Integrating COMSOL into a Mathematical Modeling Course for Chemical Engineers

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Abstract: The multiphysics simulation package COMSOL was incorporated into a course in mathematical modeling for chemical engineers. This led to three questions: Are we giving the students the appropriate background to use the software? Are we effectively teaching students how to use COMSOL? Are we teaching the students to be informed and critical users of computer packages? Our implementation for the first year of using COMSOL in the course is described, and assessment results based on examinations and student survey results are presented and analyzed. The students appear to be learning how to operate the COMSOL program quite satisfactorily, but their skills in setting up problems and in becoming discriminating users of the technology are less well developed and will motivate some changes in the curriculum for the next offering.

Keywords: education, finite element method, transport and reaction, applied mathematics.

1. Introduction

Engineering students need to learn how to formulate mathematical models of physical situations, how to obtain useful solutions to the model equations, and how to correctly interpret and present the results. For chemical engineers, the second step in this sequence frequently involves the solution of ordinary or partial differential equations describing transport phenomena and/or reacting systems. This has traditionally been accomplished by analytical methods such as Laplace transforms or Fourier series expansion in eigenfunctions. While such methods have their place, they are usually restricted to linear problems in simple geometries, whereas chemical engineering problems heavily involve nonlinear phenomena, in geometrically complex processing equipment.

We want to introduce our chemical engineering students to problem-solving with modern engineering tools, such as COMSOL, applied to more realistic problems. The place, amount and type of computing in the undergraduate chemical engineering curriculum are ongoing matters of interest [1]. It is essential that students should not lose sight of the physical and chemical phenomena being modeled, the assumptions behind the mathematical models used, or the need to verify and validate the computational methods applied to the problem [2]. Similar concerns have been raised regarding the use of process simulation software to carry out the extensive material and energy balances for a process design [3], and successful implementation of these advanced computer tools may require a re-focusing of course objectives and skills taught, and a re-structuring of the course curriculum [4]. In addition, the tendency of students to accept computational results at face value must be guarded against, and it is important to instill in students a healthy skepticism of computer results and a willingness to critically examine the results of their efforts [5].

Our mathematical modeling course is organized to follow the three steps enumerated above, and in this contribution we report on our first use of COMSOL to allow students to apply the finite element method for step 2, the solution of the governing model equations. Previous offerings of the course had used either analytical solution methods or numerical finite difference methods implemented in Excel, which also had severe limitations. We also wished to use this experience to inculcate good computing practices into the students – checking results for errors, critical assessment of results, model validation, mesh verification – as well as some principles of approximation and discretization, especially finite element methods and solution of linear systems of equations.

2. Course Implementation

The course is an advanced junior/senior level undergraduate elective, which also counts towards fulfillment of our core course requirements. WPI has 7-week terms, which means that undergraduate students carry three courses which meet at least 5 hours per week. Students have typically had calculus through differential equations, but not linear algebra. This includes some limited exposure to vectors, but not to vector/tensor calculus. The problems and examples in the course are drawn mainly from the transport and reaction area, so students are encouraged to take this course following the Fluids, Heat Transfer and Mass Transfer sequence, but the Kinetics and Reactors course is often taken concurrently.

Use of COMSOL in the course required some background in mathematical topics that the students had not all seen before. Classes were explicitly provided for matrix manipulations and vector and tensor calculus. The first third of the course covered the derivation and set-up of differential equation models for transport and reaction in chemical engineering. We covered lumped models, boundary-value problems, boundary conditions, elliptic PDEs (Laplace equation), parabolic PDEs (heat/diffusion equation), 1^{st}-order (convection) PDEs and briefly mentioned hyperbolic PDEs (wave equation). Instruction in using the COMSOL program took place in a computer lab and was based on a "watch and do" method [4] where the instructor went through a demo problem, then students tackled a worksheet problem on their own with instructor help. Further practice was provided through homework exercises, and partial assessment was achieved by an "in-lab" exam in which the students solved a problem similar to one of their homework assignments, under reasonable time constraints. Some limited background theory in the Finite Element Method was provided in the form of lectures and handouts, which ran in parallel to the COMSOL lab sessions through the latter two-thirds of the course.

Many of the in-class examples and homework problems were based on the text by Finlayson [6], although students were not required to purchase this book, as large parts of it cover use of Excel, Aspen Plus and MATLAB, which are not part of the course, in addition to FEMLAB (the earlier version of COMSOL).

3. Assessment Methods

Student reactions to the course and particularly to the inclusion of COMSOL were obtained via an end-of-course informal survey. Assessment of the degree to which the course objectives were met was made by the survey, the in-lab midterm computer exam, and short questions on the final exam.

3.1 In-lab midterm computer exam

The students were given an hour in the computer lab and asked to model the steady-state distribution of concentration of a species undergoing 1^{st}-order reaction in a tank, shown in Figure 1.

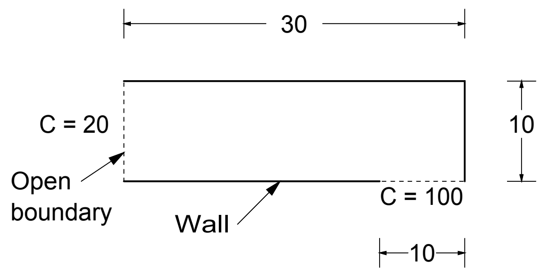

Figure 1. Schematic of steady-state 2D diffusion-reaction problem for in-lab midterm computer exam.

The PDE governing this system was given as

$$D\left(\frac{\partial^2 C}{\partial x^2}+\frac{\partial^2 C}{\partial y^2}\right)-kC=0$$

and the boundary conditions were as shown. Students were given individual values of diffusivity D and reaction rate constant k. They were asked to write the equation in vector/tensor notation, set up the equation in COMSOL and solve using the initial mesh supplied by the program, make a surface plot of the solution and superimpose contours of concentration c, check the mass balance by computing the amounts of the species entering and leaving the system, and compare to the amount consumed by reaction, and run a second calculation with changed mesh settings to get an improved mass balance.

3.2 Final exam

This one-hour exam consisted of eight short questions, made up of five questions directed towards the students understanding of various "theoretical" aspects of using finite elements to solve differential equations using COMSOL: expression of equations in vector-tensor notation, the ideas behind weighted residual and Galerkin methods, the weak form of a differential equation, system matrix assembly on an element-by-element basis for a 1D problem, matrix factorization for a linear system of equations. These were followed by three "concepts" questions designed to see whether the students understood the ideas of solution multiplicity, user error in use of computer packages, verification of computer methods, and validation of mathematical models. Further details are given below, under the Results and Discussion section.

3.3 End of course survey

In addition to the usual course evaluation administered for all WPI courses, a special survey was designed to obtain the students opinions on issues and aspects of the course and COMSOL use. The broad categories were: mathematical background, model derivation and set-up, laboratory instruction in COMSOL, finite element theory, homework and computer exercises, course structure. Details and results for those questions that involved COMSOL are presented in the following section.

4. Results and Discussion

The first three weeks of the course were spent on model development via shell balances. The associated first exam demonstrated that the students had a satisfactory grasp of the principles of deriving ordinary and partial differential equations and their boundary conditions, and were able to appreciate the physical situations to which they corresponded. The remainder of the course was directed towards numerical solution of the equations using COMSOL.

4.1 In-lab midterm computer exam

Sample student-generated concentration contour maps for the diffusion-reaction exam problem are shown in Figure 2. The correct answer is given in part (a), showing higher levels of the diffusing species at the bottom right permeable wall, and some weaker diffusion from the left boundary. The species is not present in between these due to consumption by the first-order reaction. A wide range of student responses was received for this question, and two of the more colorful are shown in parts (b) and (c), corresponding to different errors in setting up the problem.

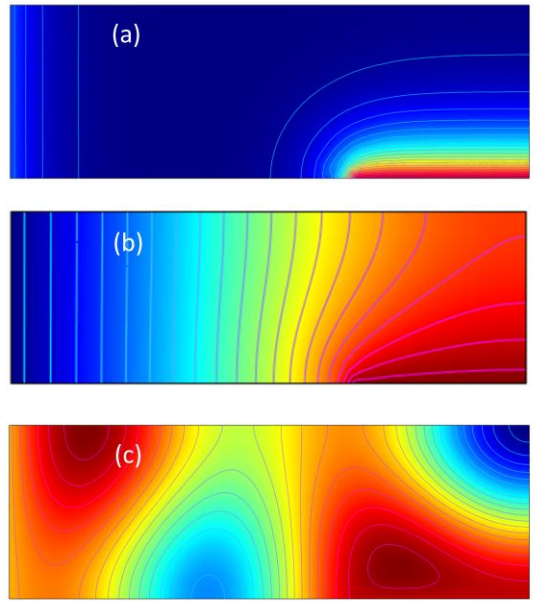

Figure 2. Sample student solutions to the in-lab midterm computer exam.

The exam results showed that nearly all students were able to set up some form of the given equation and geometry in COMSOL, and implement boundary conditions and problem constants. Some difficulties were encountered in translating the equation in component form to the vector/tensor notation used in the program (which accounted for some of the stranger concentration fields produced). Most students were able to produce some form of contour plot as requested, but many were not clear on how to use boundary integration to evaluate mass flows in and out of the domain and check the mass balance, or how to use subdomain integration with a user-defined expression to integrate the reaction rate over the subdomain. Several students were confused about how to do these manipulations in 2D, and the resulting units. These topics had been covered in-class and on homework assignments, but clearly the skills had not been acquired strongly enough.

4.2 Final exam

The theoretical background part of the course comprised six lecture classes on discretization methods (weighted residuals and the Galerkin method), finite element basics including the weak form for 2nd-order ODEs as well as natural and essential boundary conditions, computation of matrix elements with element by element matrix assembly in 1D, meshing and shape functions in 2D, artificial diffusion and the heat equation, direct methods for systems of linear equations (Gaussian elimination, LU decomposition and sparse methods), and indirect methods for systems of linear equations (Jacobi, Gauss-Seidel, preconditioning, multi-grid methods). We did not give homework assignments on these topics, as it was felt that the intense COMSOL exposure over only 4 weeks was a heavy enough workload. The first five exam questions touched on some of these topics, as well as some of the mathematical background provided in the course. Results are shown in Table 1, for the class of nineteen students.

Table 1: Final exam questions 1-5 (theory)

Question topic	Average	Standard Deviation
1. Vectors/tensors	4.68/10	1.72
2. Residual	7.53/15	5.05
3. Weak form	10.10/15	2.13
4. Matrix assembly	7.37/15	4.77
5. Matrix factorization	11.26/15	3.61

Overall, the students struggled with the theoretical material, and performed well only on the weak form question, where they had seen several examples of this derivation, and on the matrix factorization question, which was relatively easy. On the other questions, it was clear that they needed hands-on practice in using the methods described, which should be integrated with the COMSOL material.

With the last three questions an attempt was made to assess to what extent the students had assimilated several ideas of good computing practice. At several points during the course and in the COMSOL exercises, we demonstrated to the class some key ideas. They were shown an example of solution multiplicity in nonlinear differential equations (non-isothermal diffusion and reaction in a sphere) and worked a similar example for homework (non-isothermal tubular reactor). Critically checking results, and being open to the possibility of making mistakes, was stressed on several occasions. Verification by checking both domain- and mesh-independence was illustrated in demonstrations and formed a major part of at least half the COMSOL exercises, and checking of material and energy balance closure was a routine part of our procedure. Validation against simplified models was also mentioned and part of some homework exercises. Results for this part of the exam are given in Table 2, again for nineteen students.

Table 2: Final exam questions 6-8 (concepts)

Question topic	Average	Standard Deviation
6. Critical examination of numerical results	3.84/10	1.69
7. Verification of numerical method	7.42/10	2.78
8. Model validation	4.84/10	2.62

In question 6, the students were presented with a non-isothermal diffusion/reaction problem in a slab. They were given four different sets of temperature and concentration values at the slab midpoint, and told that these were the results of computer simulations. For the given values of the model constants, multiple solutions were possible and two of the sets were consistent with this interpretation. The other two sets contained physically implausible values. The question asked for an explanation of these results. Virtually the entire class missed the multiplicity idea (only one got it) despite their prior exposure to it. Most of the class offered that there must be something wrong with the input to the problem, while about one third said there was something wrong with the mesh, which was not indicated by any of their previous experience. Those who identified user error frequently cited it for all four sets, assuming all were wrong. Others identified the incorrect physical behavior, but offered no suggestions for cause or remedy, such as a sign error for a decrease in temperature in an exothermic reaction system. Clearly some of the idea of critical examination of results was communicated, but improvement is needed.

In question 7, students were asked how they would make a case for the correctness of computer simulation results for flow around a golf ball (this question was motivated by the preferred Friday afternoon activity of one of the seniors). Most of the class identified mesh refinement and changing domain size to establish mesh and domain independence. The distinction between a "better" solution with a refined mesh, and a "mesh-independent" solution was not fully understood in several instances. About a third of the class suggested running simulations with a smooth sphere, for which experimental results are available. In question 8, a non-Newtonian flow through a triangular structured packing was given, and students were asked for a definition of model validation and suggestions as to how model validation might be done. Only a third of the class mentioned experimental data, and there appeared to be confusion with verification steps, with many students again mentioning mesh refinement and closing mass balances.

4.3 End of course survey

On the final day of class the students filled out a survey on various aspects of how the class had worked. Several of the questions stemmed from ideas and complaints that had come up during the term. In Table 3 we present those parts of the survey that bear on the use and teaching of the COMSOL package. Eighteen responses were received out of nineteen students in the course.

The student responses to the survey questions on the mathematical background needed to use COMSOL indicated that in their opinions it was sufficient. While this may have been true for the matrix algebra, the in-lab and final exam questions showed that they were overly optimistic about their understanding of vectors and tensors. More practice in translating between component form and vector/tensor form was clearly indicated.

Table 3: Survey questions on COMSOL use

Question topic (1 – Strongly disagree 2 – Somewhat disagree 3 – No strong feeling 4 – Somewhat agree 5 – Strongly agree)	Average Response	Standard Deviation
Mathematics background		
1. One class on matrix algebra was enough	4.78	0.71
2. One class on vector/tensor calculus was enough	4.28	0.56
3. The background in calculus and differential equations was enough for the course	4.11	0.94
Computer in-lab instruction – more time was needed on		
1. geometry set-up in 2D	1.89	0.87
2. correspondence between COMSOL format and model equations	3.06	1.13
3. post-processing for plots	3.33	1.15
4. post-processing for boundary and domain integration	2.83	1.26
5. subdomain settings	2.33	1.10
6. boundary settings	2.33	1.15
Background theory on Finite Element Methods		
1. don't need FEM theory to use COMSOL	3.28	1.32
2. more information would make theory easier	3.33	1.05
3. theory was ok but too much in too few classes	4.39	0.89
4. needed more worked examples and homework	4.50	0.83
General aims of course and course structure		
1. better to spread COMSOL material out over entire course	3.06	1.39
2. should go back to finite differences using Excel	1.28	0.93
3. course helped me be a better/more careful computer user	4.39	0.49
4. more worked examples and homework problems on theory would aid understanding	4.28	1.10

The student responses that their calculus and differential equations background from previous courses was adequate were tempered by comments that they had not seen much of this material since their 1st or 2nd years, and retention of the material from then was a problem. They remembered having had it, but many of the details and skills had been lost.

The second category in Table 3 was intended to find out where students thought they needed most reinforcement of the existing instruction. Responses tended to be neutral, perhaps reflecting their disinclination to ask for even more material to be incorporated into the course, but in general their perceptions that they had acquired adequate skills in geometry set-up, subdomain settings and boundary settings, but needed more help with converting given model equations into COMSOL's language, and in post-processing, agreed with the exam results and with their graded work. One possible source of confusion was that COMSOL's equations are all dimensioned, whereas many of the examples and exercises taken from the text by Finlayson [6] were in dimensionless form, which sometimes caused difficulties with the units given in the user interface. In responses to other questions, the class felt that the 1-hour laboratory demo sessions were useful, but wanted them extended to two-hour sessions to allow more time for de-briefing the exercises and homework.

Responses on the issue of the theory for FEM tended to be somewhat schizophrenic. Most students agreed that more material, worked examples and homework would be beneficial, but no-one wanted to recommend that they be included! A strong body of opinion felt that the course should focus on what was needed to use COMSOL, and did not see the application of the background material. This presents a clear challenge for future versions of the course to refine the material to what is truly relevant, and to include it with the problem-solving classes in a meaningful way.

Finally, on course structure, the neutral average response to the question of spreading the COMSOL material out over the entire course hides a strongly polarized response, as shown by the standard deviation. The instructor had expected the students to be in favor of more time for the COMSOL part, but a significant number of the class felt that the first three weeks worked well as a review of model development, and did not want to change that. Clearly, any such alteration in course structure should take care to preserve the educational value of this material, while allowing more "sink time" for the computer simulation skills.

Fortunately, the students nearly unanimously preferred COMSOL to the idea of returning to Excel and using finite differences. Nobody brought up the question of to what degree they could expect to find COMSOL in the workplace. The students' numerical responses and written comments indicated a strong degree of satisfaction with the course, feeling that they had learned useful material and become better computer users in an engineering context.

5. Conclusions

The junior/senior elective mathematical modeling course at Worcester Polytechnic Institute was changed to use the finite element multiphysics package COMSOL to solve the model equations, rather than using analytical techniques or finite difference methods on a spreadsheet, as in earlier offerings. A main educational concern was the effect of the use of a "canned" package on student understanding and analysis of the results obtained.

A statistical analysis of student responses to end-of-course survey questions and exam questions was performed. The students demonstrated reasonable competence in the use of COMSOL, but their appreciation of the theory underlying the numerical method, and the problems and pitfalls of verifying and validation a computer simulation left something to be desired. Our experiences indicate that some greater focus on student preparation in vectors/tensors, integration of the finite element theory more tightly as the students learn to use COMSOL, and a stronger effort in terms of emphasizing steps of mesh refinement, comparison to data or known results for simpler cases, and more thorough scrutiny of results, are some of the changes in pedagogy indicated for the next course offering.

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