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Modelling a simple continuous-time system

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Abstract

The aim of the present paper is to give a very simple example how we can set up a mathematical model describing a not too complicated phenomenon based on measurement. It may help the beginners to model other systems too, by differential equations. At the same time we would like to enrich the possibility of demonstration in this field.

Keywords: Differential equation, mathematical model, crystal growth.

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1. Introduction

The authors of researches dealing with studying differential equations, composing them and differential equational models mention different examples as motivations for example: multiplying bacteria, radioactive decomposition (exponential growing), the nature of epidemic caused by infectious diseases, the spread of information (logistical growing). What is common in these examples is the following: it is not emphasized enough to get to know the system which is to be modeled measuring has to be done, and these measurements serve as the base of principles with the help of which we can describe the changes. In certain cases it can be reasonable to choose such a phenomenon which can easily be supported by experimental measuring and it is easier to be modeled than the others mentioned above. One of the groups of solid materials is made up by crystalline materials. Beyond the fact mentioned above, the practical importance of this may prove the studying of the process of crystallization.



Figure 1: Crystallization of Sodium Acetate in a test-tube.

2. Description and modeling of phenomenon

Due to certain properties NaAc is especially appropriate to make measuring in connection with the process in order to understand the relation which serves as the base of modelling. We pour the supersaturated solution of sodium acetate ($\text{Na}^+\text{CH}_3\text{COO}^-$ or NaAc) into the test-tube. By adding a piece of crystal we can start the process of crystallization. The speed of change is ideal (not too fast or slow) and the change can be observed well. At the same time the experiment does not require complicated tools and materials. So, this experiment can be carried out even at home. All these facts make it possible to produce measuring of the necessary promptness by using simple tools.

2.1. Mathematical model of one-dimensional case

As we wish to model the process of crystallization it seems to be natural that we consider the amount of substance $X(t)$ (number of moles) as state variable. On the base of experimental measuring we suppose that α quantity of material getting into solid phase during a given time is independent of the quantity of the solid material and the time t :

$$X(t+1) - X(t) = \alpha \quad (t \geq 0).$$

By the next point of time the quantity of the solid phase is increased by α . Let h denote the time spent between the two states, so that the problem can be described in a more general way. If we select a longer time interval then more crystals are created and vice versa so it depends on h :

$$X(t+h) - X(t) = \alpha(h) \quad (t \geq 0).$$

On the base of experience it is obvious

$$\lim_{h \rightarrow 0} \alpha(h) = 0.$$

t_i [sec]	0,0	3,0	6,0	9,0	12,0	15,0	18,0	21,0	24,0
V_i [cm ³]	0,0	1,3	3,1	4,9	6,5	8,3	10,1	11,9	13,5
ΔV_i [cm ³]	1,3	1,8	1,8	1,6	1,8	1,8	1,8	1,6	-

Table 1: The measured volume of the growing crystal.
 $\Delta V_i = V_{i+1} - V_i$ ($i = 0, \dots, 7$).

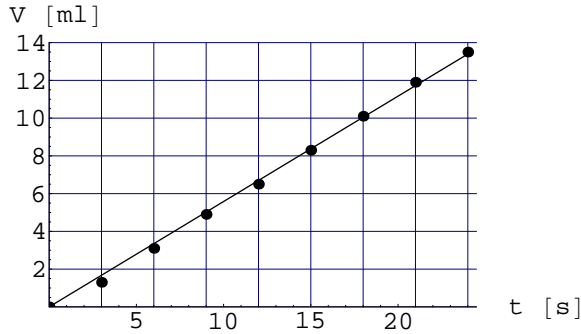


Figure 2: Linear time-dependence of the volume.
 (The measured values and the fitted line to them.)

On the base of the Table 1 and the Figure 2 we can assume that there is linear proportionality between h and the increase. During a longer period of time greater quantity of solid material is created. So $\exists \lambda_1 \in \mathbb{R}$ ($\lambda_1 > 0$), $\alpha(h) = \lambda_1 h$:

$$X(t+h) - X(t) = \alpha(h) = \lambda_1 h,$$

$$\frac{dX(t)}{dt} = \lim_{h \rightarrow 0} \frac{X(t+h) - X(t)}{h} = \lambda_1,$$

where λ_1 is independent on t and h , only it depends on a characteristic constant of the system. So the phenomenon presented by the experiment can be described by the following differential equation:

$$\frac{dX(t)}{dt} = \lambda_1 \quad (\lambda_1 > 0).$$

2.2. Exploration of the phenomenon

It is important to note that the speed of the growth of the crystal (the growth of amount of substance of solid phase during a given period of time) depends on the area of the crystal and the concentration of the liquid at a given moment.

During the experiment we produced the supersaturated solution of sodium acetate. Just like other ionic crystals sodium acetate has water molecules bound within its crystal lattice. The quantity of this water characterizes the given ionic crystals. In the case of NaAc 1 mole material has 3 moles water ($\text{NaAc}\cdot 3\text{H}_2\text{O} \equiv$ sodium acetate trihydrate). The water content of the salt escapes from the lattice during the heating and the material dissolves in this water, that is why the proportion of NaAc and the water is 1 : 3 in the supersaturated solution, too. The process of crystallization is launched by the piece of crystal put into the liquid. During the process the proportion of amounts of substances built into the lattice will be the same, so the concentration of the liquid remains constant. Regardless of the first short period of the process the surface of the increasing crystal which is in contact with the solution, also remains the same. In conclusion, the surface gets forward at an equal speed.

3. Two and three-dimensional extension of model

In the chemical point of view, the same changes can be seen in the case of the well-known hand warmer. (During the heating the supersaturated solution is produced. The launch of the crystallization is caused by the mechanical effect which can be produced by the stainless metal sheet which is in the pad.) In this case if we imagine the pad thin enough, we can idealize the phenomenon that the growth of the crystal is carried out by the following way: starting from a given point of a plain in concentric circles at an even speed. As we know, the speed of the growth depends on the size of the surface of the crystal. In our model it is proportional with circumference

$$K(t) = 2\pi R(t) \quad (3.1)$$

of the circle.

We can interpret the result of experiment that the surface of the crystal moves forward at an even speed where the $R(t)$ root is proportional with the time spent. The move of the surface of the solid material to a given direction of the space is

$$R(t) = \rho t. \quad (3.2)$$

The quantity of the material built in the solid phase is determined by the radius of the circle during h period of time:

$$\alpha(h) = X(t+h) - X(t) = \beta K(t)h.$$

(In the reality the shape of the crystal can be approached by a cylinder. The surface of its lateral is the product of the height and circumference.) We can take the length into consideration by selecting an appropriate beta constant.

By the relation of (3.1) and (3.2) we can see that $\alpha(h)$ is proportional with the time spent in each moment of time:

$$\alpha(h) = X(t+h) - X(t) = \lambda_2 t h \quad (\lambda_2 = 2\beta\pi). \quad (3.3)$$

The expression (3.3) divided by h and h tends to 0:

$$\frac{dX(t)}{dt} = \frac{X(t+h) - X(t)}{h} = \lambda_2 t.$$

So the two-dimensional growth of NaAc-crystal can be given by the differential equation:

$$\frac{dX(t)}{dt} = \lambda_2 t \quad (\lambda_2 > 0).$$

If no mechanical obstacle can be experienced in the growth of the crystal it can grow in each direction of the space then we can regard the growing crystal as sphere-symmetric and the speed of the growth is proportional with the surface

$$F(t) = 4\pi R^2(t)$$

of a sphere.

On the base of the facts mentioned above we can get the following differential equation:

$$\frac{dX(t)}{dt} = \lambda_3 t^2 \quad (\lambda_3 > 0).$$

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