Are you using POLYMATH in every Chemical Engineering Course?

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Application of Numerical Problem Solving in Chemical Engineering Coursework

A POLYMATH workshop was presented at the ASEE 2017 Chemical Engineering Summer School in Raleigh North Carolina by Drs. Cutlip and Hesketh. This workshop provided hands-on experience in using POLYMATH version 6 and the new version of POLYMathLite 1.1 for Android smartphones and tablets. In this article is a synopsis of this workshop.

POLYMATH is very easy to use! The workshop started with an example from chemical reaction engineering in which 3 simultaneous differential equations are numerically integrated. Robert Hesketh claimed that a user with no experience using POLYMATH can go through a short tutorial and within 10 minutes have a solution to this problem; an experienced user can construct this problem in less than 4 minutes. Fellow CACHE trustee Phillip Westmoreland was at this workshop and easily used POLYMATH to solve this problem in this short time period. Part of the ease in use of POLYMATH is that the user types in equations the same way that they are written on paper. For example the equation

$$\frac{d(C_A)}{dt} = -k_1 C_A \tag{1}$$

With initial condition that at $t=0 \ min$ the $C_A = 1 \ kmol/L$ can either be typed directly into POLYMATH as shown in *Figure 1* or they can use a dialog form shown in *Figure 2*.
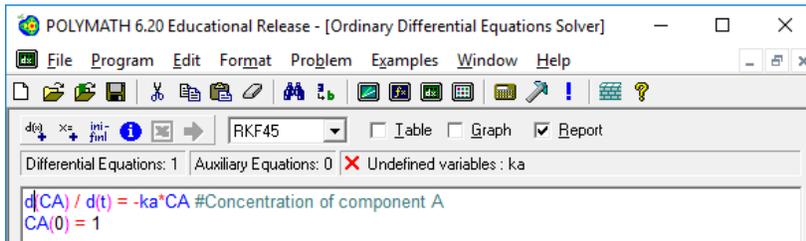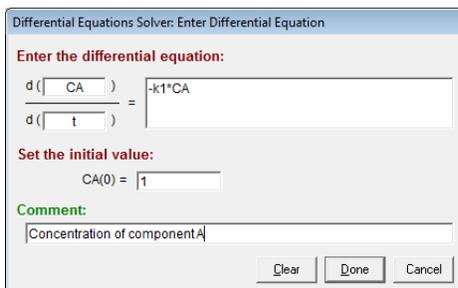

Figure 1: Equation input/modification window

Figure 2: Example entry form

The entry form is very useful for students because it reminds them that for every differential equation an initial condition must be given. Fortunately, if the user is typing in the equations without using the entry form and forgets to put in the initial condition, then an error notification is given as shown in Figure 3.
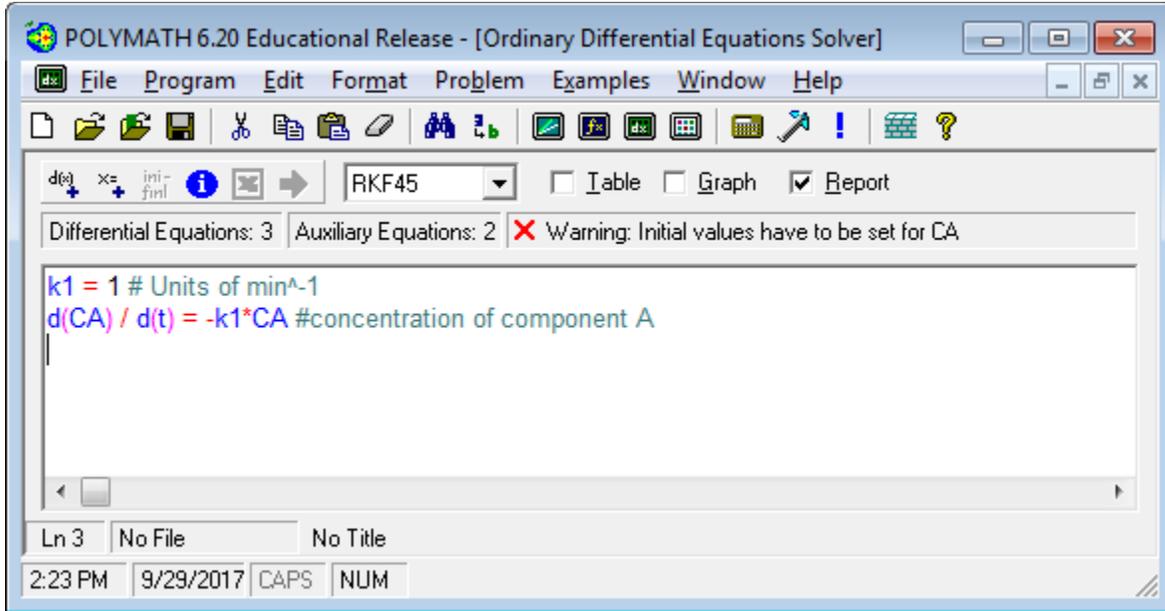

Figure 3: Error example showing the missing initial condition for the differential equation.

Why not try out POLYMATH using this pdf tutorial. If your university doesn't have a POLYMATH site license you can download a trial version at http://www.polymath-software.com/

The second part of this introduction was a session on common errors made by students in constructing a POLYMATH program and the troubleshooting features of the POLYMATH software. These errors include:

1.   What the user thinks are the same variables, but the computer uses them as different variables. This happens when you incorrectly spell a variable name or you do not match upper or lower cases. (e.g. $Tau \neq tau$ "Can't the computer read my mind?")

2.   Defining a variable more than once. Once a variable is on the left hand side of the equals sign then it is considered defined by the program.

3.   Dividing by zero

4.   Using too many parenthesis. This isn't an error, but I have found that students make mistakes in grouping terms. POLYMATH uses the standard order of operators which is exponent, multiplication/division, addition/subtraction: ^, (* or /), (+ or -) which is invoked working from left to right in an expression.

The troubleshooting features of POLYMATH help the user to write their programs and is one of the reasons it is so easy to use. For example, a special variable tracking feature in the POLYMATH window lets the user know that a variable has been used, but has not been defined as the user is typing in equations. This real time tracking is one of the reasons you can solve problems in a short period of time. So if you use ka in an equation as shown in Figure 1, and have not defined it with ka= or d(ka)/d(t)=, then this tracking feature list the ka as an undefined variable and will not start the integration until it is defined.

Integration of POLYMATH in Chemical Engineering Courses

The POLYMATH software can be used in every chemical engineering course. Most chemical engineering undergraduate students are introduced to POLYMATH in one of Scott Fogler's textbooks on Chemical Reaction Engineering. Both the Elements of Chemical Reaction Engineering and Essentials of Chemical Reaction Engineering have *living* examples in POLYMATH.

But what about other courses in Chemical Engineering? Excellent examples of problems for each chemical engineering course are contained in the textbook, "Problem Solving in Chemical and Biochemical Engineering with POLYMATH, Excel, and MATLAB (2nd Edition)." This textbook gives almost 300 problems in Thermodynamics, Fluid Mechanics, Heat Transfer, Mass Transfer, Chemical Reaction Engineering, Phase Equilibria and Distillation, Process Dynamics and Control, and Biochemical Engineering that are solved using POLYMATH.

An example of a fluids course sequence was given in which the topics using POLYMATH was outlined. In Table 1 shown below is a summary of the types of problems covered in a fluids course.

Table 1 Example Fluids Problems

ChE Course	Problem Name	Numerical Method Illustrated	Equations
Fluids	Unsteady-state tank drainage using a siphon tube (similar to POLYMATH text 8.14) *C&S8-14soln.pdf*	Solution of an first order ordinary differential equation (DEQ)	$\dfrac{dh_T}{dt} = v_{out} \dfrac{A_{out}}{A_{tank}}$ $v_{out} = f(h_T)$
	Calculations involving Friction Factors for Flow in Pipes (POLYMATH Text 8.7) and *pipeflow homework frictionfactorcalcsoln.pdf Excel Tutorial Solver Add-Ins rev4.pdf*	Solution of a system of simultaneous nonlinear algebraic equations (NLE)	$\dfrac{\Delta P}{\Delta L} = 2f_F \dfrac{\rho v^2}{D}$ $f_F = f(\varepsilon/D, Re)$ $Re = \rho v D / \mu$

ChE Course	Problem Name	Numerical Method Illustrated	Equations
Advanced Fluids	NonNewtonian fluid flow through a pipe (POLYMATH Text 8.2c) *NonNewtonian C&S 8.2 solutions & comsol.pdf* NonNewtonian fluid flow through an annulus (POLYMATH Text 8.4) *NonNewtonian C&S8.4 polymath&comsol & 3.8-8 solutions 2017.pdf*	Solution of 2 simultaneous first order ordinary differential equations with split boundary value conditions and comparison with solution using COMSOL which is an advanced finite element program	$$\frac{d(r\tau_{rx})}{dr} = -\frac{dP}{dx}r$$ $$\tau_{rx} = -K\left(\frac{dv_x}{dr}\right)\left(\left|\frac{dv_x}{dr}\right|\right)^{(n-1)}$$

It was stressed in the workshop that students need to be able to derive mathematical models of chemical engineering systems and obtain analytical solutions for simple systems. For example in a second semester fluids class students should be able to derive a momentum balance for fluid flow in a pipe and integrate this and obtain analytical solutions for Newtonian and Non-Newtonian fluids. Then students are asked to solve the same problem using POLYMATH and compare the numerical solution of the velocity profile with the analytical solution. This demonstrates that they understand the model that they have developed and now can move to more advanced geometries and configurations. An example of a lecture/homework session on this topic is shown in the presentations slides given in this link Integration of POLYMATH in ChE Courses. In this workshop it was stressed that POLYMATH is not a "canned" program in which the equations are hidden such as in COMSOL and ASPEN. The user must provide their own mathematical model which is essential in the learning process.

Another obstacle that faculty have in using POLYMATH in the classroom is that many textbooks still present models in the form of integrals and not differential equations. This was based on the numerical technique of solving these integrals using a form of quadrature (e.g. trapezoidal rule or just adding up the rectangles). For example in Geankoplis's excellent textbook titled, "Transport Processes and Separation Process Principles," the design of packed towers for gas absorption presented using integrals as shown Figure 4. In class, I use the same figure shown in Figure 5, but I derive a differential equation based on the flows in and out of the control volume shown ($\Delta V = A_c\Delta z$) resulting in the following steady-state equation.

$$\frac{d(Vy_{AG})}{dz} = -\frac{k'_y aS}{(1-y_A)_{iM}}(y_{AG} - y_{Ai}) \qquad (2)$$

$$\frac{d(Lx_{AG})}{dz} = -\frac{k'_x aS}{(1-x_A)_{iM}}(x_{Ai} - x_{AL}) \qquad (3)$$

5. *Design method for packed towers using mass-transfer coefficients.* For absorption of A from stagnant B, the operating-line equation (10.6-5) holds. For the differential height of tower dz in Fig. 10.6-9, the moles of A leaving V equal the moles entering L:

$$d(Vy) = d(Lx) \qquad \textbf{(10.6-10)}$$

where V = kg mol total gas/s, L = kg mol total liquid/s, and $d(Vy) = d(Lx)$ = kg mol A transferred/s in height dz m. The kg mol A transferred/s from Eq. (10.6-10) must equal the kg mol A transferred/s from the mass-transfer equation for N_A. Equation (10.4-8) gives the flux N_A using the gas-film and liquid-film coefficients:

$$N_A = \frac{k'_y}{(1 - y_A)_{iM}}(y_{AG} - y_{Ai}) = \frac{k'_x}{(1 - x_A)_{iM}}(x_{Ai} - x_{AL}) \qquad \textbf{(10.4-8)}$$

where $(1 - y_A)_{iM}$ and $(1 - x_A)_{iM}$ are defined by Eqs. (10.4-6) and (10.4-7). Multiplying the left-hand side of Eq. (10.4-8) by dA and the two right-side terms by $aS\, dz$ from Eq. (10.6-9),

$$N_A\, dA = \frac{k'_y a}{(1 - y_A)_{iM}}(y_{AG} - y_{Ai})S\, dz = \frac{k'_x a}{(1 - x_A)_{iM}}(x_{Ai} - x_{AL})S\, dz \quad \textbf{(10.6-11)}$$

where $N_A\, dA$ = kg mol A transferred/s in height dz m (lb mol/h).

Equating Eq. (10.6-10) to (10.6-11) and using y_{AG} for the bulk gas phase and x_{AL} for the bulk liquid phase,

$$d(Vy_{AG}) = \frac{k'_y a}{(1 - y_A)_{iM}}(y_{AG} - y_{Ai})S\, dz \qquad \textbf{(10.6-12)}$$

$$d(Lx_{AL}) = \frac{k'_x a}{(1 - x_A)_{iM}}(x_{Ai} - x_{AL})S\, dz \qquad \textbf{(10.6-13)}$$

Since $V' = V(1 - y_{AG})$ or $V = V'/(1 - y_{AG})$,

$$d(Vy_{AG}) = d\left(\frac{V'}{(1 - y_{AG})}y_{AG}\right) = V'\, d\left(\frac{y_{AG}}{1 - y_{AG}}\right) = \frac{V'\, dy_{AG}}{(1 - y_{AG})^2} \qquad \textbf{(10.6-14)}$$

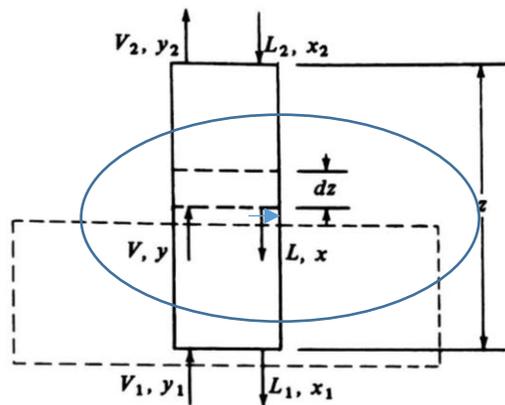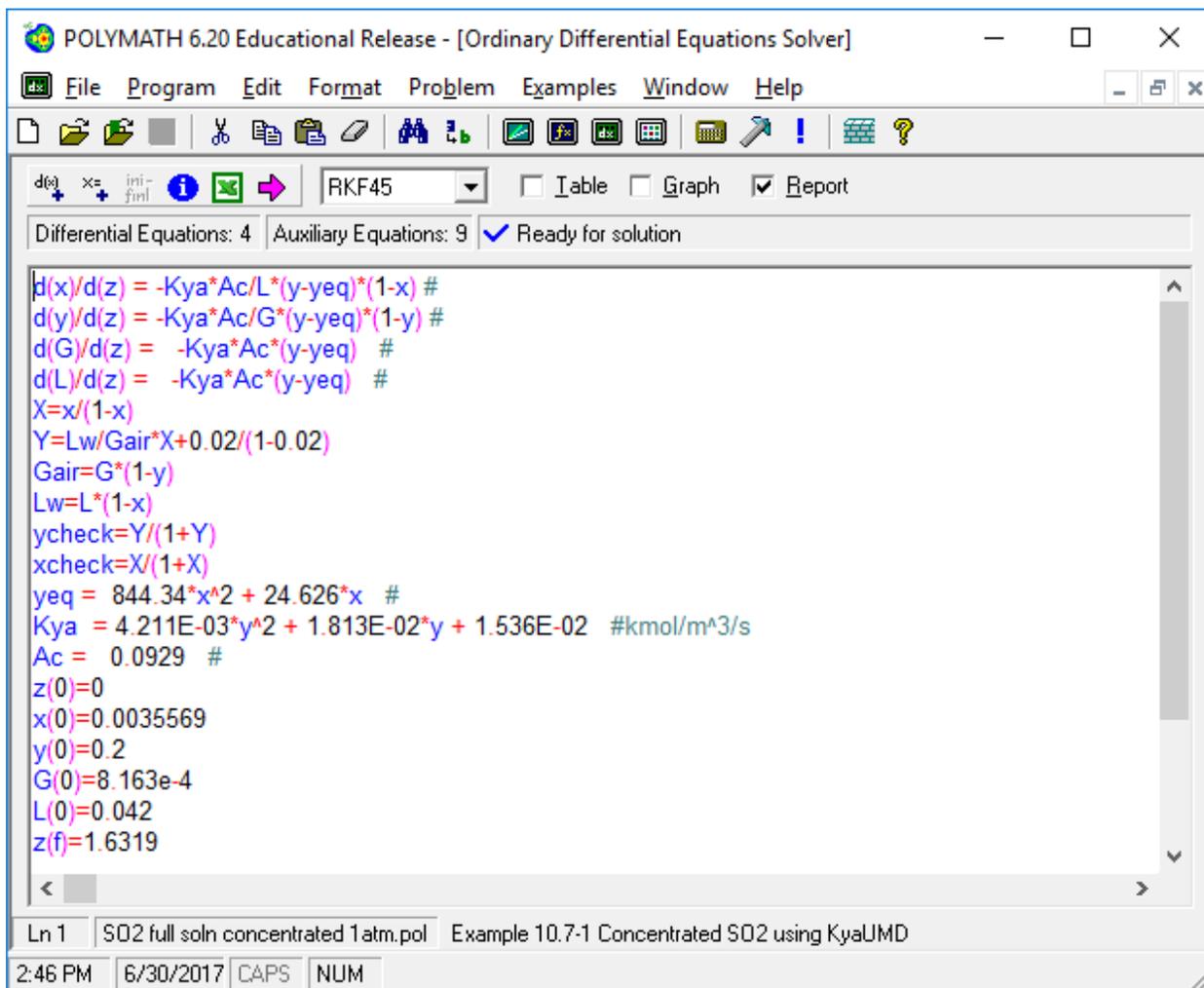*Figure 4: Gas Absorption using Integrals*

FIGURE 10.6-9.   *Material balance for a countercurrent packed absorption tower.*

Figure 5: Control Volume for ODE

This results in an absorber model for SO2 absorption in a concentration system shown below:

Figure 6: POLYMATH example for Example 10.7-1 in the Geankoplis Textbook

A copy of this presentation can be found at this link Integration of POLYMATH in ChE Courses

POLYMATH User Group Meeting at 2017 AIChE

We are interested in how you are using POLYMATH in your classrooms or research and CACHE has graciously agreed to host a breakfast meeting at the 2017 AIChE Annual Meeting. At this meeting we are inviting POLYMATH users to give us feedback on how they are using POLYMATH and to also gets some new exciting updates on new POLYMATH features. If you are interested in attending this breakfast meeting on starting at 7AM on Wednesday 1 November 2017 in the Rochester Room of the Hilton Minneapolis please send an email to Hesketh@rowan.edu. We are also interested in any feedback on this short article or on topics for future articles.