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KINETICAL SYSTEMS

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Abstract. The aim of the paper is to give some preliminary information concerning a class of nonlinear differential equations often used in physical chemistry and biology. Such systems are often very large and it is well known that where studying properties of such systems difficulties rapidly increase with their dimension. One way how to get over the difficulties is to use special forms of such systems.

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1. Kinetical system

Consider a "chemical system" $\mathcal{S}$ which is composed of n "components" $S_1, \ldots, S_n$ of "concentrations" $y_1, \ldots, y_n$. The components S_i of the system are composed of $d \leqslant n$ "base elements" $P_1, \ldots, P_d$ where the base element is understood to be a substance which does not decompose into simple substances. Therefore each component S_i is characterized as a linear combination of the base elements $P_1, \ldots, P_d$, formally

$$S_j = u_{ij} P_1 + \ldots + u_{dj} P_d, \quad j = 1, \ldots, n.$$

Coefficients of these linear combinations, usually expressed by nonnegative integers, form the rows of a matrix called in physical chemistry the "formula matrix" of the system $\mathcal{S}$.

Let us suppose that there are m "reactions" in $\mathcal{S}$ described by stoichiometric equations

$$\begin{aligned} &c_{1j} S_1 + \ldots + c_{nj} S_n \underset{d_j}{\overset{r_j}{\rightleftharpoons}} c'_{1j} S_1 + \ldots + c'_{nj} S_n, \\ &i = 1, \ldots, m;\ j = 1, \ldots, n, \end{aligned} \tag{1}$$

where nonnegative integers c_{ij}, c'_{ij} are stoichiometric coefficients of the i-th component in the j-th reaction, and r_j, d_j are non-negative functions of temperature T called "rate constants".

Assuming further that the temperature of $\mathcal{S}$ is a known time function $T(t)$ and that every reaction (1) leads after Guldberg and Waage to a time variation in the concentration of the i-th component

$$\dot{y}_i = (c_{ij} - c'_{ij}) \left[-r_j(T) \prod_{k=1}^{n} y_k^{c_{kj}} + d_j(T) \prod_{k=1}^{n} y_k^{c'_{kj}} \right],$$

the total change of the concentration of the i-th component is

$$\dot{y}_i = \sum_{j=1}^{m} (c_{ij} - c'_{ij}) \left[-r_j(t) \prod_{k=1}^{n} y_k^{c_{kj}} + d_j(t) \prod_{k=1}^{n} y_k^{c'_{kj}} \right].$$

We are now ready to formulate our system mathematically.

Definition 1.1. Let us consider $n \times m$ matrices $C = [c_{ij}]$, $C' = [c'_{ij}]$, where $c_{ij}, c'_{ij} \in \mathbb{Z}_{\geqslant 0}$ and $A = [a_{ij}] := C - C'$, $0 < L := \operatorname{rank}(A) < n$. Let $r_j, d_j \colon \mathbb{R} \to [0, \infty)$ be continuous functions and $G = [G_j]$ an m-dimensional vector such that

$$G_j(t, y) := -r_j(t) \prod_{k=1}^{n} y_k^{c_{kj}} + d_j(t) \prod_{k=1}^{n} y_k^{c'_{kj}}. \tag{2}$$

The system of equations

$$\dot{y} = AG(t, y), \quad (t, y) \in \mathbb{R} \times \mathbb{R}^n, \tag{3}$$

is called a *kinetical system*.

Remark 1. We shall always assume that the principal submatrix $A(1, \ldots, L)$ composed of the first L columns and the first L rows of A is nonsingular.

Our plan is as follows. In §2 we derive basic properties of nonnegative solutions of the non-autonomous system (3). In §3 we give a proof of existence of a critical point for the autonomous case. The main results are concentrated in §4 and they concern the asymptotic properties of a subset of (3)—the so called detailed balanced systems. The technique of proofs in this paper is based on the methods of differential inequalities, on the elementary fixed point method and on the invariance principle.

Through the paper we use the following notation:

$\mathbb{R}$—the set of real numbers.

$\mathbb{Z}$—the set of integers.

$\mathbb{R}^n$—the space of n dimensional column vectors $x = \mathrm{col}[x_1, \dots, x_n]$, $x_i \in \mathbb{R}$, $i = 1, \dots, n$.

$\mathbb{R}^n_{>0} := \{x = \mathrm{col}[x_1, \dots, x_n] \in \mathbb{R}^n : \ x_i > 0 \ i = 1, \dots, n\}$—the positive orthant.

$\mathbb{R}^n_{\geqslant 0} := \{x = \mathrm{col}[x_1, \dots, x_n] \in \mathbb{R}^n : \ x_i \geqslant 0 \ i = 1, \dots, n\}$—the nonnegative orthant.

$\mathbb{R}^{n \times m}$— the space of $n \times m$ matrices $A = [a_{ij}]$, $a_{ij} \in \mathbb{R}$, $i = 1, \dots n$, $j = 1, \dots, m$.

The previous notation is used also in the case when the set $\mathbb{R}$ is replaced by the set of integers $\mathbb{Z}$.

If $x, y \in \mathbb{R}^n$ then $x > y$ $(x \geqslant y) \iff x - y \in \mathbb{R}^n_{>0}$ $(x - y \in \mathbb{R}^n_{\geqslant 0})$.

$L(U, b) := \{y \in \mathbb{R}^n : Uy = b\}$, $b \in \mathbb{R}^d$, $U = [u_{ij}] \in \mathbb{Z}^{d \times n}$.

$H := L(U, b) \cap \mathbb{R}^n_{>0}$.

If $x \in \mathbb{R}^n$ then $\|x\|_p := \big[\sum\limits_{i=1}^n |x_i|^p\big]^{1/p}, p \in [1, \infty]$.

$B^p_n(z, \varepsilon) := \{y = [y_1, \dots, y_n] \colon \ \|z - y\|_p < \varepsilon\}$.

∂A—the boundary of the set A.

If A is an $n \times m$ matrix then $A(i_1, \dots, i_s)$ denotes the principal submatrix of A which consists of the i_1-th, …, i_s-th columns and i_1-th, …, i_s-th rows of the matrix A.

2. Global existence of nonnegative solutions of kinetical systems

In this section we consider the Cauchy problem

$$\dot{y} = AG(t, y), \quad y(t_0) = y^0, \quad (t, y) \in [0, \infty) \times \mathbb{R}^n, \tag{4}$$

where the matrix A and the vector G were introduced in Definition 1.1.

It is easy to see that

$$a_{ij} G_j(t, y) = -|a_{ij}| \left[y_i P_{ij}(t, y) - Q_{ij}(t, y)\right], \quad i = 1, \dots, n; \ j = 1, \dots, m, \tag{5}$$

where $P_{ij}(t, y)$, $Q_{ij}(t, y)$ are monoms of y such that if $y \geqslant 0$ then also $P_{ij}(t, y) \geqslant 0$, $Q_{ij}(t, y) \geqslant 0$. Indeed $a_{ij} = c_{ij} - c'_{ij}$ and if $c_{ij} = c'_{ij}$ then $a_{ij} = 0$ and (5) holds. If $c_{ij} > c'_{ij} \geqslant 0$, then $a_{ij} > 0$, $c_{ij} \geqslant 1$,

$$a_{ij} G_j(t, y) = |a_{ij}| G_j(t, y) = -|a_{ij}| \left[y_i r_j(t) y_i^{c_{ij} - 1} \prod_{\substack{k=1 \\ k \neq i}}^n y_k^{c_{kj}} - d_j(t) \prod_{k=1}^n y_k^{c'_{kj}} \right],$$

and we obtain (5) for

$$P_{ij}(t, y) := r_j(t) y_i^{c_{ij} - 1} \prod_{\substack{k=1 \\ k \neq i}}^n y_k^{c_{kj}}, \quad Q_{ij}(t, y) := d_j(t) \prod_{k=1}^n y_k^{c'_{kj}}.$$

Similarly if $a_{ij} < 0$ then we obtain (5) for

$$P_{ij}(t,y) := d_j(t) y_i^{c'_{ij}-1} \prod_{\substack{k=1\\ k\neq i}}^{n} y_k^{c'_{kj}}, \quad Q_{ij}(t,y) := r_j(t) \prod_{k=1}^{n} y_k^{c_{kj}}.$$

Assertion 2.1. *Let y denote a solution of* (4) *and $[t_0,\omega^+)$ the right maximal interval of existence for y. If there is a $t_1 \in [t_0,\omega^+)$ such that $y(t_1) \geqslant 0$, then $y \geqslant 0$ on $[t_1,\omega^+)$.*

Proof. We may suppose that $t_0 := t_1$. Let us choose $T \in (t_0,\omega^+)$ fixed and consider a sequence of mappings $\{f^j(t,y)\}_{j=1}^{\infty}$, where

$$f^j(t,y) := AG(t,y) + \frac{1}{j}[1,\ldots,1]^T, \quad j = 1,2,\ldots.$$

There is a positive integer j_0 such that for all $j \geqslant j_0$ the solution of

$$\dot z = f^j(t,z),\ z(t_0) = y^0,$$

exists on $[t_0,T]$ and owing to the uniqueness, $z^j \to y$ uniformly on $[t_0,T]$ for $j \to \infty$. Let $j \geqslant j_0$ and let $t_2 \in [t_0,T]$ be the first number such that $z_i^j = 0$.

It follows from (5) that

$$f_i^j(t,z) = -z_i \sum_k |a_{ik}| P_{ik}(t,z) + \sum_k |a_{ik}| Q_{ik}(t,z) + \frac{1}{j}.$$

Hence $\dot z_i^j(t_2) \geqslant 1/j > 0$, and in virtue of continuity of f^j the same holds also for t near to t_2. If $t_2 = t_0$, then $z_i^j(t) > z_i^j(t_2) = 0$ for $t > t_2$ near t_2. If $t_2 > t_0$, then $z_i^j(t) < z_i^j(t_2) = 0$ for $t < t_2$ near t_2, however this contradicts the definition of t_2. Altogether we have $z^j > 0$ on $[t_0,T]$ and also $y = \lim\limits_{j\to\infty} z^j \geqslant 0$ on $[t_0,T]$ as results from passing to the limit. This result is valid for all $T \in (t_0,\omega^+)$, therefore $y \geqslant 0$ on $[t_0,\omega^+)$. □

Lemma 2.2. *The equation* (3) *has at least $d := n - L$ time independent first integrals in the form*

$$\sum_{j=1}^{n} u_{ij} y_j = b_i, \quad i = 1,\ldots,d, \tag{6}$$

where u_{ij}, $b_i \in \mathbb{R}$ are suitable constants.

P r o o f. Since $0 < L = \operatorname{rank}(A) < n$ there is a real $d \times n$ matrix $U = [u_{ij}]$ such that $\operatorname{rank}(U) = d$ and $UA = 0$. Therefore

$$Uy(t) - Uy(t_0) = \int_{t_0}^{t} U\dot{y}(s)\,\mathrm{d}s = \int_{t_0}^{t} U[AG(s, y(s))]\,\mathrm{d}s = \int_{t_0}^{t} (UA)G(s, y(s))\,\mathrm{d}s = 0.$$

Hence it follows that (6) holds with

$$b_i := \sum_{j=1}^{n} u_{ij} y_j(t_0). \tag{7}$$

□

Definition 2.3. The real $d \times n$ matrix $U = [u_{ij}]$, $\operatorname{rank}(U) = d = n - L$ such that $UA = 0$ is called the *formula matrix.* If in addition

$$\begin{aligned} &u_{ij} \in \mathbb{Z}_{\geqslant 0}, \quad i = 1, \ldots, d,\ j = 1, \ldots, n, \\ &\sum_{i=1}^{d} u_{ij} > 0, \quad j = 1, \ldots, n, \end{aligned} \tag{8}$$

the matrix U is called the *nonnegative formula matrix.*

We shall need the following hypotheses:

H1 *there is at least one nonnegative formula matrix U—one of them is chosen fixed.*

Let us denote by $L(U, b)$ the subset of $\mathbb{R}^n$ satisfying (6), clearly $L(U, b)$ is a linear $L = n - d$ dimensional manifold and it is obvious from Assertion 2.1 and Lemma 2.2 that $L(U, b) \cap \mathbb{R}^n_{\geqslant} 0$ is a (positively) invariant set of (3). To ensure that this set is "sufficiently big" we assume the following:

H2 *there exists a vector $b \in \mathbb{R}^d_{>0}$ such that there is a nonnegative solution $y \in \mathbb{R}^d_{\geqslant 0}$ of* (6)*, that is the set $H := L(U, b) \cap \mathbb{R}^n_{\geqslant 0}$ is not empty. One such vector is chosen fixed.*

Our general hypotheses in the next theorem will be almost those of Assertion 2.1, the main difference being that we further assume:

H3 *$r_j(t)$, $d_j(t)$ are positive for $j = 1, \ldots, m$.*

In this case we easily obtain a bit sharper results.

Theorem 2.4. *Suppose that* (4) *satisfies* H1, H2, H3 *and y is a solution of* (4) *with the maximal interval of existence $[t_0, \omega^+)$.*

If $y^0 > 0$, then $y(t) > 0$ on $[t_0, \omega^+)$.

If $y^0 \geqslant 0$ and $y^0_i = 0$ for $i \in I \subset \{1, \ldots, n\}$, then for each $i \in I$ only one of the following possibilities takes place:

a) *$y_i(t) > 0$ on (t_0, ω^+)*

b) *$y_i(t) \equiv 0$ on $[t_0, \omega^+)$.*

Always $y_i(t) > 0$ on $[t_0, \omega^+)$ for each $i \in \{1, \ldots, n\} \setminus I$.

P r o o f. First we shall investigate the case when $y^0 > 0$. Let us consider in the contrary that there is a $T \in (t_0, \omega^+)$ such that $y_j(T) < 0$ for at least one $j \in \{1, \dots, n\}$. Then there is a largest $t_1 \in [t_0, T)$ such that $y(t) > 0$ on $[t_0, t_1)$ and $y_i(t_1) = 0$ for $i \in I$, where I is a suitable subset of $\{1, \dots, n\}$. We may assume without loss of generality that $I = \{1, \dots, p\}$, $1 \leqslant p < n$. If we denote

$$V_{ij}(t, y) := (c_{ij} - c'_{ij}) \left[-P_j(t, y) + Q_j(t, y)\right],$$

where $P_j(t, y) := r_j(t) \prod\limits_{k=1}^{n} y_k^{c_{kj}}$, $Q_j(t, y) := d_j(t) \prod\limits_{k=1}^{n} y_k^{c'_{kj}}$, then

$$\dot{y}_i(t) = \sum_{j=1}^{m} V_{ij}(t, y(t)), \quad j = 1, \dots, n.$$

If $t = t_1$, it is possible to obtain a useful classification of values of $V_{ij}(t_1, y(t_1))$ with respect to certain combinations of the coefficients c_{ij}, c'_{ij} for $i = 1, \dots, p$; $j = 1, \dots, m$. For example if $c_{1j} + \ldots + c_{pj} > 0$ and $c'_{1j} + \ldots + c'_{pj} = 0$ and $c_{ij} = c'_{ij}$ then $V_{ij}(t_1, y(t_1)) = 0$. All such important cases are contained in Table 1:

$c_{1j} + \ldots + c_{pj}$	$c'_{1j} + \ldots + c'_{pj}$		$V_{ij}(t_1, y(t_1))$
> 0	> 0		0
> 0	$= 0$	$c_{ij} = c'_{ij}$	0
> 0	$= 0$	$c_{ij} > c'_{ij}$	$c_{ij} Q_j(t_1, 0, \dots, 0, y_{p+1}, \dots, y_n)$
$= 0$	> 0	$c'_{ij} = c_{ij}$	0
$= 0$	> 0	$c'_{ij} > c_{ij}$	$c'_{ij} P_j(t_1, 0, \dots, 0, y_{p+1}, \dots, y_n)$
$= 0$	$= 0$		0

Table 1

Thus $V_{ij}(t_1, y(t_1)) \geqslant 0$ for $i = 1, \dots, p$; $j = 1, \dots, m$. At the same time it is easy to see that for each $i \in I$ two mutually exclusive cases are possible:

$$\exists j \in \{1, \dots, m\}\colon\ c_{ij} \neq c'_{ij} \wedge (c_{1j} + \ldots + c_{pj})(c'_{1j} + \ldots + c'_{pj}) = 0, \tag{9}$$

$$\forall j \in \{1, \dots, m\}\colon\ c_{ij} = c'_{ij} \vee (c_{1j} + \ldots + c_{pj})(c'_{1j} + \ldots + c'_{pj}) \neq 0. \tag{10}$$

Let us put $I = I_1 \cup I_2$ ($I_1 \cap I_2 = \emptyset$), where (9) holds for each $i \in I_1$ and (10) holds for each $i \in I_2$.

Let $i \in I_1$, then there is $j(i) \in \{1, \dots, m\}$ such that

$$V_{ij(i)}(t_1, y(t_1)) = c'_{ij(i)} P_{j(i)}(t_1, 0, \dots, 0, y_{p+1}(t_1), \dots, y_n(t_1)) > 0$$

or

$$V_{ij(i)}(t_1, y(t_1)) = c_{ij(i)} Q_{j(i)}(t_1, 0, \dots, 0, y_{p+1}(t_1), \dots, y_n(t_1)) > 0.$$

Therefore

$$\dot{y}_i(t_1) = \sum_{j=1}^{m} V_{ij}(t_1, y(t_1)) \geqslant V_{ij(i)}(t_1, y(t_1)) > 0,$$

and this inequality holds on $(t_1 - \varepsilon, t_1 + \varepsilon)$ for $\varepsilon > 0$ small enough. But this means that $y_i(t_1 - \frac{1}{2}\varepsilon) < y_i(t_1) = 0$ which contradicts the definition of t_1, also $I_1 = \emptyset$ and $I = I_2$.

Let $i \in I_2$. We can suppose, without loss of generality, that $I_2 = \{1, \dots, p\}$. Then

$$\dot{y}_i(t_1) = \sum_{j=1}^{m} V_{ij}(t_1, y(t_1)) = 0, \quad i = 1, \dots, p.$$

It is seen from Table 1 that $V_{ij}(t_1, y(t_1)) = V_{ij}(t_1,\, 0, \dots, 0, y_{p+1}(t_1), \dots, y_n(t_1))$ for $i = 1, \dots, n$; $j = 1, \dots, m$, therefore for $t = t_1$ and in general for every t^* such that $y_i(t^*) = 0$, $i = 1, \dots, p$ it is possible to write (4) in the form

$$\begin{aligned} \dot{y}_i(t^*) &= 0, \quad i = 1, \dots, p, \\ \dot{y}_i(t^*) &= f_i(t^*, 0, \dots, 0, y_{p+1}(t^*), \dots, y_n(t^*)), \quad i = p+1, \dots, n, \end{aligned}$$

where f_i is the i-th element on the right hand side of (3). Consider the problem

$$\text{(11)} \qquad \begin{aligned} &\dot{u}_i = 0, && u_i(t_1) = 0, && \text{(a)} \\ &\dot{u}_j = f_j(t, 0, \dots, 0, u_{p+1}, \dots, u_n), && u_j(t_1) = y_j(t_1), && \text{(b)} \\ &i = 1, \dots, p,\ \ j = p+1, \dots, n, \end{aligned}$$

with the unique solution $u = \operatorname{col}[u_1, \dots, u_n]$,

$$\text{(12)} \qquad \begin{aligned} u_i(t) &\equiv 0, \quad i = 1, \dots, p, \\ u_i(t) &= h_i(t), \quad i = p+1, \dots, n, \end{aligned}$$

on (ω_-^1, ω_+^1). If we substitute this solution into the right-hand side of (4), we obtain

$$\begin{aligned} f_i(t, u_1(t), \dots, u_p(t), u_{p+1}(t), \dots, u_n(t)) &= f_i(t, 0, \dots, 0, h_{p+1}(t), \dots, h_n(t)) \\ &= 0 = \dot{u}_i(t),\ \ i = 1, \dots, p, \\ f_i(t, u_1(t), \dots, u_p(t), u_{p+1}(t), \dots, u_n(t)) &= f_i(t, 0, \dots, 0, h_{p+1}(t), \dots, h_n(t)) \\ &= \dot{h}_i(t) = \dot{u}_i(t),\ \ i = p+1, \dots, n. \end{aligned}$$

and this means that (12) is the solution of (4) on $(t_1 - \delta, t_1] \subset (\omega_+^1, t_1] \cap [t_0, t_1]$ for $\delta > 0$ small enough. Therefore (4) has a couple of solutions u, y such that $u(t_1) = y(t_1)$ and $u(t_1 - 1/2\delta) = 0 \neq y(t_1 - 1/2\delta)$, which is absurd. Hence $y(t) > 0$ for $t \in [t_0, \omega^+)$.

It remains to investigate the case $y^0 \geqslant 0$, $y_i^0 = 0$ for $i \in I \neq \emptyset$. The proof, which is almost the same as in the previous case, is only outlined here for completeness.

We shall again write $I = I_1 \cup I_2$, where (9) [(10)] holds for each $i \in I_1$ [$i \in I_2$]. If $i \in I_1$, then $y_i(t_0 + \alpha) > y_i(t_0) = 0, \alpha > 0$. If $i \in I_2$, then two mutually exclusive cases are possible. Either $y_i \equiv 0$ or there exists a $t_3^i \in [t_0, \omega^+)$, $t_3^i := \inf\{t \in [t_0, \omega^+)\colon\ y_i(t) > 0\}$.

Let t_2 be the minimum of such t_3^i, $i \in I$. Consider (11) and its solution (12), this time for an initial time t_2, on $[t_2, t_2 + \gamma)$. It is easy to see that (12) is a solution of (4), too. But this contradicts the uniqueness property, therefore if $i \in I_2$ then $y_i \equiv 0$. Theorem 2.4 is proved. □

Remark 2. It follows from the proof of Theorem 2.4 that if $r_i(t)$, $d_i(t) > 0$ for $i = 1, \dots, n$, it is possible to suppose that for any nonnegative solution y of (4) we have in fact $y_i(t) > 0$ for $i = 1, \dots, n$ on (t_0, ω^+). This assumption does not lead to loss of generality, indeed it is always possible to work with the "lower dimensional system" (b)(11) (which has again the structure of a kinetical system).

Theorem 2.5. *Suppose that* (4) *satisfies* H1, H2. *If* y *is a solution of* (4) *such that* $y^0 \geqslant 0$, *then the maximal interval of existence of* y *is* $[t_0, \infty)$.

Proof. It follows from Assertion 2.1 that $y(t) \geqslant 0$ for $t \geqslant t_0$. Let us put $m := \min\{u_{ij}\colon\ u_{ij} > 0,\ i = 1, \dots, d;\ j = 1, \dots, n\}$. (8) implies that for each $j \in \{1, \dots, n\}$ there is an index $i = i(j) \in \{1, \dots, d\}$ such that $u_{i(j)j} > 0$ and we easily get from Lemma 2.2 that

$$0 \leqslant y_j(t) = \frac{1}{u_{i(j)j}} \Bigl(b_{i(j)} - \sum_{\substack{k=1\\k\neq j}}^{n} y_k(t) u_{i(j)k} \Bigr) \leqslant \frac{\|b\|_\infty}{m}, \ j = 1, \dots, n.$$

Hence

$$0 \leqslant \|b\|_1 = \sum_{k=1}^{d} b_k = \sum_{k=1}^{d} \sum_{j=1}^{n} u_{kj} y_j(t) = \max_i \Bigl(\sum_{k=1}^{d} u_{ki} \Bigr) \sum_{j=1}^{n} y_j(t)$$
$$= \Bigl\| \Bigl[\sum_{k=1}^{d} u_{ki} \Bigr]_i \Bigr\|_\infty \|y(t)\|_1.$$

Consequently we have

$$\frac{\|b\|_1}{\Bigl\| \Bigl[\sum_{k=1}^{d} u_{ki} \Bigr]_i \Bigr\|_\infty} \leqslant \|y(t)\|_1 \leqslant n \|y(t)\|_\infty \leqslant \frac{n}{m} \|b\|_\infty.$$

□

The kinetic problem (4) has especially simple structure if $m = 1$. In this case there are $n-1$ linearly independent first integrals and (4) is essentially a scalar problem. That is why the following corollary holds:

Corollary 2.6. *If the assumptions of Theorem* 2.5 *are fulfilled,* $m = 1$ *and all the functions* $r_i(t)$, $d_i(t)$ *are constant functions, then the limit* $\lim\limits_{t\to\infty} y(t)$ *exists.*

3. Autonomous case—existence of stationary points

This section is concerned with the problem of existence of nonnegative stationary points of (3) in the case when r_j, d_j are constants, i.e. (3) is in the form

$$\dot{y} = AG(y), \quad y(0) = y^0,\ y^0 \geqslant 0. \tag{13}$$

Definition 3.1. Let F be continuous on an open y-set $\Omega \subset \mathbb{R}^n$, let Ω_0 be a subset of Ω and $y^0 \in \partial\Omega_0 \cap \Omega$. The point y^0 is called an *egress point* of Ω_0 with respect to

$$\dot{y} = F(y), \tag{14}$$

if for every solution $y = y(t; 0, y^0)$ of (14), $y(0) = y^0$ there exists an $\varepsilon > 0$ such that $y(t) \notin \overline{\Omega}_0$ for $t \in (0, \varepsilon]$ [3, p. 173].

Lemma 3.2. *If F is a continuous function on an open y-set $\Omega \subset \mathbb{R}^n$, solutions of* (14) *are uniquely determined by the initial condition and $H \subset \Omega$, $H \neq \emptyset$ is a compact, convex set such that the points of ∂H are not egress points of H with respect to* (14)*, then* (14) *possesses at least one stationary point on H.*

P r o o f. It is based on the fact that the set of maps $T_a \colon H \to H$, $T_a(y^0) := y(a; 0, y^0)$ behaves like an Abelian group and on the fixed point theorem due to Brouwer. The detailed proof is omitted here because it is almost the same as the proof of Theorem 8.2 in [1, p. 48]. □

Theorem 3.3. *Suppose that* (13) *satisfies* H1 *and* H2*. Then* (13) *has a stationary point $y \in H$.*

P r o o f. The set $H = L(U, b) \cap \mathbb{R}^n_{\geqslant 0}$ is the subset of $\mathbb{R}^n$ containing all points $y = \mathrm{col}[y_1, \ldots, y_n]$ such that

$$\begin{aligned} &u_{11}y_1 + \ldots + u_{1n}y_n = b_1,\\ &u_{d1}y_1 + \ldots + u_{dn}y_n = b_d,\\ &y_1 \geqslant 0, \ldots, y_n \geqslant 0. \end{aligned}$$

Therefore H is a bounded closed convex set. Moreover, $\partial H \subset \partial L(U, b) \cup \partial \mathbb{R}^n_{\geqslant 0}$ and due to Assertion 2.1 and Lemma 2.2 the points of ∂H are not egress points with respect to the system (13). By Lemma 3.2 there is a stationary point $y \in H$. $\square$

4. Asymptotic properties

In the previous section the problem of existence of nonnegative stationary points of the system

$$\dot{y} = AG(y) \tag{15}$$

was solved without any discussion of their properties. This section concerns asymptotic properties of the system

$$\dot{y} = AG(t, y). \tag{16}$$

At the beginning we outline a rather smaller class of kinetical systems fulfilling the principle of detailed balance and point out some of the basic properties of such systems. The main results we will obtain for autonomous detailed balanced systems by using the invariance principle. In the whole section we suppose H1, H2, that is we are interested in asymptotic properties of the system

$$\dot{y} = AG(t, y), \quad (t, y) \in [t_0, \infty) \times H, \tag{17}$$

or

$$\dot{y} = AG(y), \quad (t, y) \in [t_0, \infty) \times H, \tag{18}$$

in the autonomous case. These systems are correct due to Assertion 2.1 and Lemma 2.2. In this sense we speak of critical points of (17)—that is of critical points of (16) belonging to the integral manifold H, of the stability of solutions of (17), that is of the stability of solutions with respect to the solutions belonging to the integral manifold H, similarly for the concepts of an isolated point, closure, boundary and so on.

Instead of H3 we use a stronger hypothesis:

H4 *$r_i(t)$, $d_i(t) \geqslant \xi_i > 0$ for $i = 1, \dots, m$.*

Some of the theorems also involve the following assumption:

H5 *if $y = [y_1, \dots, y_n]$ is a nonnegative solution of* (17)*, then $y_i \not\equiv 0$ on the right maximal interval of existence $[t_0, \infty)$ for $i = 1, \dots, n$.*

It follows from H5 that any nonnegative critical point y of (17) should be in fact included in $\mathbb{R}^n_{>0}$. Due to Remark 2 this hypothesis is no strong restriction.

As $\operatorname{rank}(A) = L < n$ and the columns $\operatorname{col}_1(A), \dots, \operatorname{col}_L(A)$ of the matrix A are linearly independent, there exists a unique real $L \times m$ matrix $Z = [z_{ij}]$ such that

$$\operatorname{col}_j(A) = \sum_{i=1}^{L} \operatorname{col}_i(A) z_{ij}, \quad j = 1, \dots, m, \tag{19}$$

obviously

$$z_{ij} = \frac{\det \begin{bmatrix} a_{11} & \dots & a_{1i-1} & a_{1j} & a_{1i+1} & \dots & a_{1L} \\ \vdots & & \vdots & \vdots & \vdots & & \vdots \\ a_{L1} & \dots & a_{Li-1} & a_{Lj} & a_{Li+1} & \dots & a_{LL} \end{bmatrix}}{\det \begin{bmatrix} a_{11} & \dots & a_{1L} \\ \vdots & & \vdots \\ a_{L1} & \dots & a_{LL} \end{bmatrix}}, \tag{20}$$

$$i = 1, \dots, L, \quad j = 1, \dots, m \quad .$$

Definition 4.1. System (3) is *detailed balanced* if

$$\prod_{i=1}^{L} \left[\frac{d_i(t)}{r_i(t)} \right]^{z_{ij}} = \frac{d_j(t)}{r_j(t)}, \quad j = 1, \dots, m, \tag{21}$$

where z_{ij} are the constants introduced in (19).

Of course, for $m = L$ every kinetical system (3) is detailed balanced trivially.

Definition 4.2. A critical point y^0 of a kinetical system (3) is said to be *balanced* if $G_i(t, y^0) = 0$ for each $i \in \{1, \dots, m\}$.

The previous definitions may appear to be a bit cumbersome but as we will see detailed balanced kinetical systems have very nice and natural properties especially from the point of view of applications, e.g. if the "chemical system" S described by a detailed balanced kinetical system is in a "state of equilibrium", then all its "reactions" are in a "state of equilibrium" as well.

Balanced critical points are in strong correspondence with detailed balanced systems. This connection is expressed in the following algebraic lemmas.

Lemma 4.3. *Suppose that* (16) *satisfies* H1, H2, H4. *If* (16) *possesses a balanced critical point* $y \in \mathbb{R}^n_{>0}$, *then it is detailed balanced.*

P r o o f. Let $y \in \mathbb{R}^n_{>0}$ be a balanced critical point of (16) and let $L = \operatorname{rank}(A)$. If $L = m$, the lemma is trivially satisfied. Let $L < m$, then from the assumption $G_j(t,y) = 0$, $j = 1,\dots,m$ we obtain

$$0 = G_j(t,y) = -r_j(t)\prod_{k=1}^{n} y_k^{c_{kj}} + d_j(t)\prod_{k=1}^{n} y_k^{c'_{kj}} = \left[-r_j(t)\prod_{k=1}^{n} y_k^{c'_{kj}}\right]\left[\prod_{k=1}^{n} y_k^{a_{kj}} - \frac{d_j(t)}{r_j(t)}\right],$$

hence

$$\prod_{k=1}^{n} y_k^{a_{kj}} = \frac{d_j(t)}{r_j(t)}, \quad j = 1,\dots,m.$$

According to (19) $a_{kj} = \sum_{i=1}^{L} z_{ij} a_{ki}$, $j = 1,\dots,m$; $k = 1,\dots,n$, hence for $j = 1,\dots,m$

$$\frac{d_j(t)}{r_j(t)} = \prod_{k=1}^{n} y_k^{a_{kj}} = \prod_{k=1}^{n}\prod_{i=1}^{L} y_k^{a_{ki} z_{ij}} = \prod_{i=1}^{L}\left(\prod_{k=1}^{n} y_k^{a_{ki}}\right)^{z_{ij}} = \prod_{i=1}^{L}\left[\frac{d_i(t)}{r_i(t)}\right]^{z_{ij}},$$

which means that (16) is detailed balanced. □

Lemma 4.4. *Let* (16) *be detailed balanced, satisfies* H1, H2, H4, *and let a matrix* B *consist exactly of the first* L *columns of the matrix* A. *If a point* $y \in \mathbb{R}^n_{>0}$ *is a critical point of the system*

$$\dot{y} = BG(t,y), \tag{22}$$

then it is also the critical point for the system (16).

P r o o f. In accordance with Remark 1 the principal minor $\det A(1,\dots,L)$ of the matrix A is not equal zero. If $y \in \mathbb{R}^n_{>0}$ is a critical point of (22), then $0 = BG(t,y)$ for $t \geqslant t_0$ and consequently $G_1(t,y) = \ldots = G_L(t,y) = 0$ or

$$\prod_{k=1}^{n} y_k^{a_{ki}} = \frac{d_i(t)}{r_i(t)}, \quad i = 1,\dots,L.$$

For $j = L+1,\dots,m$ we obtain

$$\begin{aligned}
G_j(t,y) &= -r_j(t)\left(\prod_{k=1}^{n} y_k^{c'_{kj}}\right)\left[\prod_{k=1}^{n} y_k^{a_{kj}} - \frac{d_j(t)}{r_j(t)}\right] \\
&= -r_j(t)\left(\prod_{k=1}^{n} y_k^{c'_{kj}}\right)\left[\prod_{k=1}^{n}\left(\prod_{i=1}^{L} y_k^{z_{ij} a_{ki}}\right) - \frac{d_j(t)}{r_j(t)}\right] \\
&= -r_j(t)\left(\prod_{k=1}^{n} y_k^{c'_{kj}}\right)\left\{\prod_{i=1}^{L}\left[\frac{d_i(t)}{r_i(t)}\right]^{z_{ij}} - \frac{d_j(t)}{r_j(t)}\right\} \\
&= 0.
\end{aligned}$$

Altogether, $G_i(t,y) = 0$ for $t \geqslant t_0$, $i = 1,\dots,m$ and y is a critical point of (15). □

Our next aim will be to show when it is possible to turn the Lemma 4.3. Therefore we shall assume that the conditions (21) are satisfied. We shall restrict ourselves to the autonomous case where LaSalle's invariance principle will demonstrate its power. At the same time we shall obtain useful information about asymptotic properties of (18).

We start our considerations with the description of properties of an auxiliary function V.

Remark 3. Let $h_i\colon \mathbb{R} \to \mathbb{R}$, $i = 1, \dots, n$ be C^1 functions and let $\tilde{V}\colon \mathbb{R}\times\mathbb{R}^n \to \mathbb{R}$ be a continuous function defined by $\tilde{V}\colon (t, y) \mapsto \sum_{i=1}^{n} \tilde{V}_i(t, y_i)$ where $\tilde{V}_i\colon \mathbb{R}\times\mathbb{R} \to \mathbb{R}$ is such that

$$\tilde{V}_i(t,x) := \begin{cases} x[h_i(t) + \ln|x|] & \text{if} \quad x \neq 0 \\ 0 & \text{if} \quad x = 0 \end{cases}$$

for $i = 1, \dots, n$. Let $f\colon \mathbb{R}\times\mathbb{R}^n \to \mathbb{R}^n$ be a continuous mapping and $(t_0, y^0) \in \mathbb{R}\times\mathbb{R}^n$ a fixed chosen point. Without loss of generality it is possible to suppose that there is a $0 \leqslant k \leqslant n$ such that $y^0 = [y_1^0, \dots, y_k^0, 0, \dots, 0]^T$ and $y_i^0 \neq 0$ for $i = 1, \dots, k$. Then for $h > 0$

$$\lim_{h\to 0+} \frac{1}{h}[\tilde{V}(t_0 + h, y^0 + hf(t_0, y^0)) - \tilde{V}(t_0, y^0)]$$
$$= \begin{cases} \sum\limits_{i=1}^{n} y_i^0 \dot{h}_i(t_0) + \sum\limits_{i=1}^{n} [h_i(t^0) + 1 + \ln|y_i^0|] f_i(t_0, y^0) & \text{if} \quad k = n \\ -\infty & \text{if} \quad k < n. \end{cases}$$

If $h_i(t) \equiv h_i \in \mathbb{R}$, $i = 1, \dots, n$ then the restriction of $\tilde{V}$ to the set $\mathbb{R}^n_{\geqslant 0}$ is a strictly convex function as follows from the fact that $\tilde{V}_i$ as a function of y_i is strictly convex on $[0, \infty)$.

4.0.1. Construction and properties of $V(y)$

Let us consider an n-parametric system of functions

$$V\colon \mathbb{R}^n_{\geqslant 0} \to \mathbb{R},$$
$$V\colon y \mapsto V(y) := \sum_{i=1}^{n} y_i(h_i + \ln y_i),\ h_i \in \mathbb{R},\ i = 1, \dots, n, \tag{23}$$

where as in Remark 3 the terms $y_i(h_i + \ln y_i)$ are replaced by 0 if $y_i = 0$, with parameters $h_i \in \mathbb{R}$ chosen in such a way that

$$\sum_{i=1}^{n} a_{ij} h_i = -\sum_{i=1}^{n} a_{ij} - \ln\frac{d_j}{r_j} \quad \text{for} \quad j = 1, \dots, m. \tag{24}$$

Remark 1 and the fact that (18) is detailed balanced, imply solvability of (24).

From (24) we get for the derivative of V along a solution of (18)

$$\begin{aligned}\dot{V}(y) &= \sum_{i=1}^{n}[(h_i+1)+\ln y_i]\dot{y}_i \\ &= \sum_{j=1}^{m}\left[\left(r_j\prod_{k=1}^{n} y_k^{c'_{kj}}\right)\left(\frac{d_j}{r_j}-\prod_{k=1}^{n} y_k^{a_{kj}}\right)\left(\ln\prod_{k=1}^{n} y_k^{a_{kj}}-\ln\frac{d_j}{r_j}\right)\right]\leqslant 0\end{aligned}$$

for $y \in \mathbb{R}^n_{>0}$. With respect to Remark 3 it is possible to extend the domain of $\dot{V}$ to $\mathbb{R}^n_{\geqslant 0}$ with $\dot{V}(y) = -\infty$ if $y \in \partial\mathbb{R}^n_{>0}$. In addition

$$\dot{V}(y) = 0 \Longleftrightarrow G_j = 0, \quad j = 1,\dots,m. \tag{25}$$

Indeed, if there is an index $j \in \{1,\dots,m\}$ such that $G_j(y) \neq 0$, then

$$\dot{V}(y) \leqslant \left(r_j\prod_{k=1}^{n} y_k^{c'_{kj}}\right)\left(\frac{d_j}{r_j}-\prod_{k=1}^{n} y_k^{a_{kj}}\right)\left(\ln\prod_{k=1}^{n} y_k^{a_{kj}}-\ln\frac{d_j}{r_j}\right) < 0.$$

The other implication is obvious.

From (25) the theorem inverse to Lemma 4.3 and Lemma 4.4 follows.

Theorem 4.5. *Suppose that* (15) *satisfies* H1, H2, H4, H5, *then:*

1. *Every stationary point of a detailed balanced system* (15) *is balanced.*
2. *If $w \in H$ is a stationary point of a detailed balanced autonomous system* (15), *then it is also a stationary point of*

$$\dot{y} = BG(y),$$

where the integer $n \times \operatorname{rank}(A)$ matrix B consists of linearly independent columns of the matrix A.

It follows from (25) that positive stationary points of (18) do not depend on the values of the constants r_j, d_j for $j = 1,\dots,n$ but only on their ratios. From this point of view it is possible to make a decomposition of the class of all systems (18) into equivalence classes where two systems are equivalent iff their stationary points are identical.

It follows from § 3 that there exists at least one stationary point of (18) even if (18) is not a detailed balanced system. In the case when (18) is a detailed balanced system it is possible to obtain stronger results by using much simpler tools than Brouwer's fixed point theorem.

Assertion 4.6. *Suppose that* (18) *satisfies* H1, H2, H4, H5. *If* (18) *is a detailed balanced system, then* (18) *has at least one balanced stationary point* $z \in H$.

Proof. If (18) has a stationary point z then by Theorem 4.5 this point is balanced. Therefore it is sufficient to prove the existence.

Since the set $H = L(U, b) \cap \mathbb{R}^n_{\geqslant 0}$ is compact and convex, the continuous and strictly convex function V assumes exactly one minimum at a point $z = [z_1, \ldots, z_n] \in H$.

It follows from the Remark 3 that the point $z \notin \partial(\mathbb{R}^n_{>0})$, hence $z > 0$ and

$$\begin{aligned} h_1 + 1 + \ln z_1 + \sum_{i=1}^{d} \lambda_i u_{i1} &= 0, \\ &\vdots \\ h_n + 1 + \ln z_n + \sum_{i=1}^{d} \lambda_i u_{in} &= 0, \\ u_{11} z_1 + \ldots + u_{1n} z_n &= b_1, \\ &\vdots \\ u_{d1} z_1 + \ldots + u_{dn} z_n &= b_d, \end{aligned}$$

where $\lambda_1, \ldots, \lambda_d \in \mathbb{R}$ are Lagrange multipliers. Using the first n equations we obtain

$$z_k = \exp\left(-1 - h_k - \sum_{i=1}^{d} \lambda_i u_{ik}\right), \qquad k = 1, \ldots, n.$$

From (24) we derive

$$\begin{aligned} \prod_{k=1}^{n} z_k^{a_{kj}} &= \prod_{k=1}^{n} \exp\left[\left(-1 - h_k - \sum_{k=1}^{d} \lambda_i u_{ik}\right) a_{kj}\right] \\ &= \exp\left[-\sum_{k=1}^{n} a_{kj} - \sum_{k=1}^{n} a_{kj} h_k - \sum_{k=1}^{n} a_{kj} \sum_{i=1}^{d} \lambda_i u_{ik}\right] \\ &= \exp\left[\ln \frac{d_j}{r_j} - \sum_{i=1}^{d} \lambda_i \sum_{k=1}^{n} u_{ik} a_{kj}\right] \\ &= \frac{d_j}{r_j}. \end{aligned}$$

Therefore $G_j(z) = 0$ for every $j \in \{1, \ldots, m\}$ and z is a balanced stationary point. $\square$

The knowledge of the function V gives us the possibility to answer questions of asymptotic properties of solutions of (18) in a neighbourhood of stationary points. The easiest way is to use the well known Chetaev's theorem [3, p. 19, 21—autonomous case]:

Theorem 4.7. *Let $\Omega \subset \mathbb{R}^n$ be an open connected set containing the origin. Let $f\colon \Omega \to \mathbb{R}^n$ be smooth enough in order that through every $x^0 \in \Omega$ there passes one and only one solution of $\dot{x} = f(x)$ and let $f(0) = 0$. If there exist $\varepsilon > 0$ (with $\overline{B}^p_n(0,\varepsilon) \subset \Omega$), an open set $\Psi \in B_n(0,\varepsilon)$ and a C^1 function $V\colon B_n(0,\varepsilon) \to \mathbb{R}$ such that*

i) *$V(x) > 0$ on Ψ,*
ii) *$\dot{V}(x) > 0$ on Ψ;*
iii) *the origin of the x-space belongs to $\partial\Psi$,*
iv) *$V(x) = 0$ on $\partial\Psi \cap B_n(0,\varepsilon)$, then the origin is unstable.*

Theorem 4.8. *Suppose that the detailed balanced system* (18) *satisfies* H1, H2, H4, H5. *If the stationary points of* (18) *are isolated, then* (18) *has exactly one stationary point uniformly stable with respect to the set H, the other stationary points* (*if they exist*) *are unstable.*

P r o o f. There exists exactly one point $z^* \in H$ such that $V(z^*) < V(z)$ for $z \in H \setminus \{z^*\}$. Evidently z^* is a balanced stationary point of (18). The stationary solution $y(t) \equiv z^*$ is (uniformly) asymptotically stable, since for sufficiently small $\varepsilon_1 > 0$ there is no other stationary point in $B_H(z^*,\varepsilon_1) := B(z^*,\varepsilon_1) \cap H$, $V \in C^1$ on $B_H(z^*,\varepsilon_1)$, $\dot{V}(z^*) = 0$, $\dot{V} < 0$ on $H \setminus \{z^*\}$ and V is convex on H.

If $z \neq z^*$ is another stationary point of (18), let us consider the function

$$\begin{aligned} &W\colon\ H \to \mathbb{R},\\ &W\colon\ y \mapsto W(y) := V(z) - V(y). \end{aligned}$$

For $\varepsilon > 0$ sufficiently small there is no other stationary point in the closed ball $\overline{B}_H(z,\varepsilon) := \overline{B}(z,\varepsilon) \cap H$ and $\Psi := \{y \in H\colon\ W(y) > 0\}$, then Ψ is an open set in H and for $y \in \Psi$ we have $W(y) > 0$, $\dot{W}(y) > 0$ and $W(y) = 0$ for $y \in \partial\Psi \cap B_H(z,\varepsilon)$ where the boundary is determined with respect to the set H. Therefore according to Theorem 4.7 z is an unstable stationary point. □

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