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ON A CLASS OF GROWTH CURVES WITH EXPONENTIALLY VARIABLE TRANSFER GENERATED BY REACTION NETWORKS. II

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Abstract: In [10] are proposed two classes of growth models, based on the specific Markov's reaction networks [1]–[2]. It is proven, that the new growth models are based on the insertion of "correcting amendments" of Bateman–Gompertz–type and Bateman–Gompertz–Makeham–type. In [9] is considered the following reaction network (for $n \geq 2$):

$$\begin{aligned}
S &\xrightarrow{k_1} P \xrightarrow{k_2} Q \\
S &\xrightarrow{k_3} P_1 \xrightarrow{k_4} Q_1 \\
&\cdots \\
S &\xrightarrow{k_{2n-1}} P_{n-1} \xrightarrow{k_{2n}} Q_{n-1} \\
P_{n-1} + X &\xrightarrow{k} nX + P_{n-1}.
\end{aligned}$$

The generation of limited growth curves with other exponentially variable transfers can be successfully expanded. It is of interest to observe the new growth model based on this reaction networks in the case where, for example, $k_1 = k_1(t), k_3 = k_3(t), \ldots, k_{2n-1} = k_{2n-1}(t)$, and $k_2 = 1, k_4 = 2, k_6 = 3, \ldots, k_{2n} = n$.

Some numerical examples, using *CAS MATHEMATICA* illustrating our results are given.

AMS Subject Classification: 41A46
Key Words: reaction networks, generalized growth model, exponentially variable transfer

1. Introduction and Preliminaries

Dynamical models consisting of a systems of "reaction" differential equations are commonly used in chemistry, there the differential equations are called *reaction equations* [3]–[8].

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In [9] Kyurkchiev considered the following reaction network (for $n \geq 2$):

$$\begin{aligned} S &\xrightarrow{k_1} P \xrightarrow{k_2} Q \\ S &\xrightarrow{k_3} P_1 \xrightarrow{k_4} Q_1 \\ &\cdots \\ S &\xrightarrow{k_{2n-1}} P_{n-1} \xrightarrow{k_{2n}} Q_{n-1} \\ P_{n-1} + X &\xrightarrow{k} nX + P_{n-1}. \end{aligned} \tag{1}$$

The proposed reaction networks (1) involve additional species interpreted as environmental resource.

Hence, the general new model can be written for the growth function in the form:

$$\begin{cases} x'(t) = kxP_{n-1}(t) \\ x(0) = x_0 \end{cases} \tag{2}$$

where for $k_i \neq k_j$; $i, j = 1, 2, \ldots, 2n$

$$P_{n-1}(t) = \frac{k_{2n-1}s_0}{k_{2n} - \sum_{i=1}^{n} k_{2i-1}} \left(e^{-\sum_{i=1}^{n} k_{2i-1}t} - e^{-k_{2n}t} \right) + p_{n-1,0}e^{-k_{2n}t}. \tag{3}$$

It is of interest to observe the new growth model based on this reaction networks in the case where, for example, $k_1 = k_1(t), k_3 = k_3(t), \ldots, k_{2n-1} = k_{2n-1}(t)$.

In this article we will get a generalized class of growth curves with exponentially variable transfer based on this reaction scheme.

2. Main Results

Considered the following reaction network:

$$\begin{aligned} S &\xrightarrow{k_1(t)} P \xrightarrow{k_2} Q \\ S &\xrightarrow{k_3(t)} P_1 \xrightarrow{k_4} Q_1 \\ &\cdots \\ S &\xrightarrow{k_{2n-1}(t)} P_{n-1} \xrightarrow{k_{2n}} Q_{n-1} \\ P_{n-1} + X &\xrightarrow{k} nX + P_{n-1}. \end{aligned} \tag{4}$$

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2.1. The case $n = 2$, $k_1(t) = k_3(t) = e^t$ and $k_2 = 1$, $k_4 = 2$

Consequently the following differential equations can be formulated

$$\begin{cases} \dfrac{ds}{dt} &= -(k_1(t) + k_3(t))s = -2e^t s \\ \dfrac{dp}{dt} &= k_1(t)s - k_2 p = e^t s - p \\ \dfrac{dp_1}{dt} &= k_3(t)s - k_4 p_1 = e^t s - 2p_1 \\ \dfrac{dx}{dt} &= kxp_1 \end{cases} \tag{5}$$

with $s(0) = s_0$; $p(0) = p_0$; $p_1(0) = p_{1,0}$; $x(0) = x_0$.

For the solution of the first equation in (5) we obtain

$$s(t) = Ce^{-2e^t}$$

and from $s(0) = s_0$ we get $C = s_0 e^2$ and

$$s(t) = s_0 e^{-2e^t+2}. \tag{6}$$

From the second equation of the system (5) we have

$$\frac{dp}{dt} + p(t) = e^t s = s_0 e^{t-2e^t+2}$$

The solution to this equation is

$$\begin{aligned} p(t) &= s_0 e^{-t} \int_0^t e^{t-2e^t+2} e^t .dt + Re^{-t} \\ &= s_0 e^{-t} \int_0^t e^{2t-2e^t+2} e^t .dt + Re^{-t} \\ &= s_0 e^{-t} \left(-\tfrac{1}{4} e^{2-2e^t}(1+2e^t) \right) |_0^t + Re^{-t} \\ &= s_0 e^{-t} \left(-\tfrac{1}{4} e^{2-2e^t}(1+2e^t) + \tfrac{3}{4} \right) + Re^{-t} \end{aligned}$$

From $p(0) = p_0$ we get $R = p_0$.

So, finally, for the solution $p(t)$ we get

$$p(t) = s_0 e^{-t} \left(-\frac{1}{4} e^{2-2e^t}(1+2e^t) + \frac{3}{4} \right) + p_0 e^{-t}. \tag{7}$$

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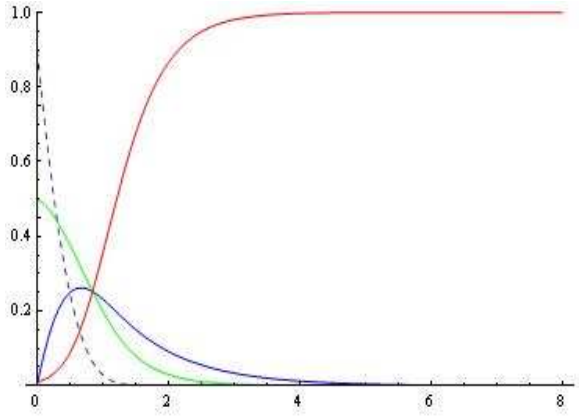

Figure 1: The functions $x(t)$–(red); $p(t)$–(blue); $p_1(t)$–(green); $s(t)$–(dashed) for $k = 9.695;\ s_0 = 0.9;\ p_0 = 0.001;\ p_{1,0} = 0.5;\ x_0 = 0.01$

For the solution $p_1(t)$ we have

$$\begin{aligned} p_1(t) &= s_0 e^{2-t} \int_0^t e^t e^{-2e^t+2} e^{2t}.dt + R_1 e^{-2t} \\ &= s_0 e^{-2t} \int_0^t e^{3t-2e^t+2}.dt + R_1 e^{-2t} \\ &= s_0 e^{-2t} \left(-\tfrac{1}{4} e^{2-2e^t}(1 + 2e^t + 2e^{2t}) \right) |_0^t + R_1 e^{-2t} \\ &= s_0 e^{-2t} \left(-\tfrac{1}{4} e^{2-2e^t}(1 + 2e^t + 2e^{2t}) + \tfrac{5}{4} \right) + R_1 e^{-2t} \end{aligned}$$

From $p_1(0) = p_{1,0}$ we get $R_1 = p_{1,0}$ and

$$p_1(t) = s_0 e^{-2t} \left(-\frac{1}{4} e^{2-2e^t}(1 + 2e^t + 2e^{2t}) + \frac{5}{4} \right) + p_{1,0} e^{-2t}. \tag{8}$$

More importantly, the solution $x(t)$ of the last equation of the differential system

$$x(t) = x_0 e^{-\frac{k}{8}(-2s_0-4p_{1,0})+\frac{k}{8}e^{-2e^t-2t}\left(e^2 s_0+2e^{2+t}s_0-e^{2e^t}(4p_{1,0}+5s_0)\right)} \tag{9}$$

generates a new growth model that we have not encountered described in the literature.

We illustrate our new model for various parameters $k, s_0, p_0, p_{1,0}$ and x_0 (see, Fig. 1–Fig. 2).

Remark. It is important to study the characteristic - "super saturation" of the model to the horizontal asymptote.

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Manipulate[Plot[{s0 * Exp[-2 * Exp[t] + 2],
   s0 * Exp[-t] * (-(1/4) * Exp[2 - 2 * Exp[t]] * (1 + 2 * Exp[t]) + 3/4) + p0 * Exp[-t],
   s0 * Exp[-2 * t] * (-(1/4) * Exp[2 - 2 * Exp[t]] * (1 + 2 * Exp[t] + 2 * Exp[2 * t]) + 5/4) + p1 * Exp[-2 * t],
   e^(-(k (3 e^2 s0 - e^2 (4 p1 + 5 s0)))/(8 e^2)) + 1/8 e^(-2 e^t - 2 t) k (e^2 s0 + 2 e^(2 + t) s0 - e^(2 e^t) (4 p1 + 5 s0)) x0}, {t, 0, 20}],
 {{k, 5.522, "k"}, 0, 2, Appearance → "Open"}, {{s0, 0.9, "s0"}, 0, 2, Appearance → "Open"},
 {{p0, 0.1, "p0"}, 0, 2, Appearance → "Open"}, {{p1, 0.1, "p1"}, 0, 2, Appearance → "Open"},
 {{x0, 0.004, "x0"}, 0, 2, Appearance → "Open"}]
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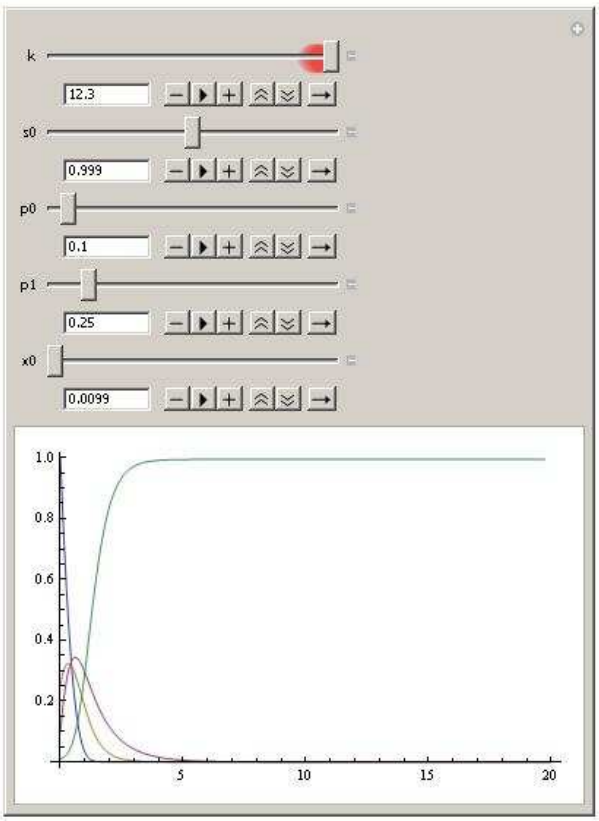

Figure 2: An example of the usage of dynamical solution of the system and their graphical representation. The plots are prepared using *CAS Mathematica*

In this connection, we note only that, for the new model (9) is fulfilled:

$$\lim_{t\to\infty} x(t) = x_0 e^{\frac{k}{4}(s_0+2p_{1,0})},$$

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2.2. The case $n = 3$, $k_1(t) = k_3(t) = k_5(t) = e^t$ and $k_2 = 1$, $k_4 = 2$, $k_6 = 3$

The model can be written for the growth function in the form:

$$\begin{cases} x'(t) = kxP_2(t) \\ x(0) = x_0 \end{cases} \tag{10}$$

where

$$P_2(t) = s_0 e^{-3t}\left(-\frac{1}{27}e^{3-3e^t}(2 + 6e^t + 9e^{2t} + 9e^{3t}) + \frac{26}{27}\right) + p_{2,0}e^{-3t}. \tag{11}$$

2.3. The case $n = 4$, $k_1(t) = k_3(t) = k_5(t) = k_7(t) = e^t$ and $k_2 = 1$, $k_4 = 2$, $k_6 = 3$, $k_8 = 4$

The model can be written for the growth function in the form:

$$\begin{cases} x'(t) = kxP_3(t) \\ x(0) = x_0 \end{cases} \tag{12}$$

where

$$\begin{aligned} &P_3(t) = \\ &s_0 e^{-4t}\left(-\tfrac{1}{128}e^{4-4e^t}(3 + 12e^t + 24e^{2t} + 32e^{3t} + 32e^{4t}) + \right. \\ &\left.\tfrac{103}{128}\right) + p_{3,0}e^{-4t}. \end{aligned} \tag{13}$$

Remarks.

1. Following the idea of Sections 2.1-2.3, the reader can explicitly formulate the solution of the proposed growth model for an arbitrary value of n.

2. Evidently, if $k_i(t) = e^{a_i t}$; $i = 1, 3, \ldots, 2n-1$, then the solutions $p_{2n-1}(t)$ are preserved as a functions of the traditional exponential integral $E_i(.)$.

3. We will explicitly note that the system of differential equations corresponding to the considered reaction network is meaningful in the field of chemistry.

For other results, see [9]–[27].

For example the appropriate lest–square fitting of the specific "real wealth data" by the model (9) yields for $k = 227.123$; $s_0 = 0.999$, $p_{1,0} = 0.01$, $x_0 = 0.000001$ (see, Fig. 3).

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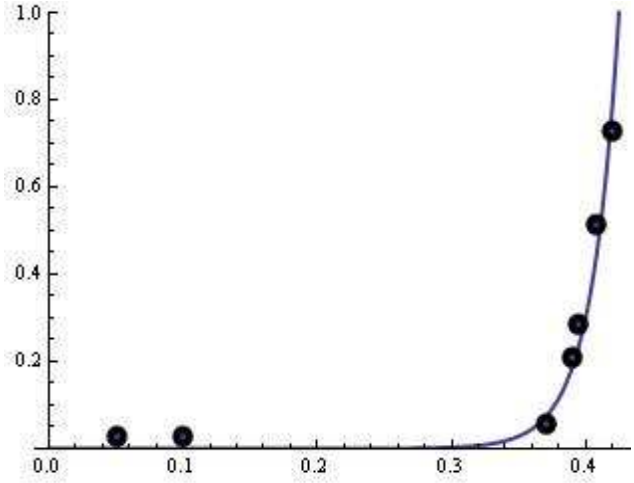

Figure 3: The fitted model (9)

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