Elements of computer modelling: 12 studies for beginners. Study 2: Main stages of modelling

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Abstract. This paper is a continuation of our foundational series on computer modelling [1] and presents the main stages of the modelling process, from initial problem formulation through computational experimentation to model validation. We examine the critical process of model creation, emphasising the necessity of simplifying assumptions and the fundamental contradiction inherent in modelling: the need to simplify whilst retaining essential features. Through practical examples using spreadsheet software, we demonstrate computational experiments with electrical circuits, both direct and alternating current, illustrating how mathematical models can be transformed into computer models for investigation. The paper addresses key technical considerations including the discretisation of continuous processes, computational errors in computer calculations, and basic numerical methods. We provide detailed algorithms for implementing these models in spreadsheet environments, making the concepts accessible to beginners. The validation process for ensuring model adequacy is discussed, along with strategies for testing models against known behaviours. This systematic approach to modelling stages provides learners with a practical framework for developing their own computer models across various domains, reinforcing the pedagogical principles established in the first study of this series.

Keywords: modelling stages, computational experiment, model validation, simplifying assumptions, discretisation, electrical circuits, spreadsheet modelling, numerical methods, model adequacy, pedagogical framework

2. Main stages of modelling

2.1. Creating a model

In practice, the starting point of modelling is some situation that poses a problem to the researcher for which an answer must be found. However, the use of words such as "problem" and "answer" in modelling can mislead the beginner. You will learn: 1) why simplifying assumptions are necessary in modelling; 2) why it is very important to distinguish between essential and secondary properties of an object; 3) what the main contradiction in modelling consists of.

2.1.1. Problem formulation and content of the answer

Real situations are very rarely clearly defined, since, as already noted above, the complex interactions of the object under study with its environment lead to significant difficulties in their description. Experience shows that in many cases it is practically impossible to immediately formulate a problem clearly enough to enable model creation based on it. The process of problem genesis, called *problem formulation*, effectively reduces to a series of successive reformulations of the condition - changes to its narrative basis by replacing real objects with their abstract images. Thus, even in the example about estimating the length of wire, we replaced buildings and the earth's

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surface with straight line segments, and only then did the problem reduce to finding the length of the hypotenuse of a right-angled triangle.

Problem formulation concludes with a textual and mathematical description of the problem condition. The verbal formulation of the problem together with explanatory drawings or diagrams is called a *conceptual* (content) model, whilst the relationships between object characteristics (parameters), written in the form of mathematical expressions, form the mathematical model. Typically, at the problem formulation stage, the types of initial data and modelling results are established.

The answer (that is, the result of model investigation) should, as already noted: a) enable the identification of new properties of the object and prediction of new results; b) facilitate decision-making; c) implement automatic control.

The answer in modelling is not necessarily what we are accustomed to in school mathematics, physics, or chemistry: x = 17, $R = 400 \Omega$, or $M = 98 \times 10^{-3}$ kg/mol, etc. Modelling results can additionally be tables of numbers, symbols or texts, corresponding diagrams, graphs, drawings, and so on.

The obtained answer must be analysed. This is performed by people (specialists), who draw the necessary conclusions.

2.1.2. Simplifying assumptions

Already at the problem formulation stage, the process of identifying the main (essential) features of the object proceeds. Some of its features appear important to the researcher, whilst others appear secondary. Rejection of features that are non-essential in the researcher's opinion leads to simplification and idealisation. The description of the object is formulated in the form of simplifying assumptions, which, together with explanatory drawings, form part of the narrative basis of the future conceptual model.

Returning again to the previously considered example about estimating the length of wire, we note that, strictly speaking, determining the wire length using the Pythagorean theorem is not entirely correct due to the sagging of the wire as an extended body that has some mass and is fixed at the ends. Using the given formula assumes that the mass, and consequently the sagging of the wire, can be neglected. For this reason, the obtained result should be considered only as an estimate of length, as stated in the condition. Simplifying assumptions always determine the existence of certain limits of applicability for any model.

2.1.3. The main contradiction in modelling

In modelling, there always exists a serious contradiction: on one hand, modelling is impossible without simplification, without neglecting secondary factors that are non-essential for some specific research, whilst on the other hand, there is always a risk of "oversimplifying" the model, discarding along with secondary features some important characteristics of the object. Equally undesirable is presenting some secondary property as important. We must agree that it is difficult to understand which properties are important and which are secondary until this object has been studied. If the object has been studied, then there is no need to develop a model. As a rule, this is the most responsible stage in creating a model.

Let us turn to another example. Accepting the assumption that the population growth of some settlement is proportional to the number of inhabitants, we obtain a mathematical model that proves correct only in a very rough approximation. If we account for the number of elderly people and children, the model undergoes corresponding complications. And if we include in consideration such factors as education level, number of working women, welfare level, etc., then the mathematical model becomes so complex that constructing and investigating it becomes quite difficult. However, even when accounting for these factors, the model may prove far from reality: after all, it does not yet account for a whole range of random factors - population migration, marriage and divorce statistics, percentage of people of reproductive age, etc.

The researcher's goal is to find the "golden mean": to create a model of the process without depriving it of its most important properties. There are no specific recommendations here. This is the sphere of personal experience, professional intuition based on it, level and quality of education, intellect and creativity of the researcher. Modelling is an art and, like any other art, it can be mastered only by constantly performing exercises, that is, by constantly solving problems, only through analysis of others' and one's own successful and erroneous actions.

2.1.4. Essential and secondary properties of an object

Different models can be assigned to each object depending on the research goal. For example, if we take such a complex system as an animal population, then a model of an individual animal as a biological being can be used to describe life processes. For modelling animal behaviour in a group, the researcher will create a different, ethological model (ethology is the science of animal behaviour and habits), and for predicting the dynamics of population size changes over time, a completely different, ecological model will be created. In this case, object properties that are essential when constructing one model may prove secondary when constructing another.

Thus, animals' communicative abilities should be considered in the behavioural model of a flock, but these abilities add almost nothing essential to the ecological model of the flock. In turn, the reproduction coefficient, essential for the ecological model, is not so important for the behavioural model.

However, secondary properties of an object can become essential when deepening or improving the model in order to make the model more adequate to the original object. In particular, in the simplest gas model called "ideal gas", the interaction of molecules at a distance is neglected, that is, their potential energy, but already in the first approximation to a real gas - the Van der Waals model - the interaction of gas molecules and their sizes become essential factors.

2.2. Computational experiment

In mathematical modelling, questions are posed to the mathematical model. And whilst in modern complex and expensive experimental installations, changing some conditions can lead to significant technical and economic costs, mathematical models are free from these disadvantages. To acquire practical skills, we will together conduct the first virtual investigation of simple electrical circuits.

The most common way of presenting a mathematical model is a system of certain equations with the data necessary for its solution: initial and boundary conditions, numerical values of coefficients in the equations, etc. By varying these, one can conduct a detailed study of processes, identify their main patterns, evaluate the influence of various factors on them, that is, obtain information analogous to that obtained during a physical experiment. However, in this case, instead of an experimental installation, we use a computer, and instead of the physical object being studied – its mathematical model. Such studies are called computational experiments. This stage constitutes the main content of solving any practical problem using a computer. Its essence most often reduces to repeating similar series of calculations when changing input data, that is, to searching for an answer to the question "What will happen if...?"

Computational experiment today is a modern technology of theoretical research based on experimentation with a mathematical model using a computer.

Research of computer mathematical models of real objects often involves identifying the type of functional dependencies between the characteristics of these objects. Such work, as already noted, is conveniently conducted in specialised modelling environments - mathematical packages adapted for certain subject areas of knowledge (technology, economics, accounting, etc.). As mentioned above, our manual is oriented towards using the universal environment familiar to all schoolchildren, called Spreadsheets, in which it is easy to construct graphs of functional dependencies.

To illustrate what has been said, let us consider two examples from physics on investigating direct and alternating current electrical circuits by studying their mathematical models.

2.2.1. Investigation of a closed direct current electrical circuit

The electrical circuit diagram is shown in figure 1.

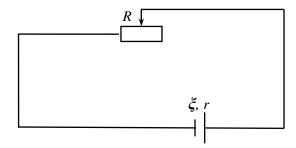


Figure 1: Closed direct current circuit.

The circuit elements are: a current source with electromotive force ξ and internal resistance r; the consumer is a variable resistor (rheostat) with resistance R. Additionally, such a circuit is customarily characterised by several more parameters: current strength I in the circuit, voltage U across the consumer terminals, consumer power P_{useful} , circuit efficiency η . We neglect the resistance of connecting wires, considering it significantly less than the sum R+r – the total circuit resistance.

The aim of the investigation is to study the dependence of the listed quantities on the consumer resistance R by creating a table and constructing corresponding graphs.

The circuit diagram in figure 1 and the two paragraphs following it are nothing other than a conceptual (content) model.

Construction of the mathematical model. The basis for constructing the mathematical model consists of the known relationships:

• Ohm's law for a complete direct current circuit: $I = \frac{\xi}{R+r}$,

as well as expressions by which the following are calculated:

- voltage across the consumer terminals: U = IR;
- useful current power: $P_{\text{useful}} = I^2 R = IU$; efficiency coefficient: $\eta = \frac{R}{R+r}$.

The characteristics of the current source – EMF ξ and internal resistance r – will be considered known and unchanging when all other circuit parameters change, that is, constants.

Thus, the mathematical model of the problem is the following system of four equations:

$$\begin{cases} I &= \frac{\xi}{R+r} \\ U &= IR \\ P_{\text{useful}} &= I^2 R \\ \eta &= \frac{R}{R+r} \end{cases}$$

where, as just noted, the quantities R, U, I, P_{useful} , η are variables, and ξ and r are

After creating the mathematical model, let us proceed to the computer model. For this, in the modelling environment - spreadsheets - we implement the following

Algorithm for further work:

1. Create a table according to the template:

	Α	В	С	D	E	F	G
1	R	I	U	Puseful	η (efficiency)	Given:	
2						ξ, V =	3
3						$r, \Omega =$	0.5
•••			•••	•••	•••		

- 2. Enter variable names (parameters) in the first row.
- 3. Fill columns F ("Given:") with names and G with input parameter values.
- 4. Record the content of cells to be filled from the keyboard key cells of the table:

Cell	Formula/Number	Comments
A2	0	
A3	=A2+0.1	
B2	=\$G\$2/(\$G\$3+A2)	copy to B3
C2	=B2*A2	copy to C3
D2	=B2*C2	copy to D3
E2	=A2/(\$G\$3+A2)	copy to E3

- 5. Copy formulas from cells B2, C2, D2, E2 to the third row, as indicated in the comments.
- 6. Select cells from area A2:E3 (second and third rows) and increase precision to two decimal places (Format cell \rightarrow "Number" tab \rightarrow type "Number", set "Decimal places" -2).
- 7. Copy all formulas from the third row to the next 45 rows.
- 8. Using data from columns A, B, C, D, E, construct graphs of the dependencies of variables I, U, P_{useful} , η on consumer resistance R (external circuit section) in one coordinate plane, as shown in figure 2.

	A	В	С	D	E	F	G
1	R	I	U	P_{useful}	η (efficiency)	Given:	
2	0.00	6.00	0.00	0.00	0.00	ξ, V =	3.00
3	0.10	5.00	0.50	2.50	0.17	$r, \Omega =$	0.50
•••	•••	•••	•••	•••	•••		

For this purpose, we select all data in columns A, B, C, D, E and access the chart wizard from the main menu. On the "Recommended Charts" tab, we choose type "Scatter", since this type ensures representation of functional dependence of the form y = y(x). By default, data from the leftmost selected column (in this case column A) become arguments, and no graph line is constructed for this data (!). Thus, by selecting five columns, we obtain four lines for the "Scatter" type, whereas for the "Line" type – five lines, including the graph x = x(x), which proves clearly superfluous. Analysing fig. 2, we can draw the following conclusions:

1) when consumer resistance R increases, current strength I in the circuit monotonically decreases to zero;

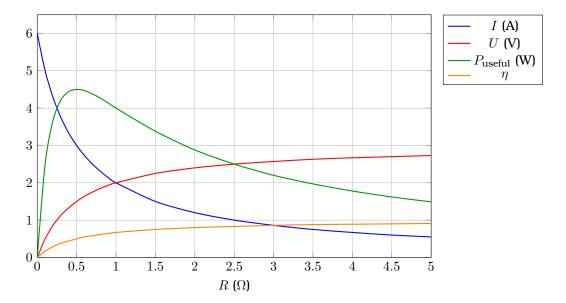


Figure 2: Graphs of dependence of I, U, P_{useful} , η on consumer resistance R.

- 2) the maximum current value corresponds to the condition $R \to 0$ this is the *short* circuit mode;
- 3) voltage U across the consumer terminals monotonically increases, approaching the value of the current source EMF ξ ;
- 4) efficiency also increases monotonically, approaching 1 (100%), however, at this point the current in the circuit equals zero, and such a mode has practically no meaning;
- 5) only useful power changes non-monotonically: its value first increases and then decreases, so that the graph of dependence $P_{useful} = P_{useful}(R)$ has a maximum, and maximum useful current power develops when $R=r=0.5~\Omega$ (when consumer resistance – the external circuit section – equals the internal resistance of the current source). However, the efficiency value is not 100%, but only 50%. This conclusion proves valid for any electrical circuits. It can be obtained without a computer, using exclusively analytical methods, but now we have the opportunity to verify this fact on a computer model.

Questions and exercises

- 1. Note: current strength I reaches maximum value when $R \to 0$ ("short circuit"). In this case, voltage U across the consumer terminals approaches zero. Under what conditions is this a very dangerous mode of electrical circuit operation, accompanied by intense heat release in various circuit elements, particularly in the current source, leading to its destruction? And when is this mode completely safe?
- 2. Model the replacement of the current source with a new one having the same EMF but with internal resistance $r = 1.0 \Omega$.
 - 2.1. How will this affect the maximum values of the variables?
 - 2.2. Repeat the computational experiment, setting the current source EMF $\xi = 5.0 \text{ V}$ and its internal resistance $r = 1.0 \Omega$.
- 3. Analytically investigate the following functions for extrema:
 - a) $P_{\text{useful}} = P_{\text{useful}}(R) = \xi^2 \frac{R}{(R+r)^2}$; b) $\eta = \frac{R}{R+r}$.

2.2.2. Investigation of an alternating current circuit section

The mathematical model is constructed based on the following relationships:

 $I_0 = \frac{U_0}{Z}$ – Ohm's law for an alternating current circuit section containing active resistance R, inductance L, and capacitance C (figure 3).

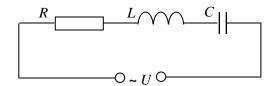


Figure 3: Diagram of the investigated alternating current circuit.

Here U_0 is the voltage amplitude across the circuit section terminals; $X_L = 2\pi\nu L;~X_C = \frac{1}{2\pi\nu C};~Z = \sqrt{R^2 + (X_L - X_C)^2}$ – formulas for inductive X_L , capacitive X_C , and total Z impedances.

Knowing the total impedance Z of the circuit, one can calculate the current amplitude: $I_0 = \frac{U_0}{Z}$.

Since complete analytical investigation of the function $I_0 = I_0(\nu)$ using differential calculus requires time, it is typically not performed in physics lessons, being limited to qualitative estimates. We will perform such an investigation in spreadsheets using an algorithm almost identical to the previous one, with subsequent graphical interpretation of results. The difference lies in the content of the key cells of the new table:

Cell	Formula
A2	=\$G\$6
A3	=A2+\$G\$7
B2	=2*3.14*A2*\$G\$4
C2	=1/(2*3.14*A2*\$G\$5)
D2	=(\$G\$3^2+(B2-C2)^2)^0.5
E2	=\$G\$2/D2*1000

The content of cells B2, C2, D2, E2 should be copied to the same columns of the third row (at this point cell A3 is already filled). Then all formulas from the third row should be copied to the next 10 rows (in this case quite sufficient).

Using data from columns A, B, C, D, E, construct graphs of the dependencies of variables X_L , X_C , Z, I_0 on the frequency ν of alternating current in one coordinate plane, as shown in figure 4b.

The graph of function $I_0 = I_0(\nu)$ in physics is called a *resonance curve*.

- 1. To simultaneously display all four graphs $X_L = X_L(\nu)$, $X_C = X_C(\nu)$, $Z = Z(\nu)$, and $I_0 = I_0(\nu)$, select all filled cells in columns A, B, C, D, E.
 - Note. If you want the legend to show the variable name next to the corresponding graph marker, selection should begin from row 1 (together with column names). If you select only the numerical part of the table, starting from the second row, then in the legend next to each marker instead of column names, inscriptions Series 1, Series 2, etc. will appear.
- 2. The graphs show that with the given circuit parameters and forced oscillation frequency $\nu \approx 50$ Hz, we have:
 - a) $X_L = X_C$; b) $Z = Z_{\min}$; c) $I = I_{\max}$.
- 3. By changing in turn the values of active resistance R (cell G3), inductance L (cell G4), and capacitance C (cell G5), investigate their influence on the appearance of each curve, including the resonance curve.

	A	В	С	D	Е	F	G
1	ν, Hz	X_L , Ω	X_C , Ω	Z, Ω	I_0 , mA	Given:	
2	25	118	455	337	44	U_0 , V =	15
3	30	141	379	238	63	$R, \Omega =$	10
4	35	165	325	160	93	<i>L</i> , H =	0.75
5	40	188	284	96	155	C, F =	1.4E-05
6	45	212	253	42	357	ν_0 , Hz =	25
7	50	236	227	13	1170	$\Delta \nu$, Hz =	5
	•••	•••	•••	•••	•••		

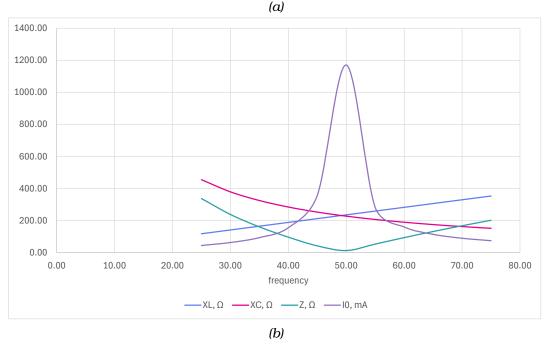


Figure 4: Construction of resonance curve: (a) table data; (b) graphs of $X_L = 2\pi\nu L$; $X_C = \frac{1}{2\pi\nu C}$; $Z = \sqrt{R^2 + (X_L - X_C)^2}$; $I_0 = \frac{U_0}{Z}$.

2.2.3. Conclusions

- 1. From the considered examples, it is evident that mathematical modelling involving a computer computer modelling opens great possibilities for graphical interpretation (representation) of complex analytical dependencies.
- 2. In the two problems, examples of *adequate use of the computer* were demonstrated when studying natural sciences, and in particular, physics. It is precisely due to this circumstance that work time is saved through automation of routine computational operations.
- 3. Computational experiment with a mathematical model makes it possible to significantly simplify the problem-solving procedure.

2.3. Checking the model for adequacy

The constructed model should be subjected to validity testing, that is, to establish how correctly its results reproduce the behaviour of the object in the investigated situations, that is, whether the correspondence of modelling results to the behaviour of the real original object is sufficiently complete. This is a peculiar "moment of truth" for the model. In this situation, we speak about *checking the model for adequacy*. A necessary sign of model adequacy is, first of all, satisfactory agreement of modelling results with known and/or sufficiently reliable observation results or field experiment data.

To check the model for adequacy, computational experiment is often directed at confirming obvious and previously known properties of the object. Such a procedure is called *model testing*. As for those cases where there is no possibility of comparing results obtained on the model with the behaviour of the object itself, testing is conducted using results provided by theory and corresponding calculations.

A model that has passed testing can be considered, if not satisfactory, then at least

Question. Is it possible to devise tests for all possible situations? What follows from this?

2.4. Computer modelling and its features

For qualitative understanding of the following text, we should clarify a number of facts that illuminate the specific features of computer modelling: those that depend on computers (the necessity of discretisation of continuous processes, errors in computer calculations), and those determined by work methods (initial concepts of numerical methods).

Almost everything discussed above could generally be done without computers. With the advent of computers, modelling possibilities rose to an incomparably higher level. As already noted, thanks to computers' ability to work with large volumes of information, and, equally importantly, the enormous (compared to other means) speed of data processing, computers have become the main working tool in modelling.

2.4.1. Features dependent on computers

From natural sciences, it is known that processes in nature can have a continuous (in space and time) character or an intermittent, jump-like character. This intermittency has a special name - discreteness.

A clear example in this regard is provided by mathematics. Thus, the set of all real numbers, when represented on the number line, is a continuous sequence of points, whilst the set of integers in this case forms a discrete sequence.

Another example can be taken from physics. To regulate current strength in an electrical circuit, rheostats are used, which usually come in two types: sliding and stepped. In sliding rheostats, resistance changes smoothly, continuously; in stepped ones - in jumps, intermittently. Depending on the design of the chosen rheostat, current strength in the circuit will change continuously, smoothly in the first case, and discretely in the second.

A digital computer, by its principle of operation, is a discrete device: information processing in it occurs intermittently, discretely under the control of so-called *clock* pulses, which ensures the possibility of implementing the required sequence of operations. Incidentally, the frequency of these pulses determines the speed of performing computational operations or, as they say, the computer's performance. Since both computer memory has finite volume and the number of operations per unit time is finite, mathematical models subject to computer processing must also be discrete and

Question. Can one strictly assert that the resistance of a sliding rheostat changes smoothly?

Discretisation of continuous processes. When we want to explain something new, it is sometimes useful to use an analogy with something familiar. Then, even if complete understanding does not appear, at least an illusion of understanding arises. As such an analogy for the method of discretising a continuous process, we will use television filming.

Imagine that using a video camera, the process of a shiny metal ball falling against

the background of a measuring tape (scale) has been recorded. Such a recording can be viewed frame by frame, replacing one frame with the next in turn.

Question. Can such a sequence of frames be considered an information model of the ball falling process?

If the recording is played in normal viewing mode, the monitor will show the falling process with sufficient smoothness (continuity) for the viewer. However, if we examine individual consecutive frames, it is easy to see that they contain no continuous process. In one frame, the ball is opposite one scale division, in the next – opposite another, and between these frames there is nothing. The smooth process of the ball falling proves to be replaced by a sequence of its individual states. Such a transition is discretisation of a continuous process.

Discretisation is the replacement of a continuous process by a sequence of its individual states.

As in the example with video recording, when discretising continuous processes, individual states are fixed with some time step. If, for example, the time step equals 0.04 s, this corresponds to a frequency of 1/0.04 = 25 frames per second, and then two adjacent frames are two process states separated from each other in time by 0.04 s.

Moving now from analogy directly to modelling, we note:

- 1. We are not going to "film" the continuous falling process at all, since we have no real process. On the contrary, we are going to model this process on a computer.
- 2. It is impossible to model continuous processes on a computer, but it is possible to calculate a sequence of individual object states with some time step. In this case, we can include any information of interest to us in the object's "state": distance from the ground, coordinate, velocity, acceleration, etc., or all of them together. Consecutive object states in this case are consecutive values of this set of quantities (parameters).

Errors in computer calculations. Let us note one more fundamental fact. Computers do not operate with real numbers of infinite precision; they work with numbers having some fixed set of digits. The number of digits in such a set is determined by hardware and software (instrumental means). Arithmetic operations performed with real numbers often lead to a specific error called rounding error. If, for example, our computer operated with real numbers containing only one decimal place, then the result of multiplying 2.1 by 3.2 would be 6.7 and not 6.72. The reasons for the origin of rounding errors allow us to understand, firstly, their inevitability, and secondly, the negative fact that they accumulate as the volume of calculations increases. To reduce these errors at least to some extent, one tries to use ready-made algorithms or develop one's own in which these errors do not accumulate noticeably.

Numerical methods. In mathematics, situations are well known where an equation has been composed, but there are no known methods for its exact analytical solution (that is, obtaining a solution in the form of an exact formula). It is not much simpler in those cases where the method of analytical solution is known, but it proves so cumbersome and costly in terms of time duration and some other computer resources that solving by this method proves ineffective. Moreover, high accuracy is far from always necessary. Therefore, mathematicians persistently work on developing so-called numerical methods for solving equations. These methods comprise the content of a separate and very important branch of mathematics called computational mathematics, which provides results with any predetermined accuracy.

Since computer modelling is nowadays a very widespread type of research activity, to satisfy the growing needs of users, software packages designed for working with

mathematical models have already been created and continue to be created – so-called specialised environments for computer modelling.

Summary

- 1. Modelling problems arise from practice, but at the moment of appearance they are not clearly formulated. Therefore, before creating a model, the process of problem formulation must always occur.
- 2. Creation of a mathematical model always begins with idealisation of the object based on simplifying assumptions. However, for the purpose of deeper study of the object, new factors (parameters) are introduced into the previous simplified version of its model from among those previously neglected but now considered essential.
- 3. If a computer may not be directly used in the process of creating a model, it will still become the final link in working with the model. Therefore, one should consider its discrete principle of operation, as well as the inevitability of rounding errors.
- 4. The central place in modelling is occupied by computational experiment, the purpose of which is to investigate model behaviour as a result of changing input data.
- 5. Since there is almost never complete confidence that the constructed model correctly reflects the phenomenon (process) it describes, checking the model for adequacy is always necessary.
- 6. The final stage in modelling is analysis of results and formulation of conclusions. One should remember that these conclusions are valid only within the accepted assumptions, and extending them beyond these limits is undesirable. If sometimes such a step is taken, in order to "look" into the past or future, this should be done extremely carefully, so as not to attribute to the object properties of a false model.
- 7. For further work with the model (its investigation by means of computational experiment), one must choose a modelling environment for each specific problem.

The simplest environment suitable for beginners is spreadsheets, which is our choice.

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