

Preface

Chemical kinetics is one of the parts of physical chemistry with the most developed mathematical description. Studying basics of chemical kinetics and successful practical application of knowledge obtained demand proficiency in mathematical formalization of certain problems on kinetics and making rather sophisticated calculations. In this respect, it is difficult or sometimes even impossible to make considerable part of such calculation without using a computer. With a mass of literature on chemical kinetics the problems of practical computing the kinetics are not actually discussed. For this reason the authors consider useful to state basics of the formal kinetics of chemical reactions and approaches to two main kinetic problems, direct and inverse, in terms of up-to-date mathematical packages Maple and Mathcad.

Why did the authors choose these packages?

The history of using computers for scientific and technical calculation can be conveniently divided into three stages:

- Work with absolute codes
- Programming using high-level languages
- Using mathematical packages such as Mathcad, Maple, Matlab,¹ Mathematica, MuPAD, Derive, Statistica, etc.

There are no clear boundaries between listed stages (*information technologies*). Working in mathematical program one may insert an Excel table,² as the need arose, or some user functions written in C language, which codes contain fragments of assembler. Besides, absolute codes are still using in calculators, which are of great utility in scientific and technical calculations. It is better to consider here not isolated stages of computer technique development but a range of workbenches that expand and interweave. This tendency results in sharp decrease of time required for creating calculation methods and mathematical models, leads to refusal of a

¹Matlab is more likely a special programming language rather than a mathematical package.

²The list of packages does not include Excel tables that are still the most popular application for computing. However, Excel just as Matlab holds the half-way position between programming languages and mathematical packages.

programmer as an additional link between a researcher and a computer, to openness of calculations, enable us to see not only result, but all formulas in traditional notation and also all intermediate data reinforced by plots and diagrams. It is openness, clearness of Mathcad calculations that makes the package attractive calculation and effective *educational* tool enabling us to use it as visualization of the basics of chemical kinetics.

Maple is justly considered to be the best package of the symbolic mathematics, particularly for analytical solution of differential equations. With this, the problems on chemical kinetics are often resolved into this task.

Mathcad and Maple were developed as program applications *alternative* to traditional programming languages. Sometimes a student or even a professional cannot solve a chemical problem because a certain step transforms it from chemistry into informatics demanding deep knowledge of programming languages. However, as a rule a chemist has no such knowledge (and does not have to). Mathcad and Maple enable us to solve a wide range of scientific, engineering, technical and training problems without using traditional programming.

A reader getting acquainted with the book content may form an opinion that the authors gave a slant towards Mathcad package and its “server development”, Mathcad Application/Calculation Server. The case is that Mathcad was initially developed as a tool for *numerical* calculations. In fact, numerical calculations lie at the center of the book. At the same time, chemical kinetics also requires *analytical*, symbolic calculations. If symbolic tools of Mathcad become insufficient for solving a particular problem we decided to take advantages of Maple – an acknowledged leader among systems of computer mathematics designed for analytical calculations.

Mathcad and Maple possess some properties allowing them to be popular both among “non-programmers” and even among aces of programming. The point is that work with these packages accelerates several times (in order) statement and solving a problem. The similar situation occurred during conversion from absolute codes to high-level programming languages (FORTRAN, Pascal, BASIC, etc.).

Even if a user knows programming languages quite well it is often appear helpful to use Mathcad on a stage of formulation and debugging of a mathematical model. One of the authors leads a team of programmers and engineers that has developed and successfully markets WaterSteamPro program package (<http://www.wsp.ru>) designed for calculations of thermal physical properties of the heat carriers at power stations. The final version of the package was written and compiled on Visual C++, but this project was hardly implemented without previous analysis of its formulae and algorithms in Mathcad, which possesses convenient visualization tools for numbers and formulae.

It should be also noted that in distinction from Excel Mathcad enables us to create calculations open for studying and further improvements.

“There is no rose without a thorn”. The main limitation of the mathematical packages was that, as a rule, they couldn’t generate executable files (exe files), which could be launched without the original program. In particular, this prevented a progressive phenomenon - dividing those sitting in front of a screen into *users* and *developers*. Usually, specialists working with mathematical programs, with

Mathcad, kept “subsistence production”: developed calculations for their own or for the a few colleagues, who can work with Mathcad. They could give their results only to those who had installed corresponding package. However, this person may not buy a ready-made file but try to create required file by his own. Actually, we consider now small calculations, which creating and checking out require time is comparable with time for searching, installing, and learning the same ready – made version. Although, rather bulky calculations find difficulty in opening the way to the market: the personal calculation can be improved or enlarged at any time but in case of somebody else’s calculation it is not. Here we can draw an analogy with another “internal Mathcad” problem. Sometimes it is easier to create a user function than find its completed version in the wilds of built-in Mathcad functions.

If a user was not acquainted with Mathcad package and did not have it in a computer it was possible to give him (her) a file only with a significant load, on condition that he (she) would install corresponding Mathcad version and would learn at least the basics of the program. Often it required to upgrade both operating system and hardware, or even to buy a new computer. It was also necessary to learn Mathcad.

Mathsoft Engineering and Education Inc., which was bought by PTC (<http://www.ptc.com>), a new owner of Mathcad package, in 2006, took actions to improve the situation. Firstly, they try to launch a free and shorten version, Mathcad Explorer, together with the eighth Mathcad release. Mathcad Explorer enabled us to open Mathcad files and calculate by them but not edit and save the documents on disks. The program itself could be downloaded from the internet free of charge. Secondly, the company actively developed tools for publication Mathcad worksheets on local networks and on the internet for studying but not for calculating. One of the main consumers of the mathematical programs is education branch in which the way to result, studying of the calculation methods, is more important than the result itself. In particular, Mathcad 2001i version, in which the letter “i” meant interactive, was designed for this.

However, all these solutions had no distant future. As was noted above, Mathcad Explorer, a rather bulky program, should be downloaded from the network and installed into a computer. In this case for solving intricate problems it is better to install Mathcad itself, which is recently possible to download from the network for prior charge, rather than a shorten version. On the other hand, it is desirable not only to view Mathcad worksheets, or rather their html or MathML copies (casts), opened on the network but also to transform them, change initial data and view (print, save) a new result. The solution of this problem, almost complete rather than partial, turned out to be possible with the help of internet again.

Mathcad Application Server (MAS) was put into operation in 2003 (it was renamed into *Mathcad Calculation Server* – MA/CS in 2006) enabling us to run Mathcad worksheets and call them *remotely* via the internet.

MA/CS technology allows us to solve the following problems:

- There is no need to install required version of Mathcad, or it’s shorten version Mathcad Explorer (see above), find somewhere, check executable files for

viruses and run them. We only have to connect computers to the Internet, access MA/CS server using Internet Explorer (version 5.5 and higher) or any browser installed in the palmtop computers or smart phones. This looks as if we work with Mathcad worksheet: we can change source data; make calculation and get a result (save and print). Calculation method (formulas in traditional notation but not in the program form; this feature makes Mathcad widespread) and intermediate data can be visible or hidden partially or completely.

- New methods of calculation, open for studying, become available instantly to all surfers of the Internet, or staff of a corporation, or researchers of a university. We should only give corresponding addresses to users. Moreover, information about suchlike calculations can appear in the databases of different search engines (yandex, google).
- Any error, misprint, imperfection and assumption in a calculation noted by an author or users can be corrected quickly. It is also easy to upgrade and extend calculations.
- The MA/CS technology does not exclude tradition capability to download Mathcad websheets from a server for their upgrading or extending. We only should make a corresponding reference in a document. There are two ways of using mcd-files. We can transfer them only for calculations on a working station having Mathcad installed and lock documents with passwords. Another way is to give them freely or sell them for work without limitations.
- The MAS technology allows us to cut down expenses for mathematical software for a corporation or a university. There is no need to install Mathcad to every computer for routine calculations, to equip all computer classrooms. Mathcad package is required now only for those who develop methods of calculations. The others can use corporation (university or open to public) MA/CS.

It was MA/CS technology that used by the authors to develop educational project on chemical kinetics: <http://twi.mpei.ac.ru/MAS/Worksheets/Chem/ChimKin>. It is possible to get access to Mathcad web sheets collection by this reference and make basic kinetic calculations in remote access mode. For this purpose a user does to have to install Mathcad on the computer.

This book was published in Russian in 2009. Due to the internet project on chemical kinetics noted above almost all its pages have been translated into English, and the book became familiar to a large number of chemists all over the world. It becomes necessary to translate the book into English and supplement it with new data that have been done by the authors.

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