two are pitchfork bifurcations, the way symmetries are broken or preserved is especially interesting. The trivial branch reflects a "higher" regularity than the symmetry condition with $\mathbf{S}$ because

$$y_1 = y_3 = y_5 \,, \quad y_2 = y_4 = y_6$$

holds. In Figure 3, symmetric solutions with respect to $\mathbf{S}$ are indicated by solid lines, and branches of asymmetric solutions are dashed, or dotted. The symmetry defined by the matrix $\mathbf{S}$ is preserved at the transcritical bifurcation points 2 and 13, but at these points the regularity responsible for $y_1 = y_3 = y_5$, $y_2 = y_4 = y_6$ is broken. Symmetry breaking of the $\mathbf{Z}_2$ symmetry takes place at the pitchfork bifurcations 7, 12, 14, 16.