STUDIA UNIVERSITATIS BABEŞ-BOLYAI, CHEMIA, L, 1, 2005

AN ALTERNATIVE APPLICATION OF FLOW GRAPH THEORY IN CHEMISTRY, PHARMACOKINETICS AND CHEMICAL ENGINEERING PROCESSES

MARIUS SOCOL and IOAN BÂLDEA

Department of Physical Chemistry, Faculty of Chemistry and Chemical Engineering of "Babeş-Bolyai" University, 11 Arany Janos, 400028, Cluj-Napoca, Romania (e-mail:ibaldea@chem.ubbcluj.ro)

ABSTRACT. An alternative method for solving homogenous and non-homogenous differential equation systems used in physical chemistry has been developed. It was applied to some dynamic processes as radical polymerization, pharmacokinetics and the flow of fluids through a tank and tank series. For this, the flow graphs principles were used. The classical method for solving these systems with flow graphs requires the Laplace transforms before depicting a flow graph and the reverse transformation after using the Mason rules for calculus. The herein presented method is simpler and more direct, eliminating the Laplace transforms in describing these processes.

Keywords: flow graph, differential equation, and dynamic processes.

INTRODUCTION

A flow graph consists of a network in which nodes (or vertices) are connected by directed edges (or branches). Each node (vertex) represents a system variable, and each edge connecting two vertices acts as a signal multiplier. An arrow placed on the edge indicates the direction of the signal flow and the multiplication factor is indicated along the edge[1,2]. This multiplication factor is named transmittance. It can be obtained from the coefficients of the equations. The signal flow graph depicts the flow of signals from one point of the system to another and gives the relationships between the signals. It represents the value of the determinant of the system[3].

Some basic principles of flow graphs were presented previously[4-6].

A flow graph example is presented in Figure 1.

Properties of flow graphs

A few important proprieties of flow graphs are as follows: A branch indicates the functional dependence of one signal on another.

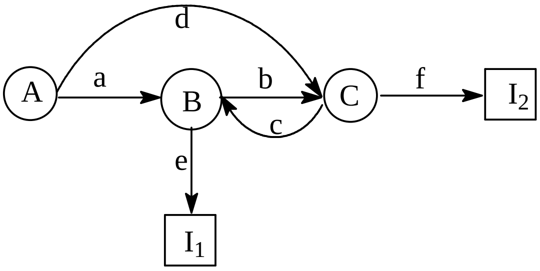


Fig. 1. An example of a flow graph." A" is an input node (source); "I_1", "I_2" are output nodes (sinks); a, b, c, d, e and f are weights of the edges; "B"," C" are the internal nodes.

A signal passes trough only in the direction specified by the arrow of the branch. A node adds the signals of all incoming branches and transmits their sum to all outgoing branches. An internal node, which has both incoming and outgoing branches, may be viewed as an output node by ignoring its outgoing branches. Note, however, that a mixed node never can be a source (input node) in this approach.

A flow graph is a diagram that represents a set of simultaneous linear algebraic situations (linear differential equations). It is used to represent an evolution of a physical system and to obtain the relationships between the system variables. By using the Cramer's method[7] with determinants one could solve the system.

For a given system a flow graph is not unique. More than one flow graphs can be drawn for a given system by writing the system equations or the corresponding determinants in a different way[3,8,9].

Homogenous Linear Differential Equations Systems

Suppose we chose to solve the following system[10-12]:

$$\begin{cases} -\dfrac{dx}{dt} = \quad a\cdot x - b\cdot y \\ -\dfrac{dy}{dt} = -c\cdot x + d\cdot y \end{cases} \quad \text{with initial conditions } x(0) = X_0 \text{ and } y(0) = 0; \qquad (1)$$

The general solutions of the system are of the form[11,12]:

$$x = A_1 e^{-\gamma_1 t} + A_2 e^{-\gamma_2 t} \quad \text{and} \quad y = B_1 e^{-\gamma_1 t} + B_2 e^{-\gamma_2 t} \qquad (2)$$

The alternative flow graph theory:

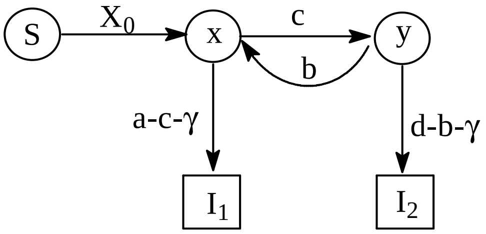


Fig. 2. The global flow graph

In this theory, the flow graphs are based on determinants[3]. The global flow graph is derived directly from the main determinant (the secular determinant), (3), by adding the initial conditions (the column of initial conditions are playing the role of source of unknowns x and y), as it was shown on the flow graphs algebra. For the classical flow graph method, the derivatives are also part of the mixed nodes and the formulas of calculus are different, as it can be seen in the numerical examples.

The consumption determinants (Δ_i), which are not unique now because they are function of γ_j, are derived from the main determinant (secular determinant), Δ:

$$\begin{array}{c|cc|} & x & y \\ x & a-\gamma & -b \\ y & -c & d-\gamma \end{array} = 0 \tag{3}$$

$$\Delta = [\gamma^2 - \gamma(a+d) + ad - bc] = (\gamma - \gamma_1)(\gamma - \gamma_2) = 0 \tag{4}$$

It means that the consumption determinants, which represent a Vandermonde determinant[10], are:

$$\Delta_i = \prod_{\substack{j=1 \\ i \neq j}}^{n} (\gamma_j - \gamma_i) \neq 0 \tag{5}$$

In this case, n = 2. The corresponding flow graph (consumption flow graph) for the main determinant is:

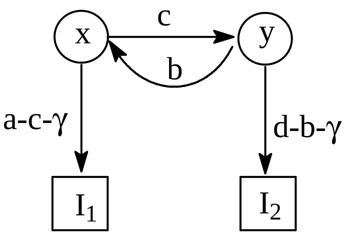


Fig. 3. The consumption flow graph

The formation determinants are obtained by replacing the columns of the secular determinant (3) by the column of free coefficients:

$$\Delta_A = \begin{array}{c|cc|} & S & y \\ x & X_0 & -b \\ y & 0 & d-\gamma \end{array} = X_0\,(d-\gamma) \tag{6}$$

The formation flow graph for *x* is depicted in Figure 4:

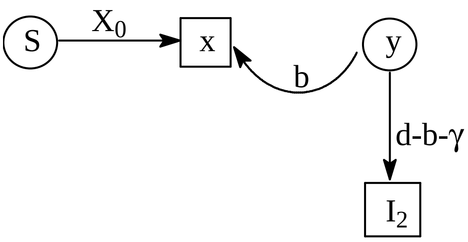


Fig. 4. The formation flow graph for x

Its gain, equivalent with the value of its determinant, is:

$$\Delta_A = X_0 b + X_0(d - b - \gamma) = X_0(d - \gamma) \tag{7}$$

The formation flow graph for *y* is depicted in Figure 5:

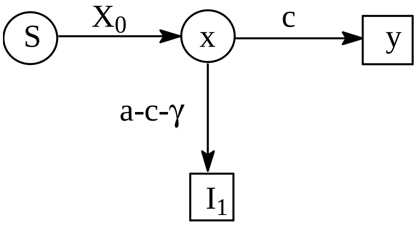


Fig. 5. The formation flow graph for y

The value of its determinant is presented below:

$$\Delta_B = X_0\, c \tag{8}$$

The pre-exponential coefficients can be calculated as:

$$\begin{gathered} A_1 = \frac{\Delta_{A_1}}{\Delta_1} = \frac{X_0(d-\gamma_1)}{(\gamma_2-\gamma_1)}; \quad A_2 = \frac{\Delta_{A_2}}{\Delta_2} = \frac{X_0(d-\gamma_2)}{(\gamma_1-\gamma_2)}; \\ B_1 = \frac{\Delta_{B_1}}{\Delta_1} = \frac{X_0\, c}{(\gamma_2-\gamma_1)}; \quad B_2 = \frac{\Delta_{B_2}}{\Delta_2} = \frac{X_0\, c}{(\gamma_1-\gamma_2)}; \end{gathered} \tag{9}$$

Non-Homogenous Differential Equations Systems

A more complicated system in which a time dependent function, f(t), acts like an input, is presented bellow[13].

The following system has to be solved:

$$\begin{cases} -\dfrac{dx}{dt} = \quad a \cdot x - b \cdot y + f(t) \\ -\dfrac{dy}{dt} = -c \cdot x + d \cdot y \end{cases} \tag{10}$$

with initial conditions

$x(0) = 0$ and $y(0) = 0$; (11)

The classical method of flow graphs[3,8,9] consists the following sequence of steps: to apply the Laplace transforms[14] in other variable (s), than Mason's rules and finally the finding of polynomial coefficients[13] and the last step reverse transforms in time variable. Our alternative method has the advantage of being simpler because it does not need the Laplace transforms. It needs only the integral of convolution[13]. The global flow graph for the system (10) is presented bellow:

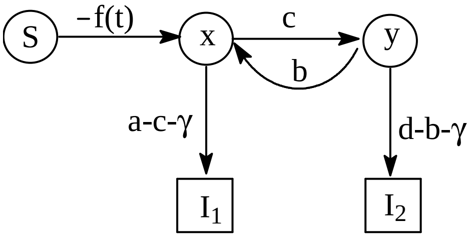


Fig. 6. The global flow graph

The role of the source is played by the input function f(t). The coefficients have the same form, but instead of X_0 we have the input function f(t).

$$A_1=\frac{\Delta_{A_1}}{\Delta_1}=\frac{-f(t)(d-\gamma_1)}{(\gamma_2-\gamma_1)};\quad A_2=\frac{\Delta_{A_2}}{\Delta_2}=\frac{-f(t)(d-\gamma_2)}{(\gamma_1-\gamma_2)};$$
$$B_1=\frac{\Delta_{B_1}}{\Delta_1}=\frac{-f(t)\,c}{(\gamma_2-\gamma_1)};\quad B_2=\frac{\Delta_{B_2}}{\Delta_2}=\frac{-f(t)\,c}{(\gamma_1-\gamma_2)};\tag{12}$$

By applying the integral of convolution, which is the link between input and output[13] it results:

$$x=\frac{-(d-\gamma_1)}{\gamma_2-\gamma_1}\int_0^t f(t-\tau)e^{-\gamma_1\tau}d\tau+\frac{-(d-\gamma_2)}{\gamma_1-\gamma_2}\int_0^t f(t-\tau)e^{-\gamma_2\tau}d\tau\tag{13}$$

and $$y=\frac{-c}{\gamma_2-\gamma_1}\int_0^t f(t-\tau)e^{-\gamma_1\tau}d\tau+\frac{-c}{\gamma_1-\gamma_2}\int_0^t f(t-\tau)e^{-\gamma_2\tau}d\tau\tag{14}$$

where the above integrals are applied to the convolution product[3,8,9,13].

Examples:

We will apply the above theory to several examples that are of interest in Chemistry of polymers, pharmaco-kinetics and Chemical Engineering.

a). ***The radical polymerisation*** is treated by using the quasi steady-state approximation method (QSSA) and the long chain approximation[15] in a batch reactor. To solve this problem it is necessary to implement a complex non-homogenous differential equation system as given bellow:

$$
\begin{array}{l}
I_2 \xrightarrow{k_d} 2I\cdot \\
I\cdot + M \xrightarrow{k_i} R_1\cdot \\
R_1\cdot + M \xrightarrow{k_p} R_2\cdot \\
R_2\cdot + M \xrightarrow{k_p} R_3\cdot \\
R_4\cdot + M \xrightarrow{k_p} R_5\cdot \\
R_5\cdot + M \xrightarrow{k_p} R_6\cdot \\
\cdots\cdots\cdots\cdots\cdots\cdots
\end{array}
\qquad
\begin{cases}
\dfrac{dI_2}{dt} = -k_d[I_2] \\
\dfrac{dI\cdot}{dt} = k_d[I_2] - k_i[I\cdot][M] \\
\dfrac{dR_1\cdot}{dt} = k_i[I\cdot][M] - k_p[R_1\cdot][M] \\
\dfrac{dR_2\cdot}{dt} = k_p[R_1\cdot][M] - k_p[R_2\cdot][M] \\
\dfrac{dR_3\cdot}{dt} = k_p[R_2\cdot][M] - k_p[R_3\cdot][M] \\
\dfrac{dR_4\cdot}{dt} = k_p[R_3\cdot][M] - k_p[R_4\cdot][M] \\
\dfrac{dR_5\cdot}{dt} = k_p[R_4\cdot][M] - k_p[R_5\cdot][M]
\end{cases}
\qquad (15)
$$

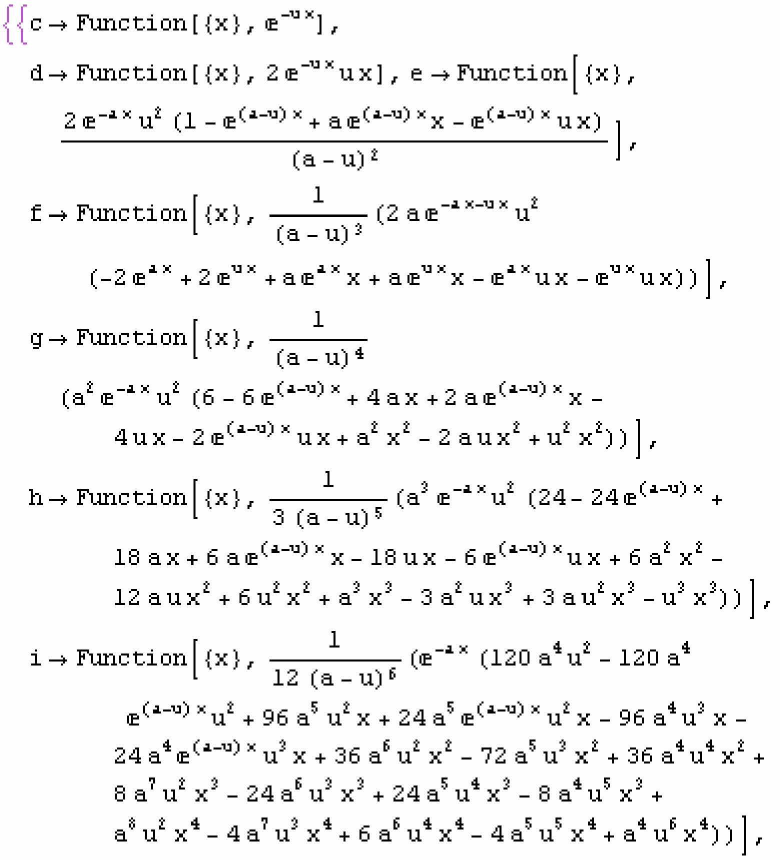
Here I_2 stands for the initiator, M for the monomer and various R_i for the increasing free radicals involved. This system has been solved using Mathematica 5.1[16];

The notations are: $[I_2]_0$ = 1mmol/L; $k_d = k_i = u = 10^{-5}$ s^{-1}; $k_p[M]_0 = a$. The monomer concentration could be considered in large excess as compared to the concentration of the increasing free radicals. Therefore, each step can be considered as obeying first-order kinetics. On the other hand, the propagation rate constants can be considered equals, at least at smaller polymerisation degree.

The script file is presented as follows:

```
DSolve[{c'[x]=-u*c[x],d'[x]=2*u*c[x]-u*d[x],e'[x]=u*d[x]-a*e[x],f'[x]=a*e[x]-

a*f[x],g'[x]=a*f[x]-a*g[x],h'[x]=a*g[x]-a*h[x],i'[x]=a*h[x]-a*i[x],j'[x]=a*i[x]-

a*j[x],k'[x]=a*j[x]-a*k[x],l'[x]=a*k[x]

a*l[x],c[0]=1,d[0]=0,e[0]=0,f[0]=0,g[0]=0,h[0]=0,i[0]=0,,j[0]=0,k[0]=0,l[0]=0},{c,d,e,f,g,

h,i,j,k,l},x]
```

The solutions are:



$$
\begin{aligned}
&\{\{c \to \text{Function}[\{x\}, e^{-u x}],\\
&d \to \text{Function}[\{x\}, 2 e^{-u x} u x],\ e \to \text{Function}\Big[\{x\},\\
&\quad \frac{2 e^{-a x} u^2 (1 - e^{(a-u) x} + a e^{(a-u) x} x - e^{(a-u) x} u x)}{(a-u)^2}\Big],\\
&f \to \text{Function}\Big[\{x\}, \frac{1}{(a-u)^3} (2 a e^{-a x - u x} u^2\\
&\quad (-2 e^{a x} + 2 e^{u x} + a e^{a x} x + a e^{u x} x - e^{a x} u x - e^{u x} u x))\Big],\\
&g \to \text{Function}\Big[\{x\}, \frac{1}{(a-u)^4}\\
&\quad (a^2 e^{-a x} u^2 (6 - 6 e^{(a-u) x} + 4 a x + 2 a e^{(a-u) x} x -\\
&\qquad 4 u x - 2 e^{(a-u) x} u x + a^2 x^2 - 2 a u x^2 + u^2 x^2))\Big],\\
&h \to \text{Function}\Big[\{x\}, \frac{1}{3 (a-u)^5} (a^3 e^{-a x} u^2 (24 - 24 e^{(a-u) x} +\\
&\qquad 18 a x + 6 a e^{(a-u) x} x - 18 u x - 6 e^{(a-u) x} u x + 6 a^2 x^2 -\\
&\qquad 12 a u x^2 + 6 u^2 x^2 + a^3 x^3 - 3 a^2 u x^3 + 3 a u^2 x^3 - u^3 x^3))\Big],\\
&i \to \text{Function}\Big[\{x\}, \frac{1}{12 (a-u)^6} (e^{-a x} (120 a^4 u^2 - 120 a^4\\
&\qquad e^{(a-u) x} u^2 + 96 a^5 u^2 x + 24 a^5 e^{(a-u) x} u^2 x - 96 a^4 u^3 x -\\
&\qquad 24 a^4 e^{(a-u) x} u^3 x + 36 a^6 u^2 x^2 - 72 a^5 u^3 x^2 + 36 a^4 u^4 x^2 +\\
&\qquad 8 a^7 u^2 x^3 - 24 a^6 u^3 x^3 + 24 a^5 u^4 x^3 - 8 a^4 u^5 x^3 +\\
&\qquad a^8 u^2 x^4 - 4 a^7 u^3 x^4 + 6 a^6 u^4 x^4 - 4 a^5 u^5 x^4 + a^4 u^6 x^4))\Big],
\end{aligned}
\tag{16}
$$

By taking into account that the following relation between rate constants holds $k_i << k_p$, then only the terms which contain exponential $e^{(a-u)x}$ should be to be considered. Therefore:

$$[R_i \cdot] = \frac{2 \cdot u^2 \cdot e^{-ut} \cdot t \cdot [I_2]_0}{a} = \frac{2 \cdot k_i^2 \cdot e^{-k_i t} \cdot t \cdot [I_2]_0}{k_p \cdot [M]} \tag{17}$$

for i = 1 to DP (degree of polymerisation).

This result is compared with that obtained by QSSA[15]:

$$R_i^{\cdot} = \frac{2 \cdot k_i \cdot [I_2]_0}{k_p \cdot [M]} \tag{18}$$

which calculates the value of all radical concentrations for initial times and is the same in any moment of time, as long as the monomer exists in the system. This system (15) is valid for the youngest radicals (initial times) when still the interruption steps are negligible. When the amount of radicals grows and the quantities of monomers decreases, the probability that interruptions occur is significant. Then the concentration of radicals obeys the QSSA rule[15].

b) ***The pharmacokinetics application.*** Another example that is quite complex and cannot be solved literarily even by the Mathematica 5.1 program[16] is given bellow:

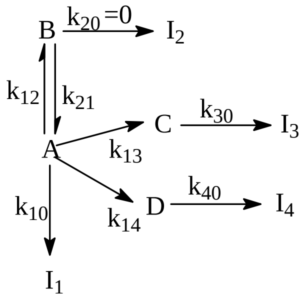


Fig. 7. The mechanism set of reactions

$$\begin{cases} -\dfrac{dx}{dt} = (k_{10} + k_{12} + k_{13} + k_{14}) \cdot x - k_{21} \cdot y - k_0 \\ -\dfrac{dy}{dt} = -k_{12} \cdot x + k_{21} \cdot y \\ -\dfrac{dv}{dt} = -k_{13} \cdot x + k_{30} \cdot v \\ -\dfrac{dz}{dt} = -k_{14} \cdot x + k_{40} \cdot z \end{cases} \tag{19}$$

This example describes the time-evolution of a medicine in a human organism. After a perfusion, the drug enters the blood or other tissues and is eliminated either by kidneys or is metabolized[17]. The *k* values represent some first-order rate constants describing the various rate of transformation. The initial conditions are: x(0) = y(0) = z(0) = v(0) = 0.

The global flow graph based on the secular determinant and the column of input function f(t) = k_0, which is a constant, has the following form:

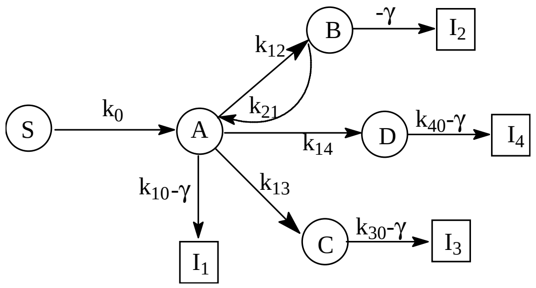


Fig. 8. The global flow graph

We symbolize x = A, y = B, v = C, z = D), representing the concentrations (quantities) of drug and its metabolites in blood or other tissues.

The consumption flow graph, which is based on secular determinant, is presented bellow:

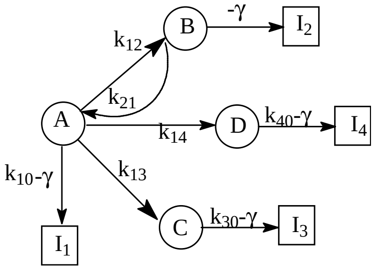


Fig. 9. The consumption flow graph

Its gain is equal with that of the secular determinant:

$$\Delta=(k_{30}-\gamma)(k_{40}-\gamma)[(-\gamma)(k_{12}+k_{13}+k_{14}+k_{10}-\gamma)+k_{21}(k_{13}+k_{14}+k_{10}-\gamma)]=0$$
$$\Delta=[\gamma^2-\gamma(k_{12}+k_{13}+k_{14}+k_{10}+k_{21})+k_{21}(k_{13}+k_{14}+k_{10})](k_{30}-\gamma)(k_{40}-\gamma)=0 \tag{20}$$

From the above equation the exponential factors, γ_1, γ_2 (the solutions of the square equation), $\gamma_3 = k_{30}$ and $\gamma_4 = k_{40}$ can be found.

The formation graph for *A* is:

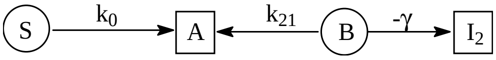


Fig. 10. The formation flow graph for A

$$\Delta_{A_i}=k_0(k_{21}-\gamma_i),\quad i=\overline{1,2} \tag{21}$$

$$A=\frac{k_0(k_{21}-\gamma_1)\int_0^t e^{-\gamma_1\tau}d\tau}{(\gamma_2-\gamma_1)}+\frac{k_0(k_{21}-\gamma_2)\int_0^t e^{-\gamma_2\tau}d\tau}{(\gamma_1-\gamma_2)}$$
$$A=\frac{k_0(k_{21}-\gamma_1)(e^{-\gamma_1 t}-1)}{(\gamma_2-\gamma_1)(-\gamma_1)}+\frac{k_0(k_{21}-\gamma_2)(e^{-\gamma_2 t}-1)}{(\gamma_1-\gamma_2)(-\gamma_2)} \tag{22}$$

The formation graph for *B* is:

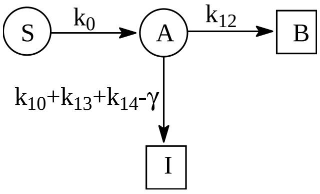


Fig. 11. The formation flow graph for B

Where *I* is the sum of all the outputs from node A.

$$\Delta_{B_i} = k_0 \cdot k_{12} \quad i = \overline{1,2} \tag{23}$$

$$B = \frac{k_0 k_{12}(e^{-\gamma_1 t} - 1)}{(\gamma_2 - \gamma_1)(-\gamma_1)} + \frac{k_0 k_{12}(e^{-\gamma_2 t} - 1)}{(\gamma_1 - \gamma_2)(-\gamma_2)} \tag{24}$$

The formation graph for *C* is:

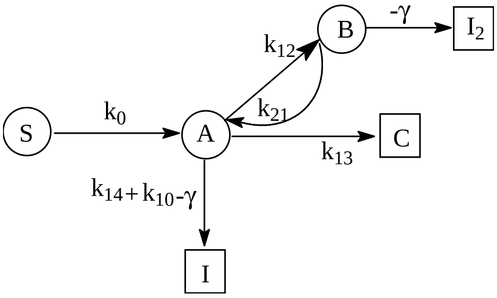


Fig. 12. The formation flow graph for C

$$\Delta_{C_i} = k_0 \cdot k_{13} \cdot (k_{21} - \gamma_i) \quad i = \overline{1,3} \tag{25}$$

$$C = \frac{k_0 k_{13}(k_{21} - \gamma_1)(e^{-\gamma_1 t} - 1)}{(\gamma_2 - \gamma_1)(\gamma_3 - \gamma_1)(-\gamma_1)} + \frac{k_0 k_{13}(k_{21} - \gamma_2)(e^{-\gamma_2 t} - 1)}{(\gamma_1 - \gamma_2)(\gamma_3 - \gamma_2)(-\gamma_2)} + \frac{k_0 k_{13}(k_{21} - \gamma_3)(e^{-\gamma_3 t} - 1)}{(\gamma_1 - \gamma_3)(\gamma_2 - \gamma_3)(-\gamma_3)} \tag{26}$$

The formation graph for *D* is:

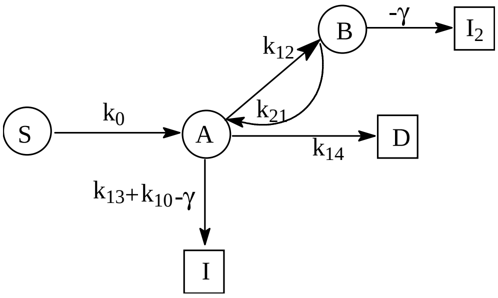


Fig. 13. The formation flow graph for D

$$\Delta_{D_i} = k_0 \cdot k_{14} \cdot (k_{21} - \gamma_i) \quad i = 1,2,4; \tag{27}$$

$$D = \frac{k_0 k_{14}(k_{21} - \gamma_1)(e^{-\gamma_1 t} - 1)}{(\gamma_2 - \gamma_1)(\gamma_4 - \gamma_1)(-\gamma_1)} + \frac{k_0 k_{14}(k_{21} - \gamma_2)(e^{-\gamma_2 t} - 1)}{(\gamma_1 - \gamma_2)(\gamma_4 - \gamma_2)(-\gamma_2)} + \frac{k_0 k_{14}(k_{21} - \gamma_4)(e^{-\gamma_4 t} - 1)}{(\gamma_1 - \gamma_4)(\gamma_2 - \gamma_4)(-\gamma_4)} \tag{28}$$

c). ***The flow through of a vessel***. In order to exemplify how the differential relation in describing dynamic system behavior is used, we have chosen a system built by a tank that is fed with a liquid that is also evacuated continuously[13]. Input and output mass flows are $F_{mi} = u(t)$ and F_{me}, respectively. The initial level of the liquid is $y(0) = H_0$, hydraulic resistance is noted by R and the section area by A, as it can be observed in figure 7. If the value of H is symbolized by y, its behavior as a function of time is calculated by a differential equation as in equation (29)[13]:

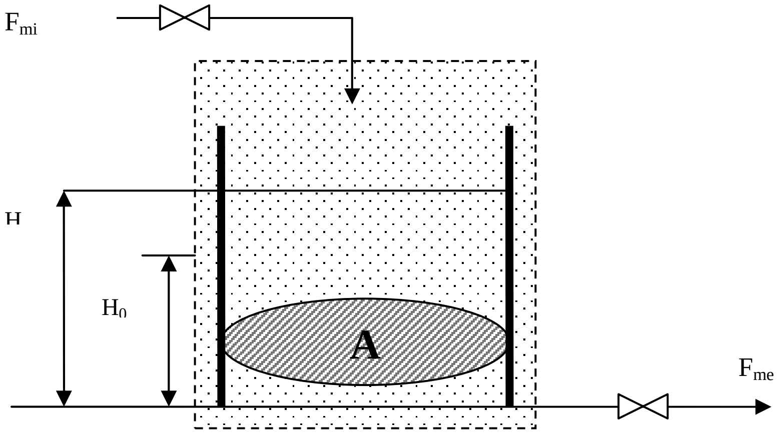


Fig. 14. Single liquid tank

$$-\frac{dy}{dt} = \frac{1}{A \cdot R} \cdot y - \frac{1}{A} \cdot u(t) \tag{29}$$

The secular determinant can be written as in equation (30):

$$\Delta = \left| \frac{1}{A \cdot R} - \gamma \right| = 0 \quad \gamma = \frac{1}{A \cdot R} \tag{30}$$

The formation flow graph for this simple system is[4-6]:

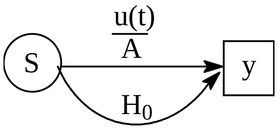


Fig. 15. The formation flow graph for *y*

It results that:

$$y = H(t) = H_0 \cdot e^{-t/A \cdot R} + \frac{1}{A} \cdot \int_0^t u(t-\tau) \cdot e^{-\tau/A \cdot R} d\tau \tag{31}$$

d). ***The flow through a tank series***. A series of two tanks, as shown in Figure 16 is considered, where $F_{vi3} = 0$. The initial conditions are:

$$H_1(0)=0,\ H_2(0)=0; \tag{32}$$

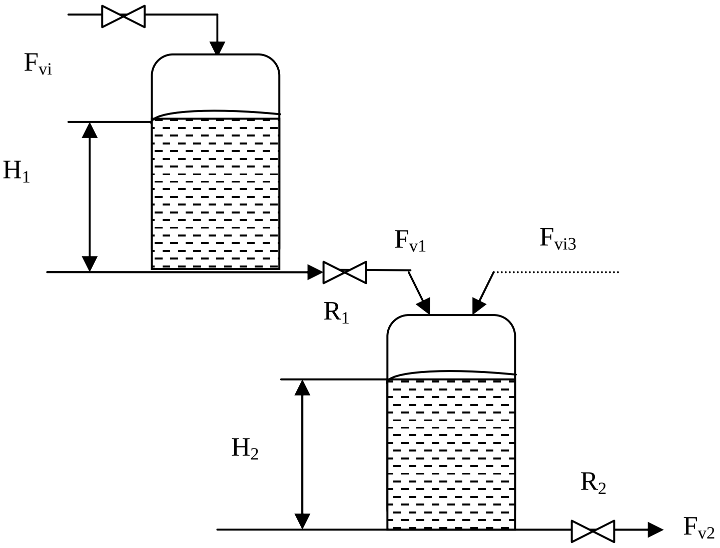


Fig. 16. Two tanks in series.

The system of differential equations describing the evolution of this series is given by:

$$\begin{cases} -\dfrac{dH_1}{dt} = \dfrac{H_1}{A_1R_1} - \dfrac{1}{A_1}\cdot u(t) \\ -\dfrac{dH_2}{dt} = -\dfrac{H_1}{R_1A_2} + \dfrac{H_2}{A_2R_2} \end{cases} \tag{33}$$

$$\Delta = \begin{vmatrix} \dfrac{1}{A_1\cdot R_1} - \gamma & 0 \\ -\dfrac{1}{R_1A_2} & \dfrac{1}{A_2R_2} - \gamma \end{vmatrix} = 0 \quad \gamma_1 = \frac{1}{A_1\cdot R_1} \text{ and } \gamma_2 = \frac{1}{A_2R_2} \tag{34}$$

The formation flow graph for *H_2* is:

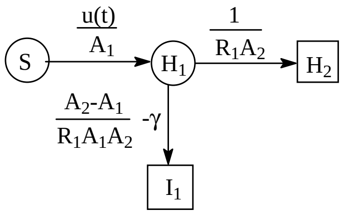


Fig. 17. The formation flow graph for H_2

The increase of the liquid height in the two tanks is[13]:

$$H_2 = \frac{1}{A_1 A_2 R_1} \cdot \frac{1}{\gamma_2 - \gamma_1} \int_0^t u(t-\tau) \cdot (e^{-\tau / A_1 \cdot R_1} - e^{-\tau / A_2 R_2}) d\tau \qquad (35)$$

$$H_2 = \frac{R_2}{A_1 R_1 - A_2 R_2} \cdot \int_0^t u(t-\tau) \cdot (e^{-\tau / A_1 \cdot R_1} - e^{-\tau / A_2 R_2}) d\tau$$

d) **The flow through a tank series with an additional feed**. The fourth example considered is treated supposing that there is a new feed $F_{vi3} = u_2(t)$ (see figure 15) and $A_1 = A_2 = A$. The corresponding differential equations are[13]:

$$\begin{cases} -\dfrac{dH_1}{dt} = \dfrac{H_1}{AR_1} - \dfrac{1}{A} \cdot u_1(t) \\ -\dfrac{dH_2}{dt} = -\dfrac{H_1}{R_1 A} + \dfrac{H_2}{AR_2} + \dfrac{1}{A} \cdot u_2(t) \end{cases} \qquad (36)$$

$$\Delta = \begin{vmatrix} \dfrac{1}{A \cdot R_1} - \gamma & 0 \\ -\dfrac{1}{R_1 A} & \dfrac{1}{AR_2} - \gamma \end{vmatrix} = 0 \quad \gamma_1 = \frac{1}{A \cdot R_1} \text{ and } \gamma_2 = \frac{1}{AR_2} \qquad (37)$$

The formation flow graph for *H_2* is:

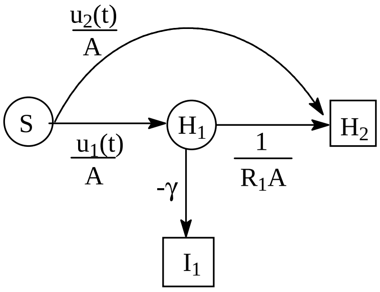


Fig. 18. The formation flow graph for H_2

It results that:

$$\Delta_{H_2} = \frac{u_1(t)}{A} \cdot \frac{1}{R_1 A} + \frac{u_2(t)}{A} \cdot (\frac{1}{R_1 A} - \gamma) \qquad (38)$$

$$H_2 = \frac{1}{A^2 R_1} \cdot \frac{1}{\gamma_2 - \gamma_1} \int_0^t u_1(t-\tau) \cdot e^{-\tau / A \cdot R_1} d\tau + \frac{1}{A} \cdot (\frac{1}{R_1 A} - \gamma_1) \cdot \frac{1}{\gamma_2 - \gamma_1} \int_0^t u_2(t-\tau) \cdot e^{-\tau / A \cdot R_1} d\tau$$

$$+ \frac{1}{A^2 R_1} \cdot \frac{1}{\gamma_1 - \gamma_2} \int_0^t u_1(t-\tau) \cdot e^{-\tau / A \cdot R_2} d\tau + \frac{1}{A} \cdot (\frac{1}{R_1 A} - \gamma_2) \cdot \frac{1}{\gamma_1 - \gamma_2} \int_0^t u_2(t-\tau) \cdot e^{-\tau / A \cdot R_2} d\tau \qquad (39)$$

CONCLUSIONS

This method seems to be very general. It applies equally well to complex chemical reactions, the description of drug time-evolution in a body or in chemical engineering. It solves systems of differential equations in a simple way. In chemistry, the image of the graph resembles with the reaction scheme or mechanism of the transformation.

REFERENCES

[1]. M. V. Diudea, O. Ivanciuc, *Topologie Moleculara*, Ed. Comprex, Cluj, 1995, p. 37.

[2]. T. Ionescu, *Grafuri. Aplicatii. Vol 1.* Ed. Didactica si Pedagogica, Bucuresti, 1973, p. 198- 207.

[3]. K. Ogata, *Modern Control Engineering,* Prentice Hall International, New Jersey, 1995.

[4]. M. Socol, I. Baldea, *Stud. Univ. Babes-Bolyai,* Chemia, XLVIII, Cluj-Napoca, 1, 2003, p. 109-128.

[5]. M. Socol, I. Baldea, *Stud. Univ. Babes-Bolyai,* Chemia, XLIX, Cluj-Napoca, 1, 2004, p. 101-110

[6]. M. Socol, I. Baldea, *Stud. Univ. Babes-Bolyai,* Chemia, XLIX, Cluj-Napoca, 2, 2004, p. 93-107.

[7]. A. C. Aitken, *Determinants and Matrices,* Oliver and Boyd, Edinburgh, 1939, Chap. 2.

[8]. N. S. Nice, *Control System Engineering,* Addison-Westley Publishing Company, 1995, p. 240-260, 268-275.

[9]. R. C. Dorf, R. H. Bihop, *Modern Control System*, Prentice Hall International, New Jersey, 2001, p. 66-80,118-158.

[10]. P. Juergen, *Reaktionskinetische Auswertung Spektroskopischer Hessdaten*, Braunschweig, 1995, p. 160-183.

[11]. M. Rosculet, *Analiza Matematica,* Ed. Didactica si Pedagogica, Bucuresti, **1984**, p. 618.

[12]. C. Udriste, *Aplicatii de algebra, geometrie si ecuatii diferentiale,* Ed. Didactica si Pedagogica, Bucuresti, **1993**, p. 264.

[13]. M. V. Cristea, S. P. Agachi, *Elemente de teoria sistemelor,* Ed. Risoprint, Cluj-Napoca, **2002**, p. 113-131.

[14]. R. V. Churchill, *Operational matematics,* McGraw-Hill, New-York, **1958**, p. 323.

[15] I. Muresan, C*himia Macromoleculelor,* Ed. Didactica si Pedagogica, Bucuresti, **1967**, p. 44.

[16]. *www.wolfram.com*

[17]. M. K. Ma, W. C. Zamboni, *Clinical Cancer Research*, 6, **2000**, p. 813-819.