Physica 19D (1986) 135–144
North-Holland, Amsterdam

ORTHOGONAL TRANSFORMS OF THE LORENZ- AND RÖSSLER-EQUATION

J. TÓTH
Computer and Automation Institute of the Hungarian Academy of Sciences, Budapest, Hungary, H-1502

and

Vera HÁRS
CHINOIN Chemical and Pharmaceutical Works Ltd., Budapest, Hungary, H-1045

Received 2 January 1985
Revised manuscript received 18 July 1985

It is shown that none of the proper or improper orthogonal transformations transforms the Lorenz-equation into a kinetic equation, i.e. into an equation representing reasonable chemistry. It is also shown that none of the proper orthogonal transformations transforms a model by Rössler into a kinetic model either. The importance of the presence of negative cross-effects is hereby emphasized.

1. Introduction

There is considerable interest in whether or not real chemical systems can exhibit chaos. The review paper by Epstein [3] describes and cites many experimental examples and asserts of certain models that the chemical relevance of differential equations is questionable.

The question which of the polynomial differential equations are chemically relevant was treated in our previous paper [6] as follows. The complex chemical reaction

$$\sum_{m=1}^{M} \alpha(m,r)X(m) \xrightarrow{k(r)} \sum_{m=1}^{M} \beta(m,r)X(m) \qquad (r=1,2,\ldots,R) \quad (1.1)$$

is usually described by the first order explicit polynomial differential equation (called the *kinetic differential equation* of (1.1))

$$\dot{c}_m(t) = \sum_{r=1}^{R} (\beta(m,r) - \alpha(m,r)) \times k(r) \prod_{m'=1}^{M} c_{m'}(t)^{\alpha(m,r)}, \quad (1.2)$$

where c_m is interpreted as the concentration of the chemical component $X(m)$: $c_m := [X(m)]$ and t is interpreted as time. An essentially simple but difficult to formulate characterization can be given of the kinetic differential equations among the polynomial differential equations. A polynomial differential equation can be considered the kinetic differential equation of a complex chemical reaction if and only if it does not contain *negative cross-effect*, i.e. if its right-hand side does not contain terms expressing the decrease of a component in processes in which the component in question does not take part (cf. [4]). As an example let us consider the Lorenz-equation [11],

$$\dot{x} = -\sigma x + \sigma y, \quad \dot{y} = rx - y - xz, \quad \dot{z} = xy - bz \qquad (\sigma, r, b \in \mathbb{R}^+), \quad (1.3)$$

where $-xz$ is a term expressing the decrease of y in a process in which y does not take part.

According to this necessary and sufficient condition (that is rather mild, see the discussion) the models with chaotic behaviour cited by Epstein [3] are nonkinetic. Furthermore, most of the chaotic

0167-2789/86/$03.50 © Elsevier Science Publishers B.V.
(North-Holland Physics Publishing Division)

models in the literature are nonkinetic too. On the other hand, it is true that Rössler [15], Schulmeister [16], Gilpin [5], Tomita and Tsuda [18], Arneodo et al. [1], and Willamowski and Rössler [21] were able to provide kinetic differential equations with chaotic behaviour.

In the present paper we should like to take a step towards algebraic-structural characterization of polynomial differential equations with chaotic behaviour from another side than it has been done by King [9]. Aiming at this we show that no proper orthogonal transformation turns the Lorenz-equation into a kinetic one. Secondly, no improper orthogonal transformation does this either. Thirdly, this statement is slightly generalized. Then it is also shown that none of the proper orthogonal transformations transform a model by Rössler into a kinetic equation either. (It is sensible to restrict ourselves to the case of *linear* transforms both because they are easy to handle and because they yield polynomial equations while a nonlinear transformation does not do this in general.)

Based upon these calculations we believe that chaotic behaviour is closely connected with the occurrence of uneliminable negative cross-effects.

2. Proper orthogonal transforms of the Lorenz-equation

The Lorenz-equation is [11]

$$\begin{aligned} \dot{x} &= -\sigma x + \sigma y, \\ \dot{y} &= rx - y - xz, \quad (\sigma, r, b \in \mathbb{R}^+) \\ \dot{z} &= xy - bz, \end{aligned}$$

or shortly

$$\dot{\boldsymbol{x}} = \boldsymbol{f} \circ \boldsymbol{x}. \tag{2.1}$$

The question is if there exists such a proper orthogonal transformation $A: \mathrm{R}^3 \to \mathrm{R}^3$ (i.e. a linear transformation with $AA^{\mathrm{T}} = I$, $\det A = 1$ or $A \in \mathrm{SO}(3)$) that $\boldsymbol{\xi} := A\boldsymbol{x}$ obeys a kinetic differential equation (i.e. an equation *without* negative cross-effects [6] such as e.g. $-xz$ is in the original system).

The differential equation for $\boldsymbol{\xi} =: (\xi, \eta, \zeta)^{\mathrm{T}}$ is

$$\dot{\boldsymbol{\xi}} = A\dot{\boldsymbol{x}} = A\boldsymbol{f} \circ \boldsymbol{x} = A\boldsymbol{f} \circ A^{-1}\boldsymbol{\xi}.$$

Let us introduce the following notations: $\mathrm{c}_x := \cos x$, $\mathrm{s}_x := \sin x (x \in [0, 2\pi))$. With these the generic proper orthogonal transformation of $\mathbb{R}^3$ may be written as a product of three plane rotations, see e.g. [2, §18]:

$$\begin{aligned} A &= \begin{bmatrix} \mathrm{c}_\alpha & \mathrm{s}_\alpha & 0 \\ -\mathrm{s}_\alpha & \mathrm{c}_\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \mathrm{c}_\beta & 0 & \mathrm{s}_\beta \\ 0 & 1 & 0 \\ -\mathrm{s}_\beta & 0 & \mathrm{c}_\beta \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \mathrm{c}_\gamma & \mathrm{s}_\gamma \\ 0 & -\mathrm{s}_\gamma & \mathrm{c}_\gamma \end{bmatrix} =: A_\alpha B_\beta C_\gamma \\ &= \begin{bmatrix} \mathrm{c}_\alpha \mathrm{c}_\beta & \mathrm{c}_\gamma \mathrm{s}_\alpha - \mathrm{c}_\alpha \mathrm{s}_\beta \mathrm{s}_\gamma & \mathrm{c}_\alpha \mathrm{c}_\gamma \mathrm{s}_\beta + \mathrm{s}_\alpha \mathrm{s}_\gamma \\ -\mathrm{c}_\beta \mathrm{s}_\alpha & \mathrm{c}_\alpha \mathrm{c}_\gamma + \bar{\mathrm{s}} & \mathrm{c}_\alpha \mathrm{s}_\gamma - \mathrm{c}_\gamma \mathrm{s}_\alpha \mathrm{s}_\beta \\ -\mathrm{s}_\beta & -\mathrm{c}_\beta \mathrm{s}_\gamma & \mathrm{c}_\beta \mathrm{c}_\gamma \end{bmatrix}, \end{aligned} \tag{2.2}$$

where $\alpha, \beta, \gamma \in [0, 2\pi)$, and $\bar{\mathrm{s}} := \mathrm{s}_\alpha \mathrm{s}_\beta \mathrm{s}_\gamma$. We shall need below $\bar{\mathrm{c}} := \mathrm{c}_\alpha \mathrm{c}_\beta \mathrm{c}_\gamma$ as well.

A is orthogonal thus $A^{-1} = A^{\mathrm{T}}$.

Thus we get at first $A^{-1}\boldsymbol{\xi}$, secondly $\boldsymbol{f} \circ A^{-1}\boldsymbol{\xi}$, and, finally, the coordinate equations of the transformed differential equation

$$\dot{\boldsymbol{\xi}} = A\boldsymbol{f} \circ A^{-1}\boldsymbol{\xi} \tag{2.3}$$

are

$$\begin{aligned}
\dot{\xi} = {} & \xi\Big[(\sigma + r)\mathrm{c}_\alpha\mathrm{c}_\beta(\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma) - b(\mathrm{c}_\alpha\mathrm{c}_\gamma\mathrm{s}_\beta + \mathrm{s}_\alpha\mathrm{s}_\gamma)^2 - \sigma(\mathrm{c}_\alpha\mathrm{c}_\beta)^2 - (\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma)^2\Big] \\
& + \eta\Big[\sigma\mathrm{c}_\alpha\mathrm{c}_\beta(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}} + \mathrm{c}_\beta\mathrm{s}_\alpha) - r\mathrm{c}_\beta\mathrm{s}_\alpha(\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma) - \mathrm{c}_\alpha\mathrm{c}_\gamma^2\mathrm{s}_\alpha + \mathrm{c}_\alpha^2\mathrm{c}_\gamma\mathrm{s}_\beta\mathrm{s}_\gamma - \mathrm{c}_\gamma\bar{\mathrm{s}}\mathrm{s}_\alpha + \mathrm{c}_\alpha\bar{\mathrm{s}}\mathrm{s}_\beta\mathrm{s}_\gamma \\
& - b\big(\mathrm{c}_\alpha\mathrm{s}_\alpha\mathrm{s}_\gamma^2 + \mathrm{c}_\alpha^2\mathrm{c}_\gamma\mathrm{s}_\beta\mathrm{s}_\gamma - \mathrm{c}_\gamma\bar{\mathrm{s}}\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{c}_\gamma^2\mathrm{s}_\alpha\mathrm{s}_\beta^2\big)\Big] + \zeta\Big[-\sigma\mathrm{c}_\alpha\mathrm{c}_\beta(\mathrm{c}_\beta\mathrm{s}_\gamma - \mathrm{s}_\beta) - r\mathrm{s}_\beta(\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma) \\
& - b\mathrm{c}_\beta\mathrm{c}_\gamma(\mathrm{c}_\alpha\mathrm{c}_\gamma\mathrm{s}_\beta + \mathrm{s}_\alpha\mathrm{s}_\gamma) + \mathrm{c}_\beta\mathrm{s}_\gamma(\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma)\Big] \\
& + \xi^2 0 - \eta^2\mathrm{c}_\beta\mathrm{s}_\alpha\mathrm{s}_\beta + \zeta^2\mathrm{c}_\beta\mathrm{s}_\alpha\mathrm{s}_\beta + \xi\eta\mathrm{c}_\alpha\mathrm{c}_\beta\mathrm{s}_\beta - \xi\zeta\mathrm{c}_\alpha\mathrm{c}_\beta^2\mathrm{s}_\alpha + \eta\zeta\big(\mathrm{c}_\beta^2\mathrm{s}_\alpha^2 - \mathrm{s}_\beta^2\big), \\
\dot{\eta} = {} & \xi\Big[-\sigma\mathrm{c}_\beta\mathrm{s}_\alpha(\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma - \mathrm{c}_\alpha\mathrm{c}_\beta) + r\mathrm{c}_\alpha\mathrm{c}_\beta(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}}) \\
& - b\big(\mathrm{c}_\alpha\mathrm{s}_\alpha\mathrm{s}_\gamma^2 + \mathrm{c}_\alpha^2\mathrm{c}_\gamma\mathrm{s}_\beta\mathrm{s}_\gamma - \mathrm{c}_\gamma\bar{\mathrm{s}}\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{c}_\gamma^2\mathrm{s}_\alpha\mathrm{s}_\beta^2\big) + \mathrm{c}_\alpha^2\mathrm{c}_\gamma\mathrm{s}_\beta\mathrm{s}_\gamma - \mathrm{c}_\alpha\mathrm{c}_\gamma^2\mathrm{s}_\alpha - \mathrm{c}_\gamma\bar{\mathrm{s}}\mathrm{s}_\alpha + \mathrm{c}_\alpha\mathrm{s}_\alpha\mathrm{s}_\beta^2\mathrm{s}_\gamma\Big] \\
& + \eta\Big[-(\sigma + r)\mathrm{c}_\beta\mathrm{s}_\alpha(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}}) - b(\mathrm{c}_\alpha\mathrm{s}_\gamma - \mathrm{c}_\gamma\mathrm{s}_\alpha\mathrm{s}_\beta)^2 - \sigma\mathrm{c}_\beta\mathrm{s}_\alpha^2 - (\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}})^2\Big] \\
& + \zeta\Big[\sigma\mathrm{c}_\beta\mathrm{s}_\alpha(\mathrm{c}_\beta\mathrm{s}_\gamma - \mathrm{s}_\beta) - r\mathrm{s}_\beta(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}}) - b\mathrm{c}_\beta\mathrm{c}_\gamma(\mathrm{c}_\alpha\mathrm{s}_\gamma - \mathrm{c}_\gamma\mathrm{s}_\alpha\mathrm{s}_\beta) - \mathrm{c}_\beta\mathrm{s}_\gamma(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}})\Big] \\
& + \xi^2\Big[-\mathrm{c}_\alpha\mathrm{c}_\beta\mathrm{s}_\beta - \mathrm{c}_\alpha^2\mathrm{c}_\beta\mathrm{c}_\gamma\mathrm{s}_\alpha\mathrm{s}_\beta^2\mathrm{s}_\gamma\Big] + \eta^2 0 + \zeta^2\mathrm{c}_\alpha\mathrm{c}_\beta\mathrm{s}_\beta + \xi\eta\mathrm{c}_\beta\mathrm{s}_\alpha\mathrm{s}_\beta + \xi\zeta\big(\mathrm{s}_\beta^2 - \mathrm{c}_\alpha^2\mathrm{c}_\beta^2\big) + \eta\xi\mathrm{c}_\alpha\mathrm{c}_\beta^2\mathrm{s}_\alpha, \\
\dot{\zeta} = {} & \xi\Big[\sigma\mathrm{s}_\beta(-\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma + \mathrm{c}_\alpha\mathrm{c}_\beta) - r\mathrm{c}_\alpha\mathrm{c}_\beta^2\mathrm{s}_\gamma - b\mathrm{c}_\beta\mathrm{c}_\gamma(\mathrm{c}_\alpha\mathrm{c}_\gamma\mathrm{s}_\beta + \mathrm{s}_\alpha\mathrm{s}_\gamma) + \mathrm{c}_\beta\mathrm{s}_\gamma(\mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma + \mathrm{c}_\gamma\mathrm{s}_\alpha)\Big] \\
& + \eta\Big[-\sigma\mathrm{s}_\beta(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}} + \mathrm{c}_\beta\mathrm{s}_\alpha) + r\mathrm{c}_\beta^2\mathrm{s}_\alpha\mathrm{s}_\gamma + b\mathrm{c}_\beta\mathrm{c}_\gamma(-\mathrm{c}_\alpha\mathrm{s}_\gamma + \mathrm{c}_\gamma\mathrm{s}_\alpha\mathrm{s}_\beta) + \mathrm{c}_\beta\mathrm{s}_\gamma(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}})\Big] \\
& + \zeta\Big[\sigma\mathrm{s}_\beta(\mathrm{c}_\beta\mathrm{s}_\gamma - \mathrm{s}_\beta) + r\mathrm{c}_\beta\mathrm{s}_\beta\mathrm{s}_\gamma - b\mathrm{c}_\beta^2\mathrm{c}_\gamma^2 - \mathrm{c}_\beta^2\mathrm{s}_\gamma^2\Big] \\
& + \xi^2\mathrm{c}_\alpha\mathrm{c}_\beta^2\mathrm{s}_\alpha - \eta^2\mathrm{c}_\alpha\mathrm{c}_\beta^2\mathrm{s}_\alpha + \zeta^2 0 + \xi\eta\mathrm{c}_\beta^2\big(\mathrm{c}_\alpha^2 - \mathrm{s}_\alpha^2\big) - \xi\zeta\mathrm{c}_\beta\mathrm{s}_\alpha\mathrm{s}_\beta - \eta\zeta\mathrm{c}_\alpha\mathrm{c}_\beta\mathrm{s}_\beta.
\end{aligned}$$

The requirement that there is no negative cross-effect implies for the coefficients of the *second order* terms:

$$\mathrm{c}_\beta\mathrm{s}_\alpha\mathrm{s}_\beta = 0, \tag{2.4}$$

$$\mathrm{c}_\beta^2\mathrm{s}_\alpha^2 \geqq \mathrm{s}_\beta^2, \tag{2.5}$$

$$\mathrm{c}_\alpha\mathrm{c}_\beta\mathrm{s}_\beta = 0, \tag{2.6}$$

$$\mathrm{s}_\beta^2 \geqq \mathrm{c}_\alpha^2\mathrm{c}_\beta^2, \tag{2.7}$$

$$\mathrm{c}_\alpha\mathrm{c}_\beta^2\mathrm{s}_\alpha = 0, \tag{2.8}$$

$$\mathrm{c}_\beta^2\mathrm{c}_\alpha^2 \geqq \mathrm{c}_\beta^2\mathrm{s}_\alpha^2. \tag{2.9}$$

Starting from (2.4) three cases seem to be possible. Either $\mathrm{c}_\beta = 0$, but then $\mathrm{s}_\beta^2 = 1$, and this contradicts to (2.5); or $\mathrm{s}_\alpha = 0$, but then $\mathrm{s}_\beta = 0$ and $\mathrm{c}_\alpha^2 = 1$, and this contradicts to (2.7); or $\mathrm{s}_\beta = 0$, but then $\mathrm{c}_\beta^2 = 1$ and $\mathrm{c}_\alpha = 0$, and this contradicts to (2.9).

3. Improper orthogonal transformations

Thus the assumption that a *proper* orthogonal transformation can remove negative cross-effects has been shown to lead necessarily to contradiction. Now let us turn to *improper* orthogonal transformations, i.e. to linear transformations B with $BB^{\mathrm{T}} = I$, $\det B = -1$. Obviously all such transformations can be decomposed into the product of a fixed improper orthogonal transformation and a proper orthogonal transformation. If reflexion to the origin is taken as the fixed improper orthogonal transformation and it is denoted by P, then

$$P = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

and for all improper B there exists a proper A such that $B = PA$. In general, if P_0 is the fixed improper orthogonal transformation then $B = P_0 P_0^{\mathrm{T}} B$, $P_0 P_0^{\mathrm{T}} = I$, thus $A := P_0^{\mathrm{T}} B$ will do.

It is obvious that on denoting the right-hand side of (2.3) by g the equation obtained under B is

$$\dot{\boldsymbol{X}} = -\boldsymbol{g} \circ (-\boldsymbol{X}) \quad (\boldsymbol{X} := B\boldsymbol{x} = PA\boldsymbol{x} = P\boldsymbol{\xi}). \tag{3.1}$$

(It is the same as the equation obtained from

$$\dot{\boldsymbol{\xi}} = \boldsymbol{g} \circ \boldsymbol{\xi} \tag{3.3'}$$

under P.)

The requirement that there is no negative cross-effect in (3.10) implies for the coefficients of the second order terms:

$$\mathrm{c}_\beta \mathrm{s}_\alpha \mathrm{s}_\beta = 0, \tag{3.2}$$

$$\mathrm{c}_\beta^2 \mathrm{s}_\alpha^2 \leqq \mathrm{s}_\beta^2, \tag{3.3}$$

$$\mathrm{c}_\alpha \mathrm{c}_\beta \mathrm{s}_\beta = 0, \tag{3.4}$$

$$\mathrm{s}_\beta^2 \leqq \mathrm{c}_\alpha^2 \mathrm{c}_\beta^2, \tag{3.5}$$

$$\mathrm{c}_\alpha \mathrm{c}_\beta^2 \mathrm{s}_\alpha = 0, \tag{3.6}$$

$$\mathrm{c}_\beta^2 \mathrm{c}_\alpha^2 \leqq \mathrm{c}_\beta^2 \mathrm{s}_\alpha^2. \tag{3.7}$$

These are the same inequalities as before except that signs are reversed. The reader may wish to check that (3.2)–(3.7) is obtained as well if the fixed improper orthogonal transformation is, say,

$$P_1 := \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Starting from (3.2) three cases seem to be possible. Either $c_\beta = 0$, but then $s_\beta^2 = 1$, and this contradicts to (3.5); or $s_\alpha = 0$, but then $c_\alpha^2 = 1$ and $c_\beta = 0$ leading to the same contradiction as before; or $s_\beta = 0$, but then $c_\beta^2 = 1$ and $s_\alpha = 0$ implying contradiction as in the second case.

Thus it has been shown that improper orthogonal transformations are also unable to eliminate negative cross-effects.

As the effect of a positive definite diagonal transformation is that a nonkinetic equation remains a nonkinetic one, it follows from our results above that the Lorenz-equation remains nonkinetic even under transformations of the form $D = MA$, where A is an arbitrary (proper or improper) orthogonal transformation, and M is a positive definite diagonal transformation.

The polar decomposition theorem by Cauchy asserts that any nonsingular transformation C can be decomposed into the product of a positive definite transformation V and an orthogonal transformation A_0, i.e.

$$C = VA_0. \tag{3.8}$$

On the other hand, according to the spectral decomposition theorem V can be decomposed into the product of two orthogonal transformations and a positive definite diagonal transformation, i.e.

$$V = TMT^{\mathrm{T}}. \tag{3.9}$$

Eqs. (3.8) and (3.9) together imply the decomposition

$$C = TMT^{\mathrm{T}}A_0 = TMA \quad (A \text{ is orthogonal}).$$

This last equation shows that in order to prove that *any* linear transformation transforms the Lorenz-equation into a nonkinetic one it would suffice to show either the general statement that proper orthogonal transformations do not affect this property or the special statement that the transform of the Lorenz-equation under a linear transformation of the form MA cannot be transformed into a kinetic equation under a proper orthogonal transformation T.

4. Proper orthogonal transforms of the Rössler equation

Rössler [14] proposed as a more realistic alternative to the Lorenz-model the following equation:

$$\begin{aligned} \dot{x} &= x - xy - z, \\ \dot{y} &= x^2 - ay, \quad (a, b, c, d \in \mathbb{R}^+) \\ \dot{z} &= bx - cy + d. \end{aligned} \tag{4.1}$$

Investigating this case some of the calculations above may be used. Let A be an arbitrary proper orthogonal transformation. Then the first expression to differ is $\boldsymbol{f} \circ A^{-1}\boldsymbol{\xi}$. The coordinate equations of the transformed differential equation are

$$
\begin{aligned}
\dot{\xi} = {} & \xi\left[\mathrm{c}_\alpha^2\mathrm{c}_\beta^2 - \bar{\mathrm{c}}\mathrm{c}_\alpha\mathrm{s}_\beta - \mathrm{c}_\alpha\mathrm{c}_\beta\mathrm{s}_\alpha\mathrm{s}_\gamma - (\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma)^2 a + (\mathrm{c}_\alpha\mathrm{c}_\gamma\mathrm{s}_\beta + \mathrm{s}_\alpha\mathrm{s}_\gamma) + \left(b\mathrm{c}_\alpha\mathrm{c}_\beta - c(\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma)\right)\right] \\
& + \eta\left[-\mathrm{c}_\alpha\mathrm{c}_\beta^2\mathrm{s}_\alpha - \mathrm{c}_\alpha^2\mathrm{c}_\beta\mathrm{s}_\gamma + \bar{\mathrm{c}}\mathrm{s}_\alpha\mathrm{s}_\beta - (\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma)a(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}}) - (\mathrm{c}_\alpha\mathrm{c}_\gamma\mathrm{s}_\beta + \mathrm{s}_\alpha\mathrm{s}_\gamma)\left(b\mathrm{c}_\beta\mathrm{s}_\alpha + c(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}})\right)\right] \\
& + \zeta\left[-\mathrm{c}_\alpha\mathrm{c}_\beta\mathrm{s}_\beta - \bar{\mathrm{c}}\mathrm{c}_\beta + (\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma)a\mathrm{c}_\beta\mathrm{s}_\gamma - (\mathrm{c}_\alpha\mathrm{c}_\gamma\mathrm{s}_\beta + \mathrm{s}_\alpha\mathrm{s}_\gamma)(b\mathrm{s}_\beta - c\mathrm{c}_\beta\mathrm{s}_\gamma)\right] \\
& + \xi^2 0 + \eta^2\left(\mathrm{c}_\beta^2\mathrm{c}_\gamma\mathrm{s}_\alpha\right) + \zeta^2\left(\mathrm{c}_\gamma\mathrm{s}_\alpha\mathrm{s}_\beta^2 - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma\right) + \xi\eta(-\bar{\mathrm{c}}\mathrm{c}_\beta) \\
& + \xi\zeta\left(-\bar{\mathrm{c}}\mathrm{s}_\alpha\mathrm{s}_\beta + \mathrm{c}_\alpha^2\mathrm{c}_\beta\mathrm{s}_\gamma\right) + \eta\zeta\left(3\mathrm{c}_\alpha\mathrm{c}_\beta\bar{\mathrm{s}}\mathrm{s}_\beta - \mathrm{c}_\alpha\mathrm{c}_\beta^3\mathrm{s}_\alpha\mathrm{s}_\gamma - 2\mathrm{c}_\beta\mathrm{c}_\gamma\mathrm{s}_\alpha^2\mathrm{s}_\beta - \bar{\mathrm{c}}\mathrm{c}_\alpha\mathrm{s}_\beta\right) + (\mathrm{c}_\alpha\mathrm{c}_\gamma\mathrm{s}_\beta + \mathrm{s}_\alpha\mathrm{s}_\gamma)d, \\
\dot{\eta} = {} & \xi\left[-\mathrm{c}_\alpha\mathrm{c}_\beta^2\mathrm{s}_\alpha + \bar{\mathrm{c}}\mathrm{s}_\alpha\mathrm{s}_\beta + \mathrm{c}_\beta\mathrm{s}_\alpha^2\mathrm{s}_\gamma - (\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}})a(\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma)\right. \\
& \left. + (\mathrm{c}_\alpha\mathrm{s}_\gamma - \mathrm{c}_\gamma\mathrm{s}_\alpha\mathrm{s}_\beta)\left(b\mathrm{c}_\alpha\mathrm{c}_\beta - c(\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma)\right)\right] \\
& + \eta\left[\mathrm{c}_\beta^2\mathrm{s}_\alpha^2 + \mathrm{c}_\alpha\mathrm{c}_\beta\mathrm{s}_\alpha\mathrm{s}_\gamma - \mathrm{c}_\beta\mathrm{c}_\gamma\mathrm{s}_\alpha^2\mathrm{s}_\beta - (\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}})^2 a - (\mathrm{c}_\alpha\mathrm{s}_\gamma - \mathrm{c}_\gamma\mathrm{s}_\alpha\mathrm{s}_\beta)\left(b\mathrm{c}_\beta\mathrm{s}_\alpha + c(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}})\right)\right] \\
& + \zeta\left[\mathrm{c}_\beta\mathrm{s}_\alpha\mathrm{s}_\beta + \mathrm{c}_\beta^2\mathrm{c}_\gamma\mathrm{s}_\alpha + a\bar{\mathrm{c}}\mathrm{s}_\gamma + a\mathrm{c}_\beta\bar{\mathrm{s}}\mathrm{s}_\gamma - (\mathrm{c}_\alpha\mathrm{s}_\gamma - \mathrm{c}_\gamma\mathrm{s}_\alpha\mathrm{s}_\beta)(b\mathrm{s}_\beta - c\mathrm{c}_\beta\mathrm{s}_\gamma)\right] \\
& + \xi^2(\bar{\mathrm{c}}\mathrm{c}_\beta) + \eta^2 0 + \zeta^2\left(\mathrm{c}_\alpha\mathrm{c}_\gamma\mathrm{s}_\beta^2 + \bar{\mathrm{s}}\right) + \xi\eta\left(-\mathrm{c}_\beta^2\mathrm{c}_\gamma\mathrm{s}_\alpha\right) \\
& + \xi\zeta\left(-\mathrm{c}_\alpha\mathrm{c}_\beta\mathrm{s}_\alpha\mathrm{s}_\gamma - \mathrm{c}_\beta\mathrm{c}_\gamma\mathrm{s}_\beta - \mathrm{c}_\alpha^2\mathrm{c}_\beta\mathrm{c}_\gamma\mathrm{s}_\beta\right) + \eta\zeta\left(\bar{\mathrm{c}}\mathrm{s}_\alpha\mathrm{s}_\beta + \mathrm{c}_\beta\mathrm{s}_\alpha^2\mathrm{s}_\gamma\right) + (\mathrm{c}_\alpha\mathrm{s}_\gamma - \mathrm{c}_\gamma\mathrm{s}_\alpha\mathrm{s}_\beta)\,d, \\
\dot{\zeta} = {} & \xi\left[-\mathrm{c}_\alpha\mathrm{c}_\beta\mathrm{s}_\beta + \mathrm{c}_\alpha\mathrm{c}_\gamma\mathrm{s}_\beta^2 - \bar{\mathrm{s}} + a\mathrm{c}_\beta\mathrm{s}_\gamma(\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma) + \mathrm{c}_\beta\mathrm{c}_\gamma\left(b\mathrm{c}_\alpha\mathrm{c}_\beta - c(\mathrm{c}_\gamma\mathrm{s}_\alpha - \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma)\right)\right] \\
& + \eta\left[\mathrm{c}_\beta\mathrm{s}_\alpha\mathrm{s}_\beta + \mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma - \mathrm{c}_\gamma\mathrm{s}_\alpha\mathrm{s}_\beta^2 + a\mathrm{c}_\beta\mathrm{s}_\gamma(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}}) - \mathrm{c}_\beta\mathrm{c}_\gamma\left(b\mathrm{c}_\beta\mathrm{s}_\alpha + c(\mathrm{c}_\alpha\mathrm{c}_\gamma + \bar{\mathrm{s}})\right)\right] \\
& + \zeta\left[\mathrm{s}_\beta^2 + \mathrm{c}_\beta\mathrm{c}_\gamma\mathrm{s}_\beta - a\mathrm{c}_\beta^2\mathrm{s}_\gamma^2 - \mathrm{c}_\beta\mathrm{c}_\gamma(b\mathrm{s}_\beta - c\mathrm{c}_\beta\mathrm{s}_\gamma)\right] + \xi^2\left[\bar{\mathrm{c}}\mathrm{s}_\alpha\mathrm{s}_\beta - \mathrm{c}_\alpha^2\mathrm{c}_\beta\mathrm{s}_\gamma\right] + \eta^2\left[-\bar{\mathrm{c}}\mathrm{s}_\alpha\mathrm{s}_\beta - \mathrm{c}_\beta\mathrm{s}_\alpha^2\mathrm{s}_\gamma\right] + \zeta^2 0 \\
& + \xi\eta\left[2\mathrm{c}_\alpha\mathrm{c}_\beta\mathrm{s}_\alpha\mathrm{s}_\gamma + \mathrm{c}_\alpha^2\mathrm{c}_\beta\mathrm{c}_\gamma\mathrm{s}_\beta - \mathrm{c}_\beta\mathrm{c}_\gamma\mathrm{s}_\alpha^2\mathrm{s}_\beta\right] + \xi\zeta\left[\mathrm{c}_\alpha\mathrm{s}_\beta\mathrm{s}_\gamma - \mathrm{c}_\gamma\mathrm{s}_\alpha\mathrm{s}_\beta^2\right] + \eta\zeta\left[-\bar{\mathrm{s}} - \mathrm{c}_\alpha\mathrm{c}_\gamma\mathrm{s}_\beta^2\right] + \mathrm{c}_\beta\mathrm{c}_\gamma d.
\end{aligned}
$$

Now exclusion of negative cross-effects in the case of second order terms does *not* lead to a contradiction as in the second section, thus a more complicated proof is needed which has been put off to the appendix. The structure of the proof is as follows:

(i) All the parameters a, b, c and d on the right-hand side of (4.2) are taken zero. Because of continuity a *necessary* condition of the absence of negative cross-effects is the solvability of the system of inequalities (A.1)–(A.18).

(ii) Most branches of a sorting of cases leads to a contradiction as in the second section.

(iii) In some cases the system of inequalities seem to have a solution. In these cases the solution candidates are to be put back into the coefficients. Then it turns out that the first order terms necessarily contain negative cross-effect if only a, b, c and d are positive.

5. Discussion

One is thus led to the conjecture that chaotic effects are closely related to the occurrence of uneliminable negative cross-effects. Fig. 1 has been devised in order to enlighten the more subtle relations between different models with chaotic solutions. It displays references to known examples as elements of different sets of differential equations which may be considered important in connection with modelling chemical kinetics.

It is possible to assume the point of view that even the models in $(P \cap W) \setminus M$ are chemically not all reasonable. (In ref. 6 we regarded the equations of $P \cap W$ as kinetic.) The result of the present paper is (shown by crossed arrows) that two specific examples, the Lorenz-equation and a model by Rössler will not be an element of $P \cap W$ after a linear transformation. This is a rather mild requirement because most people consider equations of D kinetic in accordance with the pioneering paper by Wei [20].

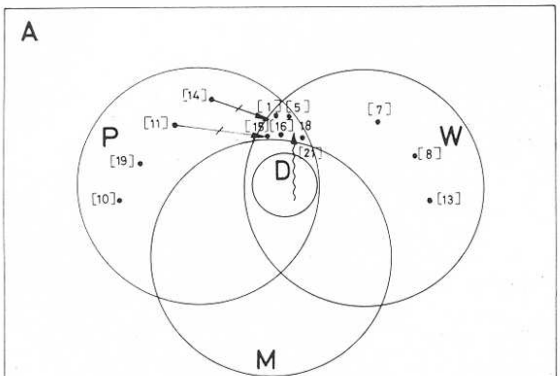

Fig. 1. Classification of differential equations with chaotic solutions. The numbers refer to the list of references, the letters to different sets of differential equations: A–autonomous, P–polynomial, M–mass conserving, W–those without negative cross-effects, D–kinetic differential equations of unconditionally detailed balanced reversible second order mass conserving reactions with mass action kinetics

The wavy arrow has been drawn in order to express that the model of Willamowski and Rössler [21] can be considered as an approximation of a model that fulfils the strictest requirements. In other words, this is the most reasonable (approximate) chaotic model from the chemical point of view.

In accordance with all the examples considered the following conjecture is proposed: if a non-kinetic differential equation shows chaotic behaviour then it cannot be transformed into a kinetic equation by any of the linear (or orthogonal) transformations.

One possible extension of the present paper could be the investigation of other specific models such as those in [9, 10] or the 4-D model by Hudson and Rössler in [7]. Another possible continuation (and a more promising one) would be a systematic classification of kinetic differential equations. It might become possible using the algebraic invariant theory of differential equations as outlined, e.g. by Sibirsky [17].

Acknowledgements

The authors thank the suggestions of Prof. O.E. Rössler. Also, we have benefited from helpful discussions with Drs. W.F. Langford and Marianna Bolla. Dr. A. Holden's and the referees' remarks were invaluable in formulating the definitive version of our paper.

Appendix

At the beginning we present complete proofs, later only sketches.

The system of inequalities expressing a necessary condition of the lack of negative cross-effects is as follows.

$$c_\alpha c_\beta(c_\gamma s_\alpha s_\beta - c_\beta s_\alpha - c_\alpha s_\gamma) \geqq 0, \tag{A.1}$$
$$-c_\alpha c_\beta(s_\beta + c_\beta c_\gamma) \geqq 0, \tag{A.2}$$
$$c_\beta^2 c_\gamma s_\alpha \geqq 0, \tag{A.3}$$
$$s_\beta(c_\gamma s_\alpha s_\beta - c_\alpha s_\gamma) \geqq 0, \tag{A.4}$$
$$c_\beta\left(3c_\alpha \bar{s} s_\beta + c_\alpha^2 c_\gamma s_\beta - 2c_\gamma s_\alpha^2 s_\beta - c_\alpha c_\beta^2 s_\alpha s_\gamma\right) \geqq 0, \tag{A.5}$$
$$c_\alpha c_\gamma s_\beta + s_\alpha s_\gamma \geqq 0, \tag{A.6}$$
$$c_\beta\left(-c_\alpha c_\beta s_\alpha + c_\alpha c_\gamma s_\alpha s_\beta + s_\alpha^2 s_\gamma\right) \geqq 0, \tag{A.7}$$
$$c_\beta s_\alpha(s_\beta + c_\beta c_\gamma) \geqq 0, \tag{A.8}$$
$$c_\alpha c_\beta^2 c_\gamma \geqq 0, \tag{A.9}$$
$$s_\beta(c_\alpha c_\gamma s_\beta + s_\alpha s_\gamma) \geqq 0, \tag{A.10}$$
$$c_\beta\left(c_\alpha s_\alpha s_\gamma + c_\gamma s_\beta + c_\alpha^2 c_\gamma s_\beta\right) \leqq 0, \tag{A.11}$$
$$c_\alpha s_\gamma - c_\gamma s_\alpha s_\beta \geqq 0, \tag{A.12}$$
$$-s_\beta(c_\alpha c_\beta - c_\alpha c_\gamma s_\beta + s_\alpha s_\gamma) \geqq 0, \tag{A.13}$$
$$s_\beta(c_\beta s_\alpha + c_\alpha s_\gamma - c_\gamma s_\alpha s_\beta) \geqq 0, \tag{A.14}$$
$$c_\alpha c_\beta(c_\gamma s_\alpha s_\beta - c_\alpha s_\gamma) \geqq 0, \tag{A.15}$$
$$-c_\beta s_\alpha(c_\alpha c_\gamma s_\beta + s_\alpha s_\gamma) \geqq 0, \tag{A.16}$$
$$c_\beta\left(2c_\alpha s_\alpha s_\gamma + c_\alpha^2 c_\gamma s_\beta - c_\gamma s_\alpha^2 s_\beta\right) \geqq 0, \tag{A.17}$$
$$c_\beta c_\gamma \geqq 0. \tag{A.18}$$

As s_β is the number occurring most often let us start the sorting of cases with the case $s_\beta > 0$.

1. $\underline{s_\beta > 0}$

In this case the system of inequalities reduces to

$$c_\alpha c_\beta(c_\gamma s_\alpha s_\beta - c_\beta s_\alpha - c_\alpha s_\gamma) \geqq 0, \tag{A.1.1}$$
$$c_\alpha c_\beta(s_\beta + c_\beta c_\gamma) \leqq 0, \tag{A.2.1}$$
$$c_\beta^2 c_\gamma s_\alpha \geqq 0, \tag{A.3.1}$$
$$c_\gamma s_\alpha s_\beta - c_\alpha s_\gamma = 0, \tag{A.4.1) + (A.12.1}$$
$$c_\beta\left(3c_\alpha \bar{s} s_\beta + c_\alpha^2 c_\gamma s_\beta - 2c_\gamma s_\alpha^2 s_\beta - c_\alpha c_\beta^2 s_\alpha s_\gamma\right) \geqq 0, \tag{A.5.1}$$
$$c_\alpha c_\gamma s_\beta + s_\alpha s_\gamma \geqq 0, \tag{A.6.1) = (A.10.1}$$
$$c_\beta\left(-c_\alpha c_\beta s_\alpha + c_\alpha c_\gamma s_\alpha s_\beta + s_\alpha^2 s_\gamma\right) \geqq 0, \tag{A.7.1}$$
$$c_\beta s_\alpha(s_\beta + c_\beta c_\gamma) \geqq 0, \tag{A.8.1}$$
$$c_\alpha c_\beta^2 c_\gamma \geqq 0, \tag{A.9.1}$$
$$c_\beta\left(c_\alpha s_\alpha s_\gamma + c_\gamma s_\beta + c_\alpha^2 c_\gamma s_\beta\right) \leqq 0, \tag{A.11.1}$$
$$c_\alpha c_\beta - c_\alpha c_\gamma s_\beta + s_\alpha s_\gamma \leqq 0, \tag{A.13.1}$$
$$c_\beta s_\alpha + c_\alpha s_\gamma - c_\gamma s_\alpha s_\beta \geqq 0, \tag{A.14.1}$$
$$c_\alpha c_\beta(c_\gamma s_\alpha s_\beta - c_\alpha s_\gamma) \geqq 0, \tag{A.15.1}$$
$$c_\beta s_\alpha(c_\alpha c_\gamma s_\beta + s_\alpha s_\gamma) \leqq 0, \tag{A.16.1}$$
$$c_\beta\left(2c_\alpha s_\alpha s_\gamma + c_\alpha^2 c_\gamma s_\beta - c_\gamma s_\alpha^2 s_\beta\right) \geqq 0, \tag{A.17.1}$$
$$c_\beta c_\gamma \geqq 0. \tag{A.18.1}$$

Let us consider the subcase when $c_\beta > 0$.

1.1. $\underline{c_\beta > 0}$

In this case the system of inequalities reduces to

$$c_\alpha(c_\gamma s_\alpha s_\beta - c_\beta s_\alpha - c_\alpha s_\gamma) \geqq 0, \tag{A.1.11}$$
$$c_\alpha(s_\beta + c_\beta c_\gamma) \leqq 0, \tag{A.2.11}$$
$$c_\gamma s_\alpha \geqq 0, \tag{A.3.11}$$
$$c_\gamma s_\alpha s_\beta - c_\alpha s_\gamma = 0, \tag{A.4.11}$$
$$3c_\alpha \bar{s} s_\beta + c_\alpha^2 c_\gamma s_\beta - 2c_\gamma s_\alpha^2 s_\beta - c_\alpha c_\beta^2 s_\alpha s_\gamma \geqq 0, \tag{A.5.11}$$
$$c_\alpha c_\gamma s_\beta + s_\alpha s_\gamma \geqq 0, \tag{A.6.11}$$
$$-c_\alpha c_\beta s_\alpha + c_\alpha c_\gamma s_\alpha s_\beta + s_\alpha^2 s_\gamma \geqq 0, \tag{A.7.11}$$
$$s_\alpha(s_\beta + c_\beta c_\gamma) \geqq 0, \tag{A.8.11}$$
$$c_\alpha c_\gamma \geqq 0, \tag{A.9.11}$$
$$c_\alpha s_\alpha s_\gamma + c_\gamma s_\beta + c_\alpha^2 c_\gamma s_\beta \leqq 0, \tag{A.11.11}$$
$$c_\alpha c_\beta - c_\alpha c_\gamma s_\beta + s_\alpha s_\gamma \leqq 0, \tag{A.13.11}$$
$$c_\beta s_\alpha + c_\alpha s_\gamma - c_\gamma s_\alpha s_\beta \geqq 0, \tag{A.14.11}$$
$$c_\alpha(c_\gamma s_\alpha s_\beta - c_\alpha s_\gamma) \geqq 0, \tag{A.15.11}$$
$$s_\alpha(c_\alpha c_\gamma s_\beta + s_\alpha s_\gamma) \leqq 0, \tag{A.16.11}$$
$$2c_\alpha s_\alpha s_\gamma + c_\alpha^2 c_\gamma s_\beta - c_\gamma s_\alpha^2 s_\beta \geqq 0, \tag{A.17.11}$$
$$c_\gamma \geqq 0. \tag{A.18.11}$$

Table I
Sorting of cases

1. $s_\beta > 0$	1.1. $c_\beta > 0$	1.1.1. $c_\gamma > 0$	1.1.1.1. $s_\alpha > 0$
			1.1.1.2. $s_\alpha = 0$
		1.1.2. $c_\gamma = 0$	
	1.2. $c_\beta = 0$	1.2.1. $s_\alpha = 0$	
		1.2.2. $s_\gamma = 0$	
		1.2.3. $s_\alpha \neq 0, s_\gamma \neq 0$*	
	1.3. $c_\beta < 0$	1.3.1. $c_\gamma < 0$	1.3.1.1. $s_\alpha = 0$
			1.3.1.2. $c_\alpha = 0$
			1.3.1.3. $c_\alpha < 0$
		1.3.2. $c_\gamma = 0$	
2. $s_\beta = 0$	2.1. $c_\alpha = 0$*		
	2.2. $c_\gamma = 0$	2.2.1. $c_\alpha = 0$	
		2.2.2. $s_\alpha = 0$*	
3. $s_\beta < 0$	3.1. $c_\beta > 0$	3.1.1. $c_\gamma > 0$	3.1.1.1. $c_\alpha > 0$
			3.1.1.2. $c_\alpha = 0$*
		3.1.2. $c_\gamma = 0$	
	3.2. $c_\beta = 0$	3.2.1. $s_\alpha = 0$	
		3.2.2. $s_\gamma = 0$	
		3.2.3. $s_\alpha \neq 0, s_\gamma \neq 0$*	
	3.3. $c_\beta < 0$	3.3.1. $c_\gamma > 0$	3.3.1.1. $c_\alpha > 0, s_\alpha > 0$
			3.3.1.2. $c_\alpha = 0, s_\alpha = 1$
			3.3.1.3. $c_\alpha = 1, s_\alpha = 0$
		3.3.2. $c_\gamma = 0$	

Two subsubcases may occur.

1.1.1. $\underline{c_\gamma > 0}$

In this case the system of inequalities leads to a contradiction as (A.3.11) implies that

$$s_\alpha \geqq 0, \qquad \text{(A.3.111)}$$

and (A.9.111) implies that

$$c_\alpha \geqq 0. \qquad \text{(A.9.111)}$$

1.1.1.1. Suppose that $\underline{s_\alpha > 0}$ holds, then (A.6.11) and (A.16.11) implies that

$$c_\alpha c_\gamma s_\beta + s_\alpha s_\gamma = 0. \qquad \text{(A.6.1111)}$$

The positivity of s_α and s_β implies that either $\underline{c_\alpha c_\gamma = s_\gamma = 0}$, but then $c_\alpha = s_\gamma = 0$, $c_\gamma = s_\alpha = 1$ and

$$c_\gamma s_\alpha s_\beta = 0. \qquad \text{(A.4.1111)}$$

holds in contradiction to the positivity of all of the factors, or

$$c_\alpha > 0 \qquad \text{(A.9.1111)}$$

and $\underline{s_\gamma < 0}$. But then

$$s_\beta + c_\beta c_\gamma = 0 \qquad \text{(A.2.1111)} + \text{(A.8.1111)}$$

should hold that is impossible because of the positivity of all of the numbers s_β, c_β, c_γ.

1.1.1.2. Suppose that $\underline{s_\alpha = 0}$ holds, then

$$c_\alpha s_\gamma = 0 \qquad \text{(A.4.1112)}$$

but c_α cannot be zero if $s_\alpha = 0$, thus $s_\gamma = 0$. Therefore $c_\gamma = 1$, thus

$$c_\alpha(s_\beta + c_\beta) = 0 \qquad \text{(A.2.1112)}$$

implying that $c_\alpha = 0$. But because of (A.9.111) $c_\alpha = 0$ must hold in contradiction to $s_\alpha = 0$.

Now let us have an overview of the cases. The cases in table I can be investigated in the same way as before except for the cases denoted by a star. Let us consider one of these, e.g. subsubcase 1.2.3. In this case $s_\beta = 1$ and the system of inequalities reduces to

$$c_\gamma s_\alpha = c_\alpha s_\gamma, \tag{A.4.123}$$

$$c_\alpha c_\gamma + s_\alpha s_\gamma \geqq 0, \tag{A.6.123}$$

$$-c_\alpha c_\gamma + s_\alpha s_\gamma \leqq 0. \tag{A.13.123}$$

(A.4.123) implies that $\alpha = \gamma$ or $\alpha = \gamma + \pi$ but $\alpha = \gamma + \pi$ is impossible because of (A.6.123). Thus $\alpha = \gamma$ and we get from (A.13.123) $s_\alpha^2 \leqq c_\alpha^2$. A short calculation after substitution shows that in this case the coefficients of the first order terms in (4.3a) are 0, $-c$ and $-b$; in (4.3b) are 0, $-a$ and 0; and in (4.3c) are $c_\alpha^2 - s_\alpha^2$, 0 and 1. Among these nine numbers the second and the third one express negative cross-effect thus showing the impossibility of transforming the Lorenz-equation into a kinetic one.

The same kind of argument can be used in all the other remaining star-denoted cases.

References

[1] A. Arneodo, P. Coullet and C. Tresser, Phys. Letters 79A (1980) 259.

[2] R. Bellman, Introduction to Matrix Analysis, (McGraw-Hill, New York, 1960).

[3] I.R. Epstein, Physica 7D (1983) 47.

[4] C. Escher, Chem. Phys. 63 (1981) 337.

[5] M.E. Gilpin, Am. Naturalist 113 (1979) 306.

[6] Vera Hárs and J. Tóth, Colloq. Math. Soc. János Bolyai 30 (1981) 363.

[7] J.L. Hudson and O.E. Rössler, in: Modelling of Patterns in Space and Time, W. Jäger and J.D. Murray, eds. (Springer, Berlin, 1984) p. 135.

[8] A.L. Kawczyński, Pol. J. Chem., to appear.

[9] R.B. King, Theoret. Chim. Acta 63 (1983) 323.

[10] W.F. Langford, Colloq. Math. Soc. János Bolyai, submitted.

[11] P. Lorenz, J. Athm. Sci. 20 (1963) 130.

[12] A.S. Pikovsky, Phys. Lett. 85A (1981) 13.

[13] O.E. Rössler, Z. Naturforsch. 31a (1976) 259.

[14] O.E. Rössler, Z. Naturforsch, 31a (1976) 1664.

[15] O.E. Rössler, in: Proc. Int. Symp. Math. Topics in Biology, Kyoto: Kyoto Res. Inst. for Math. Sci. Publs. 1978, p. 131.

[16] Th. Schulmeister, Studia Biophys. 72 (1978) 14 (microfiche).

[17] K.S. Sibirsky, Algebraic Invariant Theory of Differential Equations (Štiinca, Kiev, 1982) (in Russian).

[18] K. Tomita and I. Tsuda, Phys. Letters 71A (1979) 489.

[19] J.S. Turner, J.-C. Roux, W.D. McCormick and H.L. Swinney, Phys. Letters. 85A (1981) 9.

[20] J. Wei, J. Chem. Phys. 36 (1962) 1578.

[21] K.D. Willamowski and O.E. Rössler, Z. Naturforsch. 35a (1980) 317.