

Rectification column - mathematical modeled and computer simulated real system

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Abstract—One of the most important methods in current scientific and technological research is process of modeling and simulation of real experiment as well as modeling and simulation of real experimental device. System approach, modeling and simulation are discipline with its own theory and research methodology.

The paper focuses to the theory of the process of modeling and simulation, visualization and model validation and verification of real experiment and experimental device. Multidisciplinary approach is point out too.

Step by step there will be shown the process of creation of static and dynamic mathematical model of the real experimental device – seven storey rectification column. Mathematical model is supplemented the simulation model written in Visual Basic for Excel. Visualization is a part of the simulation model. Validation of the mathematic model as well as verification of the simulation model is shown in the paper too.

Keywords—Mathematical model, computer simulation, multidisciplinary approach, system approach, rectification column.

I. INTRODUCTION

THE terms *system*, *model*, *simulation*, *multidisciplinary approach* are important in current approach to scientific, technological and professional practice. Many universities are realizing that modeling and simulation is becoming an important tool in solving and understanding numerous and diverse problems.

Modeling and simulation, is becoming one of the academic programs of choice for students in all disciplines – see e.g. [1], [2], [3], [4]. Modeling and simulation is a discipline with its own body of knowledge, theory, and research methodology.

To engage modeling and simulation the mathematical model of the real system has to be first created. Models are approximations for the *real system*. The model is then followed by *simulation*, which allows for the repeated observation of the model. After the simulations model is *verified*, a third step takes place and that is *visualization* of the model and the real system.

The ability to define a system, to build a mathematical model and to create a simulation model develops logical thinking skills and imagination and is an inseparable part of a student's study skills for those studying the specializations "Applied Informatics". In this paper we first briefly introduce the theory of modeling and simulation as a method of multidisciplinary investigation of a real experimental device. A similar introduction can be found in [5], [6], [7].

Secondly we introduce a case study illustrating the step by step process of modeling and simulations of a real experimental device - *seven storey rectification column*. The device will be described from the real system point of view, then the static and dynamic mathematical model will be presented and finally the computer simulation model created by programming in Visual Basic for Application (VBA) will be shown. VBA is standard programming language implemented in MS Excel.

II. MODELING AND SIMULATION AS METHOD OF DEVELOPMENT OF MULTIDISCIPLINARY THINKING

A. Modeling

Modeling is a method that is often used in professional and scientific practice in many fields of human activity.

The main goal of modeling is describe the content, structure and behavior of the real system representing a part of the reality.

The models are always only approaching of the reality, because the real systems are usually more complex than the models are. The system homomorphism is applied in the process of modeling, which means that each element and interaction between the elements of the model corresponds to one element and interaction of the modeled real system, but the reverse is not true. The model is always to be understood as simplification of the original. If the relation of isomorphism is between the model and real system the original model we could not distinguish between the model and the original, which is discussed e.g. in [8].

The first step in the process of computer modeling is creation of mathematical model of the studied real system. The model can be obtained either theoretically based on basic physical properties of the system, or numerically by means of the measured values. Determination of parameters of theoretical model developed from empirical data is called system identification.

The mathematical model must adequately describe the dependency system outputs on its inputs. Models of physical systems are usually established as a system of mathematical equations as will be shown in the following paragraphs of this paper.

B. Simulation

The process of modeling is closely related to the simulation. Simulation can be understood as process of executing the

model. Simulation enables representation of the modeled real system and its behavior in real time by means of computer. The simulation enables also visualization and editing of the model.

A typical simulation model can be written both through specialized programming languages that were designed specifically for the requirements of simulations, or the simulation model can be created in standard programming languages and spreadsheets (MS Excel). In our paper the real system is simulated in Visual Basic for Application, which is programming language implemented to MS Excel.

From the above considerations, it is clear that simulation is a process that runs on the computer. In some publications, therefore, can be found the term "computer simulation". It generally is valid that computer simulation is a computer-implemented method used for exploring, testing and analysis of properties of mathematical models that describe the behavior of the real systems which cannot be solved using standard analytical tools, see e.g. [9].

The simulation models represented by executable computer program have to be isomorphic with the mathematical model that is a representation. It means that the mathematical model and simulation model have to represent the real system, its elements, internal interactions and external interaction with the environment in the same way.

Simulation has from the scientific point of view several functions – see e.g. [9].

We will focus in this paper two of them and they are:

- Replacing the real experiment;
- The development of educational process.

1) *Function of simulation - Replacement of the real experiment*

This is an important and indispensable feature of simulations and simulation model because it allows realize a situation that cannot be investigated using conventional real experimental devices. The main advantage of simulations is that simulations model allows changing of input parameters, visualization and optimization the effects of the real experiment. The simulation is usually safety and cheaper.

2) *Function of simulation - The development educational process*

The simulation is very useful from educational point of view. Using the simulation model and visualization of simulation results on the screen, students can better understand the basic processes and systems and develop their intuition. It is also essential that the teaching by means of simulation is much cheaper and faster than the teaching carried by real experiment. In some cases providing the real experiment cannot be feasible.

Despite the fact that experimental education in the laboratory cannot be completely replaced (because students acquire manual dexterity, they learn to work with real laboratory instruments, they learn to plan, implement and evaluate realistic experiment), the simulations is a part and basic methods of scientific knowledge. Students can easily

learn theoretical foundations of the laboratory tasks. The simulation model of the real laboratory task can help them to check some of the operations performed in the laboratory. This can reduce the direct lessons in the laboratory only to necessary time for their own experimental measurements. Alternatively, lessons can be realized only by the simulation models. In this case, it is important to note that students are deprived of contact with the real device, so that they will not get a full picture of the implementation of the experimental measurements.

C. *Model verification and validation*

Verification and validation are important aspects of the process modeling and simulation. They are essential prerequisites to the credible and reliable use of a model and its results [10].

1) *Verification*

In modeling and simulation, verification is typically defined as the process of determining if executable simulation model is consistent with its specification – e.g. mathematical model. Verification is also concerned with whether the model as designed will satisfy the requirements of the intended application. Verification is concerned with transformational accuracy, i.e., it takes into account simplifying assumptions executable simulation model. Typical questions to be answered during verification are:

- Does the program code of the executable simulation model correctly implement the mathematical model?
- Does the simulation model satisfy the intended uses of the model?
- Does the executable model produce results when it is needed and in the required format?

2) *Validation*

In modeling and simulation, validation is the process of determining the degree to which the model is an accurate representation of the real system. Validation is concerned with representational accuracy, i.e., that of representing the real system in the mathematical model and the results produced by the executable simulation model. The process of validation assesses the accuracy of the models. The accuracy needed should be considered with respect to its intended uses, and differing degrees of required accuracy may be reflected in the methods used for validation. Typical questions to be answered during validation are:

- Is the mathematical model a correct representation of the real system?
- How close are the results produced by the simulation executable model to the behavior of the real system?
- Under what range of inputs are the model's results credible and useful?

Validation and verification are both ultimately activities that compare one thing to another. Validation compares real system and mathematical model. Verification compares mathematical

model and executable simulation model. Sometimes validation and verification are done simultaneously in one process.

Validation of the mathematical model as well as verification of the simulation model of our real system – seven storey rectification column – are to be done simultaneously by the comparison of the dependencies of the quantities theoretically calculated from the simulation model with the dependencies of quantities experimentally measured on rectification column.

The whole process of transformation from a real system, the simulation model and its visualization is shown in Fig. 1.

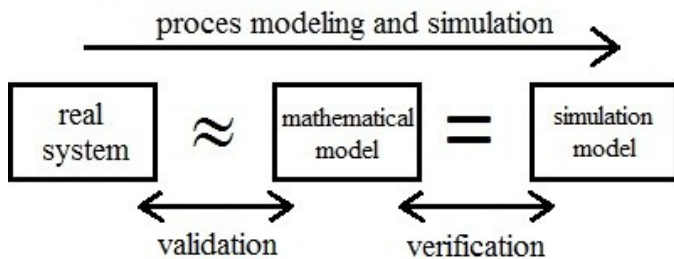


Fig. 1 Process modeling and simulation

Here again let us summarize that the mathematical model that reflects the real system has some limitations and simplifying assumptions (the real system and mathematical model are in homomorphic relation).

In contrast, the simulation model is only the computer expression of the mathematical model (the mathematical model and simulation model are in isomorphic relationship).

D. Multidisciplinary approach

Another important benefit associated with the process of modeling and simulation of real experiments is a multidisciplinary approach, without which the process of identifying the real system using mathematical and simulation model and cannot be realized. This is also emphasized in this paper.

Multidisciplinary approach generally means that specialized disciplines are applied in a study of real system. These disciplines provide partial analysis of the real system. These mono-disciplinary analyses are integrated to overall solution by integrating the solver who has basic multi-disciplines knowledge.

In our case study are integrated four disciplines, namely, experimental physics, theoretical physics, mathematics and computer science.

III. CASE STUDY – MODELING AND SIMULATION OF RECTIFICATION COLUMN

One of the research programs of the University of Hradec Kralove is development of simulation models of real devices. It is not only the work of students in resolving their theses, but also the research, whose results were published in professional journals – see e.g. [11], [12], [13].

We established general mathematical as well as computer simulation model of the rectification column, which is used for

distribution of a binary mixture of two liquids with different boiling point. The model allows simulate experimental measurements of static and dynamic properties of the column. Based on the results of simulations the single- and two-dimensional control process of the column can be designed and simulated.

The experimental device that has been used for model verification and simulation in this paper is a pilot seven-storey rectification column placed in laboratory at our university. In our particular case the methanol is separated from the methanol – water mixture.

A. Construction description

Schematic construction drawing of the seven-storey rectification column is shown on Fig. 2 – see also [11].

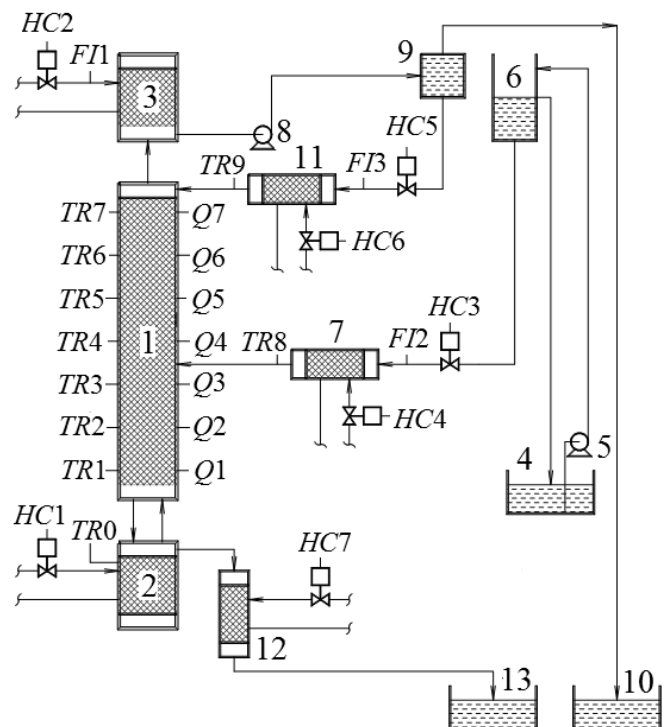


Fig. 2 Construction drawing of the seven-storey rectification column [11]

The main parts of the device are stainless steel column (1), heater (2) and condenser (3).

The rectification column (1) is stainless. Its nominal diameter is 150 mm. It has seven storeys. On each storey there is a needle from (Q1) to (Q7) for sampling. In the heater and in the all storeys there are installed platinum thermometers from (TR0) to (TR7). Signals from these thermometers are converted by resistance / voltage converter to digital signal, which is input to computer. Time constants of installed thermometers and converters are negligible with regard to the time constants of transferred characteristic of the rectification column. This is an important assumption needed for measurement and model verification of the dynamic characteristics.

Heater (2) is stainless steel, heated by the heating coils,

whose power is continuously adjustable in the range (0 ÷ 12) kW by thyristor regulator (HC1).

Condenser (3) is made of steel with copper cooling coils. Cooling water flow rate is manually set by the valve (HC2) and can be controlled with rotameters (FI1).

Injected mixture is pumped from the reservoir (4) by pump (5) to buffer tank (6). Rest injection mixture overflows back to reservoir (4). Injection flow rate is regulated by the valve (HC3) based on rotameters (FI2). The injected flow is pre-heated (7) to a temperature close to boiling point and injected to the third storey of the column. Power input heating coils in the heater is controlled by thyristor regulator (HC4). Injection temperature is measured by mercury thermometer (TR8).

The upper product is liquefied in the condenser (3), and is pumped by pump (8) into the splitter (9), where the upper product is divided into reflux and distillate. The distillate overflows to storage tank (10). Quantity of reflux is regulated by valve (HC5) based on rotameters (FI3). The reflux is pre-heated to boiling temperature in heater (11) and flows back to the 7th storey of the column. Power input heating coils in the heater is configured by thyristor regulator (HC6). Temperature of the reflux is measured by mercury thermometer (TR9).

The bottom product overflows from heater (2) through the condenser (12) into a storage container (13). Cooling water flow rate is manually configured by the valve (HC7).

Flow rates of the distillate and the distillate residuum are measured by weighing. Injection flow and distillate residuum are measured by rotameters. Concentration of the samples is determined by chromatography.

B. Technological description

It has been already mentioned that the main parts of the seven-storey rectification column are the stainless steel column (1), heater (2) and condenser (3).

Mathematical model can be created based on physical analysis of the column. Necessary physical quantities are introduced in the following text and in the Fig. 3.

Injection mixture is supplied to the m^{th} storey of the rectification column with the flow rate F and concentration x_F .

The heater contains liquid that is heated. The vapor in the heater has the concentration y_0 and flows up with the flow rate V to the upper storeys of the column. The concentration of the vapor in i^{th} storey is y_i .

Raising vapor primes the liquid with the lower boiling point. This liquid, in the form of vapor, leaves the column head (upper storey) with the flow rate V and under concentration y_n into the condenser, where n marks the order of the storey.

Here the vapor cools down, condenses and resulting liquid is partially taken as a final product in the form of a distillate with flow rate D and concentration x_D and partially flows back to the upper storey of the column as reflux with the flow rate R and concentration x_D .

The liquid flows down to the lower storeys of the column and primes the liquid with the higher boiling point. The concentration of the liquid in the i^{th} storey is x_i . Then this mixture flows from the first storey of the column into the

heater with the flow rate $F + R$ and concentration x_1 .

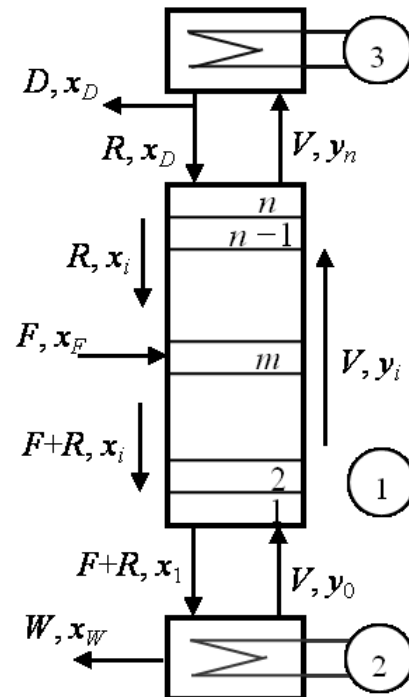


Fig. 3 Physical quantities of the rectification column

Part of the liquid transfers into vapor and this vapor flows back into the first storey of the column. The remaining part of the liquid in the heater flows out in the form of distillation residue with flow rate W and concentration x_W .

The unit of flow rates (R, F, V, D) is "mol/min", the unit of concentrations (x_D, x_W, x_i, x_F, y_i) is "mol/dm³".

In the principle the input mixture is divided into the distillate in which prevails the liquid with the lower boiling point, and distillation residue in which prevails the liquid with a higher boiling point.

IV. MATHEMATICAL MODEL

In this section the transformation of the above described real system (seven-storey rectification column) will be described. From multidisciplinary point of view the disciplines like physics and mathematics will be involved in.

Mathematical and physical analyze of the rectification column can be obtained from various complex mathematical models. Design of each model depends primarily on its subsequent use. Given that the operation of a rectification column is usually closely restricted to the operating point, it is not necessary the mathematical models describes exactly all the nonlinearities that occur within the theoretically accessible working range of the column. Therefore, the design model, always start from a number of simplifying assumptions. The bases are material and heat or only the material balance. Often these simplified models in the narrow range of the operating point are linearized.

Modeled system is schematically illustrated in Fig. 3, the meaning of used quantity symbols is explained in the previous section.

Static and subsequently the dynamic mathematical models of the tray rectification column are calculated based on the following simplifying assumptions:

- The heat transfer is ordered faster than mass transfer, which means that it is not necessary to consider the heat balance of the modeled system;
- Molar flow rates of liquid and vapor phase along the column are constant;
- Mass trap of liquid are constant in the all storeys of the column, mass trap of vapor can be neglected in comparison to the trap of liquid;
- Injection mixture flow and reflux flow are income into the column in the liquid phase at temperature equal to the boiling mixture;
- Concentrations of liquid and vapor on the floor are homogenized and both phases have the same temperature;
- The column is heated insulated system.

A. Input and output characteristic

The input variables of the mathematical model are flow rate of reflux R , the flow rate of vapor in the column V , the flow rate of injection mixture F and concentration of injection mixture x_F .

The output variables are the concentration of the distillate x_D , the concentration of distillate residuum x_W , concentration of liquid on each storey x_i , flow rate of the distillate D and flow rate of the residue W .

In terms of regulation of the rectification column it is important to monitor the dependency of concentration of the distillate x_D and the concentration of the distillate residuum x_W on flow rate of the vapor through the column V and on flow rate of the reflux R .

Increase or decrease of the values of input variables change the value of output variables - the concentrations of the distillate and the distillate residuum. Desirable effect of rectification column is increasing of concentration of the distillate and reducing the concentration of the distillate residuum. On the contrary, the adverse effect is reducing the concentration of the distillate and increasing the concentration of the distillate residuum.

Increasing the flow rate reflux R increases the concentration of the distillate x_D (desirable effect), but also increases the concentration of the distillate residuum x_W (side effect). Increasing the flow rate of vapor V reduces the concentration of the reflux x_W (desirable effect), but also reduces the concentration of the distillate x_D (side effect). The resulting control process is done by suitable compromise.

B. Static model of the column

The principle of the static model is that it allows for the values of input variables to determine the value of output variables, i.e. determine the static values of the output variables depending on values of the input values.

Mathematical model of the storey rectification column in steady state and under the simplifying assumption can be

described as a system of equations, which are based on material balance more volatile components. Following equations express the material balance in each storey of the column:

- heater:

$$(r_2 - 1)x_w = r_2x_1 - y_0 \quad (1)$$

- storeys under injection storey:

$$r_2x_i = y_{i-1} + r_2x_{i+1} - y_i \quad (2)$$

- injection storey:

$$r_2x_m = y_{m-1} + r_1x_{m+1} + (r_2 - r_1)x_F - y_m \quad (3)$$

- storeys above injection storey:

$$r_1x_j = y_{j-1} + r_1x_{j+1} - y_j \quad (4)$$

- condenser:

$$x_D = y_n \quad (5)$$

where parameters r_1 resp. r_2 can be calculated from the relations:

$$r_1 = \frac{R}{V}, r_2 = \frac{F + R}{V} \quad (6)$$

Material balance results in the following relation:

$$V = F + R = D + R \quad (7)$$

During the construction of the nonlinear mathematical model of the column should be respected non-linear concentration dependence of vapor phase y_i on the concentrations liquid phase x_i in each storey. To describe the dependence of y_i on x_i it is appropriate to describe the storey efficiency and to approximate dependence of the equilibrium concentrations of y_r on x_r of steady state liquid - vapor of the distilled mixture.

In the particular case of the distillation of methanol - water mixture can be steady state liquid - vapor approximated by experimentally observed dependence from which the value of y_i can be determined depending on the x_i :

$$y_i = \frac{1.50458x_i(3.1932 - x_i)}{1.50458x_i(3.1932 - x_i) + (0.62322 + x_i)(1 - x_i)} \quad (8)$$

Detailed solution is described e.g. in [12].

C. Dynamic model of the column

The principle of a dynamic model is to describe the time dependence of output characteristics for a step change one of the input characteristics

The dynamic model of the rectification column can be described by a set of differential equations, which are based on material balance of more volatile components in an intermediate state. Above mentioned equations of static model are complemented by terms expressing dynamics of the system:

- heater:

$$(r_2 - 1)x_w + \tau_0 \frac{dx_w}{dt} = r_2 x_1 - y_0 \quad (9)$$

- storeys under injection storey:

$$r_2 x_i + \tau_i \frac{dx_i}{dt} = y_{i-1} + r_2 x_{i+1} - y_i \quad (10)$$

- injection storey:

$$r_2 x_m + \tau_m \frac{dx_m}{dt} = y_{m-1} + r_1 x_{m+1} + (r_2 - r_1)x_F - y_m \quad (11)$$

- storeys above injection storey:

$$r_1 x_j + \tau_j \frac{dx_j}{dt} = y_{j-1} + r_1 x_{j+1} - y_j \quad (12)$$

- condenser:

$$x_D + \tau_{n+1} \frac{dx_D}{dt} = y_n \quad (13)$$

where t is time [min] and τ_i are time constant [min], which can be calculated from the equation:

$$\tau_i = \frac{G_i M_b}{V[(M_a - M_b)x_i + M_b]^2} \quad (14)$$

where G_i is mass trap of liquid on the i -th storey [g], M_a is molecular weight of the substance a [g·mol⁻¹] and M_b is molecular weight of the substance b [g·mol⁻¹].

Nonlinear dynamic model of the rectification column is composed of the set of linear differential equations.

Solution of this set of differential equations can be converted using Laplace transformation to a set of recurrent equations of the following form:

- heater:

$$x_w(k+1) = D_0 x_w(k) + \frac{1-D_0}{r_2-1} (r_2 x_1(k) - y_0(k)) \quad (15)$$

- storeys under injection storey:

$$x_i(k+1) = D_i x_i(k) + \frac{1-D_i}{r_2} (y_{i-1}(k) + r_2 x_{i+1}(k) - y_i(k)) \quad (16)$$

- injection storey:

$$x_m(k+1) = D_m x_m(k) + \frac{1-D_m}{r_2} (y_{m-1}(k) + r_1 x_{m+1}(k) + (r_2 - r_1)x_F - y_m(k)) \quad (17)$$

- storeys above injection storey:

$$x_j(k+1) = D_j x_j(k) + \frac{1-D_j}{r_1} (y_{j-1}(k) + r_1 x_{j+1}(k) - y_j(k)) \quad (18)$$

- condenser:

$$x_D(k+1) = D_{n+1} x_D(k) + (1-D_{n+1}) y_n(k) \quad (19)$$

where $x(k)$ and $y(k)$ are liquid and vapor concentrations in the beginning of the k^{th} sampling interval at time t ; $x(k+1)$ and $y(k+1)$ are liquid and vapor concentrations in the beginning of the $(k+1)^{\text{th}}$ sampling interval at time $t + \Delta t$; D are constant calculated based on following relations:

$$\begin{aligned} D_0 &= \exp\left(-\Delta t \frac{r_2 - 1}{\tau_0}\right) \\ D_i &= \exp\left(-\Delta t \frac{r_2}{\tau_i}\right) \\ D_m &= \exp\left(-\Delta t \frac{r_2}{\tau_m}\right) \\ D_j &= \exp\left(-\Delta t \frac{r_1}{\tau_j}\right) \\ D_{n+1} &= \exp\left(-\Delta t \frac{1}{\tau_{n+1}}\right) \end{aligned} \quad (20)$$

Detailed solution is described e.g. in [13].

V. SIMULATION MODEL OF THE STOREY RECTIFICATION COLUMN

Based on the derived static and dynamic models of the rectification column the simulation model was created in *Visual Basic for Application* (VBA) implemented to MS Excel. This simulation model allows simulating experimental measurements provided on the rectification column during separation of the binary liquid mixture of methanol - water. Other important result of the simulation model is that based on it the mathematical model of the seven - storey rectification column can be validate.

Despite the fact, that simulation model can be created in any programming language or simulation program, VBA have been selected, because this programming language enables saving the data directly in the MS Excel Worksheets and based on this data the appropriate quantity dependencies can be visualized by means of MS Excel Charts.

A. Programming in Visual Basic for MS Excel

All MS Office application like MS Excel, MS Access, MS Word, MS PowerPoint, MS Outlook and others, have implemented a programming language *Visual Basic for Application (VBA)*. It is an object-oriented programming language, which is based on Visual Basic.

VBA contains the same commands as Visual Basic and extra commands that operate with objects of their own parent application (with cells, selection, sheets, etc. in MS Excel). This can be regarded as the main advantage, especially in teaching of programming. Every user of MS Office has a programming language, and s/he can try to use it as s/he likes, s/he can create his/her own "little useful application", which can become the basis on which a further interest in programming develops.

VBA, although it is an object-oriented language, allows to handle the basic algorithmic tasks based on fully structured, sequential approach, which is especially helpful in the initial stages of algorithm development and programming.

1) VBA Integrated development environment

The integrated development environment (IDE) of VBA is available in MS Excel 2007 in the ribbon tab "Developer". This tab is not displayed by default. The tab "Developer" in version of MS Excel 2007 can be activated in the "Excel Options" dialog box (which is reached by clicking on the *Excel Option* button in the main menu) in the folder "Popular" – see Fig. 4. The "Show Developer tab in the Ribbon" checkbox has to be checked.

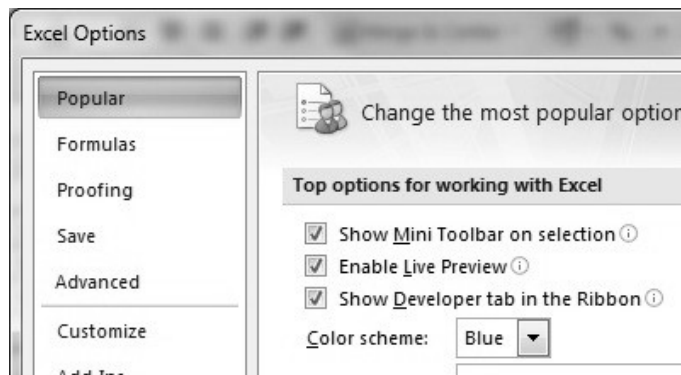


Fig. 4 Activation of Developer tab

To be able to exploit this IDE, the macro security has to be set to low. In MS Excel 2007, this setting can be performed on the "Developer tab", "Macro Security" command, where the option button "Enable all macros" has to be checked.

The IDE can be opened in two ways - either through the "Developer tab", click on "Visual Basic" command, or by pressing the keys Alt-F11.

The IDE has the Project Explorer in its left part, which shows a list of currently open projects - Workbooks, Worksheets, Modules and Forms.

In the case of sequential structured programming, the programs are saved in and run from separate *Modules*. One module can contain more programs.

In the case of object-oriented programming, the *Graphical*

user interface elements (GUI) are inserted in the *Form*. VBA includes a reduced number of GUI like *Command_Button*, *Text_Box*, *Label*, *Option_Button* and *Check_Box*.

2) Inputs / Outputs in VBA for MS Excel

The VBA for MS Excel gives different possibilities of Inputs and Outputs of variables.

Inputs:

1. The command `A = InputBox(„Input A“)` opens the input dialog box into which the user inputs the value of the variable A.
2. Command `A = Cells (R, C)` is the value of variable A read from the cell in row R and column C.
3. The *TextBox* can be used for reading the data in the object oriented approach of programming. This type of the input is used in below mentioned simulation model of the rectification column.

Outputs:

1. The command `MsgBox(A)` opens the output dialog box in which the value of variable A is output.
2. Command `Cells (R, C) = A` saves the value of variable A in a cell in row R and column C. This value can be used in following program executions.
3. The *TextBox* can be used for writing the data in the object oriented approach. This type of the input is used in below mentioned simulation model of the rectification column.

3) Variables of array type

Unlike the conventional programming languages like C #, Delphi, Visual Basic, etc., the VBA for MS Excel enables two ways of working with data stored in the form of vectors (one-dimensional variables) or matrixes (two-dimensional variables).

The first option is the same as for other languages, where the vector and matrix variables are declared in a section of variable declarations:

```
Dim A(1 To 26) As String 'Vector
```

```
Dim B(1 To 26, 1 To 26) As Long 'Matrix
```

The second option is to store one- and two-dimensional data directly into cells in Excel worksheets. The command

```
Cells(2,3) = 10
```

can be understood as an element of the matrix with the row coordinates 2 and column coordinates 3 with the value 10. The advantage of this approach with the vector and matrix data is that the values of individual elements of the vector / matrix are visible to the user.

B. Simulation application

Operation with the simulation application is intuitive based on various dialog windows – VBA Forms. The dialog windows are opened by pressing appropriate command button in the main sheet of the MS Excel application –see Fig. 5.

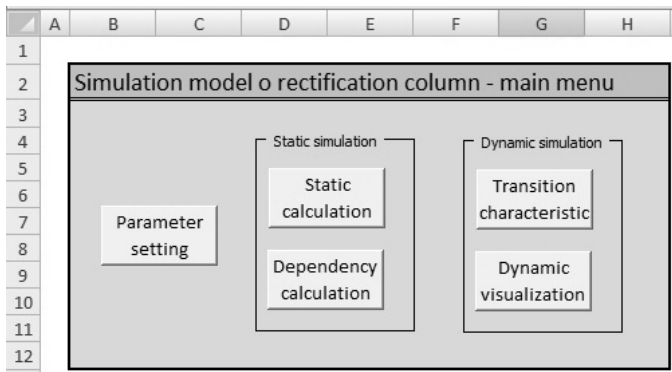


Fig. 5 Main sheet of the simulation application

Simulation application consists of five dialog windows:

- one for setting the parameters of the rectification column;
- two for calculation of the static simulation model;
- two for calculation of the dynamic simulation model.

The program was designed to simulate actual experimental device – seven storey rectification column with the injection on 3rd storey, but allows also can simulate behavior of columns with different numbers of storeys and with different locations of injection storey. It is possible also change the efficiency rate of the storey and other input parameters, see Input dialog box on Fig. 6. The parameters are stored directly in the cells of the main sheet of MS Excel application.

The dialog window "Setting of parameters of rectification column" contains several input fields:

- Number of storeys:** n - total (7), m - injection storey (3)
- Efficiency:** Under injection (0,63), Above injection (0,57)
- Mass trap:** Condenser (2200), Storey (340), Heater (13100)
- Timing:** Calculation interval of differential equation (10), Moderation of simulation time (10)

 Buttons for "OK" and "Cancel" are at the bottom left.

Fig. 6 Input dialog window for setting the parameters

C. Static simulation computer model

Given that all input variables (the flow rate of the reflux R , flow rate of the vapor in the column V , flow rate of the injector F and concentration of the injection mixture x_F) affect all output values (the concentration of the distillate x_D , the concentration of the distillate residuum x_W and concentration of liquid in each storey of the column x_i , resp. x_j) one has to decide which dependency will be simulated.

A computer program in VBA provides the following static simulations:

- static calculation of output characteristic for given input characteristic;
- calculation of static dependency of the output characteristic on input characteristic.

1) Static calculation of output characteristic

Calculation of the concentration of the distillate x_D , the concentration of the distillate residuum x_W and concentration of liquid on each storey of the rectification column x_i at given input parameters is provided by the dialog window shown on the Fig. 7, in which the input values are entered into and output values are reached from.

The dialog window "Static calculation of rectification column" is divided into three sections:

- Input data:** xF - injection concentration (0,250 mol/dm³), F - flow rate of injection (19,3 mol/min), R - flow rate of reflux (6,5 mol/min), V - flow rate of vapor (11,6 mol/min)
- Output data:** xD - concentr. of distillate (0,845 mol/dm³), D - flow rate of distillate (5,1 mol/min), xW - concentr. of residue (0,036 mol/dm³), W - flow rate of residue (14,2 mol/min)
- Survey concentration:** x7 (0,736 mol/dm³), x6 (0,603 mol/dm³), x5 (0,451 mol/dm³), x4 (0,306 mol/dm³), x3 (0,227 mol/dm³), x2 (0,175 mol/dm³), x1 (0,114 mol/dm³)

 Buttons for "OK", "Cancel", and "Calculation" are at the bottom.

Fig. 7 Input and output dialog window for static calculation

Calculation of the output characteristic of static model is given by solution of the set of the equations (1) ÷ (8). Calculation of the output characteristic x_i is in VBA executed by function:

$$\text{Static_xi}(i, x_F, F, R, V),$$

where parameter i is location of the storey and parameters x_F, F, R, V are input characteristic.

Similarly are calculated output characteristic x_D, x_W, x_j, D and W .

2) Static calculation of the dependency

This calculation enables:

- visualization of *static two-dimensional* dependency of the output characteristic on input characteristic, i.e. visualization of the changes of the concentrations (x_D, x_W, x_i and x_j) depending on the values of a selected input variables (x_F, R, F or V) or
- visualization of *static three-dimensional* dependency of the output characteristic on two input characteristics, i.e. the changes of the concentrations depending on the values of two selected input variables.

Calculation of the static dependency is done by dialog window shown on Fig. 8. This dialog window allows entering type of the dependency (two or three dimensional), entering

appropriate input value or values, i.e. the lower limit, upper limit and step of change. Radio buttons allows selection of the vary characteristic based on which the dependency is calculated. The output data are saved directly to MS Excel spreadsheet in the defined format and via the chart tools of the Excel the dependencies can be visualized.

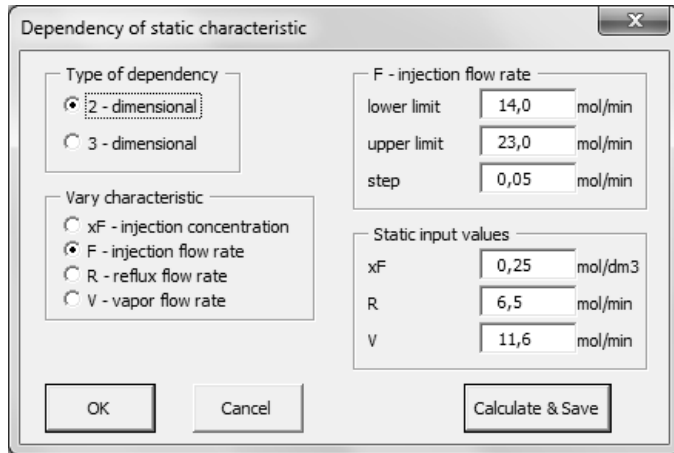


Fig. 8 Dialog window for calculation of dependency of static characteristic

Calculation of the dependency of static characteristic starts by press "Calculate & Save" command button. The following procedure is executed:

```
Private Sub CB_CalcSave_Click()
    ****input variables***
    No_of_Storeys = Sheet("Main").Cells(10, 2)
    Inject_Storey = Sheet("Main").Cells(11, 2)
    If Selection = "F" Then
        xF = TInput1.Text
        R = TInput2.Text
        V = TInput3.Text
        LowF = TLowLim.Text
        UppF = TUpLim.Text
        StepF = TStep.Text
        ****calculation and storage***
        ****of static dependemce***
        For F = LowF To UppF
            For i = 1 To Inject_Storey - 1
                xi = Static_xi(i, xF, F, R, V)
                Cells(F, i) = xi
            Next i
            xm = Static_xm(Inject_Storey, xF, F, R, V)
            Cells(F, Inject_Storey) = xm
            For j = Inject_Storey + 1 To No_of_Storeys
                xj = Static_xj(j, xF, F, R, V)
                Cells(F, j) = xj
            Next j
            xD = Static_xD(xF, F, R, V)
            Cells(F, No_of_Storeys + 1) = xD
        Next F
    End If
End Sub
```

```
xW = Static_xW(xF, F, R, V)
Cells(F, No_of_Storeys + 2) = xW
```

```
Next F
End If
End Sub
```

The output command of type $Cells(F, i) = xi$ stores calculated values directly in MS Excel sheet, from which appropriate dependency can be visualized in XY chart.

Similar procedures are created for vary input characteristic x_F , R and V .

D. Dynamic simulation computer model

A computer program in VBA provides the following dynamic simulations:

- calculation of the dynamic transition characteristics;
- visualization of the dynamic process.

1) Calculation of the transition characteristic

The transition characteristic is time dependence of the output characteristic (x_D , x_W , x_i and x_j) after the step change of one or more input variables (x_F , R , F or V).

The input dialog box for the simulation of the transition characteristics of the rectification column is shown on Fig. 9.

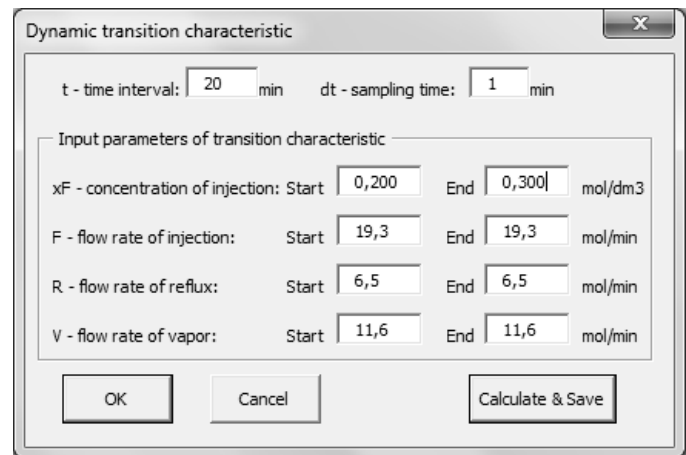


Fig. 9 Dialog window for the simulation of the dynamic transition characteristics

In this dialog box there are entered start and end values of all four input variables (x_F , R , F or V), time interval t and sampling time Δt . The output characteristic (x_D , x_W , x_i and x_j) are saved directly to MS Excel spreadsheet in the defined format and via the chart tools of the Excel the dependencies can be visualized.

Calculation of the output transition characteristic of dynamic model is given by solution of the set of the equitations (15) ÷ (20).

Calculation of the transition dynamic characteristic starts by press "Calculate & Save" command button. The following procedure is executed:

```
Private Sub CB_CalcSave_Click()
    ****input variables***
```

```

No_of_Storeys = Sheet("Main").Cells(10, 2)
Inject_Storey = Sheet("Main").Cells(11, 2)
xF1 = TxF1.Text
xF2 = TxF2.Text
R1 = TR1.Text
R2 = TR2.Text
V1 = TV1.Text
V2 = TV2.Text
F1 = TF1.Text
U2 = TF2.Text
t_interval = Tt.Text
dt = Tdt.Text
  ****inicialization part****
For i = 1 To Inject_Storey - 1
  xi = Static_xi(i, xF, F, R, V)
  Cells(1, i) = xi
Next i
xm = Static_xm(Inject_Storey, xF, F, R, V)
Cells(1, Inject_Storey) = xm
For j = Inject_Storey + 1 To No_of_Storeys
  xj = Static_xj(j, xF, F, R, V)
  Cells(1, j) = xj
Next j
xD = Static_xD(xF, F, R, V)
Cells(1, No_of_Storeys + 1) = xD
xW = Static_xW(xF, F, R, V)
Cells(1, No_of_Storeys + 2) = xW
  ****calculation and storage****
  ****of transition characteristic****
For t = 1 To t_interval Step dt
  For i = 1 To Inject_Storey - 1
    xi_old = Cells(t, i)
    xi = Dynamic_xi(i, xF, F, R, V, xi_old)
    Cells(t + 1, i) = xi
  Next i
  xm_old = Cells(t, Inject_Storey)
  xm = Dynamic_xm(Inject_Storey, xF, F, R, V, xm_old)
  Cells(t + 1, Inject_Storey) = xm
  For j = Inject_Storey + 1 To No_of_Storeys
    xj_old = Cells(t, j)
    xj = Dynamic_xj(j, xF, F, R, V, xj_old)
    Cells(1, j) = xj
  Next j
  xD_old = Cells(t, No_of_Storeys + 1)
  xD = Dynamic_xD(xF, F, R, V, xD_old)
  Cells(1, No_of_Storeys + 1) = xD
  xW_old = Cells(t, No_of_Storeys + 2)
  xW = Dynamic_xW(xF, F, R, V, xW_old)
  Cells(1, No_of_Storeys + 2) = xW

```

Next t

End Sub

Calculation of the initial values of x_i is executed by function `Static_xi(i, xF, F, R, V)`. Similarly are calculated initial values of x_D , x_W and x_j .

Calculation of the transition characteristic x_i in step $(k + 1)$ is done by function:

`Dynamic_xi(i, xF, F, R, V, xi_old)`,

where parameter i is location of the storey, parameters x_F , F , R , V are input characteristic and parameter xi_old is value of x_i in previous step k .

Similarly are calculated output characteristic x_D , x_W and x_j .

The output command of type `Cells(t + 1, i) = xi` stores calculated values directly in MS Excel sheet, from which appropriate transition dependency can be visualized in XY chart.

2) Visualization of the dynamic process

The actual process of the simulation of transition dynamic characteristics is shown in the visualization window shown on Fig. 10. By clicking the Start button the simulated experiment starts, can be stopped at any time by clicking Stop button and then resume by clicking the Start button again. The visualization window step by step displays values of all output characteristic (x_F , x_D , x_W , x_1 , x_7 , D and W) depending on input values (x_F , R , F , and V) at simulated time t . Simulated time passes much faster than real time, so the simulated experiments takes considerably less time than the experiments in the real system.

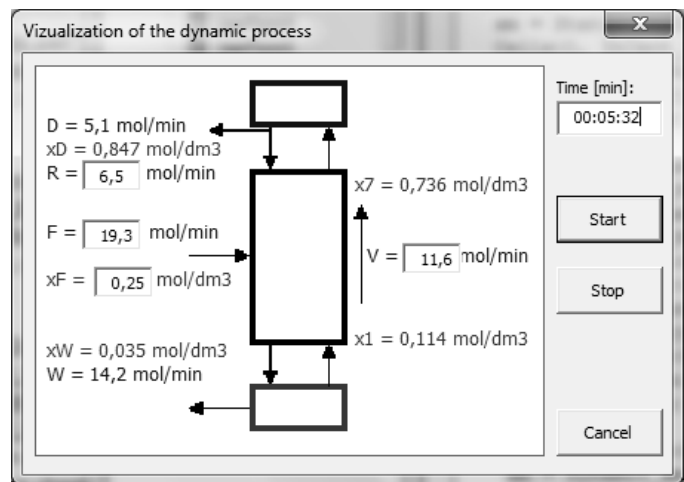


Fig. 10 Visualization window displaying time dependency of the dynamic characteristic of the experiment

VI. MODEL VERIFICATION

Validation of the static and dynamic mathematical models as well as verification of the simulation models of the rectification column was realized by comparison of dependency of the output characteristic on input characteristic derived from the simulations models with the same data dependency got from the measurement of the real experiment.

A. Verification of static model

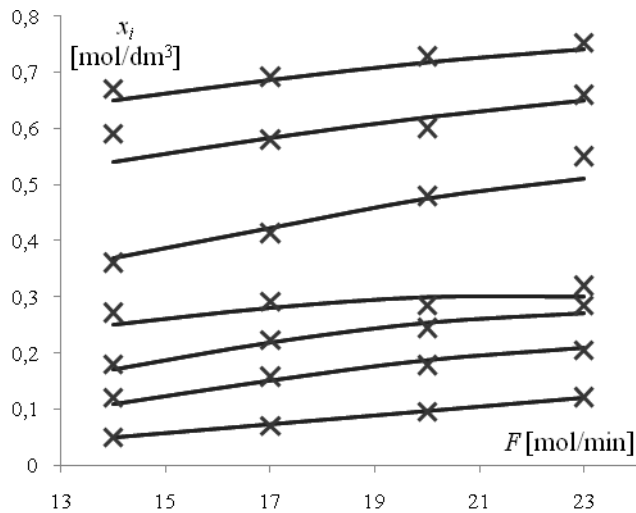


Fig. 11 Example of verification of static model

An example of verification of static model - comparing of calculated and measured dependencies is shown on Fig. 11. The lines represent the x_i dependency on F derived from the mathematical model while crosses represent the same dependence got from the measurement. The other input values were set as follows: $x_F = 0.25$ mol/dm³, $R = 6.5$ mol/min, $V = 11.6$ mol/min.

B. Verification of dynamic model

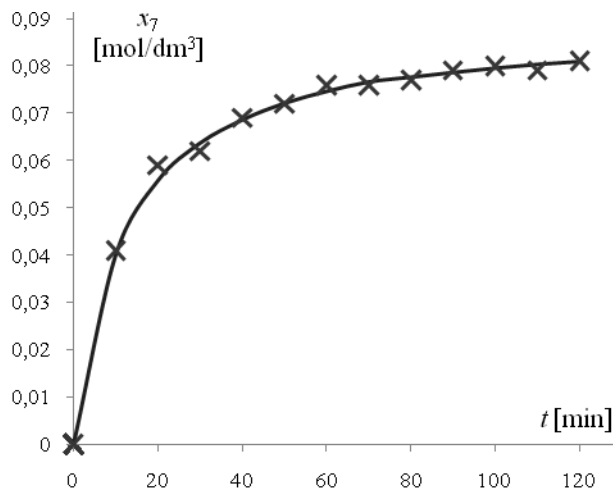


Fig. 12 Example of verification of dynamic model

An example of verification of dynamic model - comparing of calculated and measured dependencies of transition characteristic is shown on Fig. 12. The lines represent time dependency of concentration x_7 after step change of value of the flow rate of the reflux from $R = 6.49$ mol/min to $R = 7.39$ mol/min derived from the mathematical model and calculated by the transition characteristic simulation model. Crosses represent the same dependence got from the measurement.

VII. CONCLUSION

Modeling and computer simulation together with multidisciplinary approach provides new methodology of experimental research in current science – see e.g. [14].

In the paper there was offered the case study of process of modeling and simulation of real experimental device – seven storey rectification column. Step by step there is shown this process from formation of the mathematical model, creation of the simulation model in Visual Basic for Excel to visualization and verification of the model in MS Excel XY chart.

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