match no. 20 pp. 141-163 1986

A NOTE ON ESSENTIALLY POSITIVE MATRICES WHICH APPEAR IN CHEMICAL KINETICS

by

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(Received: June 1986)

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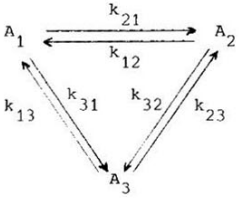
Abstract.- Matrices with positive off-diagonal elements (i.e., essentially positive matrices) appear in the analysis of systems in which n species are coupled via a complex scheme of first order reactions. The study of the spectrum of these matrices permits to infer the behavior of such systems until they reach their equilibrium states.

Key Words: location of eigenvalues, exponential of a matrix, complex monomolecular kinetics, butene.

INTRODUCTION

We will consider a system in which n chemical species are coupled via first order reactions and confined in a constant volume reactor. Suppose, for example, that we have three chemical species, A_1 , A_2 and A_3 , which are connected by the reaction scheme



where k_{ij} is supposed to be constant for each pressure and temperature. We denote by $[A_1]$, $[A_2]$, $[A_3]$ the concentrations of these species at the time t , and by $k_{ij}[A_j]$ the rate of formation of A_i from A_j , expressed in moles per unit of time.

We can assume that the energy balance in the reactions does not perturb the pressure and temperature conditions, by means of an efficient thermostatation, if necessary. So, it is reasonable to suppose that the concentrations vary according to the following linear differential system

$$\frac{d[A_1]}{dt} = -(k_{21} + k_{31})[A_1] + k_{12}[A_2] + k_{13}[A_3] \quad ,$$

$$\frac{d[A_2]}{dt} = k_{21}[A_1] - (k_{12} + k_{32})[A_2] + k_{23}[A_3] \quad ,$$

$$\frac{d[A_3]}{dt} = k_{31}[A_1] + k_{32}[A_2] - (k_{13} + k_{23})[A_3] \quad .$$

The numbers $k_{ij} > 0$, $1 \leq i,j \leq 3$, $i \neq j$, are the *rate constants* of these three composed reactions. They are determined experimentally.

Such a system can be generalized for n chemical species, each of which is coupled to every other species by chemical reaction to give

$$\frac{d[A_1]}{dt} = -\sum_{j=1}^{n} k_{j1}[A_1] + k_{12}[A_2] + \ldots + k_{1n}[A_n] \quad ,$$

$$\frac{d[A_2]}{dt} = k_{21}[A_1] - \sum_{j=1}^{n} k_{j2}[A_2] + \ldots + k_{2n}[A_n] \quad ,$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$

$$\frac{d[A_n]}{dt} = k_{n1}[A_1] + k_{n2}[A_2] + \ldots - \sum_{j=1}^{n} k_{jn}[A_n] \quad .$$

The total sum of the concentrations

$$[A_1] + [A_2] + \ldots + [A_n]$$

is *constant*; that is to say

$$[A_1](t) + [A_2](t) + \ldots + [A_n](t) = C$$

for all $t \geq 0$.

We will use the following notations:

$$x_i(t) := [A_i](t) \quad , \quad 1 \leq i \leq n \quad ; \quad x(t) := \begin{pmatrix} x_1(t) \\ \vdots \\ x_n(t) \end{pmatrix} \quad , \quad \dot{x}(t) := \begin{pmatrix} \frac{dx_1}{dt}(t) \\ \vdots \\ \frac{dx_n}{dt}(t) \end{pmatrix}$$

and

$$(1) \qquad K := \begin{pmatrix} -\sum_{j=1}^{n} k_{j1} & k_{12} & \cdots & k_{1n} \\ k_{21} & -\sum_{j=1}^{n} k_{j2} & \cdots & k_{2n} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ k_{n1} & k_{n2} & \cdots & -\sum_{j=1}^{n} k_{jn} \end{pmatrix}$$

Hence, the differential system can be expressed

$$(2) \qquad \dot{x} = Kx \quad .$$

The *problem* consists on calculating the limit concentrations of the equilibrium state (if there exists), which is attained after a sufficiently long time. The sum of the concentrations, C, as well as the rate constants $k_{ij} > 0$, $1 \leq i,j \leq n$, $i \neq j$, are supposed to be known. Given the initial concentrations $x_1(0) = c_1, \ldots, x_n(0) = c_n$, we are interested in studying the asymptotic behaviour of the solution of the problem

$$(3) \qquad \begin{aligned} & \dot{x} = Kx \\ & x(0) = c := (c_1, \ldots, c_n)^T \qquad (^T \text{ denotes transpose}) \\ & x_1(t) + \ldots + x_n(t) = C \end{aligned}$$

Namely, we wish to know if there exists the

$$\lim_{t \to \infty} x(t)$$

and then:

1) to compute its value, v , and

2) to establish the relation between v and the initial conditions.

If A is an $m \times n$ real matrix, we write $A \geq 0$ whenever all the elements a_{ij} of A are ≥ 0 , and $A >> 0$ if all the a_{ij} are > 0 . $A > 0$ means $A \geq 0$ and $A \neq 0$

The matrix K is *essentially positive*; that is $K + sI \geq 0$ for all real s sufficiently large. Then, for all $t \geq 0$,

$$e^{Kt} := \sum_{j=0}^{\infty} \frac{(Kt)^j}{j!} \geq 0 \qquad ([1] \text{ p.146}).$$

Moreover, K is an irreducible matrix ([1] p. 27, [3] p. 46) as all its elements are different from zero. Therefore, ([1] p. 146) it follows that

$$e^{Kt} >> 0$$

for all $t > 0$.

It is well known that the solution of (3) is given by

$$x(t) = e^{Kt}c \quad . \tag{4}$$

In consequence, if $c > 0$ then $x(t) >> 0$ for all $t > 0$. $x(t)$ is always in the part of the hyperplane

$$x_1 + \ldots + x_n = C$$

intercepted by the nonnegative orthant in $\mathbb{R}^n$. See the figure 1 for $n = 3$. In fact, since the sum of the elements of each column of K is zero it follows that

$$\frac{d}{dt}(x_1(t) + \ldots + x_n(t)) = 0$$

for all $t \geq 0$; thus,

$$x_1(t) + \ldots + x_n(t)$$

is constant on $0 \leq t < \infty$. But $x_1(0) + \ldots + x_n(0) = C$, therefore

$$x_1(t) + \ldots + x_n(t) = C$$

on $0 \leq t < \infty$.

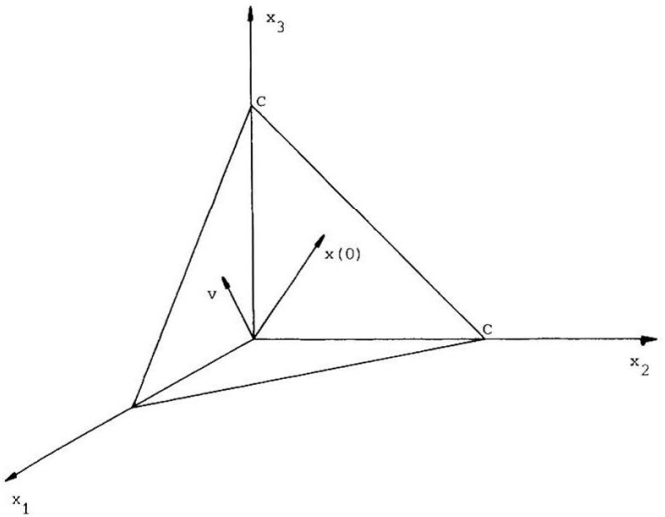


Fig. 1

We are more interested in the *direction* of the solution vector $x(t)$ than in its *length*. This is the main question for some linear differential systems which appear in *chemical kinetics* and *pharmacokinetics*. See [9].

The response to the settled questions requires the study of the matrix K . We shall do it in the next section. Previously, we point out that an incomplete and partially erroneous study of problem (3) was given in [6].

This exposition followed closely to [7]. Later we shall indicate the aspects which we criticize of these references.

SPECTRAL PROPERTIES OF ESSENTIALLY POSITIVE MATRICES

We enunciate the following classical result which will be very useful for us. It is a theorem about the location of the eigenvalues of a matrix.

THEOREM (Gershgorin, 1931)([4] p. 114). *Consider the* $n \times n$ *complex matrix*

$$A = \begin{pmatrix} a_{11} & \cdots & a_{1j} & \cdots & a_{1n} \\ \vdots & & \vdots & & \vdots \\ a_{j1} & \cdots & a_{jj} & \cdots & a_{jn} \\ \vdots & & \vdots & & \vdots \\ a_{n1} & \cdots & a_{nj} & \cdots & a_{nn} \end{pmatrix} .$$

Let

$$R_j := \sum_{\substack{i=1 \\ i \neq j}}^{n} |a_{ij}| \qquad (j = 1, \ldots, n)$$

Then every eigenvalue of A *lies in at least one of the disks*

$$|z - a_{jj}| \leq R_j \qquad (j = 1, \ldots, n)$$

The proof is the same as that of ([4] p. 114), taking into account that A^T has the same eigenvalues as A.

We also need the Perron-Frobenius theorem for positive matrices ([3] p. 49):

THEOREM (Perron 1907, Frobenius 1912). *Let* A *be an* $n \times n$ *positive matrix, i.e.* $A >> 0$. *Then* A *has a positive eigenvalue* r *which is a simple root of its characteristic polynomial and greater than the modulus of any other eigenvalue.* A *has an eigenvector* $x := (x_1, \ldots, x_n)^T$ *corresponding to* r, *which has components* $x_i > 0$ *for all* $i = 1, \ldots, n$.

We shall also use the concept of M-matrix (M due to Minkowski). Let $\mathbb{R}^{n \times n}$ be the space of the $n \times n$ real matrices and denote by $Z^{n \times n}$ the class

$$\{A = (a_{ij}) \in \mathbb{R}^{n \times n} \mid a_{ij} \leq 0 \ , \quad i \neq j\} \quad .$$

Obviously every matrix A of this class can be expressed in the form

$$A = sI - B \quad , \qquad s > 0 \ , \ B \geq 0 \quad . \tag{5}$$

Recall that the spectral radius of an $n \times n$ complex matrix C is the maximum value of the modulus of all the eigenvalues of C. It is denoted by $\rho(C)$.

DEFINITION. Any matrix $A \in Z^{n \times n}$ which can be expressed in the form (5) with $s \geq \rho(B)$, is called an *M-matrix*.

We are already in conditions to establish the main result of this note.

THEOREM 1. *Let* K *be the* n x n *real matrix given by* (1). *Then* 0 *is a simple eigenvalue of* K , *the remaining eigenvalues of* K *have negative real part and there exists an eigenvector of* K *associated to* 0 *whose components are positive.*

PROOF. By adding the n-th , (n-1)-th , . . . , 2-nd rows of K to its 1-st one, the resulting matrix has the same determinant as K and, thus

$$|K| = \begin{vmatrix} 0 & 0 & \cdots & 0 \\ k_{21} & -\sum_{j=1}^{n} k_{j2} & \cdots & k_{2n} \\ \vdots & \vdots & & \vdots \\ k_{n1} & k_{n2} & \cdots & -\sum_{j=1}^{n} k_{jn} \end{vmatrix} = 0$$

Taking into account that the determinant of K is equal to the product of the eigenvalues of K , it follows that 0 is an eigenvalue of K .

By the Gershgorin theorem, all the eigenvalues of K lie in the union of the disks

$$\left| z + \sum_{j=1}^{n} k_{jp} \right| \leq \sum_{j=1}^{n} k_{jp} \qquad (p = 1,\ldots,n)$$

(we recall that $k_{jj} := 0$, $j = 1,\ldots,n$) .

So, all the non-null eigenvalues of K are complex numbers with negative real part. Indeed, these disks are contained in the semiplane $\mathrm{Re}(z) \leq 0$ and their only point in common with the imaginary axis is $z = 0$.

If we set $A := -K$ then $A \in Z^{nxn}$ and we can write $A = sI - B$ with $s > 0$ and $B > 0$. Moreover, if $\lambda_1,\lambda_2,\ldots,\lambda_n$ are the eigenvalues of K then $-\lambda_1,-\lambda_2,\ldots,-\lambda_n$ are the eigenvalues of A . On the other hand, as

(6) $$|\lambda I - A| = (-1)^n |(s-\lambda)I - B| \quad ,$$

if $\mu_1,\ldots,\mu_n$ are the eigenvalues of B, then $s-\mu_1,\ldots,s-\mu_n$ are the eigenvalues of A. Since 0 is an eigenvalue of A, s is an eigenvalue of B. So,

$$s \leq \rho(B).$$

Now, by the Perron-Frobenius theorem, $\rho(B)$ is a simple eigenvalue of B. Hence $s-\rho(B)$ is an eigenvalue of A and therefore $s<\rho(B)$ is not possible because all the non-null eigenvalues of A have positive real part. Hence $s=\rho(B)$. And this enable us to derive that 0 is a simple eigenvalue of A. In fact, $\rho(B)$ is a simple root of the characteristic polynomial of B

$$|\mu I - B| \quad ;$$

which yields

(7) $$|\mu I - B| = (\mu - \rho(B))q(\mu)$$

$q(\mu)$ being a polynomial such that $q(\rho(B)) \neq 0$.

By replacing μ by $s-\lambda$ in polynomial identity (7) and taking into account (6), it follows that

$$|\lambda I - A| = (\lambda - (s-\rho(B)))q_1(\lambda) \quad ,$$

where

$$q_1(\lambda) := (-1)^{n+1} q(s-\lambda)$$

and, thus,

$$q_1(s-\rho(B)) = (-1)^{n+1} q(\rho(B)) \neq 0 \quad .$$

Therefore $s - \rho(B)$ is a simple root of $|\lambda I - A| = 0$. As $0 = s - \rho(B)$, 0 is a simple eigenvalue of A and K .

Finally, as $A = sI - B$ with $s = \rho(B)$, A is an M-matrix . Moreover A is singular and irreducible, whence there exists a vector $v >> 0$ such that $Av = 0$ ([1], Theorem (4.16)(2), p. 156). Thus,

$$Kv = 0 \quad ,$$

and the theorem is proved .

REMARK 1. Since 0 is a simple eigenvalue of K we have that dim Ker $K = 1$, Ker $K := \{x \in \mathbb{R}^{nx1} \mid Kx = 0\}$ being the null-space of K . Hence there exists an unique vector $v = (v_1, \ldots, v_n)^T$ such that $Kv = 0$, $v_1 + \ldots + v_n = C$ and $v_i > 0$ for $i = 1, \ldots, n$

ASYMPTOTIC BEHAVIOR OF THE SOLUTIONS

We are going to discuss the existence and value of the

$$\lim_{t \to \infty} x(t)$$

where $x(t) = e^{kt}c$ is the solution of (3). For this, we are going to use the Jordan normal form of K ([5] p.236), that we denote by J.

It is well known there exists an nxn invertible complex matrix P such that

$$P^{-1}KP = J, \tag{8}$$

where J is block diagonal matrix

$$J = \begin{pmatrix} J_1 & & & & \\ & J_2 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & J_u \end{pmatrix}$$

and each J_i being an $n_i x n_i$ matrix of the form

$$\begin{pmatrix} \lambda_i & 1 & 0 & \cdots & 0 \\ 0 & \lambda_i & 1 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & 1 \\ 0 & 0 & 0 & \cdots & \lambda_i \end{pmatrix}$$

if $n_i > 1$, or (λ_i) if $n_i = 1$ (i=1,...,u).

J_i is called the i-th Jordan block. It may be that $\lambda_i = \lambda_j$ although $i \neq j$. Here $\lambda_1, \ldots, \lambda_u$ are the eigenvalues of K.

From (8) it follows that

$$e^{Kt} = Pe^{Jt}P^{-1} = P \begin{pmatrix} e^{J_1 t} & & & & \\ & e^{J_2 t} & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & e^{J_u t} \end{pmatrix} P^{-1}$$

It is known that ([10] p.389)

$$e^{J_i t} = e^{\lambda_i t} \begin{pmatrix} 1 & t & \frac{t^2}{2!} & \cdots & \frac{t^{n_i-1}}{(n_i-1)!} \\ 0 & 1 & t & \cdots & \frac{t^{n_i-2}}{(n_i-2)!} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}$$

for $i = 1,\ldots,u$.

Choose $\lambda_1 = 0$. As λ_1 is a simple eigenvalue of K, $J_1=(0)$ is 1×1 and $\lambda_i \neq 0$ for all $i=2,\ldots,u$. Besides, an eigenvector of K associated with 0 can be chosen as the first column of the matrix P ([5] p.236); that is to say

$$(9) \qquad K \begin{pmatrix} p_{11} \\ p_{21} \\ \cdot \\ \cdot \\ \cdot \\ p_{n1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix}$$

If m is an integer ≥ 0 and λ is a complex with negative real part, then $t^m e^{\lambda t} \to 0$ as $t \to \infty$. Therefore it follows from Theorem 1 that there exists the

$$\lim_{t \to \infty} e^{Kt} c = P \begin{pmatrix} 1 & 0 & . & . & . & 0 \\ 0 & 0 & . & . & . & 0 \\ . & . & & & & . \\ . & . & & & & . \\ . & . & & & & . \\ 0 & 0 & . & . & . & 0 \end{pmatrix} P^{-1} c =$$

$$\begin{pmatrix} p_{11} & 0 & . & . & . & 0 \\ p_{21} & 0 & . & . & . & 0 \\ . & . & & & & . \\ . & . & & & & . \\ . & . & & & & . \\ p_{n1} & 0 & . & . & . & 0 \end{pmatrix} P^{-1} c =: \tilde{v} = \begin{pmatrix} \tilde{v}_1 \\ . \\ . \\ . \\ \tilde{v}_n \end{pmatrix} .$$

Taking into account that $e^{Kt} >> 0$ for all $t > 0$, $x(t)$ is a real vector and $x(t) >> 0$ for all $t > 0$. Given that

$$\tilde{v}_i = \lim_{t \to \infty} x_i(t) ,$$

is follows that $\tilde{v}_i \geq 0$ and

$$\tilde{v}_1 + \ldots + \tilde{v}_n = \lim_{t \to \infty} (x_1(t) + \ldots + x_n(t)) = C .$$

Furthermore,

$$K \tilde{v} = K \begin{pmatrix} p_{11} & 0 & . & . & . & 0 \\ p_{21} & 0 & . & . & . & 0 \\ . & . & & & & . \\ . & . & & & & . \\ . & . & & & & . \\ p_{n1} & 0 & . & . & . & 0 \end{pmatrix} P^{-1} c =$$

$$\left(K \begin{pmatrix} p_{11} \\ p_{21} \\ . \\ . \\ . \\ p_{n1} \end{pmatrix}, K \begin{pmatrix} 0 \\ 0 \\ . \\ . \\ . \\ 0 \end{pmatrix}, \ldots, K \begin{pmatrix} 0 \\ 0 \\ . \\ . \\ . \\ 0 \end{pmatrix} \right) P^{-1} c = 0 \; P^{-1} c = 0 ,$$

by virtue of (9).

Due to the Remark 1, from $K\,\tilde{v} = 0$, $\tilde{v}_1 + \ldots + \tilde{v}_n = C$ and $\tilde{v}_i \geq 0$ we deduce that $\tilde{v}$ is completely determinated and $\tilde{v}_i > 0$ for all $i = 1,\ldots,n$. Thus, $\tilde{v}$ does not depend on the initial conditions $x(0) = c$.

EQUILIBRIUM. In particular, the constant vector-valued function $x(t) := \tilde{v}$ defined for all $t \geq 0$ is a solution of (3). It is the solution which verifies $x(0) = \tilde{v}$, due to the uniqueness of the solutions in an initial conditions problem. In such a case, the concentrations of the chemical species, $x_1(t), \ldots, x_n(t)$, will not vary with the time. $\tilde{v} = (\tilde{v}_1,\ldots,\tilde{v}_n)^T$ is the *equilibrium state* of system (2).

REMARK 2. In ([6] p. 230-232) it is asserted that if $a := (a_1,\ldots,a_n)^T >> 0$ is a vector such that

$$K\,a = 0 \qquad \text{and} \qquad a_1 + \ldots + a_n = 1 \quad ,$$

and we define $D := \text{diag}\,(a_1,\ldots,a_n)$, then the matrix $K\,D$ is symmetric. There, this result is deduced from the "principle of microscopic reversibility" or "principle of detailed balancing", which enables to write

$$k_{ji}\,a_i = k_{ij}\,a_j \quad .$$

Next, the author defines $P := \text{diag}\,(\sqrt{a_1},\ldots,\sqrt{a_n})$ and he considers the matrix

$$\tilde{K} := P^{-1}\,K\,P \quad .$$

Using again this chemical-physical principle he proves that $\tilde{K}$ is symmetric and, therefore, all the eigenvalues of K are real .

Now, if

$$(10) \qquad K := \begin{pmatrix} -4 & k_{12} & 1 \\ 2 & -(k_{12}+3) & 1 \\ 2 & 3 & -2 \end{pmatrix}$$

and $0 < k_{12} < 1$, it is easy to see that K has two complex eigenvalues with non-null imaginary part. Thus, the reasoning of [6] must be wrong.

Also in [6] it is assumed that K is diagonalizable, which is not always true. For example, when $k_{12} = 1$ in (10), K is not diagonalizable. In fact, K has two distinct eigenvalues, 0 simple, -5 double, but the proper subspace associated with -5 has dimension 1 .

APPLICATION TO THE CASE OF THE HYDROCARBON BUTENE.

Consider the hydrocarbon of formula C_4H_8 called *butene* (family of the alkenes). This hidrocarbon has three *isomers* called 1-butene, *cis*-2-butene and *trans*-2-butene according to the disposition of the atoms in the molecule. See figure 2 ([12] p. 506).

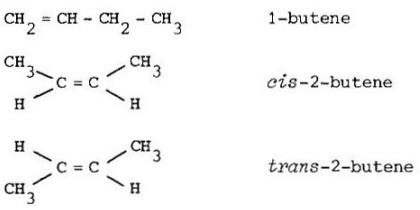
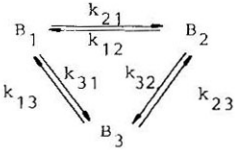


Fig. 2

Denote by $B_1, B_2 B_3$ these isomers. At fixed pressure and temperature, they coexist in general in gaseous state, and they interchange into one another according to the reactions



Call $[B_1](t)$, $[B_2](t)$, $[B_3](t)$ the concentrations of the three substances at the time t. It is reasonable to suppose that they vary following the linear differential system

$$\begin{pmatrix} \frac{d[B_1]}{dt} \\ \frac{d[B_2]}{dt} \\ \frac{d[B_3]}{dt} \end{pmatrix} = \begin{pmatrix} -(k_{21}+k_{31}) & k_{12} & k_{13} \\ k_{21} & -(k_{12}+k_{32}) & k_{23} \\ k_{31} & k_{32} & -(k_{13}+k_{23}) \end{pmatrix} \begin{pmatrix} [B_1] \\ [B_2] \\ [B_3] \end{pmatrix},$$

where the numbers $k_{ij} > 0$, $1 \leq i,j \leq 3$, $i \neq j$ are the rate constants.

The total concentration of butene, $[B_1]+[B_2]+[B_3]$, is constant. Call it C.

It follows from the results of the previous sections that:

1) There exists the

$$(11) \qquad \lim_{t\to\infty} \begin{pmatrix} [B_1] \\ [B_2] \\ [B_3] \end{pmatrix} =: \begin{pmatrix} [B_1]_\infty \\ [B_2]_\infty \\ [B_3]_\infty \end{pmatrix} \quad , \text{ and}$$

2) that it is given by

$$[B_1]_\infty = \mu(k_{13}k_{12}+k_{13}k_{32}+k_{23}k_{12}) \quad ,$$

$$[B_2]_\infty = \mu(k_{21}k_{13}+k_{21}k_{23}+k_{31}k_{23}) \quad ,$$

$$[B_3]_\infty = \mu(k_{21}k_{32}+k_{31}k_{12}+k_{31}k_{32}) \quad ,$$

where μ is equal to

$$\frac{C}{k_{13}k_{12}+k_{13}k_{32}+k_{23}k_{12}+k_{21}k_{13}+k_{21}k_{23}+k_{31}k_{23}+k_{21}k_{32}+k_{31}k_{12}+k_{31}k_{32}}$$

Obviously, $[B_1]_\infty$, $[B_2]_\infty$, $[B_3]_\infty$ do not depend on the initial concentrations.

Let us suppose that one wishes to study this case (n=3) in elementary terms. That is to say, avoiding the Perron-Frobenius theorem, the M-matrices and the Jordan normal form. Such a study can be done throughout the next arguments:

As in Theorem 1 one easily proves that 0 is an eigenvalue of the 3x3 matrix K . If $\lambda_1=0$, λ_2 , λ_3 are the eigenvalues of K, then

$$|\lambda I_3 - K| = \lambda^3 - (\lambda_1+\lambda_2+\lambda_3)\lambda^2 + (\lambda_1\lambda_2+\lambda_1\lambda_3+\lambda_2\lambda_3)\lambda - \lambda_1\lambda_2\lambda_3 \ .$$

By identifying the coefficients of λ^2 and λ in these two polynomials, we find that

$$-(\lambda_2+\lambda_3) = k_{21}+k_{31}+k_{12}+k_{32}+k_{13}+k_{23} \quad ,$$

and

$$\lambda_2\lambda_3 = k_{13}k_{12}+k_{13}k_{32}+k_{23}k_{12}+k_{21}k_{13}+k_{21}k_{23}+k_{31}k_{23}+$$
$$+ k_{21}k_{32}+k_{31}k_{12}+k_{31}k_{32} \quad .$$

So,

$$\lambda_2 + \lambda_3 < 0$$
$$\lambda_2 \lambda_3 > 0 \qquad (12)$$

since $k_{ij} > 0$ $(i,j = 1,2,3, \ i \neq j)$.

Hence $\lambda_2 \neq 0$ and $\lambda_3 \neq 0$, whence 0 is a simple eigenvalue.

Suppose that $\lambda_2 = \alpha_2 + i\beta_2$ with $\alpha_2, \beta_2 \in \mathbb{R}$:

1st.- If $\beta_2 \neq 0$, then $\lambda_3 = \overline{\lambda}_2 = \alpha_2 - i\beta_2$. Thus $2\alpha_2 = \lambda_2 + \lambda_3 < 0$, which yields $\alpha_2 < 0$.

2nd.- If $\beta_2 = 0$, then λ_2 and λ_3 are real. Moreover by (12), they are negative. Then either $\lambda_2 \neq \lambda_3$ or $\lambda_2 = \lambda_3$.

In any case, λ_2 and λ_3 have negative real part.

If K is not diagonalizable, one can use the Hamilton-Cayley theorem to establish that

$$e^{Kt} = e^{\lambda_2 t}\{I_3 + t(A - \lambda_2 I_3)\} + \frac{1 - e^{\lambda_2 t}}{\lambda_2^2}(A - \lambda_2 I_3)^2 + \frac{t\, e^{\lambda_2 t}}{\lambda_2}(A - \lambda_2 I_3)^2$$

where 0 and λ_2 (double) are the eigenvalues of K ([11] p. 257-259). And with this formula one can prove the existence of the given eigenvector of K associated with 0.

FINAL REMARKS

1. If the matrix K has some element k_{ij} equal to zero, it could be taken a new matrix K' with the element k'_{ij} of the entry (i,j) nearly equal to zero. This is possible due to the continuity of e^{Kt} and of the eigenvalues of K with respect to the matrix K.

2. The convergence of all positive solutions of (2) to an unique limit as $t \to \infty$, can be also deduced from a theorem of G. Birkhoff and L. Kotin [13]. This theorem is related with a time-depending coefficient system similar to (2). It makes use of the Hilbert projective metric on the space of directions.

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Revised September 5, 1986