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THE QUALITATIVE ANALYSIS OF A DYNAMICAL SYSTEM MODELING THE FORMATION OF TWO-LAYER SCALES ON PURE METALS

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ABSTRACT. F. Gesmundo and F. Viani have modeled the growth rates of two-oxide scales by the system:

$$\frac{dq_1}{dt} = m\frac{K_1}{2q_1} - \frac{m-1}{m}\frac{K_2}{2q_2}, \qquad \frac{dq_2}{dt} = -m\frac{K_1}{2q_1} + \frac{K_2}{2q_2}.$$

We provide a complete qualitative analysis of (1.1) by making use of known results about the general n-dimensional dynamical system:

$$\frac{dp_i}{dt} = -\sum_{j=1}^{n}\frac{a_{ij}}{p_j}, \quad p_i(t) > 0, \qquad i = 1, \dots, n.$$

We show that for $m > 1$, the Gesmundo-Viani system admits a unique parabolic solution $q_i(t) = c_i\sqrt{t}$, $c_i > 0$. This parabolic solution attracts all other solutions. Every solution extends uniquely to a solution on $[0, +\infty)$, such that the extended solution is eventually monotonically increasing. Finally, the trajectory of any solution coincides with a trajectory of the following linear system:

$$\frac{dq_1}{dt} = -\frac{m-1}{m}\frac{K_2}{2}q_1 + m\frac{K_2}{2}q_2, \qquad \frac{dq_2}{dt} = \frac{K_2}{2}q_1 + m\frac{K_1}{2}q_2.$$

1. INTRODUCTION

A metal oxide is a compound containing oxygen and metal. For instance, common rust is caused by the oxidation of metal. Certain pure metals can form different oxides, and oxidation of such metals produces a multilayer oxide scale on the metal, where the oxide layer containing the highest concentration of metal is in contact with the surface of the metal, while the oxide layer containing the highest concentration of oxygen is in contact with the gas or oxygen to which the surface of the metal is exposed. In the article [2], F. Gesmundo and F. Viani analysed the parabolic growth of two-layer oxide scales on those metals which can form two oxides. They obtained the following nonlinear two-dimensional

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dynamical system as a model for the growth of such scales:

$$\begin{aligned} \frac{dq_1}{dt} &= m\frac{K_1}{2q_1} - \frac{m-1}{m}\frac{K_2}{2q_2}, \\ \frac{dq_2}{dt} &= -m\frac{K_1}{2q_1} + \frac{K_2}{2q_2}. \end{aligned} \tag{1.1}$$

Here $K_i > 0$ $(i = 1, 2)$ are rate constants, $m > 0$ is a parameter, and $q_i > 0$ is the weight of oxygen contained in oxide i per unit area.

"This system of first-order nonlinear differential equations cannot easily be solved by standard methods" [2, p. 224]. Nevertheless, in their paper, Gesmundo and Viani succeed in using a heuristic argument to show that there exist positive constants c_1, c_2 such that $q_i(t) = c_i\sqrt{t}$, $i = 1, 2$, is a solution of (1.1)—such a solution is said to be a *parabolic solution*. However, they do not delve further into the analysis of the solutions of (1.1).

In [1], H. C. Akuezur, M. W. Hirsch, and the author of this paper studied the following generalization of the system (1.1)

$$\frac{dq_i}{dt} = -\sum_{j=1}^{n} \frac{a_{ij}}{q_j}, \quad q_i(t) > 0, \qquad i = 1, \dots, n. \tag{1.2}$$

In that paper we establish that under mild algebraic conditions on the constant matrix $A = (a_{ij})$, in the long-run the trajectories of (1.2) are well-behaved in the sense that every solution $\mathbf{q} = (q_1, \dots, q_n) : [0, a] \to \mathbf{R}^2$, $0 < a < +\infty$, can be extended to a solution on $[0, +\infty)$, such that $\lim_{t\to+\infty} p_i(t) = +\infty$, $i = 1, \dots, n$. Moreover, the difference between any two solutions is bounded as a function of t. Finally, if A is irreducible and tridiagonal, then all solutions are eventually monotone increasing on $[0, +\infty)$.

In the present paper, we use the analysis of (1.2) to provide a complete qualitative analysis of the nonlinear system (1.1) in the case where m is in the interval $(1, +\infty)$: We show that for $m > 1$, the system (1.1) admits a unique parabolic solution $q_i(t) = c_i\sqrt{t}$, $c_i > 0$, $i = 1, 2$. Every solution extends uniquely to a solution on $[0, +\infty)$, such that the extended solution is eventually monotonically increasing. The parabolic solution attracts all other solutions. Finally, the trajectory of any solution coincides with a trajectory of the following system:

$$\begin{aligned} \frac{dq_1}{dt} &= -\frac{m-1}{m}\frac{K_2}{2}q_1 + m\frac{K_2}{2}q_2, \\ \frac{dq_2}{dt} &= \frac{K_2}{2}q_1 + m\frac{K_1}{2}q_2. \end{aligned} \tag{1.3}$$

The following notation will be used:

$$\begin{aligned} \mathbf{R}^2_+ &= \{(q_1, q_2) \in \mathbf{R}^2 \mid q_1, q_2 \geq 0\}, \\ \mathbf{R}^2_{++} &= \{(q_1, q_2) \in \mathbf{R}^2 \mid q_1, q_2 > 0\}. \end{aligned}$$

The following is a detailed description of our analysis of the nonlinear system (1.1):

Theorem I. *Assume that* $m > 1$ *in the dynamical system* (1.1). *Then the following statements hold.*

(i) *Every solution of* (1.1) *of the form*

$$\mathbf{p} = (p_1, p_2) : [0, a) \to \mathbf{R}^2_{++}, \qquad 0 < a < +\infty,$$

extends uniquely to a solution of (1.1) *of the form*

$$\mathbf{p} = (p_1, p_2) : [0, +\infty) \to \mathbf{R}^2_{++},$$

such that

$$\lim_{t \to +\infty} p_i(t) = +\infty, \qquad i = 1, 2.$$

Moreover, the extended solution $\mathbf{p}$ *is eventually monotone increasing on* $[0, +\infty)$.

(ii) *Let* $\mathbf{p}_0 \in \mathbf{R}^2_{++}$, *and let* $\mathbf{p} : [0, +\infty) \to \mathbf{R}^2_{++}$ *be the solution of* (1.1) *which starts at* $\mathbf{p}_0$. *Let* $\mathbf{r} = (r_1, r_2) : [0, +\infty) \to \mathbf{R}^2$ *be the solution of* (1.3) *which also starts at* $\mathbf{p}_0$. *Then* $\mathbf{p}$ *and* $\mathbf{q}$ *have the same trajectory in* $\mathbf{R}^2_{++}$; *and at any point on this common trajectory,* $\mathbf{p}$ *and* $\mathbf{q}$ *move in the same direction. Moreover, it is a saddle point of the system* (1.3), *and hence* $(0, 0)$ *is also a saddle point of the system* (1.1).

(iii) *There exists a unique parabolic solution of* (1.1) *of the form*

$$\mathbf{q} = (q_1, q_2) : [0, +\infty) \to \mathbf{R}^2_{++}, \quad q_i(t) = c_i\sqrt{t}, \qquad c_i > 0, \ i = 1, 2, \ t > 0.$$

Let λ *and* δ *be defined as follows*:

$$\lambda = \frac{1}{2}\sqrt{\left(mK_1 + \frac{m-1}{m}K_2\right)^2 + K_1K_2} - \frac{1}{4}\left(mK_1 + \frac{m-1}{m}K_2\right),$$
$$\delta = \frac{mK_1}{\left(2\lambda + \frac{m-1}{m}K_2\right)}.$$

Then c_1, c_2 *are given by*

$$c_1 = \sqrt{mK_1 - \left(\frac{m-1}{m}\right)\delta K_2}, \qquad c_2 = \frac{c_1}{\delta}.$$

(iv) *If* $\mathbf{p} : [0, +\infty) \to \mathbf{R}^2_{++}$ *is any solution of* (1.1), *then the trajectory of* $\mathbf{p}$ *is asymptotic to the linear trajectory of the parabolic solution of* (1.1). *This linear trajectory is given by*

$$r_1 = \delta r_2, \quad (r_1, r_2) \in \mathbf{R}^2_+.$$

The main result from [1] which we will use to prove Theorem I is the following lemma. (Recall that a real $n \times n$ matrix $A = (a_{ij})$ is *irreducible* if for each distinct pair of indices i, j with $1 \le i \ne j \le n$ there exists a finite sequence $i = k_0, \dots, k_m = j$ such that $a_{k_{r-1}, k_r} \ne 0$, $r = 1, \dots, m$.)

Lemma I. *Assume that the* $n \times n$ *matrix* $A = (a_{ij})$ *in* (1.2) *satisfies the conditions*:

(i) $\det A \ne 0$ *and* $a_{ij} \ge 0$, *for* $i \ne j$;
(ii) A *is irreducible*;
(iii) *for all* $\mathbf{x} = (x_1, \dots, x_n) \in \mathbf{R}^n_+$, *if* $x_i \sum_{j=1}^n a_{ij}x_j = 0$ *for* $i = 1, \dots, n$, *then* $\mathbf{x} = 0$;
(iv) *every real eigenvalue of* A *is negative.*

Then every solution of (1.2) *of the form*

$$\mathbf{q} = (q_1, \dots, q_n) : [0, a] \to \mathbf{R}^n_{++}, \qquad 0 < a < +\infty,$$

extends uniquely to a solution

$$\mathbf{q} : [0, +\infty) \to \mathbf{R}^n_{++},$$

and

$$\lim_{t \to +\infty} q_i(t) = +\infty, \qquad i = 1, \dots, n.$$

Moreover, if $\mathbf{r}(t) = (r_1(t), \dots, r_n(t)) : [0, +\infty) \to \mathbf{R}^n_{++}$ *is any other solution of* (1.2), *then*

$$\sup_{0 \le t < +\infty} \|\mathbf{q}(t) - \mathbf{r}(t)\| < +\infty,$$

and hence

$$\lim_{t \to +\infty} \frac{q_i(t)}{r_i(t)} = 1, \qquad i = 1, \dots, n.$$

Finally, if the matrix A *is tridiagonal, then every solution* $\mathbf{q}(t) : [0, +\infty) \to \mathbf{R}^n_{++}$ *of* (1.2) *is eventually monotone increasing on* $[0, +\infty)$.

2. Preliminaries

In this section we present the background material which is needed in the proof of Theorem I.

Lemma 2.1. *Let* $K_1, K_2 > 0$ *and* $m > 1$. *Define the* 2×2 *matrix* $A = (a_{ij})$ *by*

$$A = \begin{pmatrix} -\dfrac{mK_1}{2} & \dfrac{m-1}{m}\dfrac{K_2}{2} \\ \dfrac{mK_1}{2} & -\dfrac{K_2}{2} \end{pmatrix}.$$

Then A *satisfies conditions* (i)–(iv) *of Lemma* I.

Proof. Condition (i) of Lemma I is easily verified. Because $a_{12}, a_{21} \neq 0$, condition (ii) is immediate. Condition (iii) follows from the fact that $a_{12}, a_{21} \neq 0$ and $\det A \neq 0$. Finally, (iv) follows from direct calculation. □

Lemma 2.2. *Let* $\mathbf{p} = (p_1, p_2) : [0, +\infty) \to \mathbf{R}^2_{++}$ *be the solution of* (1.1) *which starts at the point* $\mathbf{p}_0 \in \mathbf{R}^2_{++}$, *and let* $\mathbf{r} = (r_1, r_2) : [0, +\infty) \to \mathbf{R}^2$ *be the solution of* (1.3) *which starts at the same point. Then the trajectory of* $\mathbf{p}$ *is contained in the trajectory of* $\mathbf{r}$. *Moreover, the solutions* $\mathbf{p}$ *and* $\mathbf{q}$ *move in the same direction at any point on the trajectory of* $\mathbf{p}$.

Proof. Let e, f, g, h be defined by

$$e = m\frac{K_1}{2}, \qquad f = -\frac{(m-1)}{m}\frac{K_2}{2},$$
$$g = -m\frac{K_1}{2}, \qquad h = \frac{K_2}{2}.$$

Because $\mathbf{p}$ is a solution of (1.1), we have

$$\frac{dp_2}{dp_1} = \frac{\dot{p}_2}{\dot{p}_1} = \left(\frac{g}{p_1} + \frac{h}{p_2}\right) \Big/ \left(\frac{e}{p_1} + \frac{f}{p_2}\right) = \frac{hp_1 + gp_2}{fp_1 + ep_2}.$$

But r_1, r_2 also satisfy this differential equation; therefore, because $\mathbf{r}$ and $\mathbf{p}$ start at the same point, we see that the trajectory of $\mathbf{p}$ is contained in the trajectory of $\mathbf{r}$.

The second part of the lemma follows from the fact that if $s, t \in [0, +\infty)$, with $\mathbf{r}(s) = \mathbf{p}(t)$, then $\dot{\mathbf{r}}(s) = \lambda \dot{\mathbf{p}}(t)$, where $\lambda = [p_1(t)p_2(t)]^{-1}$. □

Lemma 2.3. *Let $m > 1$ in the linear dynamical system* (1.3); *then the origin is a saddle point for the system. Let $\mathbf{p} : [0, +\infty) \to \mathbf{R}^2$ be the solution of* (1.3) *that starts in $\mathbf{R}^2_{++}$. Let λ be the positive root of the characteristic polynomial of the system* (1.3), *and let λ' be the negative root of this polynomial. Define α and β by*

$$\alpha = m\frac{K_1}{2}, \qquad \beta = \frac{-(m-1)}{m}\frac{K_2}{2}.$$

There exists constants $C_1 \neq 0$ and C_2 such that for $t \in [0, +\infty)$, $\mathbf{p}(t) = (p_1(t), p_2(t))$, where

$$p_1(t) = \alpha(C_1 e^{\lambda t} + C_2 e^{\lambda' t}),$$
$$p_2(t) = (\lambda - \beta)C_1 e^{\lambda t} + (\lambda' - \beta)C_2 e^{\lambda' t}.$$

Moreover, the trajectory of $\mathbf{p}$ is asymptotic to the line

$$(\lambda - \beta)q_1 = \alpha q_2, \qquad (q_1, q_2) \in \mathbf{R}^2_+.$$

Proof. Standard techniques from the theory of systems of linear differential equations suffice to establish this lemma. □

3. Proof of Theorem I

We are now ready to prove Theorem I. By Lemma 2.1, we may apply Lemma I to the dynamical system (1.1). Condition (i) of Theorem I is then a direct consequence of this application.

To prove (ii) of Theorem I, let $\mathbf{p} = (p_1, p_2) : [0, +\infty) \to \mathbf{R}^2_{++}$ be the solution of (1.1) which starts at the point $\mathbf{p}_0 \in \mathbf{R}^2_{++}$, and let $\mathbf{r} = (r_1, r_2) : [0, +\infty) \to \mathbf{R}^2$ be the solution of (1.3) which starts at the same point. By Lemma 2.2, the trajectory of $\mathbf{p}$ is contained in the trajectory of $\mathbf{r}$, and the solutions $\mathbf{p}$, $\mathbf{r}$ move in the same direction at any point on the trajectory of $\mathbf{p}$. By (i) of Theorem I, we have

$$\lim_{t \to +\infty} p_i(t) = +\infty, \qquad i = 1, 2.$$

Consequently, $\mathbf{p}$ and $\mathbf{r}$ have the same trajectory. Lemma 2.3 implies that the origin is a saddle point of (1.3), and hence it is also a saddle point of (1.1).

For the proof of (iii), let $\mathbf{p} = (p_1, p_2)$ and $\mathbf{q} = (q_1, q_2)$ be parabolic solutions of (1.1), where

$$p_i(t) = a_i\sqrt{t}, \quad q_i(t) = b_i\sqrt{t}, \qquad a_i > 0, b_i > 0, \ i = 1, 2, \ t > 0.$$

By Lemma I, we have $1 = \lim_{t\to+\infty} p_i(t)/q_i(t) = a_i/b_i$, $i = 1, 2$. Therefore, $\mathbf{p} = \mathbf{q}$. Now let c_1, c_2 have the values given in (iii) of Theorem I. Then a direct calculation shows that if $\mathbf{q} = (q_1, q_2) : (0, +\infty) \to \mathbf{R}^2_{++}$, where $q_i(t) = c_i\sqrt{t}$, $i = 1, 2$, then $\mathbf{q}$ is a solution of (1.1). This proves (iii).

Finally, to prove (iv), let $\mathbf{p}_0 \in \mathbf{R}^2_{++}$, and let $\mathbf{p} : [0, +\infty) \to \mathbf{R}^2_{++}$ be the solution of (1.1) which starts at $\mathbf{p}_0$. Let $\mathbf{r} : [0, +\infty) \to \mathbf{R}^2_+$ be the solution of (1.3) which starts at $\mathbf{p}_0$. By (ii), $\mathbf{p}$ and $\mathbf{r}$ have the same trajectory, and by Lemma 2.3, the trajectory of $\mathbf{r}$ is asymptotic to the line $(\lambda - \beta)u_1 = \alpha u_2$, $(u_1, u_2) \in \mathbf{R}_+^2$. Therefore, the trajectory of $\mathbf{p}$ is asymptotic to the same line. Because $\delta = \alpha/(\lambda - \beta)$, (iv) holds.

Remark. The values c_1, c_2 given in (iii) are obtained heuristically as follows. Assume that $q_i(t) = c_i\sqrt{t}$, $i = 1, 2$, is a parabolic solution of (1.1). Then (by Lemma 2.2 and Lemma 2.3) the point $(c_1\sqrt{t}, c_2\sqrt{t})$ is on the line $(\lambda - \beta)p_1 = \alpha p_2$, $(p_1, p_2) \in \mathbf{R}_+^2$. Hence, $c_1/c_2 = \alpha/(\lambda - \beta) = \delta$, i.e., $c_2 = c_1/\delta$. Because q_i, $i = 1, 2$, is a solution of (1.1), we have

$$c_1 = m\frac{K_1}{c_1} - \frac{m-1}{m}\frac{K_2}{c_2},$$
$$c_2 = -m\frac{K_1}{c_1} + \frac{K_2}{c_2}.$$

The first equation and $c_2 = c_1/\delta$ imply that $c_1^2 = mK_1 - [(m-1)/m]\delta$. $\square$

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