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ARTICULO ORIGINAL

Transversality of mathematical modelling techniques in Pharmacy by means of a spreadsheet

Transversalidad de las técnicas de modelado matemático en Farmacia con la ayuda de una hoja de cálculo

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RESUMEN

La implantación del EEES en las titulaciones en Farmacia va a significar la potenciación del autoaprendizaje por parte del alumno. Esto va a poner a prueba la capacidad de aplicar conocimientos adquiridos en unas materias, para entender y conocer otras. Entre dichos conocimientos, se encuentran las técnicas de modelado matemático, incluidas en el campo de las Matemáticas. El presente artículo reflexiona acerca de la utilidad de las populares hojas de cálculo como software dirigido al alumno.
Un alumno de Farmacia, probablemente, tendrá que realizar cálculos matemáticos y representaciones gráficas con datos experimentales, muy especialmente en las prácticas de algunas de sus asignaturas. La utilización de un software es, en este sentido, especialmente importante, no sólo en la fase de aprendizaje de dichos conocimientos matemáticos en la correspondiente asignatura del título, sino a la hora de disponer de una herramienta que facilite su aplicación en otras. ¿Qué software podemos elegir para el alumno? A pesar de que existen multitud de candidatos, una hoja de cálculo reúne una serie de características que la hacen idónea para un alumno de Farmacia: corto tiempo de aprendizaje, amplia disponibilidad en distintas plataformas y flexibilidad para poder realizar una gran diversidad de tareas, entre otras propiedades.
Finalmente, como ejemplo se presenta una página Web, http://www.ugr.es/~focana/farmaspreadsheet.htm, que facilita material para ayudar al alumno de Farmacia a aprovechar las posibilidades que ofrecen las hojas de cálculo Excel (Microsoft Office) y Calc (OpenOffice.org) en el estudio de sus asignaturas en Farmacia.

ABSTRACT

The implementation of the EHEA in Pharmacy studies will lead to foster student self-learning. This way the student abilities to apply knowledge, learned in some subjects, to search knowledge in any other will be tested. Among such applicative knowledge, we can consider the mathematical modelling techniques, included in the field of Mathematics. This article draws attention to the usefulness of popular spreadsheets for Pharmacy students interested in the application of mathematical modelling techniques.
Roughly speaking, a pharmacy student will probably have to perform mathematical calculations and

experimental data visualizations, especially in the practice syllabus of some of his subjects. The use of software is important in this respect, not only in the learning step of the mathematical concepts in the corresponding math subject, but also in its application to other Pharmacy subjects. What application software can be chosen for the students? Although there are many candidates, a spreadsheet offers some capabilities that make it ideal for a Pharmacy student: short learning time, wide availability on different computer platforms and flexibility to carry out a variety of computational tasks.
Finally, we present a Web page which provides self-learning material to Pharmacy students for harnessing the potential offered by the spreadsheets Excel (Microsoft Office) and Calc (OpenOffice.org) in the study of their subjects in Pharmacy.

PALABRAS CLAVE: modelo matemático, representación gráfica, hoja de cálculo, transversalidad.

KEYWORDS: Pharmacy, mathematical model, data visualization, spreadsheet, transversality.

INTRODUCCIÓN

Lifelong learning is one of the main paradigms implicitly considered in the design of the well known European Higher Education Area (EHEA). Roughly speaking, it gathers those learning activities with the aim of improving knowledge, skills and competence. Behind this paradigm, we can find an answer implemented by European education policies to the scale of current economic, scientific and social changes in Europe. In some sense, lifelong learning based policies promote adaptation attitudes in the European society in order to strength Europe’s competitiveness and improving the employability (1).

Such knowledge-based adaptation capabilities can also be found in the well-known lemma “learning to learn”, which has been considered in the new Pharmacy degrees in Spain. Taking into account the wide range of changes in the pharmaceutical sciences nowadays, this lemma emphasizes the information search processes, which leads to points out their importance as part of the knowledge to be included in Pharmacy curricula.

Among such information search processes in Pharmacy, we can consider the mathematical modelling techniques, which are usually contained in the syllabus of its Math-like subject, named Biometry in the new degree in Pharmacy to be taught in Granada. Such modelling techniques are not only key topics in the math subject, but also are procedures which are constantly used in other subjects in the Pharmacy degree, mainly in their practice or experimental topics. Briefly, both mathematical calculations and experimental data visualization are skills to be often applied by students along the Pharmacy curriculum.

The aforementioned features of modelling techniques in Pharmacy lead to establish that such techniques are included in the transversal contents of Pharmacy degrees, i.e., such as is also known in education literature, they are one of the cross curricular components in Pharmacy degrees. In fact, the current adaptation of the Pharmacy degrees in Spain to the EHEA has been guided by considering Mathematics included in their set of basic scientific fields. However, the transversality of modelling techniques in Pharmacy is not an easy goal in practice, due to, on the one hand, the complexity of the involved mathematical concepts and, on the other hand, the hardness of the requested graphics and computing procedures when such techniques are applied in practice in Pharmacy.

This paper argues that the transversality of modelling techniques in Pharmacy studies could be enhanced by easing its applicability. In turn, one way of achieving this target consists of selecting a well suited software program to aid students to automate the procedures involved in mathematical calculations and data visualizations. As is known, this is a multiple choice problem wherein lots of factors can be considered: cost, time learning, efficiency, etc. In fact, this problem and the involved factors are discussed in what follows. In our case, taking into account the features of Pharmacy studies, we will propose the spreadsheets as an interesting software candidate to enhance the transversality of the mathematical modelling techniques.

This paper is sketched out as follows. Section 2 shows the transversality features of mathematical modelling techniques in Pharmacy curriculum, which motivates the discussion of selecting an optimal application software to be used in practice. Section 3 presents a software candidate, the spreadsheets, and discusses why they are an interesting choice for learning mathematical modelling techniques in Pharmacy. Finally, Section 4 illustrates how the ideas developed in this paper have been put into practice in Pharmacy studies in Granada by considering simultaneously both Excel and Calc (2).

MATHEMATICAL MODELLING TECHNIQUES: A TRANSVERSAL SUBJECT IN PHARMACY

Let us think about the mathematical modelling concepts involved across Pharmacy curriculum. Roughly speaking, they can be in summary clustered as follows:

- mathematical formulae calculation,
- calculus of a real function of one variable (derivative, integral, etc.),
- graphics of a real function of one variable,
- idem for a real function of two variables,
- basic Statistics,
- visualization of experimental data,
- regression.

These mathematical concepts are usually included in the like-math subject contained in the Pharmacy degrees in Spain. Moreover, some of the aforementioned concepts are considered in the development of some subjects on Pharmacy, what points out the transversality feature of the mathematical modelling techniques. Though in a non representative way, Figures 1 and 2 illustrate the application of mathematical modelling techniques in some problems studied in Pharmacy.

- Study of the dissolution profiles for two drug formulations, where several characteristics are computed for the two curves (4).

- Estimation of the Freundlich adsorption isotherm of oxalic acid on charcoal activated, where a non-linear model is estimated from experimental data.
- Estimation of the Michaelis-Menten kinetics curve of the phosphatase enzyme after using Lineweaver–Burk and the Eadie-Hofstee diagrams, where a non-linear model is estimated from experimental data by following two equivalent linear models.
- Determination of the equivalence point in strong acid/strong base titration by using (four methods) the pH curve, the first-derivative pH curve, the second-derivative pH curve and by Gran's method (5), where Calculus and regression concepts are considered.

This transversality feature should drive the curriculum design of such a math-like subject. Indeed such a feature must determine not only the syllabus of such a subject, but also the skills to apply the mathematical concepts by using information and communication technologies (ICTs). To be specific, an application software provides to the student an interesting tool both to understand the mathematical concepts, taught in such a math-like subject, and to apply in a efficiently way such concepts in Pharmacy studies, enhancing the transversality of such knowledge (6). For instance, in the degree of Pharmacy at Granada, the practice syllabus of the math-like subject is developed by using a software application. In this sense, the development of a computer-based subject in Pharmacy must be driven not only to handle the chosen application software, but also to the output interpretation, where to link between concepts and output evidences must be established. Because of this, the level of complexity to handle the considered application software should be minimized in a first stage, maximizing the time expended on interpreting mathematical outputs.

Finally, the use of a computer as a learning tool leads to the problem to be solved, at least partly, in this paper: what's the best software application for a Pharmacy student? For this non-unique solution problem, lots of software candidates could be considered. However, some factors must be taken into account to choice an optimal application software for the application of mathematical modelling techniques in Pharmacy studies. The following section tries answering the proposed question.

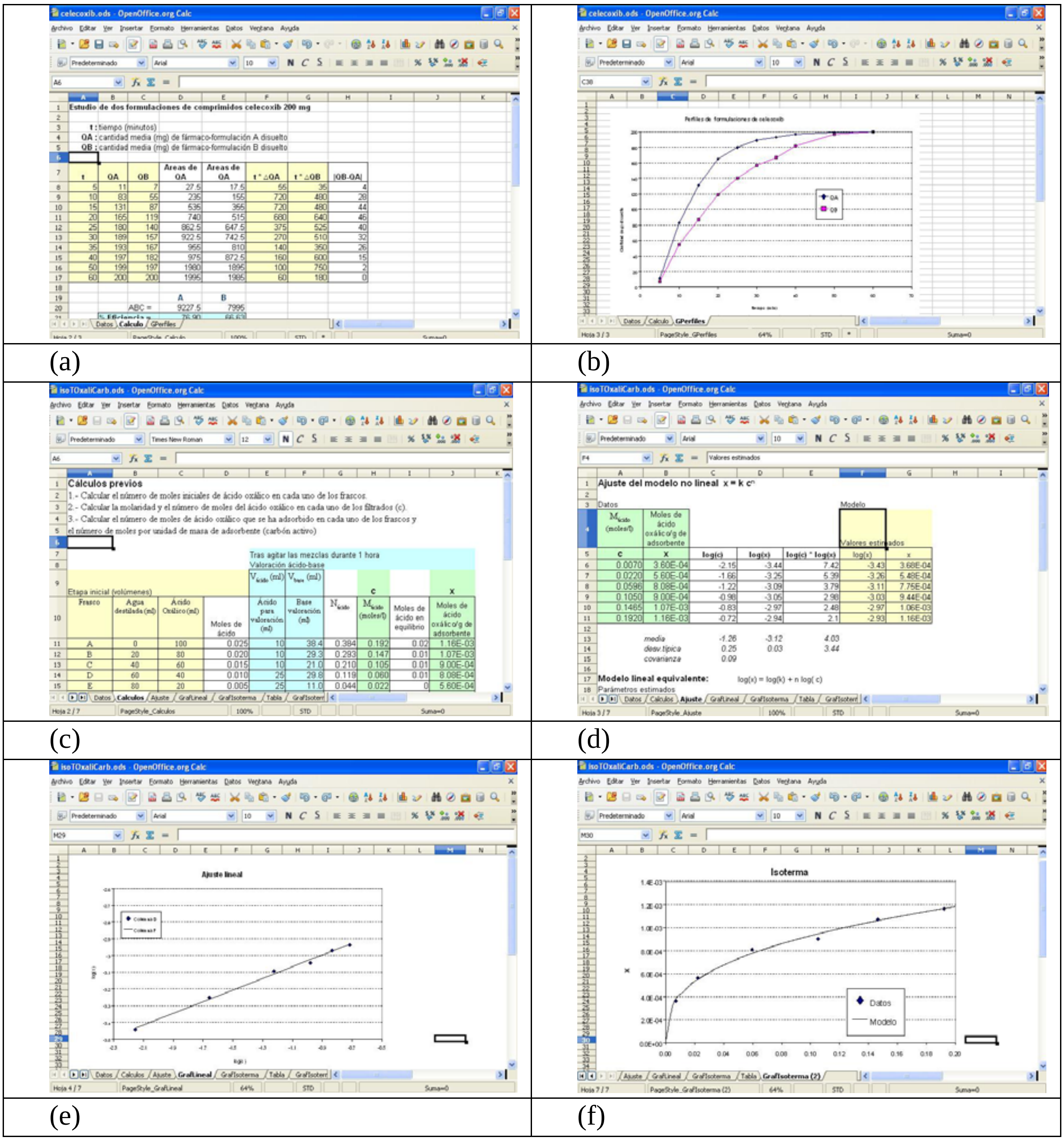
SPREADSHEETS: A CLASS OF SOFTWARE CANDIDATES

Spreadsheets are a type of software applications very popular in end-user PCs. Nowadays they are usually included in an office package, typically combined with other software applications (word processor, presentation program, etc.). Perhaps the best way of introducing this kind of software is by referring to some popular spreadsheets known by the reader: Excel, Calc, etc., though there were also several historical predecessors, for instance, Lotus-1-2-3. The connection between mathematics and spreadsheets can be noticed in the fact that the first spreadsheet, developed by Pardo and Remi, could not be patented in the U.S. Patent and Trademark Office, because it was initially considered a purely mathematical invention (NB: mathematical inventions can not be patented in USA).

First of all, spreadsheets are only one of the software candidates to enhance transversality of mathematical modelling techniques. Indeed there are a lot of software application candidates addressed to the mathematical calculation and visualization of experimental data.

However, a spreadsheet holds, in our view, a number of features that make it ideal as one of the top of the list of software applications for a Pharmacy student. Among such features, we can enumerate the following ones.

Figure 1. (a)-(b): Comparative study of the dissolution profiles for two Celecoxib formulations. (c)-(f): Freundlich adsorption isotherm of oxalic acid on charcoal activated: estimation procedure (step-by-step) and associated experimental data with plots of the estimated models.



1. Spreadsheets do not require excessive time for learning the basic concepts to get a beginner user level. Moreover, those spreadsheets providing a GUI (graphic user interface) assist the user with help functionalities. This is an interesting feature for Pharmacy students, as their average profile does not hold a specialized background on ICTs.

2. Regardless of their graphic settings, most of the spreadsheet GUIs exhibit many similarities between them (for instance, compare Excel or Calc). Thus, a user of a spreadsheet can become, with little effort, a potential user of any other spreadsheet, at least with a basic level. Hence, as this feature assures a significant level of interchangeability of spreadsheets, any student could even choose with no heavy effort a different spreadsheet for that available in his University teaching network. Hence, the spreadsheet chosen by the University does not impose critical bounds to the student learning or to the future use of any spreadsheet by him.

3. Spreadsheets are widely available under different operating systems on PCs, particularly under windows-like systems. Usually, a spreadsheet is contained in the popular office suites installed in almost all PCs. Possibly, a Pharmacy student can find an office suite almost everywhere (in the classroom, the lab, his home, etc.).

4. Taking into account the economic cost for the use of a spreadsheet, their prices are in a wide range: from a spreadsheet under some kind of free software licence or freeware agreement, to some other one which requires pay-per-use. This feature is a key factor not only for students, but also for institutions.

5. Spreadsheets provide a high degree of flexibility, as it allows the user to perform a variety of tasks, whether mathematical calculations or graphical representations of data (6). In order to easy their use, the most of them even provide a GUI where all their computational and graphics functionalities are easily managed. Taking into account the diversity of mathematical operations to be carried out by a Pharmacy student in a practice experience, this feature makes the spreadsheet an useful and easy-to-use tool in a wide range of tasks.

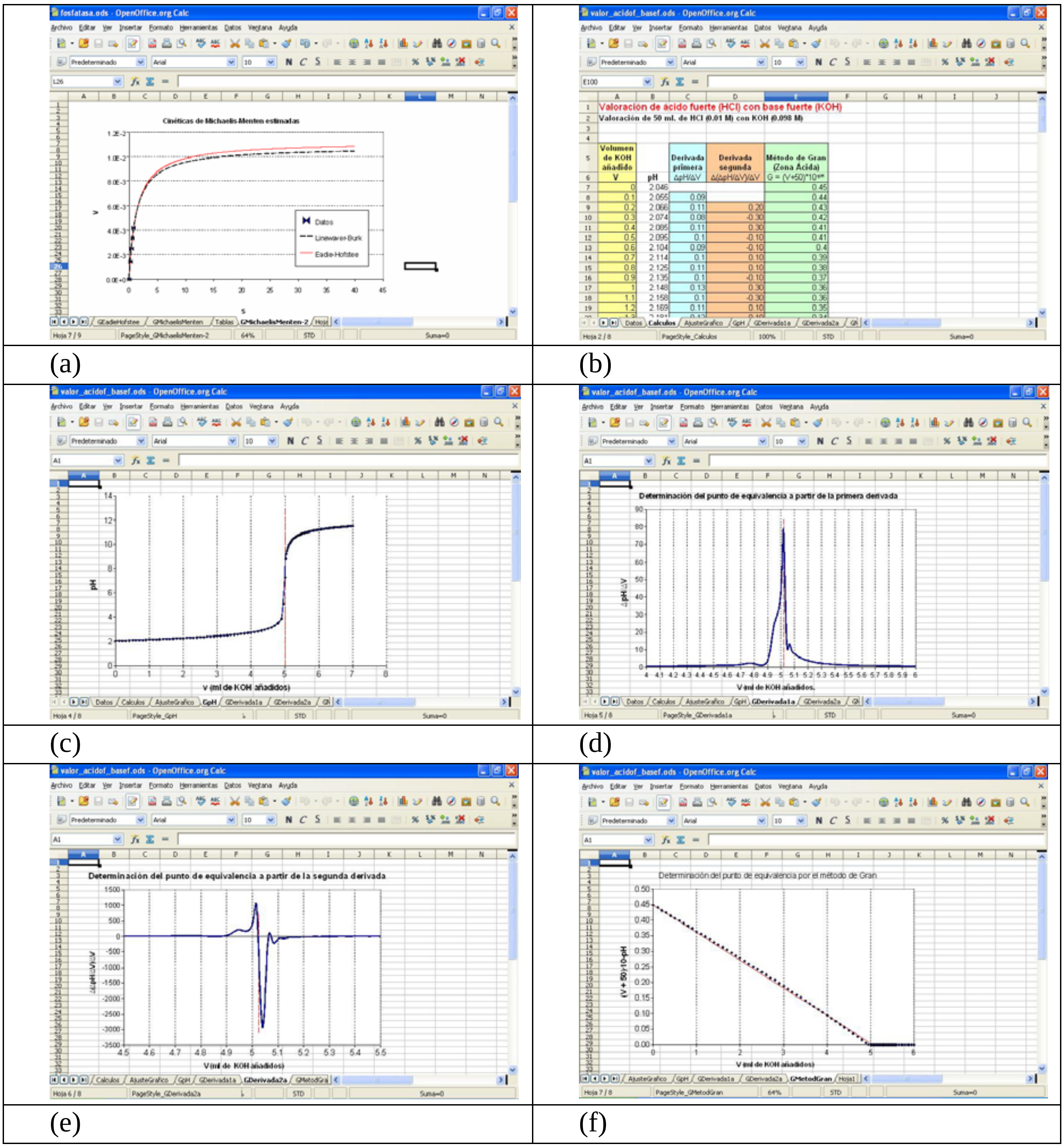
6. From a learning point of view, a spreadsheet offers an added value as its use emulates the "process of hand calculation".When a spreadsheet is used by a student to implement a certain process, it requires, and then it empowers, that the steps making up such a process must be understood by the student. Indeed, in a spreadsheet the student must organize calculations and graphic operations involved in the target-process in a way which is much closed to the classical hand-made strategy, but achieving much more computational efficiency.

7. Collaborative work is a learning paradigm in some of the learning guides of subjects in the EHEA adapted degrees. This relies on the idea consisting of learning is conceived not only as an individual experience, but also as a collective experience. This way, collaborative works constitute a test for carrying out medium scale projects and, then, a framework where knowledge and ideas are critically exchanged by students. In this regard, it is very interesting the new tool Google Spreadsheets (launched in 2006), which is included in Google Docs. This new tool is a web-based platform that makes it easier for student to manage and share spreadsheets online (7). It thus could enable Pharmacy students collaborating on worksheet-based projects, no matter where they are or when they need to access them. Consequently, the spreadsheet way of working is extended beyond the students' PC through the WWW.

These features make spreadsheets a very interesting learning tool in Pharmaceutical Sciences. However, we can not conclude that this type application software can be considered as the best software for mathematical modelling (8). Indeed there exists a wide range of alternative applications software which can be used for mathematical modelling, i.e.

Statgraphics, SPSS, S, R, etc. However, in the framework given by the Pharmaceutical degrees, the spreadsheet provides an easy-to-use and flexible software tool to be used in the majority of mathematical modelling projects addressed in Pharmacy degrees.

Figure 2. (a) Plot of the estimated Michaelis-Menten kinetics curve of the phosphatase enzyme after using Lineweaver–Burk and the Eadie-Hofstee diagrams, and scatterplot of the considered experimental data. (b)-(f) Determination of the equivalence point in strong acid/strong base titration by using (three methods) the pH curve, the first-derivative pH curve, the second-derivative pH curve and the Gran's method.



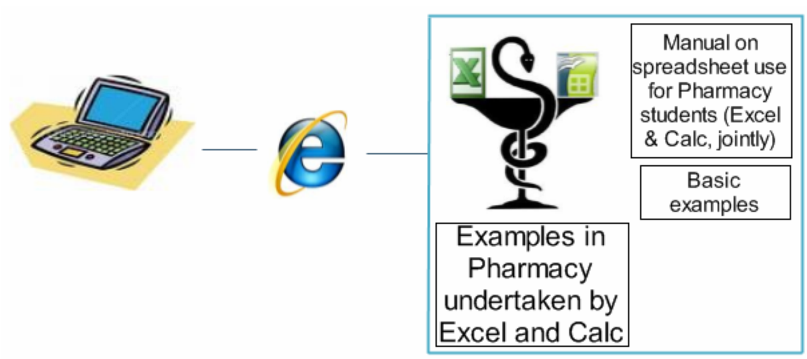
1. Online support for Pharmacy students

The ideas presented in this paper have been drawn from the teaching activities of a multidisciplinary group of professors in the Faculty of Pharmacy of Granada. Its activity were carried out through several informal collaborative initiatives, which consisted of testing the use of several applications software to develop some learning activities with a significant component on mathematical modelling addressed to Pharmacy students. Taking into account the average Pharmacy student profile, the option given by a spreadsheet emerged as one of the most appropriate to be considered for such students. Afterwards, this collaborative work was driven through the teaching project entitled "Self-learning material on mathematical modelling techniques using spreadsheet for Pharmacy students" (10).

The aforementioned project conceived such a student not only as a spreadsheet user, but also as a user who wants to apply mathematical modelling techniques in a Pharmacy project. In order to easy access to the material developed under this project, a Web page was also designed at http://www.ugr.es/~focana/farmaspreadsheet.htm. Among the available spreadsheets, two were considered in this project: Excel, which is included in the proprietary package Microsoft Office, and Calc, integrated in the free package by OpenOffice (2). The motivation for this duality relies on the wide spectrum of student's interest.

Finally, this project exemplified the capabilities of spreadsheets to enhance the transversality of mathematical modelling techniques in Pharmacy studies.

Figure 3: Flow diagram of a Website providing self-learning material on a spreadsheet for Pharmacy students (10).



REFERENCES

1. Commission of the European Communities. A Memorandum on Lifelong Learning. Brussels: CEC; 2000.
2. OpenOffice.org en Español, http://es.openoffice.org.
3. http://www.bologna-berlin2003.de/pdf/MemorandumEng.pdf
4. Montejo Rubio MC. Parámetros amodelísticos: comparación de perfiles. In: Antonio Aguilar Ros, coordinador. Biofarmacia y farmacocinética: ejercicios y problemas resueltos. Barcelona : Elsevier; 2008.
5. Petrucci RH, Harwood WS and Herring FG. Química General. Madrid: Prentice Hall; 2003.
6. Berk KN and Carey P. Análisis de datos con Microsoft Excel. Mexico: Thomson Editores; 2001.
7. Google Announces Google Docs & Spreadsheets. Official Google Press Release 2006-10-11. http://www.google.com/intl/en/press/annc/docsspreadsheets.html. Retrieved 2010-4-20.
8. McCullough BD. On the accuracy of statistical procedures in Microsoft Excel 2003. Computational Statistics & Data Analysis 2005; 49(4): 1244-1252.
9. Valderrama Bonnet, Mariano J. Modelos Matemáticos en las Ciencias Experimentales. Madrid: Ediciones Pirámide; 1995.
10. Ocaña FA, Escabias M, Jiménez F, Matilla A, Navarrete R, Ocaña FM, Rodríguez P and Valderrama MJ. Material de autoaprendizaje de técnicas de modelado matemático en Farmacia mediante hoja de cálculo, 2009. http://www.ugr.es/~focana/farmaspreadsheet.htm