



Automation of Control's Process of Macro of Microsoft Excel File for Data Processing of Chemical Experiments

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ABSTRACT

In this paper, an approach for experimental data processing using Microsoft Excel was proposed. The experimental data was automatically transferred to a common file using the developed macro. An application was developed to accelerate the operation of the macro and reuse it. The structure of the macro was described in the paper. The created approach can be applied in tasks that require the storage of a large statistical data volume. Testing of approach was carried out on the results of chemical experiments.

Keywords: Storage of Large Data Volume, Automation, Experiment Processing, Macro.

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INTRODUCTION

Any scientific study is accompanied by an experiment. The experiment is the same experience with certain conditions. The main purpose of the experiment was testing the validity of the formulated hypothesis, as well as revealing the characteristics of the objects under study. The experiment can be carried out in natural (full-scale experiment) and artificial (computational experiment) conditions. The experiments are conducted in scientific laboratories and in industry, in medical clinics and agricultural fields, in outer space and in the depths of the ocean. In each case, the experiments are accompanied by a large received data volume. The examples of these experiments are data on the exchange rate during the year, data on air temperature in some areas, the results of the strength of the concrete samples for compression and more. Now, the analysis of experimental results is inconceivable without using computers and software packages. Using computer programs allows performing primary data processing with the ability of

graphical representation and data analysis using statistical methods. Thus, the task of automating the experimental data processing using an application program has been relevant.

MATERIALS AND METHODS

In this study, the process of automating the processing of experimental data on the synthesis of styrene-butadiene copolymer was considered. Styrene-butadiene rubber was obtained as a result of copolymerization in continuous stirred tank reactors. The resulting copolymer was processed into rubber during vulcanization. The choice of the investigated process was due to the fact that among the large-capacity synthetic rubbers of general purpose, the most common was styrene-butadiene rubber. It accounts for about 50% of the world's synthetic rubber's production, and 75% of the consumption of such rubbers falls on the production of passenger car's tires.

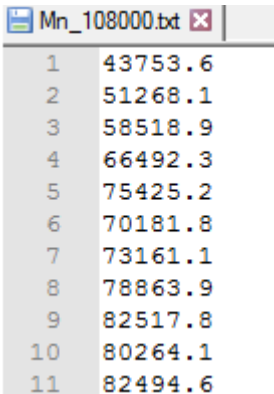
The study of the process and characteristics of the formed product under industrial conditions was labor intensive. To solve the problem, the methods of mathematical modeling were used. Earlier, in [1, 2] the kinetic scheme of the inves-

tigated process was described. In [3], the approach to simulation of the process was offered, and the algorithm was developed. The algorithm was based on the Monte Carlo method. The Monte Carlo method simulates a random process – creation of copolymer's macromolecules at particle level. Such an imitation of the process makes it possible to easily obtain the molecular weight's and viscosity's characteristics of the resulting product at any time.

It has been known that, in industry the process under study has been carried out in a continuous mode simultaneously in several reactors. All the reactors have been united in cascade. The process has been accompanied by continuous feeding of new reagents into the reactor and continuous output of interaction products. This has been due to a significant reduction in costs for operating of reactors, an increase in the total operating time, the stability of the technological regime, and the stability of the product. Therefore, in constructing the model, each particle of the system was characterized by the residence time in the reactor in accordance with a random distribution [4, 5].

Using the developed algorithm, the authors created a software package for data simulation. The software package was designed for carrying out computational experiments on the simulation of a continuous process of copolymerization in a cascade of stirred tank reactors. The software package made it possible to solve the direct problem of determining the molecular weight's and viscosity's characteristics of the product, as well as to investigate the composition distribution of the formed copolymer. In particular, the number average and weight average molecular weight of the copolymer, the polydispersity index, the intrinsic viscosity and Mooney viscosity, monomers conversion, weight content of monomers in copolymer, microheterogeneity index, etc. are determined. Information on the consumption of the components of the reaction mixture could also be obtained. The results were stored in text files. The name of each file contained a prefix. Each prefix corresponded to a product's characteristic (Mn, Mw, etc.) and the

current time (in seconds). All information was stored in a file according to a given characteristic for each reactor of the cascade for each hour of the experiment. For example, the file Mn_108000.txt contained data of the number of the average molecular weight of the styrene-butadiene copolymer. These data were obtained within 30 hours of the simulation of the process (Fig. 1). Thus, after a computational experiment, a large volume of unprocessed statistical data was accumulated.



Row	Value
1	43753.6
2	51268.1
3	58518.9
4	66492.3
5	75425.2
6	70181.8
7	73161.1
8	78863.9
9	82517.8
10	80264.1
11	82494.6

Fig. 1. The example of a text file with the results of an experiment

Statistical data must be collected in a common file. Due to the wide distribution of Microsoft Office products, it will be expedient to use the Microsoft Excel product. The file format allowed presenting data simultaneously in a tabular and graphical form. This provided the researcher to evaluate the dynamics of product characteristics.

For example, the file for storing the results of the experiment was created. In the file, there were sheets with fields for all the possible characteristics of the product. And a sheet called "Portion parameters" was also created. This sheet contained information about the compliance of the characteristics of the copolymer, prefixes in the names of text files, and the names of sheets in the Microsoft Excel file (the fragments of the table have been shown in Fig. 2). The information about the folder was indicated in one of the cells of the sheet. This folder stored text files with the results of the experiment.

Mask	Mn	
Sheet name	Mn	
Path	D:\Stat\	
Sheet name	Mask	Characteristic
Mn	Mn	Number-average molecular weight
Mw	Mw	Weight-average molecular weight
Conversion	Conv	Conversion
Chain transfer agent consumption	Reg	Chain transfer agent consumption
Initiator consumption	In	Initiator consumption
Butadiene consumption	ButC	Butadiene consumption
Styrene consumption	StC	Styrene consumption
Composition	But	Mass content of butadiene
Composition	St	Mass content of styrene

Fig. 2. Fragments of the Microsoft Excel template file

Manually copying the experimental data by the user into a template file consisted of the following steps: open a text file, copy the data, go to the template file, insert the data into the selected area, and close the text file. Due to the large data volume of the computational experiment, the independent data entry into a common Microsoft Excel file will take a long time. Therefore, the primary data processing of the same type of text files must be organized using a macro. A macro is a program from a list of commands that are automatically executed by the application in place of the user [6]. The built-in programming language Microsoft Excel Visual Basic for Applications (VBA) was used to develop the macro [7]. The macro code for automatic data entry is shown in Fig. 3.

RESULTS AND DISCUSSION

The action of the macro allowed automating the transfer of information from text files to a template file for a specific characteristic. The choice of characteristics was determined by the user. When the characteristic changed, the macro must be restarted. There was another problem,

that was the creation of a macro by users. Therefore, the next step was to create a software module (application). This module should automate the re-execution of the macro.

To implement the application, the researchers used the Microsoft Visual Studio development environment and the C# programming language with the Microsoft Excel Object Library [8]. The software product interface is shown in Fig. 4. When working with the application, the user must specify the path to the Microsoft Excel template file, the path to the folder with the files – the results of the experiment – and then select the characteristics. The application automatically analyzed the list of available data in the specified folder, and made the corresponding sheets available.

After selecting the parameters, pressing the "Start Macro" button created a copy of the specified Microsoft Excel file. Then, the macro worked in the sheets of the file.

Fig. 5 shows an example of a Microsoft Excel file before the application ran (only the data of the industrial experiment were shown on the graphs). Fig. 6 – a file, which contains the results of the computer experiment after the automated filling.

```

Sub Данные()
    Dim coll As Collection, dirPath, maskSearch
    dirPath = Worksheets("Параметры порции").Cells(24, 2).Value
    maskSearch = Worksheets("Параметры порции").Cells(19, 2).Value + "_*.txt"
    wsname = Worksheets("Параметры порции").Cells(20, 2).Value
    numbColl = Worksheets("Параметры порции").Cells(22, 2).Value
    j = Worksheets("Параметры порции").Cells(23, 2).Value
    Set coll = FilenamesCollection(dirPath, maskSearch, 1)
    Application.ScreenUpdating = False
    For i = 1 To coll.Count
        filePath = coll(i)
        thisfile = dirPath + Dir(filePath)
        fileNumber = FreeFile
        numbColl = numbColl + j
        Open thisfile For Input As #fileNumber
        Ctr = Worksheets("Параметры порции").Cells(21, 2).Value
        Do
            Line Input #fileNumber, Data
            Ctr = Ctr + 1
            Worksheets(wsname).Cells(Ctr, numbColl).Value = Data
        Loop While EOF(1) = False
        Close #fileNumber
    Next
End Sub

Function FilenamesCollection(ByVal FolderPath As String, Optional ByVal Mask As String = "", _
    Optional ByVal SearchDeep As Long = 999) As Collection

    Set FilenamesCollection = New Collection
    Set FSO = CreateObject("Scripting.FileSystemObject")
    GetAllFileNamesUsingFSO FolderPath, Mask, FSO, FilenamesCollection, SearchDeep
    Set FSO = Nothing: Application.StatusBar = False
End Function

Function GetAllFileNamesUsingFSO(ByVal FolderPath As String, ByVal Mask As String, ByRef FSO, _
    ByRef FileNamesColl As Collection, ByVal SearchDeep As Long)
    On Error Resume Next: Set curfold = FSO.GetFolder(FolderPath)
    If Not curfold Is Nothing Then
        Application.StatusBar = "Поиск в папке: " & FolderPath

        For Each fil In curfold.Files
            If fil.Name Like "*" & Mask Then FileNamesColl.Add fil.Path
        Next
        SearchDeep = SearchDeep - 1
        If SearchDeep Then
            For Each sfol In curfold.SubFolders
                GetAllFileNamesUsingFSO sfol.Path, Mask, FSO, FileNamesColl, SearchDeep
            Next
        End If
        Set fil = Nothing: Set curfold = Nothing
    End If
End Function

```

Fig. 3. Macro code for transferring data from text files

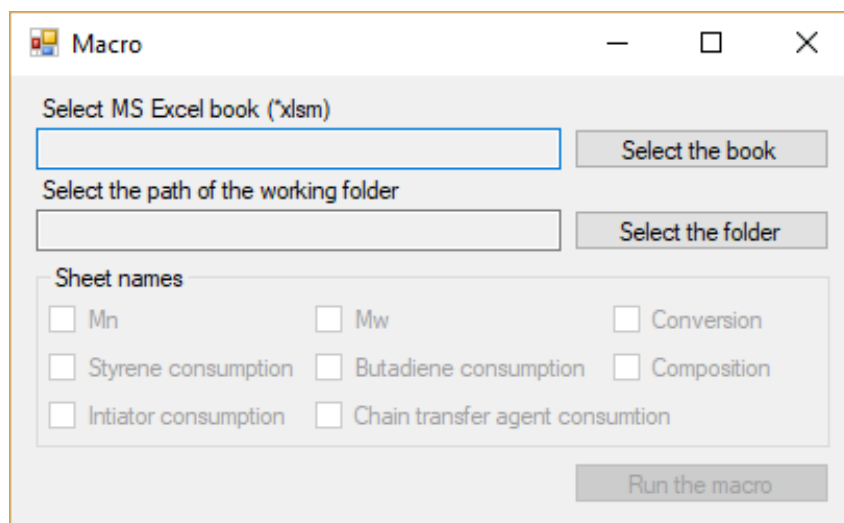


Fig. 4. The application interface

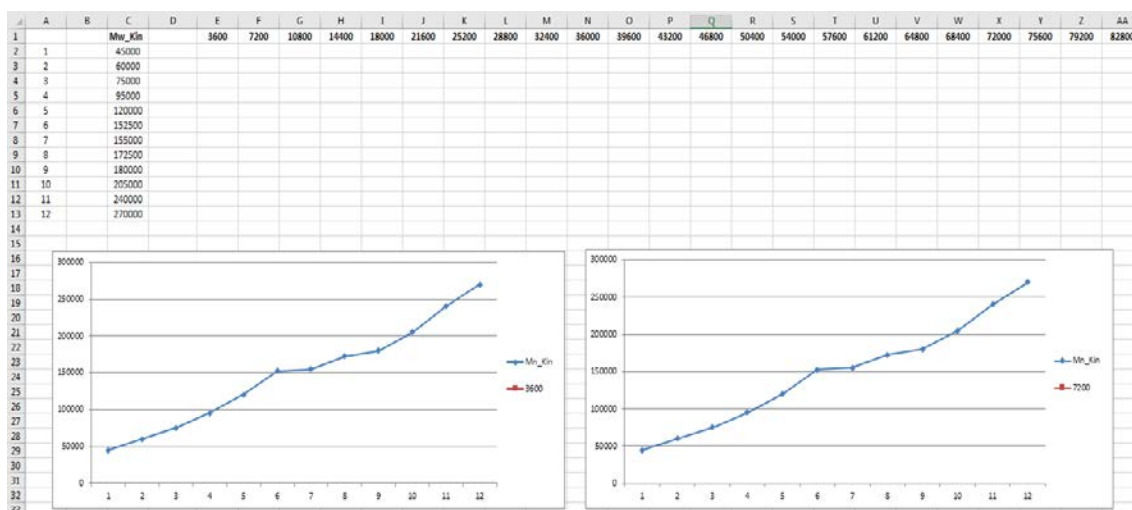


Fig. 5. Sheet's structure for storing experiment's results in a template file

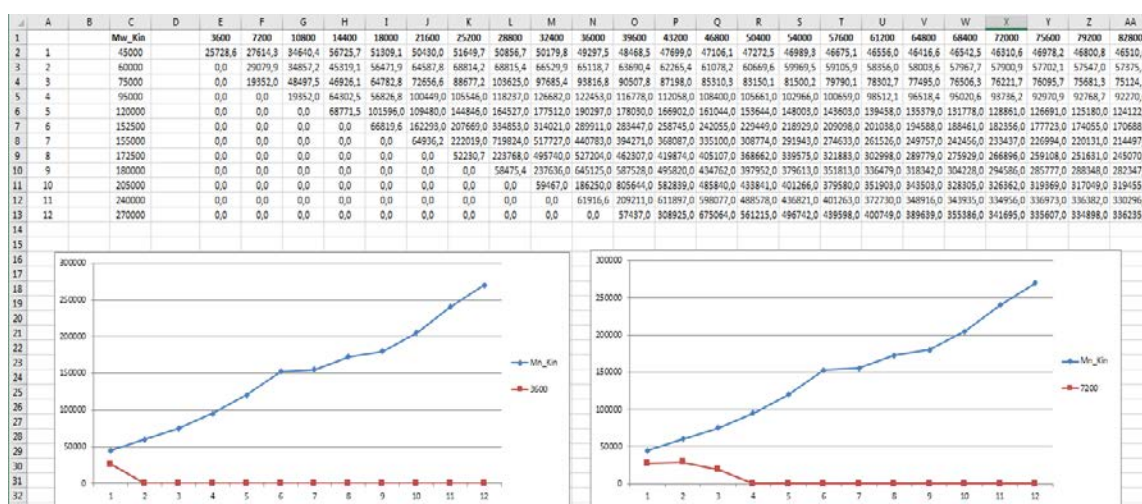


Fig. 6. Results of writing data to a template file

CONCLUSION

The macro was created in the paper. It allowed automating the process of transferring data from text files of the same structure to a common template file. The application was developed to work with the macro. This software product allows multiple launching of the macro without additional user involvement. The application was tested using data from a computational experiment for the synthesis of a styrene-butadiene copolymer. The generated common file can be used to analyze the influence of technological parameters and the formula of the reaction mixture on the characteristics of the copolymer [9]. The developed application can be applied for making decision for similar problems arising in other branches of science.

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