

## **Spatial Pattern Formation in Compartmental Reaction-Electrodiffusion Systems with Concentration-Dependent Diffusivities\***

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**Abstract** Reaction-electrodiffusion equations with concentration-dependent diffusivities are given in their compartmental representation. Microscopic and global electroneutrality limit are considered respectively. Conditions for the emergence of Turing structures in continuous systems are derived. The formation of Turing patterns after diffusive instability of a homogeneous concentration distribution in a chain of compartments is shown numerically for two nonlinear model reaction systems. The nonlinear polynomial concentration dependence of diffusion influences amplitudes and symmetry of the spatial structures.

### **1. Introduction**

The theory of reaction-diffusion equations has found many applications in developmental biology, ecology, physiology etc., for reviews compare e.g. Murray 1977, Okubo 1980, Segel 1980, Meinhardt 1982, Britton 1986. The term "reaction" is used as a synonym for reactive interactions of chemical substances as well as for inter- and intraspecific interactions of biological species. The term "diffusion" includes the description of random and/or constrained movements of chemical as well as biological species. Those reactive and diffusive interactions are described by generally nonlinear partial differential equations (PDE) and the states of the biological or biochemical system of interest correspond to transient or stationary solutions of these equations. A great variety of spatial, temporal, and spatio-temporal solutions has been obtained. Since the basic paper by Turing (1952) the role of physiological gradients (Child, 1941; Kühn, 1965) and their stabilization by reaction and diffusion of biochemical substances during biological pattern formation has been of increasing interest (Gmitro and Scriven, 1966; Wolpert, 1969; Crick, 1970; Frankel, 1974; Kauffman et al., 1978; Hunding, 1981; Malchow and Feistel, 1982; Meinhardt, 1982; Murray, 1982; Malchow and Schimansky-Geier, 1985; Nagorcka et al., 1987). Because biochemical reactions are interactions of charged particles the ionic character of the reactants is included in the theoretical investigation of the system kinetics here. The importance of internal and external electric fields for morphogenetic processes has been emphasized already

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\*Dedicated to Professor Ei Teramoto on occasion of his retirement.

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by several authors (Jaffe, 1968; Plonsey, 1969; Jorné, 1975; Larter and Ortoleva, 1981; Ebeling and Feudel, 1983; Malchow et al., 1983; Pohl and Lamprecht, 1985; Toko et al., 1985; Malchow, 1988). Conditions for the emergence of Turing structures in reaction-electrodifffusion systems with constant diffusion have been derived by Jorné (1975) for the strong microscopic electroneutrality (MEN) limit and by Ebeling and Feudel (1983) for the weaker global electroneutrality (GEN) limit. The results of Jorné have been extended recently to the case of arbitrary concentration-dependent diffusion. It has been shown that the inclusion of concentration dependence of diffusion controls the amplitudes of the spatial distribution (Malchow, 1988). The inclusion of concentration dependence of diffusion is not only essential in ionic reaction-diffusion systems but also in other physical, chemical, and biological systems. Density-dependent migration and its effect on spatial segregation in prey-predator systems has been of special interest (Shigesaka et al., 1979; Minura and Kawasaki, 1980; Teramoto and Shigesada, 1981).

Because of the difficulties often arising while dealing with nonlinear PDE or for modelling special processes as e.g. cell-cell communication it is sometimes useful to investigate spatially discrete instead of continuous systems. The space is divided into a finite number of homogeneous, wellmixed, lumped compartments with mass exchange. The processes inside these coupled compartments can be described by ordinary differential equations (ODE). Useful introductions to compartmental modeling have been given by Atkins (1969), Jacquez (1972), Godfrey (1983) and an application to selforganization in multiple-unit systems by Babloyantz (1986).

In this paper ch. 2 is devoted to systems with MEN, ch. 3 to systems with GEN. In chs. 2.1 and 3.1 conditions for the emergence of Turing instabilities in continuous systems are given. The obtained regions of critical ratios of diffusion coefficients are applicable to the following numerical study of the corresponding compartmental systems. A set of ODE describing ionic reaction and concentration-dependent diffusion in a compartmental system for the MEN is derived in ch. 2.2. In ch. 2.3 a special ternary model reaction system (Malchow, 1988) is solved numerically under Turing instability conditions for polynomial concentration dependence of diffusion.

The assumption of MEN is dropped in ch. 3 and the condition of GEN is taken into consideration. Compartmental equations are derived in ch. 3.2. A binary model reaction system due to Ebeling and Feudel (1983) is treated numerically in ch. 3.3. The arising voltages are computed by the method of Hafemann (1965). The control of amplitudes and symmetry of the Turing structures by the concentration dependence is shown for systems with MEN as well as with GEN.

## 2. Reaction-Electrodifffusion Equations in the Microscopic Electroneutrality Limit

The time course of ionic reactive and diffusive interactions can be described by parabolic partial differential equations of the form

$$(\partial/\partial t)X_i(\mathbf{r},t) = f_i(X) - \nabla j_i(\mathbf{r},t); \quad i=1, 2, \dots, n. \quad (2.1)$$

Here  $X_i(\mathbf{r}, t)$  is the concentration of ions of kind  $i$  at time  $t$  and position  $\mathbf{r}$  whereas the  $f_i$  are the generally nonlinear reaction functions. The flux  $j_i(\mathbf{r}, t)$  reads

$$j_i(\mathbf{r}, t) = -D_i(\mathbf{X}) \nabla X_i(\mathbf{r}, t) + M_i(\mathbf{X}) X_i(\mathbf{r}, t) \mathbf{E}(\mathbf{r}, t); \quad i=1, 2, \dots, n; \quad (2.2)$$

with the macroscopic electric field  $\mathbf{E}(\mathbf{r}, t)$  satisfying the Poisson equation. The concentration-dependent diffusivities  $D_i(\mathbf{X})$  and mobilities  $M_i(\mathbf{X})$  are connected by the Einstein relation

$$M_i(\mathbf{X}) = z_i F D_i(\mathbf{X}) / RT; \quad i=1, 2, \dots, n; \quad (2.3)$$

where the  $z_i$  are the charge numbers,  $F$  is the Faraday constant,  $R$  the gas constant and  $T$  the temperature. Introducing the reference values for time  $t_0$ , concentration  $X_0$ , length  $L_0$ , diffusion  $D_0 = L_0^2/t_0$  and electric field  $E_0 = RT/FL_0$  one obtains in dimensionless quantities

$$(\partial/\partial t) X_i(\mathbf{r}, t) = f_i(\mathbf{X}) + \nabla [D_i(\mathbf{X}) X_i(\mathbf{r}, t) - z_i D_i(\mathbf{X}) X_i(\mathbf{r}, t) \mathbf{E}(\mathbf{r}, t)]; \quad i=1, 2, \dots, n. \quad (2.4)$$

For the MEN limit and  $n=2$  this system can be treated by the concept of ambipolar diffusion (Ebeling, 1967; Falkenhagen, 1971; Arndt and Roper, 1972; Malchow and Schimansky-Geier, 1985), for  $n>2$  this simplification is not possible at all but the corresponding system of  $n$  equations can be reduced to order  $(n-1)$ , the  $n$ th concentration value follows simply from the electroneutrality condition

$$\sum_{i=1}^n z_i X_i(\mathbf{r}, t) = 0, \quad X_n(\mathbf{r}, t) = -\sum_{i=1}^{n-1} (z_i/z_n) X_i(\mathbf{r}, t). \quad (2.5)$$

Using (2.5) the electric field is related to the concentration gradients by

$$\mathbf{E}(\mathbf{r}, t) = \frac{\sum_{k=1}^{n-1} z_k [D_k(\mathbf{X}) - D_n(\mathbf{X})] \nabla X_k(\mathbf{r}, t)}{\sum_{k=1}^{n-1} z_k [z_k D_k(\mathbf{X}) - z_n D_n(\mathbf{X})] X_k(\mathbf{r}, t)}, \quad (2.6)$$

so that (2.4) can be rewritten and reads

$$\begin{aligned} (\partial/\partial t) X_i(\mathbf{r}, t) = & f_i(\mathbf{X}) \\ & + \nabla \{ D_i(\mathbf{X}) \nabla X_i(\mathbf{r}, t) - t_i(\mathbf{X}) \sum_{k=1}^{n-1} (z_k/z_i) [D_k(\mathbf{X}) - D_n(\mathbf{X})] \nabla X_k(\mathbf{r}, t) \} \end{aligned} \quad (2.7)$$

with the transference numbers (Falkenhagen, 1971)

$$t_i(\mathbf{X}) = \frac{z_i^2 D_i(\mathbf{X}) X_i(\mathbf{r}, t)}{\sum_{k=1}^{n-1} z_k [z_k D_k(\mathbf{X}) - z_n D_n(\mathbf{X})] X_k(\mathbf{r}, t)}; \quad i=1, 2, \dots, n-1. \quad (2.8)$$

Introducing the self- and cross-diffusion coefficients (Jorné, 1975)

$$D_{ii}(\mathbf{X}) = [1 - t_i(\mathbf{X})] D_i(\mathbf{X}) + t_i(\mathbf{X}) D_n(\mathbf{X}), \quad (2.9)$$

$$D_{ij}^{i \neq j}(\mathbf{X}) = -(z_j/z_i) t_i(\mathbf{X}) [D_j(\mathbf{X}) - D_n(\mathbf{X})];$$

$$i=1, 2, \dots, n-1; \quad j=1, 2, \dots, n-1; \quad (2.10)$$

eq. (2.7) can be written as a general reaction-diffusion equation with concentration-dependent diffusion matrix  $\mathbf{D}$  including non-vanishing off-diagonal elements

$$(\partial/\partial t) \mathbf{X}(\mathbf{r}, t) = \mathbf{f}(\mathbf{X}) + \nabla [\mathbf{D}(\mathbf{X}) \nabla \mathbf{X}]. \quad (2.11)$$

## 2.1 CONDITIONS FOR THE EMERGENCE OF TURING STRUCTURES IN CONTINUOUS TERNARY SYSTEMS

Now the existence of a homogeneous steady state  $X^s$  with  $(\partial/\partial)X^s=0$ ,  $f(X^s)=0$  is assumed. Investigating its stability against small fluctuations

$$x(r, t) \propto \exp\{pt + ikr\} \quad (2.12)$$

one finds in linear analysis the characteristic equation for the eigenvalues  $p$  determining stability

$$\det |a_{ij} - k^2 D_{ij}(X^s) - \delta_{ij}p| = 0 \quad (2.13)$$

with

$$a_{ij} = \left[ \frac{\partial f_i}{\partial X_j} \right]_{X=X^s} - \frac{z_j}{z_i} \left[ \frac{\partial f_i}{\partial X_n} \right]_{X=X^s};$$

$$i=1, 2, \dots, n-1; \quad j=1, 2, \dots, n-1. \quad (2.14)$$

By definition of a Turing instability the solution is assumed to be stable for  $k=0$ , i.e. the real parts of all eigenvalues are less than zero:

$$\operatorname{Re} p_i(k=0) < 0; \quad i=1, 2, \dots, n-1; \quad (2.15)$$

whereas instability occurs for finite  $k>0$ , i.e. at least one real part becomes greater than zero:

$$\operatorname{Re} p_m(k>0) > 0; \quad 1 \leq m \leq n-1;$$

$$\operatorname{Re} p_i(k>0) < 0; \quad \forall i \neq m. \quad (2.16)$$

If this is specified for ternary systems ( $n=3$ ) one obtains the well-known condition for maintaining stability at  $k=0$ :

$$a_{11} + a_{22} < 0; \quad a_{11}a_{22} - a_{12}a_{21} > 0. \quad (2.17)$$

One finds the necessary condition

$$D_{22}a_{11} + D_{11}a_{22} > D_{21}a_{12} + D_{12}a_{21} \quad (2.18)$$

and finally the sufficient condition

$$D_{22}a_{11} + D_{11}a_{22} - D_{21}a_{12} - D_{12}a_{21} \geq 2\{(D_{11}D_{22} - D_{12}D_{21})(a_{11}a_{22} - a_{12}a_{21})\}^{1/2} \quad (2.19)$$

for inducing Turing instabilities (Malchow, 1988). These are the equivalents of the formulas for neutral two-component systems found by Segel and Jackson (1972). It is to be seen that even negative cross-diffusion can increase the region of instabilities, i.e. cross-diffusion-induced instabilities become possible.

## 2.2 COMPARTMENTAL SYSTEMS

A compartmental formulation of eq. (2.7) is derived now. The simplest case of Cartesian coordinates in one dimension is considered. It can be extended easily to other geometries and/or higher dimension. The space is divided into  $m$  compartments with equal volume and characteristic length  $d$ . The flux between the compartments  $k$  and  $(k-1)$  is characterized by the exchange coefficients  $P_{ik}$  for the pure diffusion

exchange and  $B_{ijk}$  for the exchange caused by electric field interactions. The index  $i$  is a mark for the kind of ion,  $k$  is the number of the compartment and  $j$  a summation index to be seen below. The definition of these exchange coefficients is related to the treatment of space-dependent diffusion by DeAngelis et al. (1986). The system is sketched in Fig. 1:

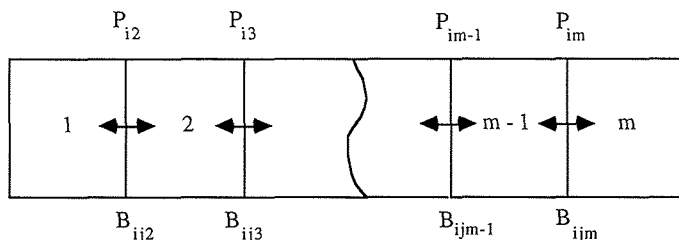


Fig. 1. Sketch of the compartmental system used in Ch. 2 (compare text).

With these definitions eq. (2.7) can be written in its compartmental formulation

$$\begin{aligned}
 (\partial/\partial t)X_{ik} = & f_i(X_k) + P_{ik+1}X_{ik+1} + P_{ik}X_{ik-1} - (P_{ik+1} + P_{ik})X_{ik} + \\
 & - \sum_{j=1}^{n-1} [B_{ijk+1}X_{jk+1} + B_{ijk}X_{jk-1} - (B_{ijk+1} + B_{ijk})X_{jk}] \quad (2.20)
 \end{aligned}$$

with

$$P_{ik} = (1/2d^2) [D_i(X_k) + D_i(X_{k-1})], \quad (2.21)$$

$$B_{ijk} = (z_j/2d^2z_i) \{ t_i(X_k)[D_j(X_k) - D_n(X_k)] + t_i(X_{k-1})[D_j(X_{k-1}) - D_n(X_{k-1})] \}, \quad (2.22)$$

and

$$\begin{aligned}
 t_i(X_k) = & \frac{z_i^2 D_i(X_k) X_{ik}}{\sum_{l=1}^{n-1} z_l [z_l D_l(X_k) - z_n D_n(X_k)] X_{lk}}; \quad i=1, 2, \dots, n-1; \\
 & k=1, 2, \dots, m. \quad (2.23)
 \end{aligned}$$

These equations are valid for all compartments except at the ends where the boundary conditions must be satisfied.

### 2.3 NUMERICAL TREATMENT OF A TERNARY MODEL REACTION SYSTEM WITH POLYNOMIAL CONCENTRATION DEPENDENCE OF DIFFUSION

A ternary model reaction system has been introduced recently (Malchow, 1988). The charge numbers are  $z_1 = -1$ ,  $z_2 = z_3 = +1$ . After substitution  $X_1 = X_2 + X_3$  because of MEN the pseudo-two-component system to be considered reads in dimensionless quantities without flux terms

$$\begin{aligned}
 \frac{\partial X_2}{\partial t} = & -\alpha X_2 + X_2^2 X_3 - X_2 [X_2 + X_3] + \beta, \\
 \frac{\partial X_3}{\partial t} = & \alpha X_2 - X_2^2 X_3, \quad (2.24)
 \end{aligned}$$

where  $\alpha$  and  $\beta$  are functions of reaction rates and concentrations of substrates and products. The only stationary solution

$$X_1^s = \frac{\beta}{\sqrt{\beta-\alpha}}; \quad X_2^s = \sqrt{\beta-\alpha}; \quad X_3^s = \frac{\alpha}{\sqrt{\beta-\alpha}} \quad (2.25)$$

is always stable against homogeneous fluctuations but can be destabilized by crossing critical ratios ( $D_3/D_2$ ).

The concentration dependence of diffusion is chosen as a polynomial of third order (Malchow, 1988):

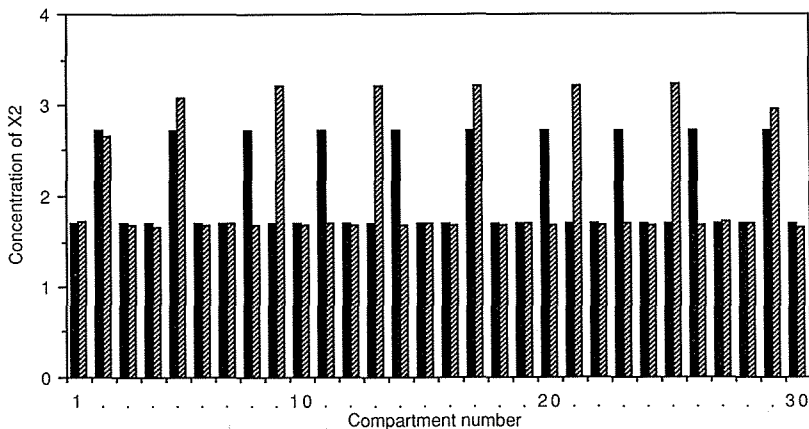
$$D_i = D_{i0} \{ 1 + S(A_i X_i + B_i X_i^2 + G_i X_i^3) \} \quad (2.26)$$

with

$$A_i = -\frac{(X_i^s)^2}{m_i}; \quad B_i = \frac{1+m_i}{m_i} X_i^s; \quad G_i = -1; \quad i=1, 2, 3; \quad (2.27)$$

where  $D_{i0} > 0$  and  $m_i > 1$  are specific constants for each ion. This choice of  $A_i$ ,  $B_i$ , and  $G_i$  yields  $D_i > D_{i0}$  for  $X_i < X_i^s$  and vice versa for small deviations from the stationary state.  $S$  is only a technical parameter switching the concentration dependence on or off.

Eqs. (2.24) and (2.26) are inserted into (2.20) now assuming a chain of 30 compartments with Neumann boundary conditions. The resulting system of 60 ODE's is integrated by Gear's method after finding instability regions from (2.18) and (2.19). Fig. 2 shows a typical numerically stable result. It is seen that the inclusion of concentration dependence of diffusion not only influences the amplitudes of the spatial distribution but also breaks its spatial symmetry. Contrast sharpening by concentration-dependent diffusion has been obtained recently for continuous space using the same model reaction system and determining the spatial distribution near the Turing bifurcation point analytically (Malchow, 1988).



**Fig. 2.** Turing structure for the MEN limit. Black columns ( $S=0$ ): Constant diffusion. Hatched columns ( $S=10^{-2}$ ): Concentration-dependent diffusion. Parameters:  $\alpha=12$ ;  $\beta=16$ ;  $D_{10}=0.03$ ;  $D_{20}=0.002$ ;  $D_{30}=0.5$ ;  $d=1$ .

### 3. Reaction-Electrodiffusion Equations without Microscopic Electroneutrality Limit

The assumption of microscopic charge neutrality is self-contradictory because experimentally measured potential differences could not appear if there would be no charge separation. However, Hafemann (1965) proved the approximate validity of the MEN assumption for time scales on which experiments are performed. Following the same author and Ebeling and Feudel (1983) this assumption is eliminated and charge distributions are computed.

#### 3.1 CONDITIONS FOR THE EMERGENCE OF TURING STRUCTURES IN CONTINUOUS BINARY SYSTEMS

Starting again with the continuous system (2.1) the Poisson equation

$$E(\mathbf{r}, t) = -\nabla \phi; \quad \nabla E(\mathbf{r}, t) = -\Delta \phi(\mathbf{r}, t) = -\frac{1}{\varepsilon_1} \sum_{i=1}^n z_i X_i(\mathbf{r}, t), \quad (3.1)$$

with potential  $\phi$  and dimensionless dielectric constant

$$\varepsilon_1 = \frac{RT}{F^2} \frac{1}{L_0^2 X_0} \varepsilon \varepsilon_0 \quad (3.2)$$

is inserted explicitly into the flux term (2.2). As in ch. 2.1 the stability of a homogeneous steady state  $X^s$  against fluctuations (2.12) is investigated now. One finds the characteristic equation for the eigenvalues

$$\det |a_{ij} - (z_i z_j / \varepsilon_1) D_i(X^s) X_i^s - \delta_{ij} [k^2 D_i(X^s) + p]| = 0 \quad (3.3)$$

with

$$a_{ij} = \left[ \frac{\partial f_i}{\partial X_j} \right]_{X=X^s}; \quad i=1, 2, \dots, n; \quad j=1, 2, \dots, n. \quad (3.4)$$

As in the MEN limit (Jorné, 1975; Malchow, 1988) the inclusion of concentration dependence of diffusion does formally not alter the results of linear stability analysis for constant diffusion given by Ebeling and Feudel (1983). Introducing the abbreviation

$$\tilde{a}_{ij} = a_{ij} - \frac{z_i z_j}{\varepsilon_1} D_i(X^s) X_i^s; \quad i=1, 2, \dots, n; \quad j=1, 2, \dots, n; \quad (3.5)$$

one finds the following conditions for the emergence of Turing structures specified for binary systems:

i) for  $k=0$ :  $a_{11} + a_{22} < 0, \quad a_{11} a_{22} < 0, \quad (3.6)$

ii) for finite  $k > 0$ :

-necessary  $D_2(X^s) \tilde{a}_{11} + D_1(X^s) \tilde{a}_{22} > 0; \quad D_1(X^s) \neq D_2(X^s) \quad (3.7)$

or explicitly

$$D_2(X^s) a_{11} + D_1(X^s) \tilde{a}_{22} - \frac{1}{\varepsilon_1} D_1(X^s) D_2(X^s) [z_1^2 X_1^s + z_2^2 X_2^s] > 0, \quad (3.8)$$

-sufficient

$$D_2(X^s)\tilde{a}_{11} + D_1(X^s)\tilde{a}_{22} \geq 2\{D_1(X^s)D_2(X^s) [\tilde{a}_{11}\tilde{a}_{22} - \tilde{a}_{12}\tilde{a}_{21}] \}^{1/2}. \quad (3.9)$$

The second inequality in (2.17) does not longer hold for binary systems because of  $a_{11} = a_{21}$  and  $a_{12} = a_{22}$ . In this case only (3.6) determines stability for  $k=0$ . Eqs. (3.7) and (3.9) correspond exactly to the conditions found by Segel and Jackson (1972) for neutral systems but extended to concentration-dependent electrodiffusion in the GEN limit. However, it is readily seen from (3.8) that the inclusion of the electric field interactions reduces the region of Turing instabilities, i.e. the electric field stabilizes the homogeneous distribution. The instability region can decrease further but also increase again due to the concrete concentration dependence of diffusion.

### 3.2 COMPARTMENTAL SYSTEMS WITH INTERNAL ELECTRIC POTENTIAL DIFFERENCES

Introducing exchange coefficients  $P_{ik}$  for pure diffusion and  $B_{ik}$  for the exchange due to electric field interactions as in ch. 2.2 one finds the compartmental formulation of (2.4):

$$\begin{aligned} (\partial/\partial t)X_{ik} = & f_i(X_k) + P_{ik+1}X_{ik+1} + P_{ik}X_{ik-1} - (P_{ik+1} + P_{ik})X_{ik} \\ & + B_{ik+1}\phi_{k+1} + B_{ik}\phi_{k-1} - (B_{ik+1} + B_{ik})\phi_k, \end{aligned} \quad (3.10)$$

with

$$P_{ik} = (1/2d^2) [D_i(X_k) + D_i(X_{k-1})] \quad (3.11)$$

and

$$B_{ik} = (z_i/2d^2) [D_i(X_k)X_{ik} + D_i(X_{k-1})X_{ik-1}], \quad (3.12)$$

or explicitly with the abbreviations  $f_i(X_k) = f_{ik}$ ,  $D_i(X_k) = D_{ik}$

$$\begin{aligned} \partial X_{ik}/\partial t = & f_{ik} \\ & + \frac{1}{2d^2} \sum_{l=k-1}^{k+1} \{ [D_{il} + D_{ik}] (X_{il} - X_{ik}) + z_i [D_{il}X_{il} + D_{ik}X_{ik}] (\phi_l - \phi_k) \}; \\ & i=1, 2, \dots, n; \quad k=1, 2, \dots, m. \end{aligned} \quad (3.13)$$

For constant diffusion the latter equation reduces to the expression found by Ebeling and Feudel (1983).

The potential differences appearing in (3.13) are determined by the method due to Hafemann (1965). It is assumed all of the charge in compartment  $k$  to lie on a plane at the midpoint of the compartment. The surface charge density  $\sigma_k$  on this plane is

$$\sigma_k = d \sum_{i=1}^n z_i X_{ik} \quad (3.14)$$

with

$$\sum_{k=1}^m \sigma_k = 0, \quad (3.15)$$

because the system as a whole has no net charge. The planes are located at  $r_1, r_2, \dots, r_m$  respectively. The electric field intensity  $E$  at a point  $r$  between  $r_k$  and  $r_{k+1}$  is



$$E(r) = \frac{1}{\varepsilon_1} \sum_{j=1}^{k(r)} \sigma_j, \quad (3.16)$$

where the summation includes the charges on the left side of  $r$  only. Fig. 3 shows a sketch of the considered compartmental system with charged planes.

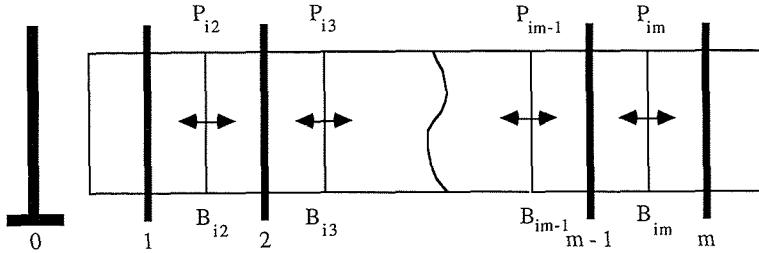


Fig. 3. Sketch of the compartmental system used in Ch. 3 (compare text).

The potential difference  $\Phi$  across a system of infinite planes of uniform surface charge with a reference electrode of potential  $\phi_0$  is given by

$$\Phi = \phi_m - \phi_0 = \frac{d^2}{\varepsilon_1} \sum_{j=1}^m j \sum_{i=1}^n z_i X_{ij}. \quad (3.17)$$

From this expression one finds finally for the potential differences between adjacent compartments

$$\phi_k - \phi_{k-1} = \frac{d^2}{\varepsilon_1} \sum_{j=k}^m \sum_{i=1}^n z_i X_{ij}; \quad k=1, 2, \dots, m. \quad (3.18)$$

For  $m=2$  this coincides with the potential difference of a plate capacitor used by Ebeling and Feudel (1983) for a two-compartment system. Eqs. (3.13) and (3.18) describe the compartmental system completely except the ends which have to satisfy the boundary conditions.

### 3.3 NUMERICAL TREATMENT OF A BINARY MODEL REACTION SYSTEM WITH POLYNOMIAL CONCENTRATION DEPENDENCE OF DIFFUSION

The model reaction used here is due to Ebeling and Feudel (1983). The charge numbers are  $z_1 = +1$ ,  $z_2 = -1$  and the kinetic equations read in dimensionless quantities without flux terms

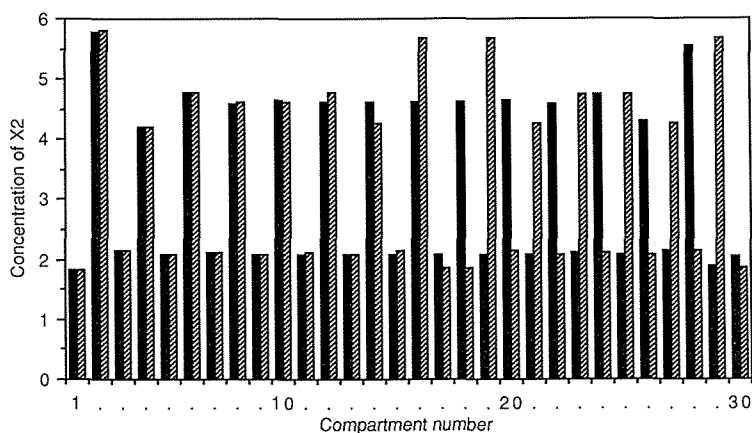
$$\frac{\partial X_1}{\partial t} = 1 - X_1 X_2 + \alpha X_1^2 = \frac{\partial X_2}{\partial t}. \quad (3.19)$$

This system has one homogeneous steady state

$$X_1^s = X_2^s = (1 - \alpha)^{-1/2} \quad (3.20)$$

which is without diffusion always stable for  $\alpha < 1$  but can be destabilized crossing

critical ratios ( $D_1/D_2$ ) for  $(1/2) < \alpha < 1$ . The concentration dependence of diffusion is assumed to be the same as in ch. 2.3. Instability regions are found from (3.7) and (3.9). A numerically stable integration result can be seen in Fig. 4 for 30 compartments and Neumann boundary conditions. As for systems in the MEN limit the inclusion of nonlinear concentration dependence of diffusion influences amplitudes and symmetry of the spatial distribution.



**Fig. 4.** Turing structure for the GEN limit. Black columns ( $S=0$ ): Constant diffusion. Hatched columns ( $S=10^{-4}$ ): Concentration-dependent diffusion. Parameters:  $\alpha=0.75$ ;  $D_{10}=0.01$ ;  $D_{20}=0.2$ ;  $d=2$ ;  $L_0=10^{-6}$ ;  $X_0=10^{-7}$  mol cm $^{-3}$ ;  $T=300$  K.

### Discussion

Compartmental reaction-electrodifusion equations have been derived for concentration-dependent diffusion in systems with MEN as well as with GEN limit. The conditions for the emergence of Turing structures in continuous systems have been extended to the case of concentration-dependent diffusion. After finding instability regions from the latter conditions the compartmental equations have been integrated by Gear's method for a ternary model system in the MEN limit as well as for a binary model in the GEN limit. In both cases the concentration dependence of diffusion controls not only the amplitudes of the spatial distribution but can also break the symmetry of the Turing structures.

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