Effective Low-Cost Numerical Problem Solving Software
for ChE Education in Developing Countries

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Engineering education increasingly involves problem solving that requires numerical solutions of complicated systems of equations and/or regressions/curve fitting of extensive data. Software required for these types of problems can be expensive for academic departments, and typically it can also be very expensive for individual graduates when they start their professional careers.

Many engineering programs in developing have limited resources to provide this type of software for their faculty and students, and the latest personal computers that enable this software problem solving are in limited supply.

A possible solution to this challenge in the advancement of global engineering education is to be enabled by philanthropic cooperation of a non-profit educational corporation, the CACHE Corporation[1] (Computer Aids for Chemical Engineering Education) and Polymath Software[2]. These two organizations have been cooperating to provide low-cost site licenses of POLYMATH to mainly chemical engineering departments since 1990, with currently some 120 site licenses in use by universities world wide with most institutions being located in the USA.

A new initiative that provides these site licenses, at no cost to interested engineering departments or programs in developing countries is presented in this paper. This initiative will enable interaction numerical problem solving on a wide range of personal computers with Microsoft[3] operating systems of Windows 2000[3] through Windows 7[3]. These site licenses will allow distribution of individual copies of the software to all students, faculty and staff. In addition, the software may be installed in engineering computer labs and laboratories. Initial distribution of this software is being focused in Africa a this time.

POLYMATH Software – A Brief Overview

POLYMATH enables the user to apply effective numerical analysis techniques during interactive problem solving on personal computers with Microsoft operating systems. This software is extremely easy to use as there is no command language to remember. Results are presented in tabular or graphical formats for easy understanding and for incorporation into papers and reports. Capabilities now include a color-coded full-screen editor and allow for solution of problems involving Linear Equations, Nonlinear Equations, Differential Equations, Data Analysis and various types of Regression. Capabilities of POLYMATH are summarized in Table 1. The installation file is relative small, about 17 Mb, and the installed code requires only 9 Mb.

POLYMATH Software – A Very Simple Example

Let's consider a simple example of a model of a well-mixed batch reactor that is described by a system of ordinary differential equations. The batch reactor initially has only

reactant A. The reactions are first order and irreversible. This example will be solved with all three software packages.

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

Table 1 – POLYMATH Educational Version

- Linear Equations - up to 100 simultaneous equations.
- Nonlinear Equations - up to 30 simultaneous nonlinear and 40 explicit algebraic equations
- Differential Equations - up to 30 simultaneous ordinary differential and 40 explicit algebraic equations
- Data analysis and Regression - up to 300 data points with capabilities for linear, multiple linear, and nonlinear regressions
- Automatic Creation of Excel Spreadsheet Solution for Problem (include unique ODE_Solver Add-In for solving simultaneous first-order differential equations)
- Generation of Ordered MATLAB[4] Code for Problem

The differential mass balances on a batch reactor yield

$$\frac{dC_A}{dt} = -k_1 C_A \qquad \text{I. C. } C_A\big|_{t=0} = 1$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B \qquad \text{I. C. } C_B\big|_{t=0} = 0$$

$$\frac{dC_C}{dt} = k_2 C_B \qquad \text{I. C. } C_C\big|_{t=0} = 0$$

$$k_1 = 2 \qquad k_2 = 3$$

POLYMATH Solution – A Brief Look

Entry of this sample problem is accomplished within the POLYMATH full screen editor as shown in Figure 1. Note that entry is facilitated for new users by use of templates for the input of differential equations or explicit algebraic equations.
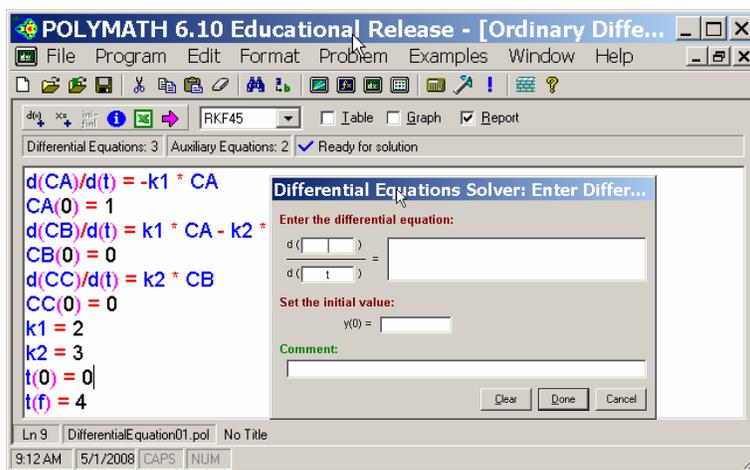

Figure 1 – Entry of Differential Equations into POLYMATH

Selection of the desired integration algorithm and the desired output followed by a mouse click on the highlighted arrow yields the numerical solution. The graph output option gives the expected result shown in Figure 2. Additional options for a Table of results and for a Report of the problem solution are not shown. The POLYMATH program can handle system of nonlinear ordinary differential equations with a variety of standard integration algorithms including those for stiff systems.
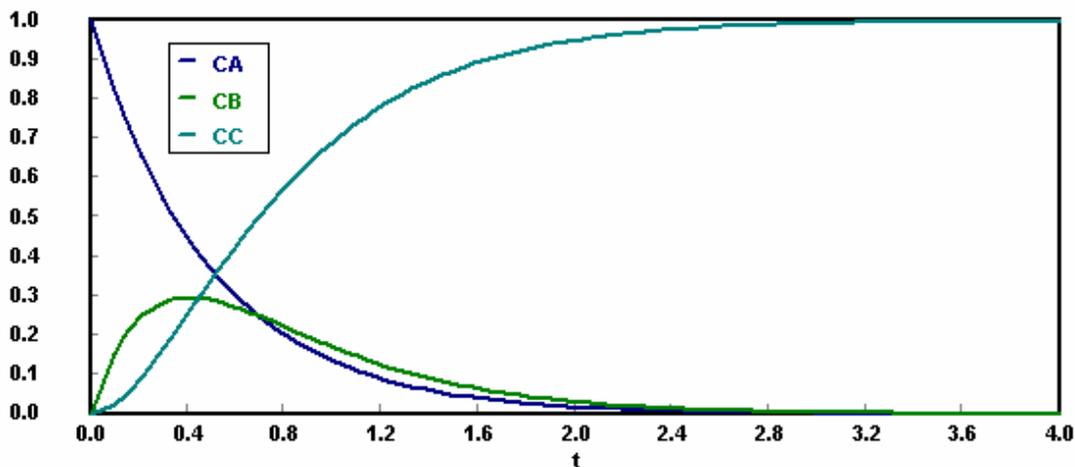

Figure 2 – Graph Output of the Differential Variables from POLYMATH

Exporting Problems from POLYMATH for Solution in Excel[2] – A Brief Look

Problems that can be solved completely in POLYMATH can also be automatically exported to Excel for solution. (A working spreadsheet is generated.) A POLYMATH ODE_Solver Add-In is included with POLYMATH for solving ordinary differential equations in Excel. Available Excel capabilities are used wherever they are available. For example, the provided Add-In *solver* is used to solve systems of simultaneous nonlinear equations in Excel.

The Excel solution for this sample problem is achieved by clicking the Excel icon from the POLYMATH editor. This then automatically exports the problem to an open Excel spreadsheet as shown in Figure 3. Note that all intrinsic functions and logical variables are automatically converted and placed in the Excel spreadsheet. The POLYMATH variable names and equations are shown for the convenience of the user. Since Excel does not have a differential equation solver, an Add-In, ODE_Solver.xla, is provided along with POLYMATH that will solve simultaneous ordinary differential equations. This additional software runs completely independently of POLYMATH.

The Excel solution is automatically generated in a new worksheet as shown in Figure 4. Note that a Table is given that summarizes the solution over the integration interval. Also output of the desired variables by tabulated column give the user options for use or plotting within Excel.
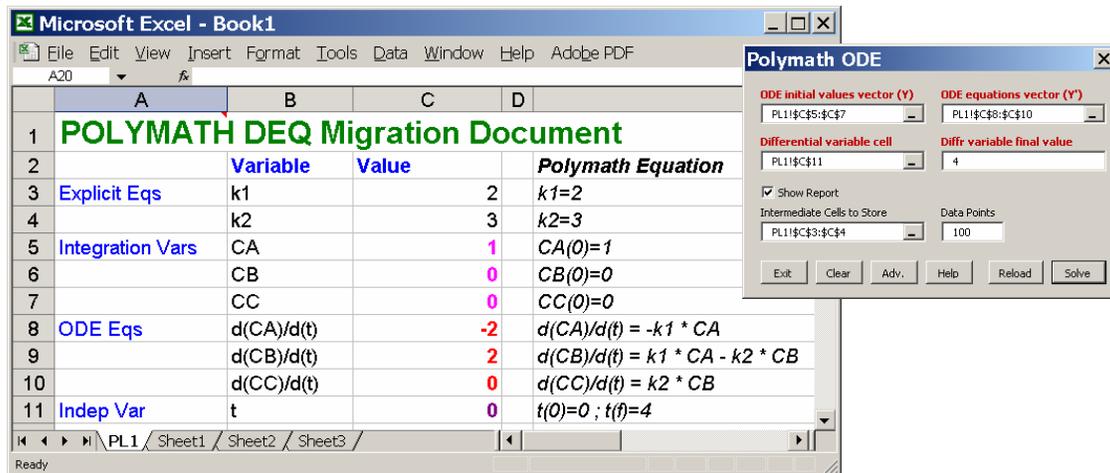
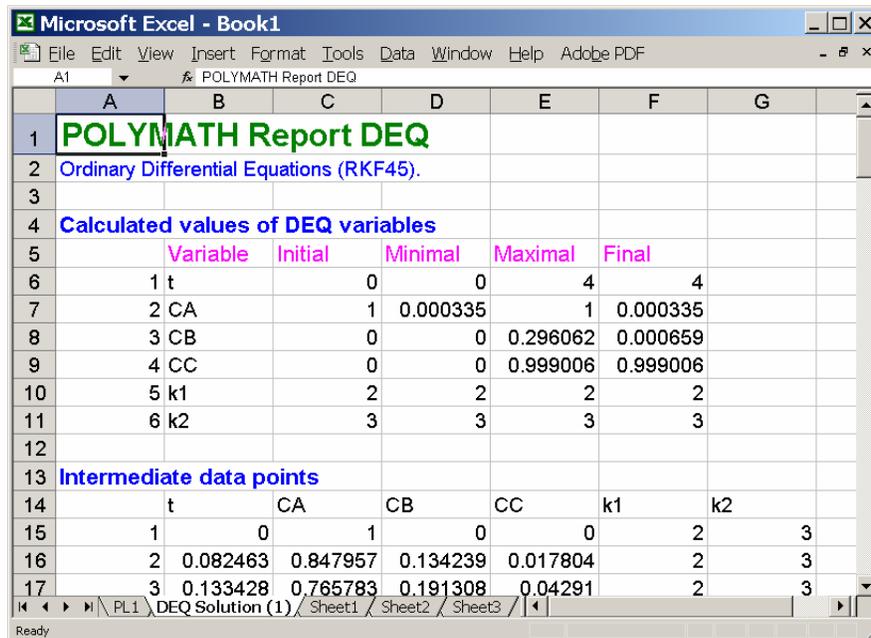Figure 3 – Excel Spreadsheet with POLYMATH ODE_Solver Add-In

Figure 4 – Worksheet Automatically Generated During Sample Problem Solution

Exporting Problems from POLYMATH to MATLAB for Solution – A Brief Look

The MATLAB solution for this sample problem is obtained by setting an option within POLYMATH that will output the problem code for MATLAB to utilize. This option leads to code which contains the translation of the intrinsic functions and logical expressions from POLYMATH into MATLAB code automatically. The generated code for this sample problem is shown in Figure 5 as is provided at the end of the POLYMATH program report.
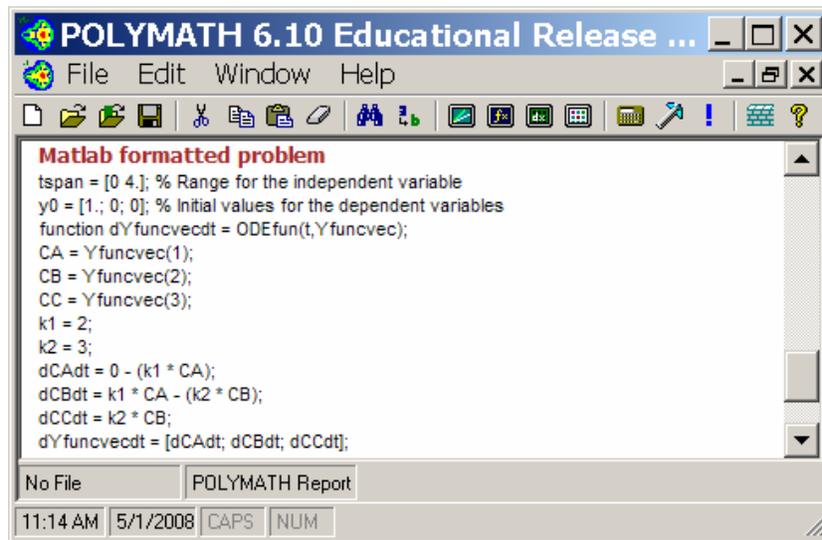
Figure 5 – POLYMATH Generated MATLAB Code

Incorporation of the generated code into a supplied MATLAB Template for simultaneous ordinary differential equation gives the m-file given in Figure 6 where the yellow bars indicate the placement of the code generated by POLYMATH.

```
1    function MATLAB01
2  - clear, clc, format short g, format compact
3  - tspan = [0 4.]; % Range for the independent variable
4  - y0 = [1.; 0; 0]; % Initial values for the dependent variables
5  - disp(' Variable values at the initial point ');
6  - disp([' t    = ' num2str(tspan(1))]);
7  - disp('          y                dy/dt        ');
8  - disp([y0 ODEfun(tspan(1),y0)]);
9  - [t,y]=ode45(@ODEfun,tspan,y0);
10 - for i=1:size(y,2)
11 -     disp([' Solution for dependent variable y' int2str(i)]);
12 -     disp(['          t              y' int2str(i)]);
13 -     disp([t y(:,i)]);
14 -     plot(t,y(:,i));
15 -     title([' Plot of dependent variable y' int2str(i)]);
16 -     xlabel(' Independent variable (t)');
17 -     ylabel([' Dependent variable y' int2str(i)]);
18 -     pause
19 - end
20   %- - - - - - - - - - - - - - - - - - - - - -
21   function dYfuncvecdt = ODEfun(t,Yfuncvec);
22 - CA = Yfuncvec(1);
23 - CB = Yfuncvec(2);
24 - CC = Yfuncvec(3);
25 - k1 = 2;
26 - k2 = 3;
27 - dCAdt = 0 - (k1 * CA);
28 - dCBdt = k1 * CA - (k2 * CB);
29 - dCCdt = k2 * CB;
30 - dYfuncvecdt = [dCAdt; dCBdt; dCCdt];
```

Figure 6 – Code for MATLAB m-file

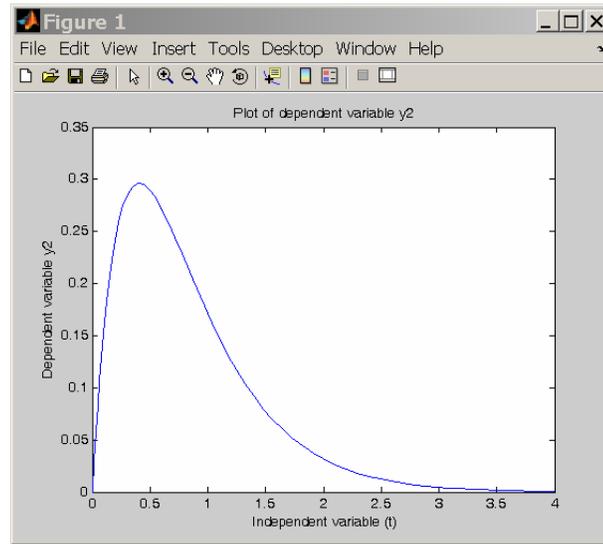The working m-file gives both tabular results (not shown) and graphical results (partly shown in Figure 7).

Figure 7 – Partial Graphical Results as Generated by MATLAB for Concentration of B

Integrating the Use of POLYMATH, Excel, and MATLAB

The POLYMATH software enables a programming and problem solving environment that also can utilize Excel and MATLAB as is shown in Figure 8. In this environment, the problem is first entered into POLYMATH and then can be automatically exported to Excel. From the initial POLYMATH program, the capability to generate MATLAB code enables the creation of a problem m-file.
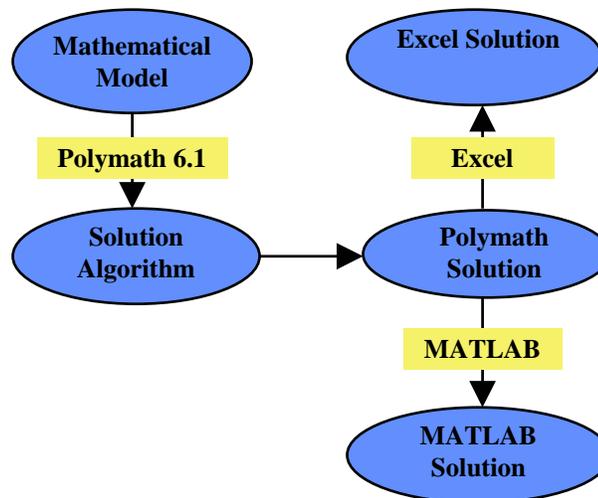

Figure 8 – Desktop Programming/Problem Solving Environment

This environment can be provided in a computer laboratory or to students and faculty for use on their own personal computers. The POLYMATH site license allows distribution of POLYMATH to all students, faculty, and staff plus use in all computer labs. Excel is widely available as a component of the Microsoft Office software, and this is usually available in computer labs and on individual computers. MATLAB provides inexpensive site licenses to most colleges and universities and also markets student versions.

Recent African Initiatives

A major connection with all of the engineering programs in Nigeria was made as a result of the presentation of a POLYMATH workshop at the 7th Annual ASEE Global Colloquium on Engineering Education[5] in Cape Town, South Africa in October of 2008. One of the attendees was Felix Atume who is the Registrar of Council for the Regulation of Engineering in Nigeria, COREN. This organization accredits all the academic engineering programs in Nigeria and also maintains required registration of all practicing engineers in the country. This connection to COREN in South Africa resulted in this author being invited to Nigeria in February of 2009 to present a six-hour workshop to most of the deans and the various department heads, not just chemical engineering, of the 28 engineering programs in the country (~ 110 individuals).

The workshops in Nigeria were supported by the preparation of a web site that provided all of the participants with access to the all of the workshop materials. This also included the installation files for POLYMATH software so that the software could be freely distributed to students, faculty and staff. Also the software can be installed on any computers in the college or university. The MathWorks, Inc. also generously provided a two-month license for MATLAB to the participants. In addition, a CD-ROM with all the workshop materials was given out to each of the faculty participants at the workshop to take back to their home departments.

In September of 2009, the website was updated and the new POLYMATH software installation file that will execute for another year was made available. The workshop materials were given in Acrobat pdf files that contain the actual program files that are used during the workshop. Thus faculty members are able to present workshops using these materials. There have been some preliminary discussions regarding some additional workshops for COREN to be held in Nigeria in February of 2010.

Future African Initiatives

Among other connection made at the ASEE Global Symposium was one with Prof. Funso Falade who is the current President of the African Engineering Education Association[6]. There may be a possible opportunity for a workshop and/or presentation at the next biannual meeting in September of 2010. It is hoped that this conference would be a good venue to promote the use of POLYMATH in developing countries in the African continent.

Assessment of Current Activities

There is strong encouragement from presentations, workshops and contacts that have been made at international meetings regarding the use of POLYMATH in many engineering

disciplines within academic institutions. The necessary connections and interactions do require some international travel and the delivery of workshops and presentations within countries where POLYMATH and other related software can be used to enhance the problems solving capabilities of engineering students who have some even very limited access to personal computers. The use of Internet web sites as well as CD-ROMs and DVDs helps to disseminate the software and related educational materials. Hopefully this will contribute to the improvement of engineering education in developing countries. Much future work continues to be necessary in this area.

Conclusions

- POLYMATH Software provides personal computers with extensive interactive software that can be widely used for engineering and scientific problem solving.
- The automatic export of problems from POLYMATH to Excel enables the efficient use of this spreadsheet software in the solution of a variety of problems.
- The generation of ordered MATLAB code by POLYMATH enables this high-level and programmable software to solve many problems and enable extensions to higher level capabilities where programming is involved.
- POLYMATH software is well received by faculty in developing countries in various engineering disciplines in addition to chemical engineering.
- Future use of POLYMATH site licenses for developing countries will continue to be promoted by POLYMATH Software and the CACHE Corporation, particularly to departments in developing countries, including those with limited financial resources.
- Efforts to widen the use of POLYMATH and related software in engineering problem solving will continue to be made by workshops and presentations at appropriate meetings and by the preparation and dissemination of materials via the Internet and by CD-ROMs and DVDs.

References

1. CACHE Corporation, http://www.cache.org/. CACHE, which stands for Computer Aids for Chemical Engineering, is a not-for-profit organization whose purpose is to promote cooperation among universities, industry and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession. CACHE was initially sponsored by the Commission on Education of the National Academy of Engineering and funded by the National Science Foundation. The current Executive Officer of CACHE is Professor Thomas F. Edgar of the University of Texas at Austin.
2. Polymath Software, http://www.polymath-software.com/. The various POLYMATH programs allow the user to apply effective numerical analysis techniques during interactive problem solving on personal computers. The CACHE Corporation provides site licenses for POLYMATH to colleges and universities.
3. Microsoft Corporation, http://www.microsoft.com. Windows 95, Vista, Excel, and Microsoft Office are products and trademarks of the Microsoft Corporation.
4. MATLAB is a product and trademark of The MathWorks, Inc., http://www.mathworks.com.
5. 7th Annual ASEE Global Colloquium on Engineering Education, http://asee.org/conferences/international/2008/index.cfm.
6. African Engineering Education Association (AEEA), http://www.aeea.co.za/.