Utilization of Mathematical Software Packages in Chemical Engineering Research and Design

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ABSTRACT

Engineers in the chemical industry are extensively using computers, but surprisingly only a very small percentage use mathematical software packages as was found in a recent survey by Davis et al. (1995). The authors of that survey suggested a possible explanation that "the industry tends to develop specialized users of scientific computing packages and that they, in turn, serve the needs of other engineers." The need of most engineers to turn to this specialized group for solving even moderately complicated design and analysis problems make their work much less efficient than it could be if they could effectively utilize software packages.

It is important to examine this under utilization of mathematical software packages by most engineers. Until recently, the textbooks used in undergraduate chemical engineering education did not emphasize numerical solution techniques because it was believed that computer solutions are more effective than the traditional techniques only for complex and complicated

problems. Indeed, until the emergence of interactive mathematical software packages (such as POLYMATH, MATLAB, MATHEMATICA), this approach was justified. If a computer solution required programming, in FORTRAN for example, the effort required and the level of expertise needed excluded all but complex, large-scale problems from computer solution. But the incorporation of advanced numerical and optimization capabilities into popular spreadsheet programs and the emergence of the user-friendly, interactive mathematical software packages has changed the situation. In order to enable most engineers to improve their productivity by effectively using advanced problem solution tools, new computer-based solution techniques for common design and analysis problems must be incorporated into the textbooks and industrial practice.

We have been working in recent years on developing various materials that can help the shift from traditional design techniques to those which utilize numerical methods on personal computers. Our book that contains extensive examples that require the use of computer for their solution for most required chemical engineering courses has been published (Cutlip and Shacham, 1999). The examples and assignments formulated in the book demonstrate the benefits of the use of the mathematical software packages in solving realistic engineering problems. Additionally, criteria for comparing mathematical software for engineering problems solving has been developed (Shacham et al., 1998, Shacham et al., 1996). Ten representative problems from various Chemical Engineering subject areas were selected, and this set of problems was solved using six numerical software packages (Excel, MAPLE, MATHCAD, MATLAB, MATHEMATICA and Polymath). The problems and solutions for the various packages are available from the Internet or FTP (Cutlip et al., 1998).

Our main conclusion from the aforementioned activities is that there are a wide variety of design and analysis problems that most engineers can solve effectively using the mathematical software packages, without needing help from computer specialists. This paper will illustrate this conclusion by the presentation of typical design problems from various subject areas of Chemical Engineering (i. e. heat, mass and momentum transfer, reaction engineering) which require various numerical techniques for solution (i.e. ordinary and partial differential equations, differential-algebraic systems). Representative solutions of these design problems will be used to demonstrate that effective solutions can be by most engineers using available software packages with much less effort than is required using traditional design techniques.

REFERENCES

1. Davis, J.F., G. E. Blau and G.V. Reklaitis, “Computers in Undergraduate Chemical Engineering Education: A Perspective on Training and Application”, **Chem. Engr. Ed.** (1), 50-55(1995).

2. Cutlip, M. B. and Shacham, M. *Problem Solving in Chemical Engineering with Numerical Methods.* Prentice Hall, Upper Saddle River, New Jersey, 1999.

3. Shacham, M., M. B. Cutlip, and N. Brauner, "General Purpose Software for Equation Solving and Modeling of Data", pp. 73-84 in Carnahan, B. (Ed), *Computers in Chemical Engineering Education*, CACHE Corporation, Austin, TX, 1996.

4. Shacham, M., N. Brauner and M. Pozin, "Comparing Software for Interactive Solution of Systems of Nonlinear Algebraic Equations", **Computers Chem. Engng**., Vol. 22, 321-323(1998).

5. Cutlip, M.B., Hwalek, J. J., Nuttal, H.E., Shacham, M., Brule, J., Widman, J., Han, T., Finlayson, B., Rosen E. M. and Taylor, R., “A Collection of 10 Numerical Problems in Chemical Engineering Solved by Various Mathematical Software Packages”, **Comput. Appl. Eng. Educ.** 6, 169-180(1998).
(Internet at http://www.polymath-software.com/ASEE/)

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