Instructor Notes for ABC Kinetics©

Jorge A. Carrazana García
Universidad de Santiago de Compostela
Facultad de Ciencias de Lugo
Departamento de Quimica Fisica
Lugo 27002. Spain.
Telef.: +34-982-285 900 Ext. 24132
e-mail: uscqfjcg@cesga.es

Archive	Contents
ABCKinetics7.zip	ABC_Kin.hbk and folder ABC_Kin with all the files of the e Book for version 7 of Mathcad
ABCKinetics11.zip	ABC_Kin.hbk and folder ABC_Kin with all the files of the e Book for version 11 of Mathcad
ABCKinetics_htm.zip	e Book image in html format
ABCKinetics_pdf.zip	e Book image in pdf format

Using the pdf image.

Once extracted from the corresponding compressed archive, is ready to print. For viewing the file **ABCKinetics.pdf** Adobe Acrobat or Adobe Acrobat Reader is needed.

Steps for using the "Web page" version of the book, are:

1. Unzip the archive **ABCKinetics_htm.zip** to an empty folder.
2. Open the file **ABC_Chemical_Kinetics_Ini.htm** with the Internet browser: MS Internet Explorer or Netscape Communicator.

Mathcad is not necessary for viewing the "Web page" version of the book, because it is mathematically inactive. Nevertheless, the hypertext properties are conserved because the active links in the Mathcad e-book still work in its html image. In the Web version the interactivity consists in browsing around the different pages.

Steps for using the "live" Mathcad e-book are:

1. Unzip the archive ABCKinetics7.zip or ABCKientics11.zip to an empty folder. After that, this folder will contain the file **ABC_Kin.hbk** and the subfolder **ABC_Kin** with all the e-book files inside.
2. Open Mathcad (version 7 or later for ABC_Kin_7, or version 11/2001i or later for ABC_Kin_11).
3. Execute the menu command **Help/ Open book**.
4. Search for the file **ABC_Kin.hbk** and open it.

Notes:

The user will have two ways for browsing through the book: (1) linearly, using the buttons on the book control palette along the top of the Mathcad window, or (2) non-linear exploration, clicking in the links activated in the Table of Contents, in the bottom of each worksheet and anywhere the user see a "roman underlined" text region. As detailed in the legend below the Table of Contents, some icons in the worksheets have associated hyperlinks too.

Like QuickSheets and the Resource Center, these e-books are a collection of live Mathcad worksheets hyperlinked and protected. The user can interact with the models shown and perform the numerical and graphical experiments. Normally, the changes are discarded when the book is closed and the next time the book is opened, it will show the original worksheet again. If the user chose to save the changes or annotate the book, Mathcad creates an annotated copy of the electronic book and it opens that copy, rather than the original, every time the book is opened in the future. The original state of the book is also saved so it is always possible to restore it.

Finally, no mater how much RAM a PC has, it is never enough. If a group of hyperlinked worksheets are opened successively with Mathcad, the moment will come when the PC memory is full. The next worksheet called will be charged incomplete and run time errors appear. On the other hand, if the group of worksheets is used in the electronic book format (via Help/ Open book menu command) Mathcad handles the memory in a more effective way; the complete set of worksheets can be browsed without these kinds of problems.

For solving the additional exercises in the worksheets it is recommended that the user work in an empty Mathcad worksheet, opened at the side of the e-book window. Relevant equations and graphs can be copied and pasted from the e book and finally the work can be saved as an independent worksheet with a unique file name.

Fonts

It is advisable to have installed the "MathSoft Text" font. Without this, the system shows the text in "Arial". This font occupies more space and it disarranges several regions of the documents, changing enough the aspect of the document so that reading and using the document may be tedious. This font difficulty affects mainly the web page version but may affect the Mathcad version’s ease of use.

Abstract/Summary:

The system formed by three chemical species "A", "B" and "C" related to each other by elementary reactions, reversible or not, is broadly used in Chemical kinetics as a first step in the study of the so-called "complex reactions". This model presents an appropriate

combination of mathematical complexity and chemical applicability that transforms it into a didactic resource of great educational value at various levels of Chemical Kinetics, Physical Chemistry or even basic General Chemistry, where reaction rates and mechanisms are of interest.

In this collection of worksheets, a step-by-step study of the "ABC" system is accomplished with the aid of Mathcad. Work in real math notation, interactive graphs and symbolic processing allows useful equations to be obtained, transformed and live applied, with the result of clarifying the study goals and objectives. By perturbing the values and immediately observing the effect can visually enhance the significance of the different model parameters. The proposed exercises not only consolidate the concepts and skills but also extend the analysis by applying the models and methods to other similar systems.

The organization of all the material a Mathcad electronic book format makes its use easy. The user can learn working with the interactive models, can annotate the book and, at the same time, the original information is conserved and stable. The PC's memory handling is more efficient when a group of Mathcad worksheets are part of an electronic book rather than used as individual sheets. The "live" book is presented for its use with the versions 7 and 11 of Mathcad. Non-interactive images of the book, in "pdf" and "html" formats are provided too.

Goal: Provide a systematic and interactive study of the "ABC" reaction scheme in order to help students to understand important methods and concepts of Chemical Kinetics.

Objectives: With the assistance of Mathcad, this study is accomplished in seven, non-necessarily consecutive steps, after which the student should be able to:

1. Obtain analytical equations for the reaction rates in function of time and use the mass balance to show the relation between them in a particular reaction scheme.
2. Apply the mathematical methods for function analysis to kinetic equations, obtaining important information for describing a reaction system.
3. Solve indeterminate forms in kinetics equations, using Calculus methods and automatic symbolic processing.
4. Evaluate, by means of an interactive graph, the Steady State Approximation, applying it to the system A-B-C where the exact analytical solution is known.
5. Evaluate, by means of an interactive graph, the Steady State and pre-Equilibrium Approximations, applying them to the system A=B-C where the exact analytical solution is known.
6. Evaluate, numerically and by means of an interactive graph, the usefulness of Mathcad ODE-solver in Chemical Kinetics, applying it to the system A=B-C with known analytical solution.
7. Model a general system that includes most of the "simple" and "complex" reactions studied in Chemical Kinetics and solve it using the Mathcad numerical ODE-solver, showing the results by means of an interactive graph.

Even when each worksheet in the book is part of an interconnected group, the different objectives can be worked individually. For this reason every theme is separately introduced and analyzed, and has its own exercises and references. This is graphically showed as rows in the book's Table of Contents. Alternatively, a vertical progression in the Table of Contents implies changes in the objective pursued and, eventually, a more general model under study.