Problem-centered Course in Numerical Methods

Bruce A. Finlayson
University of Washington

Introduction. The following educational elements were all included in one course: oral and written communication, design, generation of multimedia lessons, use of sophisticated computer software, group learning, and learning by objective. An undergraduate elective course on numerical methods and modeling has been reorganized to focus on the problem of reducing automobile pollution. The course has essentially been turned upside down. In the past, each problem was posed, and the need for its solution explained. Then the general equations were reduced to the point that a viable model was achieved. Several such problems were treated in each quarter. In the revised course, one societal problem is posed, namely automobile pollution, and a catalytic converter is chosen as one solution. The first models are very simple, but are within the reach of the students at the start of the course. Then these models are used to show the need for including additional phenomena, which necessitates more complicated numerical methods. In this way the students practiced ‘just in time learning’. Their motivation was increased, and their success at solving difficult problems was higher.

Overview. The course began with an assignment of an essay on the scope of the automobile pollution problem, thereby giving them experience in written communication. One side benefit for the professor is the large number of unusual sources of information the students find. This was the first time in this professor’s experience that material on a CD-ROM encyclopedia was used as a reference in an assignment. The course went through the same topics as in the past: methods to solve algebraic equations, initial value problems, boundary value problems, and partial differential equations. However, each type of equation arose in some manner in the catalytic converter for an automobile. The programs MATLAB and EXCEL were used to solve the various numerical models. The models were improved week by week, and after seven weeks the models were much more sophisticated and powerful than had been achieved in prior courses. Then a design problem was posed. Solution of the design problem involved using the model, working in groups, and presenting the design in written and oral format. At one point in the course the class considered doing experiments to test various catalysts, but this was abandoned as too time consuming.

Mathematical Models. In order to make the course manageable the problem was simplified somewhat. The class treated only carbon monoxide (CO), since the details to treat propylene, methane and other components just add complicated bookkeeping that doesn’t improve understanding. The CO kinetics were from Oh and Cavendish.

A variety of models were used, as listed here. The approach was to assign homework problems for each model that invoked some numerical procedure. The models are organized so that by the end of the course all
numerical topics are covered. The first model was for a steady CSTR at constant temperature, which permitted discussion of methods to solve a single nonlinear algebraic equation.

\[
Q (c - c_{in}) = -\frac{V k_2 c}{(1 + K_1 c)^2}
\]

Next an unsteady CSTR at constant temperature was treated to introduce solving ordinary differential equations as initial value problems.

\[
\varepsilon V C_{tot} \frac{dy}{dt} = Q C_{tot} (y_{in} - y) - \alpha V r(y, T)
\]

The model was then expanded to be steady but with heat effects included, and the Newton-Raphson method was introduced to solve sets of non-linear equations.

\[
Q C_{tot} (y_{in} - y) = \alpha V r(y, T)
\]

\[
Q C_{tot} \dot{M} C_{pg} (T - T_{in}) = \alpha V (-\Delta H_{rxn}) r(y, T)
\]

\[
r = \frac{k_1 y 0.05}{T (1 + K_1 y)^2}, \quad k_1 = 6.70 \times 10^{10} \exp (-12556/T), \quad K_1 = 65.5 \exp (961/T)
\]

In preparation for studying stiff equations, a heat-transfer-only model was used.

\[
V[(1-\varepsilon)\rho_s C_{ps} + \varepsilon \rho_f C_{pg}] \frac{dT}{dt} = Q C_{tot} \dot{M} C_{pg} (T_{in} - T) + \alpha V (-\Delta H_{rxn}) r(Y)
\]

and this was compared with the transient model for chemical reaction and mass transfer with the temperature fixed. The students could then see that the time scales of heat transfer and mass transfer/reaction were very different. Next a stiff problem was posed and solved using a non-stiff integrator (Runge-Kutta method).

\[
\varepsilon V t_{tot} \frac{dy}{dt} = Q C_{tot} (y_{in} - y) - \alpha V r(y, T)
\]

\[
V[(1-\varepsilon)\rho_s C_{ps} + \varepsilon \rho_f C_{pg}] \frac{dT}{dt} = Q C_{tot} \dot{M} C_{pg} (T_{in} - T) + \alpha V (-\Delta H_{rxn}) r(y, T)
\]

Then stiff integrators were discussed, and the same problem was solved with them. The students experienced the value of a stiff solver for ordinary differential equations instead of just hearing their professor talk about it. The need for stiff equation solvers was very evident after the students had used the usual methods to solve a stiff problem and had to wait for their computer to finish! Next a quasi-static approximation was made, and with this approximation the non-stiff integrators can again be used.

\[
Q C_{tot} (y_{in} - y) - \alpha V r(y, T) = 0
\]

\[
V[(1-\varepsilon)\rho_s C_{ps} + \varepsilon \rho_f C_{pg}] \frac{dT}{dt} = Q C_{tot} \dot{M} C_{pg} (T_{in} - T) + \alpha V (-\Delta H_{rxn}) r(y, T)
\]

Chemical engineers of course know the importance of mass/heat transfer resistance in chemical reactors, and this problem demands such phenomena be included in the model. The final quasi-static model with mass/heat
transfer resistance is
\[
(1-\varepsilon) \frac{d T_s}{dt} = h S V (T - T_s) + \alpha V (-\Delta H_{\text{rxn}}) r(y_s, z_s, T_s)
\]

with
\[
z = z_{in} + \frac{1}{2} (y - y_{in})
\]

This model requires solving sets of algebraic equations inside the ordinary differential equation solver. An alternative would be to use a differential-algebraic solver, but these were not available in MATLAB and are not as robust in this case. The strategy is to introduce things one at a time – the students’ debugging skills are adequate for one difficulty at a time. At that point they had a working model of a CO oxidizer in a CSTR. Then the inlet conditions were allowed to change with time.

**Design.** Finally a design problem was posed with a 250 second abbreviated federal test cycle. The design objective was to eliminate 95% of the CO in this cycle. The class was divided into eight two-person groups. By this time in the course, the entire class knew that about 95% of the pollution coming out of a converter comes out in the first two to three minutes when the converter and engine are cold. Lo and behold, when the designs came back they all found they couldn’t achieve the design objectives without pre-heating the catalyst or using an adsorber or a flame! One of the groups came back with that conclusion and said they had reached it before they found out that was a strategy being discussed in industry, and they were very proud of themselves! This design problem could also be tied to the essay they wrote at the start of the course, making the whole experience more real than in other courses.

**Evaluation.** The course was run for nominally ten weeks, with two lectures per week and one day for discussion of the homework. The discussion of homework allowed the instructor to expand on it and give additional details and insights. These insights are more meaningful to the student when they are illustrated for a problem they have worked on.

In any revision, things have to be left out. Statistics and parameter estimation could not be covered in as much depth. Partial differential equations were also less important (for the CSTR model the class used), so that was deemphasized. The use of the finite element method for solving two- and three-dimensional transport problems could not be covered, and the orthogonal collocation method was not discussed. However, the method of lines (for the finite difference method) was easily introduced because good written material with worked examples was available (and had been used in earlier classes)\(^2\). When organized around the type of numerical problems solved, the number of lectures devoted to different topics in successive years is shown in Table I, which suggests not too great a difference. Other class periods were spent discussing phenomena, class presentations, going on a field trip to Microsoft, and taking tests. However, the difference is made evident in
Tables II and III, which lists the many fields covered in prior years, compared with one main one in the revised course. It is clear that many fewer topics were treated in the revised course.

Table I. Number of Lectures Devoted to Different Topics

<table>
<thead>
<tr>
<th>Topic</th>
<th>1994</th>
<th>1995</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameter Estimation</td>
<td>3</td>
<td>left out</td>
</tr>
<tr>
<td>Algebraic Equations</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>Ordinary Differential Equations as Initial Value Problems</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Ordinary Differential Equations as Boundary Value Problems</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>Partial Differential Equations</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>Finite Element Method</td>
<td>1</td>
<td>left out</td>
</tr>
<tr>
<td>Class Discussion of Homework and Extensions</td>
<td>8</td>
<td>6</td>
</tr>
</tbody>
</table>

Table II. Abdication Fields Treated (in varying depth) in 1994

- Mass Balance with Recycle
- Hot Water Heaters (radiation and convection)
- Heat Transfer (microscopic)
- Kinetics (including parameter estimation)
- Reactors: CSTR, axial dispersion, plug flow
- Reactors: S0, reactor, CO oxidation, fermentation
- Diffusion and Reaction in Porous Media
- Solid Elasticity

Table III. Application Fields Treated in 1995

- Reactors: CSTR, plug flow, monolith
- Reactors: CO oxidation
- Heat Transfer (microscopic)
- Heat and Mass Transfer Resistance

However, a major theme of the course was that you have to learn to check your work: show how you know you’ve solved the problem you think you have and how you know the accuracy of the numerical solution. The author believes that this is the single most important skill the students will remember after six months. For example, the details of solid elasticity, which was only invoked in one homework problem, will not be remembered. However, everyone knows about the ‘two minute problem’ and everyone knows how to check the computer work. After all, using modern packages, the computer package is doing 90% of the work, and it behooves us to be sure our 10% is right. The topic of checking your work can be covered for boundary value problems and partial differential equations (and were covered on the final) even though everyone in class is not an expert in the mechanics of solving them. Again, the guiding theme was always: learn only what you need to solve the problem at hand.

Tests. The tests in the two classes were similar. In 1995 the hour test was a take-home test requiring computer work, whereas the 1994 hour test was in class and had questions related to computer work. Other than that they were similar. There were questions on estimating accuracy of numerical solutions on the final in both years. In 1995 the final was closed book and more analysis was required, but the level of numerical
sophistication was comparable in both years. The difficulty of the tests was comparable, as nearly as possible. The scores in 1995 were much higher.

**Cooperation.** One important part of the course is the cooperative spirit that developed among the students and instructor. There was much more of a problem solving spirit than a competitive drive to achieve the highest grade. Each week the instructor would pose more and more complicated models, after justification that the new phenomena needed to be included based on the simpler models. Then the students would work that homework and turn it in. The instructor would then give the solution, make available his code, for those who didn’t get it quite right, so they would have something to compare against. In contrast to previous courses, where students just throw away feedback, they used this, because they knew that they were going to have to use it in the next model. What developed during the course was a cooperative spirit as we built better and better models. At the end, they worked in design groups and used their models to tackle the final problem – the first two minutes when the car was cold. The cooperative spirit worked both ways: the students taught the instructor how to differentiate and integrate on the computer, for example. The lesson on computer differentiation came after an interesting experience. One of the non-isothermal models involved solving two nonlinear algebraic equations in two unknowns. Practitioners know that oxidation reactions can be very hard to solve, and iterative algorithms can easily fail to converge. Of the 16 people in class, only 3 were able to differentiate the equations correctly, as needed by the Newton-Raphson method, and all 3 of those used the computer. The other 13 did know the concept of the derivative, and carried out many details correctly, but there were probably 30 steps in the derivation. If each step was not correct the algorithm would not work. Only the computer users did the problem correctly. This experience has led the instructor to wonder if the undergraduate education might be shortened or made more efficient by removing some of the drill: cover the basic idea and let the computer do the mechanics.

**Multimedia Lessons.** Student groups were also assigned to prepare a lesson on the computer, using either Macromedia Director or the html markup language. A one-page handout was prepared that listed the most essential instructions for Director and one class was spent demonstrating the instructions by using a portable projector in the Department. Lessons were prepared on how to solve algebraic equations, how to solve ordinary differential equations, how to solve stiff equations, and a lesson was made to explain to sixth graders what a catalytic converter did and chemical engineers’ role in it. Interaction with personnel at Microsoft was used to improve the lessons. The lessons are installed on the local computer network so that students who have not taken the class can use them in a ‘how to’ fashion. One exciting development was to witness the creativity the students showed while creating their lesson. The instructions are simple enough that they can do dramatic things easily, and this encourages them to develop better lessons. It may be that the creativity and trial-and-error engineering that used to be exercised working on students’ cars and bicycles is now being exercised on the computer.

**Conclusion.** Student enthusiasm was high and a cooperative learning atmosphere was created. While everyone is not as much an expert in the details of all the methods as in past years, the instructor feels every one of them has the overall background needed to sit down with notes and books and learn the missing details.
Offsetting this loss of detail is a recognition of how to make and check models that can be used to solve problems of practical and public importance.

Nomenclature.

\[ c \quad \text{CO concentration (kg.mol/m}^3\text{)} \]
\[ C_{pg} \quad \text{heat capacity (J/kg K)} \]
\[ C_{tot} \quad \text{total concentration (kg.mol/m}^3\text{)} \]
\[ h \quad \text{heat transfer coefficient (J/m}^2\text{Ks)} \]
\[ -\Delta H_{rxn} \quad \text{heat of reaction (J/kg.mol)} \]
\[ k_2 \quad \text{reaction rate constant (s}^{-1}\text{)} \]
\[ k_r \quad \text{reaction rate constant (kg.mol K/m}^2\text{s)} \]
\[ K_1 \quad \text{term in reaction rate (–)} \]
\[ k_m \quad \text{mass transfer coefficient (m/s)} \]
\[ M \quad \text{molecular weight of mixture} \]
\[ r \quad \text{rate of reaction (kg.mol/m}^2\text{s)} \]
\[ Q \quad \text{flow rate of gas (m}^3\text{/s)} \]
\[ S \quad \text{surface area per unit volume (m}^2\text{/m}^3\text{)} \]

Greek letters

\[ \alpha \quad \text{catalytic area per unit volume (m}^2\text{/m}^3\text{)} \]
\[ E \quad \text{void fraction (–)} \]
\[ p \quad \text{density (kg/m}^3\text{)} \]

Subscripts

\[ f,g \quad \text{fluid or gas} \]
\[ \text{in} \quad \text{inlet value} \]
\[ s \quad \text{solid} \]

References

[3] Most of the automobile pollution coming from cars with exhaust treatment systems (post 1979) occur during the first two minutes before the catalytic treatment has been heated up.
[4] The handout on Director will be sent via e-mail to anyone who requests it, using the most current version. The address is: finlayson@cheme.Washington.edu.

Biographical Information

BRUCE A. FINLAYSON obtained a B.A. in 1961, a M.S. in 1963 from Rice University and a Ph.D. in 1965 from the University of Minnesota. He is the Rehnberg Professor of Chemical Engineering and Chair at the University of Washington, a member of the National Academy of Engineering, a Fellow of the American Institute of Chemical Engineers, and received the Martin Award from the Chemical Engineering Division of the ASEE.