

# **THE CACHE CORPORATION**

## **WHAT IS CACHE?**

CACHE 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.

## **CREATION OF THE CACHE CORPORATION**

During the 1960s the rapid growth of computer technology challenged educators to develop new methods of meshing the computer with the teaching of chemical engineering. In spite of many significant contributions to program development, the transferability of computer codes, even those written in FORTRAN, was minimal. Because of the disorganized state of university-developed codes for chemical engineering, fourteen chemical engineering educators met in 1969 to form the CACHE (Computer Aids for Chemical Engineering) Committee. The CACHE Committee was initially sponsored by the Commission on Education of the National Academy of Engineering and funded by the National Science Foundation. In 1975, after several successful projects had been completed, CACHE was incorporated as a not-for-profit corporation in Massachusetts to serve as the administrative umbrella for the consortium activities.

## **CACHE ACTIVITIES**

All CACHE activities are staffed by volunteers including both educators and industrial members and coordinated by the Board of Trustees through various Task Forces. CACHE actively solicits the participation of interested individuals in the work of its ongoing projects. Information on CACHE activities is regularly disseminated through CACHE News, published twice yearly.

Individual inquiries should be addressed to:

CACHE Corporation  
P. O. Box 7939  
Austin, Texas 78713-7939  
(512) 471-4933  
FAX: (512) 295-4498  
cache@uts.cc.utexas.edu

<http://www.cache.org>

## **CACHE NEWS**

The CACHE News is published twice a year and reports news of CACHE activities and other noteworthy developments of interest to chemical engineering educators. Persons who wish to be placed on the mailing list should notify CACHE at the aforementioned address. Contributions from CACHE representatives are welcome. This issue was edited by Christine Bailor with contributions from a number of CACHE members and representatives.

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[herb\\_britt@aspentech.com](mailto:herb_britt@aspentech.com)

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[colakymc@ucarb.com](mailto:colakymc@ucarb.com)

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[kim\\_sangtae@lilly.com](mailto:kim_sangtae@lilly.com)

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[steven\\_simroth@merck.com](mailto:steven_simroth@merck.com)

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[siirola@eastman.com](mailto:siirola@eastman.com)

## **Mitsubishi Chemical Corporation**

Miho Hanafusa

[2306475@cc.m-kagaku.co.jp](mailto:2306475@cc.m-kagaku.co.jp)

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Dear Colleague:

It gives me great pleasure to introduce the current issue of CACHE News to you. It contains several thoughtful, timely, and valuable articles written by some of the distinguished members of our profession for everyone's benefit. Building on its nearly 35 years of excellence in serving the chemical engineering community, CACHE continues to serve with several exciting new initiatives. Of particular importance are the task forces in the areas of systems biology, computational fluid dynamics and software engineering in addition to ongoing efforts such as the molecular modeling activity. You will learn more about these initiatives in these pages in the current as well as future issues. We are also very pleased with the success of the FOCAPO 2003 conference organized by Professor Ignacio Grossmann of Carnegie Mellon University and Dr. Conor McDonald of DuPont earlier this year. We are eagerly looking forward to the FOMMS 2003 conference in a couple of months in Colorado. This is the second one in this series and all indications point to a very successful event in the making. There is more as described in the conferences section. These conferences are extremely important for our profession as they bring leaders in various areas together from all over the world to make a status assessment and set the directions for the immediate future in research, education and engagement with the industry.

Thus, CACHE continues to serve our profession in many different ways. On behalf of the organization I thank you and your institution for your continued support.

Best regards,

Venkat Venkatasubramanian  
President  
CACHE Corporation

## Comments from the Editors

As readers of CACHE News are aware, a thorough re-examination and re-design of the undergraduate curriculum in chemical engineering is currently under way at ChE departments throughout the U.S. (for example, <http://web.mit.edu/cheme/>). In this issue Tom Edgar looks at this issue from the perspective of Process Control.

Several articles and reports -- provided from the CACHE Task Forces -- address progress in computational fluid dynamics, molecular modeling, bio-systems, new CACHE initiatives, and the industrial affiliates program.

Upcoming CACHE Foundation Conferences in Operations or Design (FOCAPO 2003 AND FOCAPD 2004), and Molecular Modeling and Design (FOMMS 2003) conferences are detailed to help in your planning to attend these conferences

Two articles in this issue discuss FEMLAB/Matlab. Bruce Finlayson's article -- "*On the proper use of computational fluid dynamics for senior research projects and beginning graduate fluids mechanics courses*" -- details some of his experiences with this Computational Fluid Dynamics (CFD) Package. Edward Rosen -- "*Learning FEMLAB/MATLAB for chemical engineering – unsteady-state heat conduction in a one-dimensional slab*" -- illustrates how it can be used to solve a simple classical problem. Your co-editors of CACHE News believe that one-, two-, and three-dimensional computational dynamics software will soon become a major component of undergraduate chemical engineering education. More articles on this subject will appear in future CACHE News issues.

The editors welcome articles – specially those concerning Fluent and FEMLAB software -- from our readers.

Edward Rosen  
Scott Fogler  
Peter Rony

# Computational Fluid Dynamics

*Jennifer Sinclair Curtis – Purdue University*

The Computational Fluid Dynamics (CFD) Task Force is working to develop methods and tools for incorporating CFD in undergraduate education. CFD is the numerical solution of the differential momentum balance and continuity equation and is sometimes accompanied by the solution of turbulent transport equations, the differential energy balance, or species continuity equations.

In the academic setting, CFD has historically been used as a research tool. However, with advancements in the capabilities, user-friendliness, and speed of simulations, CFD can now also be used as an educational tool. Understanding of concepts in transport and reaction engineering classes can be enhanced through visualization. Students can see developing flow, temperature, or concentration profiles. The CFD graphics bring “life” to the lecture or homework assignment. CFD can be used as a computational laboratory where students can explore the effects of changes, for example, fluid properties, geometry of system, and operating conditions. Students can also investigate 2-D and 3-D problems that can not be solved analytically. In 1-D situations, they can compare their simulation results to analytical solutions obtained in class, results from empirical correlations, or their own laboratory data.

When using CFD students need to think through the modeling of the process and answer questions such as:

Is 2-D acceptable?

What boundary conditions should be applied?

What inputs and parameters need to be specified?

Where are large gradients anticipated and where should a finer grid be used?

As a supplement to CFD, students also can be introduced to numerical solution techniques for non-linear coupled differential equations or more advanced turbulence models.

Through the introduction of CFD in ChE education, students become familiar with a tool for design, scale-up and optimization of flow processes. More companies are using CFD for a range of single-phase and multiphase applications. Without learning CFD in their undergraduate education, it is very easy for students to complete their transport course sequence with the impression that if the flow problem can not be solved analytically or there are no empirical correlations, there are no methods to address the problem.

Recent efforts with the Fluent program FLOWLAB have focused on developing a series of CFD problems that can be applied seamlessly into an undergraduate fluid mechanics course. These problems were distributed at the recent 2002 ASEE Summer School. If you would like a copy of these problems, please contact CFD Task Force leader, Jennifer Sinclair Curtis at [jlids@ecn.purdue.edu](mailto:jlids@ecn.purdue.edu).



# Activities of the Molecular Modeling Task Force

**David Kofke**

*Department of Chemical Engineering  
University at Buffalo, The State University of New York*

The Molecular Modeling Task Force (MMTF) was formed by CACHE in 1996 and charged with the task of developing resources and activities that assist the introduction of molecular modeling methods into the chemical engineering curriculum and ultimately into chemical engineering practice. The task force is headed by Peter Cummings, and its membership includes CACHE trustees Warren Seider, David Kofke and Phil Westmoreland along with 16 other representatives from the molecular modeling research community. A full list is available at the MMTF web site, <http://zeolites.cqe.nwu.edu/Cache/>

Meetings of the MMTF have been facilitated by the generous support of the Department of Chemical Engineering at the Colorado School of Mines. The group last met there nearly two years ago, in March 2001, but many of the original activities of the Task Force are continuing or are reaching fruition. In this article we describe the latest news.

## **FOMMS 2003**

One of the major activities of the MMTF has been the establishment of a new triennial series of international conferences, Foundations of Molecular Modeling and Simulation (FOMMS). The scope of the conference series is theory and applications of computational quantum chemistry and molecular simulation, and the forum is unique in its aim to bring together industrial and academic researchers from the quantum to the process scale. The inaugural meeting was organized by Peter Cummings and Phil Westmoreland at Keystone Resort (CO) in July 2000, and is widely viewed as a great success. Now the next one in the series is nearly upon us. It is being organized by Jim Ely and will take place July 6-11, 2003 again at Keystone. The web site for the meeting is <http://www.mines.edu/academic/chemeng/fomms/>

The content of the meeting is balanced between molecular simulation and computational chemistry. All talks are invited, and two poster sessions will provide opportunities for attendees to present their work. One afternoon will be devoted to a software/hardware demonstration session for providers to showcase their products and services. There will be large blocks of time available for informal discussions, and receptions will be held to facilitate interaction between conference participants. Each invited talk will represent a state-of-the-art review and will be rigorously reviewed and edited. All papers (both posters and invited) will be published in a combination of the journals *Molecular Physics* and *Molecular Simulation*.

The schedule of sessions and speakers is listed here:

**Sunday, July 6**

**Keynote Address:** Dominic Tildesley, Unilever

**Monday, July 7**

***Industrial Applications (morning session)***

Joseph Golab, BP  
Cristina Thomas, 3M  
Sami Karaborni, Merck

***Biological Applications (evening session)***

Sangtae Kim, Eli Lilly  
[Ken Dill, UCSF](#)

**Tuesday, July 8**

***Polymeric Materials (morning session)***

[Ron Larson, UMich](#)  
[Masao Doi, Nagoya](#)  
[Doros Theodorou, Patras](#)

***Nanoscience and Nanotechnology (evening session)***

[Alain Fuchs, UParis-LCP](#)  
[Anabella Selloni, Princeton](#)

**Wednesday, July 9**

***Electronic Materials (morning session)***

[Krishnan Raghavachari, IU](#)  
[Dimitrios Maroudas, UMass](#)  
[Roberto Car, Princeton](#)

***Advances in Molecular Simulation Techniques (evening session)***

[Dave Kofke, UB/SUNY](#)  
Patrick Warren, Unilever

**Thursday, July 10**

***Reaction Engineering (morning session)***

[Thanh Truong, Utah](#)  
[Matt Neurock, UVA](#)  
[Tony Rappé, CSU](#)  
[Bill Green, MIT](#)

**Friday, July 11**

***Future Vision (morning session)***

[Alex Bell, UCB](#)  
[Costas Pantelides, Imperial College](#)  
Ellen Stechel, Ford

## Molecular Simulation Modules

Another major activity of the MMTF is the development of molecular simulation modules for undergraduate and graduate instruction. Each module consists of an interactive molecular simulation and written supporting material related to it. The molecular simulation is written in the Java programming language, and in most cases it can be run as an applet in a web browser. In all cases the simulation can instead be downloaded and run as an application on the user's machine. The supporting material provides an introduction to the concepts demonstrated by the applet, with some detailed background about what is being modeled. There are also examples describing the use of the simulation, and exercises suitable to use as homework assignments.

We have designed a consistent web-based interface that organizes all of the material in each module. We have developed scripts using *perl* that ease the job of putting the written material into this common format. The developer of a module must construct simple text files, perhaps with HTML markup that permits inclusion of figures and tables. Then he or she runs the files through the *perl* script, which adds HTML formatting and links to put the set of files into the common configuration. We then upload the files to our module site for anyone to access. This site is perhaps best accessed through the *etomica* site. *Etomica* is a Java-based support environment we have developed for the modules project, and which has now been expanded for other applications: go to <http://www.ccr.buffalo.edu/etomica> and click on the "modules" link in the navigation bar on the left.

To exemplify the interface, we present the following screen shot from the introduction page for the piston-cylinder module :

»MolecularSimulationModules« "PistonCylinder"

Introduction Background Examples Problems Simulator

### PistonCylinder: Introduction

This module presents an interactive molecular simulation of a piston-cylinder apparatus. The piston-cylinder apparatus is a standard tool used to conceptualize and illustrate thermodynamic concepts involving heat, work, and internal energy. The module may be used also to study equations of state, reversibility, and corresponding states concepts. These ideas form the core of thermodynamics, and this module illustrates how they arise from the aggregate motions of many molecules, each behaving according to simple classical mechanics.

The simulated apparatus is a container (cylinder) with one movable wall (the piston), within which are 100 spherical molecules undergoing simple molecular dynamics. The piston moves in response to collisions with the molecules. The external pressure on the piston may be adjusted, and the system may be set as isothermal or adiabatic; the instantaneous and average density adopted by the system is presented. A dynamic plot is available showing graphically the response of the system to changes in state. Many different quantitative and qualitative experiments can be performed to explore the thermodynamic behavior of the system. The observed behavior is clearly seen as a consequence of the collective molecular motions.

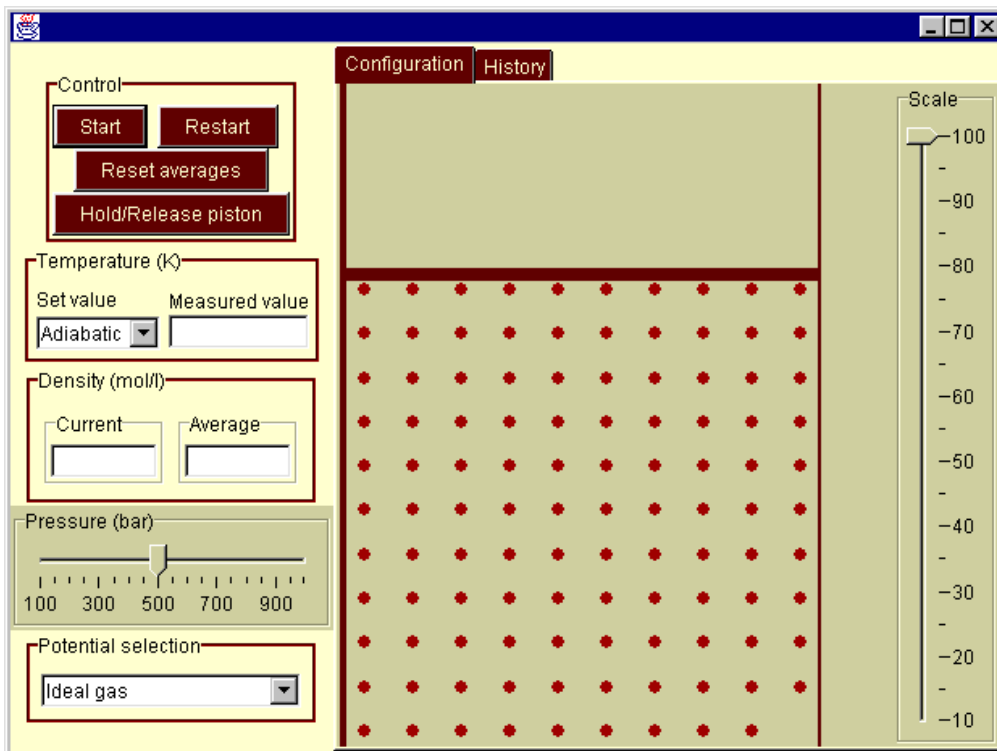
This module is applicable to thermodynamics courses at both the undergraduate and graduate levels.

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This particular module presents an interactive molecular simulation of a piston-cylinder apparatus. The text on the introduction page describes its purpose, "The piston-cylinder

apparatus is a standard tool used to conceptualize and illustrate thermodynamic concepts involving heat, work, and internal energy. The module may be used also to study equations of state, reversibility, and corresponding states concepts. These ideas form the core of thermodynamics, and this module illustrates how they arise from the aggregate motions of many molecules, each behaving according to simple classical mechanics.”

Here is a screen shot from the piston-cylinder simulation itself:



Again, as per the introduction, “The simulated apparatus is a container (cylinder) with one movable wall (the piston), within which are 100 spherical molecules undergoing simple molecular dynamics. The piston moves in response to collisions with the molecules. The external pressure on the piston may be adjusted, and the system may be set as isothermal or adiabatic; the instantaneous and average density adopted by the system is presented. A dynamic plot is available showing graphically the response of the system to changes in state. Many different quantitative and qualitative experiments can be performed to explore the thermodynamic behavior of the system. The observed behavior is clearly seen as a consequence of the collective molecular motions.”

Following is a list of other phenomena and concepts for which modules are completed or planned for this year:

- Chemical reaction equilibrium
- Osmosis
- Diffusion
- Molecular dynamics
- Normal modes of a solid
- Chemical reaction kinetics



- Dissipative particle dynamics
- Surface tension
- Crystal viewer
- Joule-Thomson expansion
- Self assembly
- Chemical potential
- Multicomponent phase equilibrium
- Heat transfer
- Atomic billiards
- Viscosity

The success in using Java for development of these modules has led us to expand its capabilities further, and the Java-based codes are now the primary tool used for research applications in the author's group. Further development of the code for these purposes is being supported by a new 4-year grant from NSF, via the ITR program.

**Proposal for new  
CACHE Task Force  
on  
Computing, Biosystems, and Chemical Engineering Education**

**Task Force Organizers**

Frank Doyle - *University of Delaware*

Sangtae Kim - *Eli Lilly*

**Summary Statement**

In recognition of the changing nature of the chemical engineering discipline, a task force is proposed to address the new challenges in computing in chemical engineering education that arise in the areas of biosystems (functional genomics, bioinformatics, proteomics, computational biology, pattern discovery, systems biology, etc.). The timing is critical, many of the major chemical engineering departments in the U.S. are revising their undergraduate curriculum to address new technological challenges in biosystems. At the same time, industry is looking to recruit chemical engineering graduates with combined skills in computing/modeling and biosystems.

At the present time, CACHE does not have a focused effort in this area, owing largely to a lack of trustees in the bio area. This task force would aim to take on the challenge of archiving or creating computer-based modules for biological problems that can be integrated into traditional core courses (mass balance, thermo, fluids, control, design, etc.). Some such modules already exist in the CACHE products portfolio. More ambitious objectives may be possible with leveraged NSF funding (mirroring the successes of the molecular modeling task force).

This task force will address means for involving the present (and potential future) industrial affiliates in this task force activity. With Sangtae Kim as a co-organizer, we can reach Lilly. Other likely collaborators include Dow, Merck, and DuPont. Industrially motivated problems would be a valuable contribution to any module development.

A side benefit of this activity would be the recruitment of energetic new trustees in the bio area. There is also a significant professional development opportunity for the members of this task force as they take a role in shaping education in this emerging area.

**Related Synergistic Activities**

- AICHE has an initiative at the Board level to examine the future of biotechnology & bioengineering (Sangtae Kim is on that committee)

- There was a session at the 2002 Annual Meeting on Bioinformatics in Chemical Engineering Education (co-chaired by Frank Doyle)
- Bioengineering sessions at the recent ASEE Summer School for ChE Faculty  
The CACHE website is accumulating content in bioengineering curriculum

### **Current Status**

1. In addition to Frank Doyle and Sangtae Kim, the following individuals have been suggested for the proposed task force, and each has agreed to serve on the ad hoc committee:

Professor Vassily Hatzimanikatis, Northwestern  
Professor Mike Henson, U. Massachusetts  
Dr. Bob Leipold, Entelos  
Professor Costas Maranas, Penn State  
Professor Babatunde Ogunnaike, U. Delaware  
Dr. Julia Ross, U. Maryland Baltimore County  
Dr. Chen Su, Eli Lilly

2. An initial meeting convened at the 2002 AIChE Annual Meeting. Brainstorming on the question of curriculum content was followed by the suggestion of identifying 2-3 computational modules that would be effective for several of the core undergraduate courses in the chemical engineering curriculum. The group is currently preparing a list of sample modules for the following core courses:

Separations  
Reaction Engineering  
Process Control  
Process Design

3. Findings will be reported at the Summer Trustees meeting, along with a formal proposal for the task force.

## **An Invitation to Participate in the**

### **CACHE**

#### **Industrial Affiliates Program**



#### **About CACHE**

CACHE is a not-for-profit organization whose objectives are to make chemical engineering instruction more effective and to enhance the familiarity of students, educators, and practitioners with computer-based tools and technology. CACHE interacts with over 140 chemical engineering departments from domestic as well as foreign academic institutions.

The CACHE Committee was founded in 1969 under the sponsorship of the Commission on Education of the National Academy of Engineering and was initially funded by the National Science Foundation. It was later incorporated as a not-for-profit educational organization, CACHE Corporation. A Board of Trustees of eminent educators and industrial practitioners having skills and knowledge of computing technologies in chemical engineering oversees CACHE programs. The academic trustees are notable for their interest in the advancement of chemical engineering education. Many have written textbooks that are among the most popular books in chemical engineering.

#### **CACHE Products and Services**

CACHE services include:

- Development, testing, and distribution of educational software to chemical engineering departments.
- Assessment and dissemination of new developments in chemical engineering.
- Operation of internationally recognized research conferences in computer-related technologies such as process design, process control, process operations, molecular modeling and artificial intelligence. The conference proceedings are important archival references in the area of computing and systems technology and related fields.

CACHE products address a variety of educational needs in chemical engineering. These include reviews of new educational computing technologies, surveys of computing

practices in industry and academia, and computer programs, some of which have been integrated with popular chemical engineering textbooks.

CACHE serves as a focal point for new thrusts in chemical engineering education and sponsors demonstrations and programs with other professional societies such as AIChE and ASEE. Projects are carried out through Task Forces under the guidance of the CACHE Trustees. Current task forces are involved in content development in the areas of molecular modeling and simulation, computational fluid dynamics, biosystems, and web-based courses.

The CACHE website ([www.cache.org](http://www.cache.org)) provides a portal to a variety of web-based courses, the Fall and Spring issues of CACHE News, faculty openings, and a number of other services.

### **Industrial Affiliate Program**

The Industrial Affiliates Program is of mutual benefit to both CACHE and companies participating as industrial affiliates. For CACHE, it provides much-needed industrial input about the educational needs for chemical engineering graduates and also financial support for its activities. For the industrial affiliates, it gives an opportunity to participate in undergraduate educational programs and simultaneously derive some promotion benefits. Available opportunities for Industrial Affiliates are:

- **Educational**
  - Providing input to undergraduate computer-related education issues (including recommended educational requirements)
  - Creating case studies and educational modules
  - Writing articles in CACHE News
  
- **Promotional**
  - Access to the CACHE website
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- **Other**
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  - Complimentary copy of all unrestricted CACHE publications (case study, report, conference proceedings, etc.)
  - Interaction with leading educators/researchers

## **How to be an Industrial Affiliate**

The maximum benefit of Industrial Affiliates Program is derived through mutual interaction between the CACHE organization and the Industrial Affiliate company. This is best served through one (or more) contact person(s) at the Industrial Affiliate company who will participate in the educational and promotional opportunities listed above.

An Industrial Affiliate may participate at a number of levels:

- Annual dues of \$1,500. All Industrial Affiliate benefits for one year. This includes subsidiaries of global corporations.
- Financial support of a specific CACHE event such as a conference or reception at a level of \$1,500 or greater. All Industrial Affiliate benefits for one year and recognition for five years.
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# On the Choice of VBA

*Edward M. Rosen*  
EMR Technology Group

## Introduction

Choosing a suitable computer language to teach undergraduate chemical engineering students has been the topic of debate for some time. Generally the debate has been embedded in the more general issue of how much computer training is needed to prepare the undergraduate student for work in industry or graduate school.

Edgar (1) indicated five abilities that the B.S. Ch.E. graduates should have. He notes that programming language expertise is not included in his list and discusses a number of numerically oriented programs that are available for equation solving, optimization, process simulation and other mathematical capabilities. He suggests programs such as Matlab, Mathematica and Maple are suitable alternatives for numerical analysis as a required course.

In support of the idea that programming training is not needed, Davis et. al. (2) indicated that most engineers in industry feel that such training is not expected.

There is a downside to the above, however. In the research environment of graduate school a programming proficiency is often critical to the research. When a programming skill is needed in the corporate workplace, industry will often argue that the skill can be hired outside via a consultant. Though this may be the case, once the job is done by a consultant there is no one available to understand, maintain and extend the work. The outside consultant's work then is wasted. In addition, the consultant is often not really familiar with the application as is the full time staff member. It is the author's observation that having a programming skill within a company is a real advantage both to the employee and the company.

There is also a downside to the teaching of a number of different tools to the student as he/she passes through various courses. The student rarely has time to learn any of the programs very well. Few tools can be learned without continual use. As a result the tool loses its potential effectiveness.

There is, in addition, a downside to teaching a student to program in FORTRAN, C , C++ or Visual Basic so as to enable the student to address a variety of problems. Each of the languages takes a long time to learn and takes a considerable effort to apply to a particular problem.

## **The VBA Choice**

Building on the use of the Excel spreadsheet program (3) is an attractive alternative. Excel has emerged as a general standard spreadsheet program and is the one program that the student has learned and applies on a regular basis. What can be taught is Excel's macro language Visual Basic for Applications (VBA).

There are already a large number of available spreadsheet programs that can be used throughout the curriculum. The VBA language itself is procedural and object oriented. It provides a means of calling routines in other languages (FORTRAN, C, Matlab, Mathcad).

A possible scenario would be to offer a two-hour credit course in the freshman level that introduces the use of spreadsheets, the VBA language and numerical methods. The student could use the capabilities of Excel with VBA to meet essentially his entire undergraduate computing needs (4,5). Use of a process simulator (e. g. Aspen Plus, HYSYS) may be useful as a supplement.

A long recognized advantage of the spreadsheet is that it enables the student to thoroughly understand an algorithm or a computational procedure. From a teaching point of view this is much better than using a series of black boxes.

Spreadsheets are widely used in industry. The author has used the VBA language in a range of research and development projects. Industrial personnel respond well to the use of spreadsheets.

VBA comes with applications other than Excel. It is the same language used in all of Microsoft's Office Application in addition to programs such as AUTOCAD and Microsoft's Project. Once VBA is learned in one application it can be used in others.

There are currently no college textbooks that point to the use of VBA in homework problems. The appearance of such textbooks would be of considerable benefit. Use of other books (6, 7, 8, 9), however, can be made. The Internet has a large number of VBA oriented sites.

## **References**

1. Edgar, T. F. "Chemical Engineering Education and the Three C's: Computing, Communication, and Collaboration"  
*CACHE News*, Fall 2000

2. Davis, J. F., Taylor, R., Hyrmak, A. "CACHE 1997 Computing Survey – Final Analysis" , May 18, 1998.
3. Rosen, E. M. "The Case for Excel and Visual Basic for Applications"  
*CACHE News*, Spring 1998.
4. Clough, D. and Carnahan, B. Workshop 18: Integrating Computing across the Curriculum via Spreadsheets, *ASEE Chemical Engineering Post Summer School Summer 2002, Boulder, Colorado*.
5. Rives, C. and Lacks, D. J. "Teaching Process Control With A Numerical Approach Based on Spreadsheets", **Chemical Engineering Education**, Vol 36, 2002 p 242
6. Walkenbach, J., *Excel 2000 Power Programming with VBA*, IDG Books , Foster City 1999
7. Getz, K and Gilbert, M., *VBA Developer's Handbook*, Sybex, San Francisco 1997
8. Cummings, Steve *VBA for Dummies*, Hungry Minds, New York (2001)
9. Hart-Davis, Guy, *Mastering VBA 6* , Sybex, San Francisco (2000)

# ChE Curriculum of the Future: Re-evaluating the Process Control Course

Thomas F. Edgar

Department of Chemical Engineering  
University of Texas  
Austin, TX 78712

I recently attended a department chairs workshop in Orlando, FL (“New Frontiers in Chemical Engineering Education”, 1/27-29/03), where a group of about 45 faculty wrestled with how to make the Ch.E. curriculum more relevant for today’s graduates. One of the major undercurrents of this workshop (which will have follow-on workshops later this year) was to determine what role biological science and engineering will play in the future curriculum. A corollary to this question was if new courses are added to the curriculum, what can be removed? Clearly all departments face a variety of local constraints that result in relatively inflexible paths to the degree (with a hard constraint on the total number of credit hours... a zero-sum game).

After the first breakout sessions, different groups reported a long and varied list of proposed changes to the curriculum. Notably, a few groups reported that the subject of process control was high on the “hit list”. While process control was not perceived as the only option, I was not expecting to see it in such an egregious position. This caused me to begin thinking about why the value of process control to academic chemical engineers is apparently not as high as I thought it was. Of course, my views are strongly influenced by the fact that I have spent 35 years teaching , writing textbooks, and doing research in this field.

I inquired of my colleagues at the workshop why process control had reached such a “lowly state” in their eyes, and I began to get a few clues as to why this may be the case. With the emphasis today on “bio, nano, enviro, and info” at funding agencies such as NSF, NIH, and DOD, it is not clear where process control researchers fit into this

agenda. Hiring faculty at research-oriented departments has certainly moved in the same direction as the available funding (which includes the disproportionate effect of the Whitaker Foundation in the bio area). Faculty in these areas are oriented towards discovery-type research, far from the details of making commercial quantities of products.

A related article (“Refocusing Chemical Engineering”) was published in the January, 2002 issue of Chemical Engineering Progress, Ed Cussler et al. declared that a number of fields like thermodynamics, reaction engineering, transport, and control can be relegated to the scrap heap of “mature technologies” that will not have much future impact in the gain in knowledge. Ed et al. proposed dropping courses on control and optimization at the end of the article but add several disclaimers: “First, we accept without question the importance of process optimization to commodity chemicals. Secondly, we recognize that process control has a key role in ensuring the success of those other cornerstones of competitive advantage in specialty product manufacture; safety, consistency and quality. Our third hesitation stems from our unwillingness to sacrifice any of our technical core to less-quantitative business ideas. Still, we recognize that a large part of our future is going to be in areas where different skills are needed”. So, Ed, what discipline will staff chemical manufacturing in the future, mechanical engineers? The semiconductor industry already discovered that chemical engineers are the best process engineers (“process” interpreted very broadly). Or is manufacturing as we know it not going to exist in 2020? See [www.cache.org/vision/index.html](http://www.cache.org/vision/index.html) for one perspective on how it will change (Vision 2020).

A third strike against academic process control as an important technological contributor was the recent article published by long time practitioner Greg Shinskey (retired from Foxboro) in IEC Research, Vol. 41(16) p. 3745 (2002). Greg states there has been little or no progress in 35 years in closing the industrial-academic gap in process control, causing B.S. graduates to be unprepared for industrial assignments. This is reminiscent of statements I heard at technical meetings 30 years ago that “control research is dead”. Obviously it rose from the ashes in the 1970s and has been alive and

well for the past 20 years. Of course Greg Shinskey also believes that any useful analysis can be done on the back of an envelope, which suggests that academics in many fields of chemical engineering are not engaged in meaningful work. It is interesting that Shinskey and Cussler express opposing views. Shinskey argues that nothing important has been accomplished, whereas Cussler states that so much has been accomplished there are no major improvements expected in the future. To use an analogy articulated by an industrial colleague, Shinskey says we have been driving in the wrong direction (but we can turn the car around), while Cussler says the car is out of gas and drivers are no longer needed.

Industrial chemical engineers seem to have little doubt that process control is important to keeping modern chemical plants operating, a view that was articulated by several industrial attendees at the Frontiers workshop. So maybe the disconnect is how the typical faculty member views where employment opportunities will reside in the future, say in 2020. If chemical engineers are not involved in making value-added “stuff” at a desired quality level, the contribution of chemical engineering to the national economy will undoubtedly be greatly reduced. What do we expect B.S. chemical engineers to be doing then?

Other observations that emerged at the workshop were that a systems viewpoint is very important for chemical engineers and separates them from chemists, biologists, and other engineers. It was pointed out that unsteady-state behavior and feedback control are important concepts in living systems, and any organism that is at steady-state is dead (arguing for an understanding of dynamic process models). Also chemical engineers have to deal with a wide range of scales, from molecular to macro, even enterprise levels, which suggests that mathematical models are important. So that seems to bode (no pun intended) well for keeping process control in the curriculum. However, another view that emerged at the workshop was that we could insert a little bit of process control in five or six courses. Realistically, that approach may not be effective and could be easily diminished in any course by individual faculty option.

So why does the process control course cause fear and loathing among our non-control colleagues? First, like design, it is usually taught by a small subset of faculty in a typical department (as opposed to other core courses in thermo, transport, unit operations, etc.). It perhaps is one of the “short straws” in teaching assignments. Second, process control is perceived by many faculty to be an applied mathematics course that heavily focuses on Laplace transforms, analytical solutions to linear differential equations, linear algebra, frequency response, optimization, and the like, without much practical content beyond tuning a PID controller. Computer simulation takes a back seat to theoretical analysis. This is the way many faculty taught undergraduate process control 20 or more years ago, but some departments may not have changed the emphasis or content of the course. In fact the availability (since 1998) of computer-based tools such as Simulink in MATLAB or Control Station (by Doug Cooper) has completely changed the way in which process control can be taught.

The topics I cover when I teach process control include dynamic behavior (with about one lecture on Laplace transforms and analytical solutions to ODEs), physical and empirical modeling, computer simulation, measurement and control hardware technology, basic feedback and feedforward control concepts, and advanced control strategies. Many of these topics can be presented to reflect applications in biochemical or materials engineering. More emphasis could be placed on modeling, optimization, and data analysis/statistics in a revised course. Unfortunately existing textbooks (including mine) mostly use examples from continuous processes in petrochemical plants (vs. batch specialty products). This shortcoming can be addressed near-term by using the world wide web to disseminate new course materials that augment existing books. A new committee organized under the CACHE Corporation and led by CACHE trustees Frank Doyle, Sangtae Kim, and Tunde Ogunnaike is focusing on developing biosystems course materials in the areas of design, control, kinetics, and separations. There already is a good start for such a website in the Teaching Resource Center at [www.cache.org](http://www.cache.org). One outcome of the Frontiers workshops being held in 2003 will likely be a proposal to NSF to fund the development of educational modules to supplement existing textbooks in all core areas.

Most educators agree that a systems viewpoint is valuable for chemical engineering graduates. Dynamics, feedback, and stability are intellectual underpinnings required for understanding many new and complex systems of interest to chemical engineers. Control, like design, can be taught in a way so that students must integrate knowledge from other core ChE courses in process modeling and analysis of process behavior. There are not many courses in the curriculum that fulfill these needs. Constructive change is critical to the health of our profession, so I invite all faculty, especially those from the computing and systems community, to join this discussion to revitalize our curriculum.

[note: a shorter version of this article was published in Chemical Engineering Education, Spring, 2002]



# Using VBA As An Alternative

by  
*Edward Rosen, EMR Technology*

## Introduction

Many routine calculations carried out using stand-alone systems such as MathCad (1) can be carried out as well in Excel using its macro language Visual Basic for Applications (VBA). The advantages of doing this are discussed in (2). This communication reviews (3) some of the details involved in a VBA implementation of the integration of an n-dimensional system of differential equations.

## Earth's Carbon Cycle

A model of the earth's carbon cycle is discussed in (4). The differential equations describing the model together with their initial values are given in Tables 1 and 2. A plot of deforestation ( $F_d(t)$ ) and fossil fuels data ( $F_f(t)$ ) is given in graphical form in Figure 1 (taken from Reference 4). The task is to integrate the differential equations from the year 1850 to 1990. Of particular interest is the growth of atmospheric carbon dioxide over that period of time.

## The Excel Spreadsheet

The spreadsheet of the model is given in Figure 2. The step size for the integration (h) and the number of equations to be solved (n) are specified under System Parameters (C5, C6). The model parameters starting in C12 are defined to the left of the main table. The main table begins in location F12 with the year 1850. The initial values of the eight dependent variables are specified on the same line. The value of the CO<sub>2</sub> (P12) concentration is calculated from the value of M1.

The spreadsheet invokes the array function procedure Intc (Figure 3) starting in the year (1850 + h). The initial invocation with the output selected in H13:O13 is

$$= \text{Intc} ( \$D\$6, \$D\$7, \$G13, \$H13:\$O13, \$D\$13)$$

Ctrl+Shift+Enter is pressed.

This corresponds to the general calling sequence

$$= \text{Intc} ( h, n, x, y, prm)$$

where

h = step size  
n = number of equations  
x = independent variable  
y = dependent variable vector  
prm = parameter vector

Entries for the following years are copied from the entry for  $1850 + h$ .

### **The VBA Integration and Interpolation Routines**

VBA has access to a large number of routines but lacks two that are needed for this application: an n-dimensional integration routine and a one-dimensional interpolation routine that can be extrapolated.

For the integration, the array function Intc invokes the rk4a function. This is a 4<sup>th</sup> order Runge-Kutta routine utilizing a fixed step size, h (Figure 4). The routine was modified by Pedro L. Claveria (5) from the EMR Technology Library (6). The parameter vector prm was passed from the spreadsheet to rk4a via the Intc function.

Data for  $F_f(t)$  and  $F_d(t)$  (at 1850, 1860, 1870, etc) was read directly from the plot of Figure 2 in Reference (4). The data was entered using the array function of VBA (7) and is used in the function dydx (Figure 5) which defines the right hand sides of the differential equations. The  $F_r(t)$  data (for the reforestation) was taken as zero (Reference (4)).

The interpolation function Interp (Figure 6) was used to interpolate quadratically within the arrays yr, AFFt, AFDt and AFRt

The general calling sequence is

= Interp (nl, x, fx, arg)

where

nl = 1 for linear interpolation, 2 for quadratic interpolation  
x = the independent variable vector  
fx = the dependent variable vector  
arg = the independent variable vector

The years 1991 to 2000 in Figure 2 represents an extrapolation.

## **Executing the Spreadsheet**

The reader may download the spreadsheet

Earth Carbon Cycle.xls

which is available in this issue of CACHE News. The VBA may be brought up by hitting Alt+F11. By modifying the data in dydx for  $F_f(t)$ ,  $F_d(t)$  and  $F_r(t)$  (AFFt,AFDt,AFRt for years 1850 to 1990) different atmospheric carbon dioxide levels can be predicted for future years (as suggested in Reference (4)).

## **Results and Conclusions**

Table 3 compares the results of the spreadsheet/VBA computations with that given in Reference (4). The results compare favorably considering the different ways the data for  $F_f(t)$  and  $F_d(t)$  are handled. (In this study interpolation is used on data read from a chart. In Reference (4) curve fitting was employed on original data). Another source of difference may be due to the different integration routines used in this study and that used from MathCad (1).

Excel offers a viable alternative for carrying out routine calculations such as integrating initial value differential equations. This may be done with VBA code or other languages such as FORTRAN (8,9).

## **References**

1. MathCad, <http://www.mathcad.com>
2. Rosen, E. M. "On the Choice of VBA", *CACHE News*, No 56 Spring 2003
3. Rosen, E. M. "The Case for Excel and Visual Basic for Applications", *CACHE News*, No 46 Spring 1998 p 5
4. Schmitz, R. A. "The Earth's Carbon Cycle", *Chemical Engineering Education*, Vol 36, No. 4 Fall, 2002, pp 296
5. Pedro Luis Claveria Vila, Private Communication (circa, April 2002)
6. EMR Technology Group Library, CACHE Corporation
7. Walkenbach, John *Excel 2000 Power Programming with VBA* IDG Books Worldwide, Inc , Foster City, CA. 1999 p 255
8. Rosen, E. M. "Calling FORTRAN Subroutines from Excel 7.0" *CACHE News*, No 47, Fall 1998

9. Rosen, E. M. "On the Use of IMSL Routines in Excel 7.0"  
*CACHE News* No 49, Fall 1999

Table 1

Earth's Carbon Cycle Differential Equations

$$dM_1 / dt = -(k_{12} + k_{13})M_1 - k_{15}M_8 \frac{M_1 - g}{M_1 + \Gamma} + k_{21}M_2^{b_2} + k_{31}M_3^{b_3} + k_{51}M_5 + k_{61}M_6 + F_f(t) + F_d(t) - F_r(t)$$

$$dM_2 / dt = k_{12}M_1 - (k_{23} + k_{24})M_2 - k_{21}M_2^{b_2} + k_{42}M_4$$

$$dM_3 / dt = k_{13}M_1 + k_{23}M_2 - k_{34}M_3 - k_{31}M_3^{b_3} + k_{43}M_4$$

$$dM_4 / dt = k_{24}M_2 + k_{34}M_3 - (k_{42} + k_{43})M_4$$

$$dM_5 / dt = k_{15}M_8 \frac{M_1 - g}{M_1 + \Gamma} - (k_{51} + k_{56})M_5 - F_d(t) + F_r(t)$$

$$dM_6 / dt = k_{56}M_5 - k_{61}M_6$$

$$dM_7 / dt = -F_f(t)$$

$$dM_8 / dt = \frac{-[k_d F_d(t) - k_r F_r(t)]}{M_{5,ref}}$$

**Table 2**  
**Numerical Values and Units for Model Constants**

<u>Symbol</u>	<u>Value</u>	<u>Units</u>
k <sub>12</sub>	0.0931	y <sup>-1</sup>
k <sub>13</sub>	0.0311	y <sup>-1</sup>
k <sub>15</sub>	147	y <sup>-1</sup>
k <sub>21</sub>	7.05006E-26	PgC <sup>(1-β<sub>2</sub>)</sup> y <sup>-1</sup>
k <sub>23</sub>	<b>0.0781</b>	y <sup>-1</sup>
k <sub>24</sub>	<b>0.0164</b>	y <sup>-1</sup>
k <sub>31</sub>	2.31615E-21	PgC <sup>(1-β<sub>3</sub>)</sup> y <sup>-1</sup>
k <sub>34</sub>	<b>0.714</b>	y <sup>-1</sup>
k <sub>42</sub>	<b>0.00189</b>	y <sup>-1</sup>
k <sub>43</sub>	<b>0.00114</b>	y <sup>-1</sup>
k <sub>51</sub>	<b>0.0862</b>	y <sup>-1</sup>
k <sub>56</sub>	<b>0.0.0862</b>	y <sup>-1</sup>
k <sub>61</sub>	<b>0.0333</b>	y <sup>-1</sup>
β <sub>2</sub>	<b>9.4</b>	
β <sub>3</sub>	<b>10.2</b>	
?	62	PgC*
G	198	PgC
k <sub>d</sub>	<b>0.230</b>	
k <sub>r</sub>	1.0	
M <sub>5,ref</sub>	580	

\*PgC, 1 Pg = 10<sup>15</sup> g

Conversion Factor: 2.218 PgC/ppmv

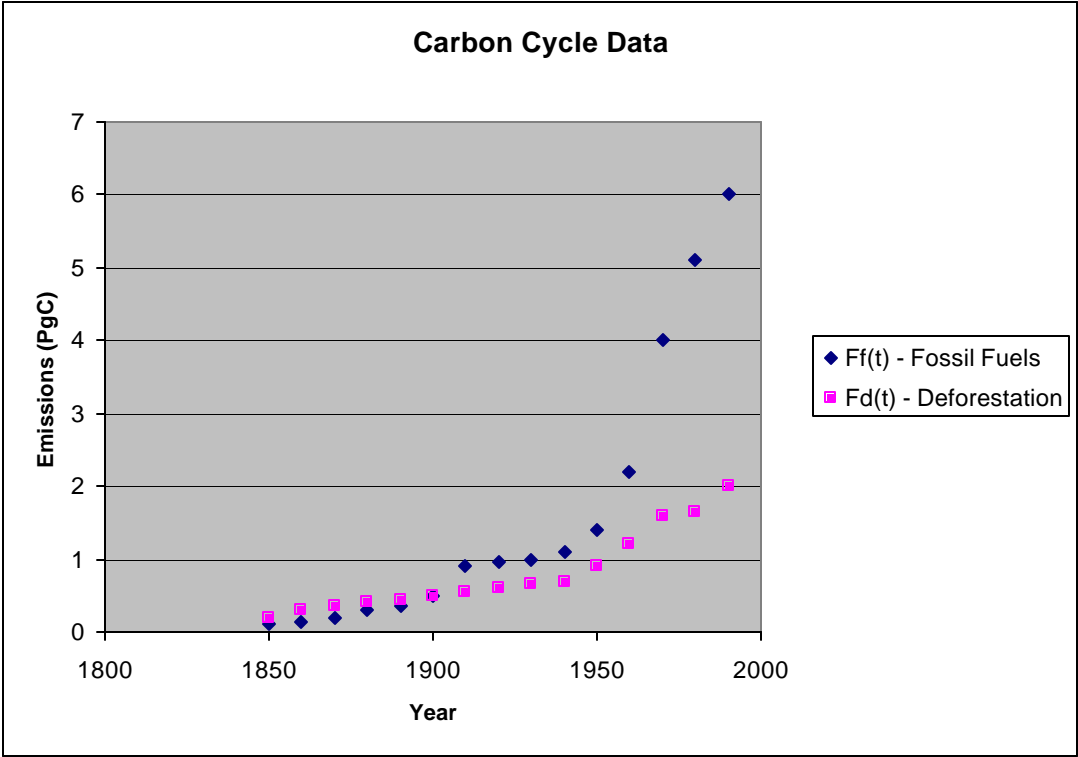


Figure 1  
Fossil Fuels and Deforestation Emissions

A/1	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
2		Earth's Carbon Cycle from Schnitz CEE Vol 36 No 4 Fall 2002														
3																
4																
5		System Parameters		Units												
6		h		1 years												
7		n		8 Number of Equations												
8																
9		Parameters														
10																
11	prm	Symbol	Value	Units	Year	M1	M2	M3	M4	M5	M6	M7	M8			CO2 (ppmv)
12																
13		1 k12	0.0931	y <sup>-1</sup>	1850	612.0	730.0	140.0	37000.0	580.0	1500.0	5300.0	1.0000000			287.6
14		2 k13	0.0311	y <sup>-1</sup>	1851	612.5	730.0	140.1	36999.9	579.7	1500.0	5299.9	0.9999182			287.8
15		3 k15	147	y <sup>-1</sup>	1852	612.9	730.0	140.1	36999.8	579.4	1500.0	5299.8	0.9998317			272.3
16		4 k21	7.05E-26	PgC <sup>(1-beta2)</sup> /y	1853	613.3	730.0	140.1	36999.7	579.1	1500.0	5299.7	0.9997407			288.2
17		5 k23	0.0781	y <sup>-1</sup>	1854	613.7	730.0	140.2	36999.6	578.9	1500.0	5299.6	0.9996452			288.4
18		6 k34	0.0164	y <sup>-1</sup>	1855	614.0	730.1	140.2	36999.6	578.8	1499.9	5299.4	0.9995456			288.5
19		7 k31	2.32E-21	PgC <sup>(1-beta2)</sup> /y	1856	614.4	730.1	140.2	36999.5	578.6	1499.9	5299.3	0.9994420			288.7
20		8 k34	0.714	y <sup>-1</sup>	1857	614.7	730.2	140.2	36999.5	578.5	1499.8	5299.2	0.9993347			288.9
21		9 k42	0.00189	y <sup>-1</sup>	1858	615.0	730.2	140.2	36999.4	578.4	1499.7	5299.0	0.9992238			289.0
22		10 k43	0.00114	y <sup>-1</sup>	1859	615.3	730.2	140.2	36999.4	578.3	1499.6	5298.9	0.9991095			289.2
23		11 k51	0.0862	y <sup>-1</sup>	1860	615.6	730.3	140.2	36999.4	578.3	1499.5	5298.8	0.9989921			289.3
24		12 k56	0.0862	y <sup>-1</sup>	1861	615.9	730.3	140.2	36999.3	578.2	1499.5	5298.6	0.9988721			289.4
25		13 k61	0.0333	y <sup>-1</sup>	1862	616.2	730.3	140.2	36999.3	578.1	1499.4	5298.4	0.9987502			289.6
26		14 beta2	9.4	y <sup>-1</sup>	1863	616.5	730.4	140.2	36999.3	578.1	1499.3	5298.3	0.9986262			289.7
27		15 beta3	10.2	y <sup>-1</sup>	1864	616.8	730.4	140.2	36999.3	578.1	1499.2	5298.1	0.9985003			289.8
28		16 gamma	62	PgC	1865	617.0	730.4	140.2	36999.2	578.0	1499.1	5298.0	0.9983724			290.0
29		17 lambda	198	PgC	1866	617.3	730.5	140.2	36999.2	578.0	1499.0	5297.8	0.9982426			290.1
30		18 kd	0.23		1867	617.6	730.5	140.2	36999.2	578.0	1498.9	5297.6	0.9981107			290.2
31		19 kr	1		1868	617.8	730.5	140.2	36999.2	577.9	1498.8	5297.4	0.9979769			290.3
32		20 M5, ref	580		1869	618.1	730.5	140.2	36999.2	577.9	1498.7	5297.2	0.9978411			290.5
33					1870	618.4	730.6	140.2	36999.2	577.9	1498.6	5297.0	0.9977033			290.6
					1986	738.1	742.7	142.4	37053.9	579.3	1493.7	5111.9	0.9597859			346.9
					1987	741.4	743.1	142.5	37055.5	579.5	1493.9	5106.2	0.9590549			348.4
					1988	744.8	743.4	142.5	37057.2	579.7	1494.1	5100.4	0.9583076			350.0
					1989	748.2	743.7	142.6	37058.9	579.8	1494.3	5094.5	0.9575428			351.6
					1990	751.6	744	142.7	37060.6	580.0	1494.5	5088.5	0.9567595			353.2
					1991	755.1	744.4	142.7	37062.4	580.1	1494.7	5082.5	0.9559562			354.8
					1992	758.6	744.7	142.8	37064.3	580.2	1495.0	5076.4	0.9551320			356.5
					1993	762.2	745.1	142.8	37066.1	580.3	1495.2	5070.2	0.9542856			358.2
					1994	765.9	745.4	142.9	37068.1	580.4	1495.4	5063.9	0.9534158			359.9
					1995	769.5	745.7	143.0	37070.0	580.5	1495.7	5057.6	0.9525213			361.6
					1996	773.3	746.1	143.0	37072.0	580.5	1495.9	5051.2	0.9516011			363.4
					1997	777.1	746.5	143.1	37074.1	580.5	1496.1	5044.7	0.9506540			365.2
					1998	780.9	746.8	143.2	37076.2	580.4	1496.3	5038.2	0.9496787			367.0
					1999	784.8	747.2	143.2	37078.3	580.4	1496.5	5031.5	0.9486740			368.8
					2000	788.7	747.5	143.3	37080.5	580.3	1496.7	5024.9	0.9476388			370.6

Figure 2  
 Spreadsheet for Earth  
 Carbon Cycle

```

Option Base 1
Public Function Intc(h, n, x, y, prm)

Dim xx As Single
Dim Irtn As Integer
Dim I As Integer

nn = n + 1

ReDim yy(1 To n) As Single
ReDim ddd(1 To nn) As Single
ReDim fff(1 To n)

xx = x

For I = 1 To n
yy(I) = y(I)
Next I

Irtn = rk4a(n, h, xx, yy, prm)

xx = xx + h

ddd(1) = xx

For I = 2 To nn
ddd(I) = yy(I - 1)
Next I

Intc = ddd

End Function

```

**Figure 3**

**Listing of VBA Array Function Intc**



```

        Public Function rk4a(n, h, x, y, prm)
,
'Modified from Pedro L. Claveria abril/2002
'based in EMR Technology Group Library
,
,
'n = number of equations
'h = step size for integration
'x = independent variable
'y = vector of dependent variables
'prm = vector parameters

ReDim ccc(n), fff(n)
ReDim k1(n), k2(n), k3(n), k4(n)
ReDim y2(n), y3(n), y4(n)

'Calculation of k1
muda1 = dydx(x, y, prm, fff)
For I = 1 To n: k1(I) = fff(I): Next
'Calculation of k2
For I = 1 To n: y2(I) = y(I) + 0.5 * h * k1(I): Next
muda2 = dydx(x + h / 2, y2, prm, fff)
For I = 1 To n: k2(I) = fff(I): Next
'Calculation of k3
For I = 1 To n: y3(I) = y(I) + 0.5 * h * k2(I): Next
muda3 = dydx(x + h / 2, y3, prm, fff)
For I = 1 To n: k3(I) = fff(I): Next
'Calculation of k4
For I = 1 To n: y4(I) = y(I) + h * k3(I): Next
muda4 = dydx(x + h, y4, prm, fff)
For I = 1 To n: k4(I) = fff(I): Next

'New values of the dependent variables
For I = 1 To n
    ccc(I) = y(I) + (h / 6) * (k1(I) + 2 * k2(I) + 2 * k3(I) + k4(I))
Next I

For I = 1 To n
    y(I) = ccc(I)
Next I

rk4a = 0

End Function

```

**Figure 4**

**Listing of VBA Function Procedure rk4a**

```

Public Function dydx(x, y, prm, fff)

'x = independent variable
'y = vector of dependent variables
'prm = parameter vector
'fff = dy/dx

Dim AFFt As Variant
Dim AFDt As Variant
Dim AFRT As Variant
Dim Ayr As Variant

Dim NL As Integer
Dim xx As Single

Dim t1, t2, t3, t4 As Single

yr = Array(1850,1860,1870,1880,1890,1900,1910,1920,1930,1940, _
           1950, 1960, 1970, 1980, 1990)

AFFt = Array(0.1, 0.15, 0.2, 0.3, 0.35, 0.5, 0.9, 0.95, 1#, 1.1, _
            1.4, 2.2, 4#, 5.1, 6#)

AFDt = Array(0.2, 0.3, 0.35, 0.4, 0.45, 0.5, 0.55, 0.6, 0.65, 0.7, _
            0.9, 1.2, 1.6, 1.65, 2#)

AFRT = Array(0#, 0#, 0#, 0#, 0#, 0#, 0#, 0#, 0#, 0#, 0#, 0#, _
            0#, 0#, 0#)

NL = 2
xx = x

FFt = Interp(NL, yr, AFFt, xx)
FDt = Interp(NL, yr, AFDt, xx)
FRt = Interp(NL, yr, AFRT, xx)

t1 = -(prm(1) + prm(2)) * y(1) - prm(3) * y(8) * (y(1) - prm(16)) _
      / (y(1) + prm(17))
t2 = prm(4) * y(2) ^ prm(14)
t3 = prm(7) * (y(3) ^ prm(15)) + prm(11) * y(5) + prm(13) * y(6)
t4 = FFt + FDt - FRt

fff(1) = t1 + t2 + t3 + t4

t1 = prm(1) * y(1) - (prm(5) + prm(6)) * y(2)
t2 = -prm(4) * y(2) ^ prm(14) + prm(9) * y(4)

fff(2) = t1 + t2

```

**Figure 5**

**Listing of VBS Function Procedure dy/dx (page 1)**

```

t1 = prm(2) * y(1) + prm(5) * y(2) - prm(8) * y(3)
t2 = -prm(7) * y(3) ^ prm(15) + prm(10) * y(4)

fff(3) = t1 + t2

fff(4) = prm(6) * y(2) + prm(8) * y(3) - (prm(9) + prm(10)) * y(4)

t1 = prm(3) * y(8) * (y(1) - prm(16)) / (y(1) + prm(17))
t2 = -(prm(11) + prm(12)) * y(5) - FDt + FRt

fff(5) = t1 + t2

fff(6) = prm(12) * y(5) - prm(13) * y(6)

fff(7) = -FFt

fff(8) = -(prm(18) * FDt - prm(19) * FRt) / prm(20)

dydx = 0
End Function

```

**Figure 5**  
**Listing of VBS Function Procedure dy/dx (page 2)**

```

Public Function Interp(nl, x, fx, arg)

Public Function Interp(n, x, fx, arg)

'Written by EMRosen 6/19/97
'Copyright (c) by EMR Technology Group

'Modified 8/15/97 For Extrapolation

' nl is the order of interpolation -1 for Linear, 2 for second order
' x is the x array of numbers to be used -
' the name for the range is used in the call
' fx is the array corresponding values of f(x) -
' the the first element of the range may be used
'arg is the x argument
' The return is the value of f(arg)

xarg = arg

'Nc is the total array length
Nc = Application.Count(x)
'MsgBox "Value of Nc=" & Nc

If (xarg < x(1)) Then
    Num = 1
    GoTo Setn:
End If

If (xarg >= x(Nc) And n = 1) Then
    Num = Nc - 1
    GoTo Setn:
End If

If (xarg >= x(Nc) And n = 2) Then
    Num = Nc - 2
    GoTo Setn:
End If

'Num is the index of the element in the range less than or equal to arg
Num = Application.Match(arg, x, 1)

Setn:

If (n = 2 And Nc < 3) Then
    Interp = 0
    Exit Function
End If

If (n = 1 And Nc < 2) Then
    Interp = 0
    Exit Function
End If

```

**Figure 6**  
**Listing of VBS Function Procedure Interp (Page 1)**

```

xarg = arg

x1 = x(Num)
fx1 = fx(Num)

x2 = x(Num + 1)
fx2 = fx(Num + 1)

If (n = 2 And Nc >= Num + 2) Then GoTo Second:

If (n = 2 And Nc < Num + 2) Then GoTo Third:

Term1 = (xarg - x2) / (x1 - x2)
Term2 = (xarg - x1) / (x2 - x1)

Interp = Term1 * fx1 + Term2 * fx2

Exit Function
Second:

x3 = x(Num + 2)
fx3 = fx(Num + 2)
GoTo Continue:

Third:

x1 = x(Nc - 2)
fx1 = fx(Nc - 2)

x2 = x(Nc - 1)
fx2 = fx(Nc - 1)

x3 = x(Nc)
fx3 = fx(Nc)

Continue:
Term1 = (xarg - x2) * (xarg - x3) / ((x1 - x2) * (x1 - x3))
Term2 = (xarg - x1) * (xarg - x3) / ((x2 - x1) * (x2 - x3))
Term3 = (xarg - x1) * (xarg - x2) / ((x3 - x1) * (x3 - x2))

Interp = Term1 * fx1 + Term2 * fx2 + Term3 * fx3

End Function

```

**Figure 6**  
**Listing of VBS Function Procedure Interp (Page 2)**

Table 3

Comparison of Solutions at 1990

	<u>Reference 4</u>	<u>This Work</u>
M <sub>1</sub>	753	751.6
M <sub>2</sub>	744	744.0
M <sub>3</sub>	143	142.7
M <sub>4</sub>	37071	37060.5
M <sub>5</sub>	577	580.0
M <sub>6</sub>	1489	1494.5
M <sub>7</sub>	5086	5088.5
M <sub>8</sub>	0.952	0.9568

# On the Proper Use of Computational Fluid Dynamics for Senior Research Projects and Beginning Graduate Fluid Mechanics Courses

Bruce A. Finlayson  
Rehnberg Professor of Chemical Engineering  
University of Washington  
Seattle, WA 98195-1750  
finlayson@cheme.washington.edu

## Abstract

This paper demonstrates how to introduce computational fluid dynamics (CFD) to undergraduates in a research setting and graduate students in a beginning fluid mechanics course. Of course the students must learn to use the CFD program, but FEMLAB™ has made that very easy. Thus, the burden is on the user and instructor to insure that the students have a way to validate their results. Shown here are the preliminary steps the author has used:

- solving simple problems to compare with textbook examples;
- learning to make the equations non-dimensional and report the results in a consistent, meaningful manner;
- using mesh refinement to validate the numerics;
- comparing results to published and known results.

Also shown here are some of the remarkable results achieved:

- pressure coefficients for slow flow to augment those for turbulent flow;
- entry length and approach length correlations to enlarge the body of design information;
- orifice calculations to correct errors in the literature;
- calculations to help graduate students estimate (and then calculate) the impact of assumptions;
- examination of patents in microfluidics.

## Introduction

Computational Fluid Dynamics (CFD) programs are getting better and better (i.e. easier to use) and it is important to teach students what they can do, and what they cannot do. This paper will describe experience using a CFD program that is particularly easy to use, FEMLAB™. Undergraduate chemical engineering students at the University of Washington have used this in senior research projects, and beginning graduate students have used it in the fluid mechanics course. When the material is presented sequentially, and the professor has some knowledge of CFD (to get out of tight spots), students can learn to solve the problem they want to solve, document that process, and assess the accuracy of their solution independent of any experiment. Because of the recent interest in microfluidics, most simulations are for laminar flow, at a variety of Reynolds numbers.

## Undergraduate Research Projects

The procedure for teaching students how to use CFD programs is described. An essential element of the process is to make the steps small and manageable, with the eventual goal clearly specified. A sample goals statement is given in Figure 1 for a beginning researcher and Figure 2 for someone who has worked with me in previous quarters.

### **Figure 1. Predicting Pressure Drop across Orifices in Laminar Flow**

Ch.E. 499 Project for Febe Kusmanto, Sp, 2002

The goal is to predict the pressure drop across orifices when the flow is laminar. This project continues one started last spring. The published literature has a mistake in it (the student last year found this, with help from me). We want to prepare a good summary of what the data should look like, based on an old paper (which I have, from the Journal of Fluid Mechanics, JFM), and then do numerical calculations as a function of thickness of the orifice and Reynolds number to further validate our results. If done well, this could lead to a published paper.

The beginning steps will be:

1. Learn to use pde toolbox on the PCs in 125
  2. Run some example cases using FEMLAB in BNS 125
  3. Learn to nondimensionalize the equations, and transfer between computer results, dimensionless results, and dimensional results.
  4. Set up the problem in FEMLAB, for flow in a cylinder with an orifice of finite thickness. Solve it as a function of Reynolds number, for different thicknesses (from the paper).
  5. Prepare correlations of the dimensionless pressure drop versus Reynolds number, for different geometries. Compare with the JFM paper and with the experimental data (and also with the bogus report.)
  6. Write a final report, convert to PowerPoint presentation, prepare Web display.
- 

The second step is to learn to use the program. The programs are demonstrated by the instructor, and a handout is given for the program pdetool™ (which operates on top of Matlab™ and was a precursor to FEMLAB™), as shown in Figure 3. With this demo and handout, all students, undergraduate and graduate, have been able to use the programs successfully, without instructor help.



## Figure 2. Mixing of Miscible Fluids in Microfluidic Devices

Ch.E. 499 Project for Marlina Lukman, Spring, 2002

The overall goal this quarter will be to study the mixing of miscible fluids in microfluidic devices. Conceptually, consider two different fluids coming in the two ports of a 'T'. Then they flow down together through the stalk of the 'T'. Since they are miscible, they will diffuse into each other. When the fluids have different viscosities, one must use a mixing rule to determine the viscosity as a function of concentration. We will do this and compare mixing with and without these mixing rules.

This is an outline of the objectives/tasks:

1. For a 'T' mixer in planar geometry, solve for flow when the physical properties of the two fluids are the same.
2. Add diffusion to that.
3. Using correlations and books, develop a mixing rule for two chemicals.
4. Solve the problem when the viscosities and densities are a function of concentration.
5. As time permits, see how this mixing is enhanced as the Reynolds number changes, as the ratio of viscosities changes, as the density ratio changes.
6. Write a final report, convert to PowerPoint presentation, prepare Web display.

Together we will have to decide what chemicals we want to use, and the best mixing rule.

---

## Figure 3. Ch. E. 475 - Tutorial for using Matlab/PDE Toolbox to solve elliptic boundary value problems

**Open Matlab** and give the command **pdetool**. (This only works if one has the professional version with pde toolbox. This is installed in BNS 125.)

### **draw**

click on the square icon and draw a rectangle  
for the inner rectangle, do again  
to make a hole, use R1 – R2  
double click on the object to set exact dimensions

### **boundary mode** - choose $\partial\Omega$ icon

click on one boundary  
or shift click on all boundary segments with the same boundary condition  
double click on the last one, and set the boundary condition

### **mesh**

click once on triangle icon  
click on divided triangle icon to refine the mesh

**pde**

choose specification - to check the differential equation

=

click on = to solve the problem

**plot**

set parameters to choose the type of plot

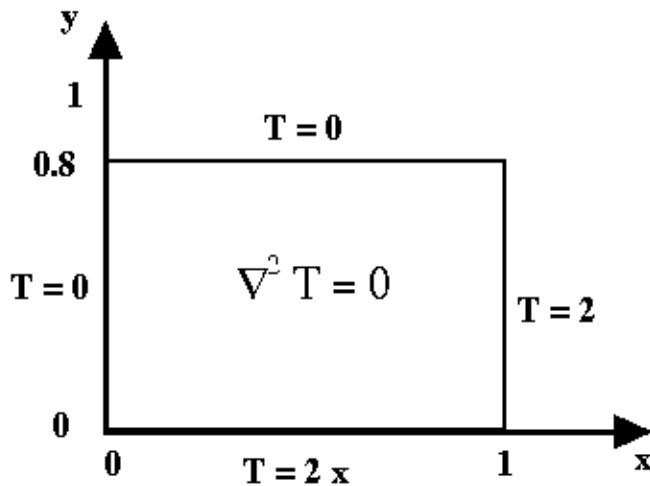
You can go back and refine the mesh (click the more refined mesh symbol) and resolve the problem. This gives you an indication of the accuracy of the solution.

If you want detailed information about the solution, you must save the solution to the MATLAB command workspace (it is called u), and save the element information (it is called p e t).

**Save your work frequently!**

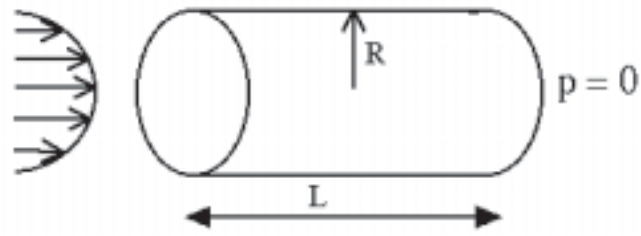
---

Shown in Figures 4 and 5 are two problems that are assigned. The student is to solve them, make plots of them, and report back to the instructor. This exercise gives the student confidence, since they are able to solve the problems, although maybe the comparison to their textbook is difficult the first time. It also gets them ‘over the hump’ on how to access the program, use it, save their results, print figures, etc. A printed copy of the mesh is always required, to emphasize the importance of mesh refinement. Figure 4 involves geometries that are not quite square, and boundary conditions that are not uniform. Figure 5 involves cylindrical geometry.



Put 2 \* x into the BC window rather than a number.

**Figure 4. Heat Transfer Problem**



Put  $u = u_0 \left[ 1 - \left( \frac{r}{R} \right)^2 \right]$  as boundary condition.

Compare with Hagen-Poiseuille law in your textbook.

**Figure 5. Flow in Capillary**

The next lesson that must be learned is how to make the equations nondimensional, and how to report results that others can use. My checklist is:

- What velocity is 1.0 in the computer?
- What distance is 1.0 in the computer?
- What boundary conditions did you use?
- What is the Reynolds number, and where did you use it (see below)?

The Navier-Stokes equations are

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u}$$

To make them non-dimensional, we divide each quantity by a standard dimension, denoted by the subscript s.

$$\mathbf{u}' = \frac{\mathbf{u}}{u_s}, \quad p' = \frac{p - p_0}{p_s}, \quad \mathbf{x}' = \frac{\mathbf{x}}{x_s}, \quad \nabla' = x_s \nabla, \quad \nabla'^2 = x_s \nabla^2$$

The primed variables have no dimensions. The standard dimensions are constants, and hence carry through any differentiation operation. Substituting for  $\mathbf{u}$  and  $p$  in the Navier-Stokes equations gives

$$\frac{\rho u_s^2}{x_s} \mathbf{u}' \cdot \nabla' \mathbf{u}' = -\frac{p_s}{x_s} \nabla' p' + \frac{\mu u_s}{x_s^2} \nabla'^2 \mathbf{u}'$$

There are now two versions for the next steps, the first one natural for laminar flow and the second one natural for turbulent flow.

In version 1, for laminar flow

$$\text{Divide by } \frac{\mu u_s}{x_s^2}, \quad \text{use } \frac{p_s x_s}{\mu u_s} = 1$$

$$\frac{\rho u_s x_s}{\mu} \mathbf{u}' \cdot \nabla' \mathbf{u}' = - \nabla' p_1' + \nabla'^2 \mathbf{u}'$$

$$\text{Re} = \frac{\rho u_s x_s}{\mu}, \quad p_s = \frac{\mu u_s}{x_s}$$

and the equation is

$$\text{Re} \mathbf{u}' \cdot \nabla' \mathbf{u}' = - \nabla' p_1' + \nabla'^2 \mathbf{u}'$$

Here the pressure from the computer (the primed variable) is multiplied by the viscosity times the standard velocity and divided by the standard distance to obtain the real pressure in Pascals, e.g. The reason this form of nondimensionalization is useful for laminar flow (particularly for microfluidic flows) is that for small Reynolds number the whole solution is independent of Reynolds number, including the dimensionless pressure drop. (The actual transition where Reynolds must be taken into account depends upon you accuracy standards:  $\text{Re} \leq 0.1$  is good enough,  $\text{Re} = 1$  may be, and  $\text{Re} = 10$  has some effect of the Reynolds number.)

In version 2, for turbulent flow

$$\text{Divide by } \frac{\rho u_s^2}{x_s}, \quad \text{use } \frac{p_s}{\rho u_s^2} = 1$$

$$\mathbf{u}' \cdot \nabla' \mathbf{u}' = - \nabla' p_2' + \frac{\mu}{\rho u_s x_s} \nabla'^2 \mathbf{u}'$$

$$\text{Re} = \frac{\rho u_s x_s}{\mu}, \quad p_s = \rho u_s^2$$

and the equation is

$$\mathbf{u}' \cdot \nabla' \mathbf{u}' = - \nabla' p_2' + \frac{1}{\text{Re}} \nabla'^2 \mathbf{u}'$$

Here the pressure from the computer (the primed variable) is multiplied by the density times the standard velocity squared to obtain the real pressure in Pascals, e.g. The reason this form of the nondimensionalization is useful for turbulent flow is that at high Reynolds number the pressure is proportional to density times velocity squared, and thus the dimensionless pressure drop is a constant. (The actual transition where this is true, though, is an extremely high Reynolds number, say  $10^6$ , but it is a useful rule of thumb.)

The equations in the computer are given as

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \eta \nabla^2 \mathbf{u}$$

$$\text{Either } \rho = \text{Re} \text{ and } \eta = 1 \text{ or } \rho = 1 \text{ and } \eta = \frac{1}{\text{Re}}$$

determines how  $p$  is converted to real numbers.

A convenient way to differentiate between the computer variables and other formulations is to write the equations in the following form.

$$\rho_c \mathbf{u}_c \cdot \nabla_c \mathbf{u}_c = -\nabla_c p_c + \eta_c \nabla_c^2 \mathbf{u}_c$$

The next lesson to be learned is how to present your results. Students are accustomed to calculating the Reynolds number based on the average velocity in a pipe and diameter of a pipe. What do you do if you make the standard distance the radius of the pipe, i.e. your computer geometry goes from zero at the centerline to 1.0 at the wall? Students need to learn how to take the computer results and change them into the conventions we all use. One example that is helpful in doing that is the following: suppose we have two pipes coming together to join and go down a single pipe. What is the Reynolds number? Obviously, how one presents this case is a matter of convention, since one can talk about the Reynolds number in each of three pipes. Once that problem is posed, students understand that the conditions must be specified very clearly. This brings back my checklist:

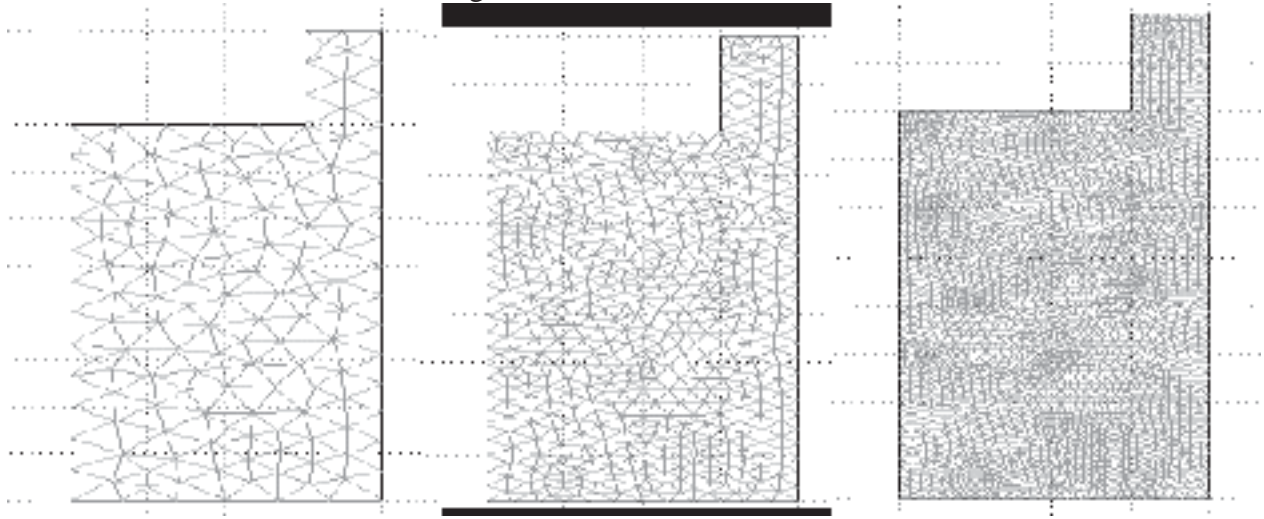
- What velocity is 1.0 in the computer? (This is the standard velocity, and can be converted to words.)
- What distance is 1.0 in the computer? (This is the standard distance, and can be converted to words.)
- What boundary conditions did you use? (This helps define the problem.)
- What is the Reynolds number, and where did you use it? (This determines how to go

from the computer pressure to the real pressure.)

In a group meeting, we go through some examples in which the computer conditions and results are given, and the students are asked to give the average velocity in m/s, the diameter in m, and the pressure (in Pascals) once enough information is given to do so. While I've never done so, it would be instructive to assign the problem of solving the same problem using the two different formulations and showing that the velocities are the same, the dimensionless pressure drops are different, but the pressure drop derived in Pascals is the same. Now the students are ready to solve 2D and 3D flow problems.

The last topic to understand is mesh refinement. Early in the program, the instructor decided not to worry about explaining the finite element method, but to emphasize the fact that the results are an approximation which gets better the more elements there are. Consequently, students were asked to compute the same problem with different meshes and report how some aspect (like pressure drop)

changed. Now a PowerPoint presentation is given about the finite element method in order to give students a better idea of how the problem is solved; this does not go deeply into the details of the Galerkin method (which requires the divergence theorem and 2D/3D math). Typical mesh refinements from FEMLAB are shown in Figure 6.



**Figure 6. Three meshes**

### Sample Results from Undergraduate Research Projects

Results are shown here that were derived by undergraduate students: pressure coefficients in 2D/3D situations, pressure drops across orifices with finite width, entry and approach lengths in contraction flows, and flow and diffusion with a concentration-dependent viscosity.

Shown in Figure 7 is a page from Bird, Stewart, Lightfoot [1]. It shows the viscous dissipation coefficient for pressure drop in turbulent flow. This coefficient is similar to the pressure coefficient described below. To calculate the overall pressure drop for turbulent flow in a piping network, one combines the pressure drop for flow through straight pipe with the pressure drop through the bends, valves, and contractions, etc. Undergraduates working with me are developing the same information for laminar flow. Notice that the viscous dissipation coefficient naturally goes with the second form of nondimensionalization, since it is normalized with respect to velocity squared.

Figure 8 shows how the pressure coefficient is defined in the two cases. Figure 9 shows how that coefficient will vary with Reynolds number in the two cases, the left one using as pressure standard the viscosity times velocity over distance, and the right one using one half the kinetic energy. (All these are for laminar flow). The pressure contours in a rounded corner (between flexible flat plates) is shown in Figure 10. The pressure loss is divided into three parts: the pressure drop in the straight pipe before the bend, the pressure drop in the straight pipe after the bend, and the pressure drop in the bend. The pressure drop in the bend is correlated with the parameters of the problem as shown in Figure 11.

Three-dimensional cases can be done, too, but the computer network at the University of Washington is quite old, and slow. Thus, it is important to be able to learn essential things on good

TABLE 7.4-1  
BRIEF SUMMARY OF FRICTION LOSS FACTORS FOR USE WITH EQ. 7.4-10.  
(Approximate Values for Turbulent Flow)<sup>a</sup>

Obstacles	$e_s$
<i>Sudden Changes in Cross-Sectional Area<sup>b</sup></i>	
Rounded entrance to pipe	0.05
Sudden contraction	$0.45(1 - \beta)$
Sudden expansion <sup>c</sup>	$\left(\frac{1}{\beta} - 1\right)^2$
Orifice (sharp-edged)	$2.7(1 - \beta)(1 - \beta^2) \frac{1}{\beta^2}$
<i>Fittings and Valves</i>	
90° elbows (rounded)	0.4-0.9
90° elbows (square)	1.3-1.9
45° elbows	0.3-0.4
Globe valve (open)	6-10
Gate valve (open)	0.2

<sup>a</sup> Taken from H. Kramers, *Physische Transportverschijnselen*, Technische Hogeschool, Delft, Holland (1958), pp. 53-54.  
<sup>b</sup>  $\beta = (\text{smaller cross sectional area})/(\text{larger cross sectional area})$   
<sup>c</sup> See derivation from the macroscopic balances in Example 7.5-1. When  $\beta = 0$ ,  $\hat{E}_s = \frac{1}{2}\langle \bar{v} \rangle^2$  where  $\langle \bar{v} \rangle$  is the velocity *upstream* from the enlargement.

Figure 7. Friction Loss Factors, from BSL

At high Re :  $\Delta P = K \rho \langle u \rangle^2 / 2$

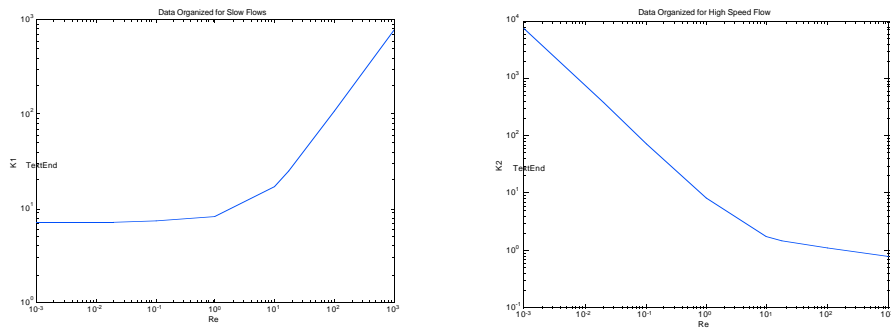
Ex : for 90° elbows  $K = 0.75$

At low Re :  $\Delta P = K \mu \langle u \rangle / x_s$

non-dimensionlize:  $\Delta P' p_s = K \mu / x_s u_s \langle u \rangle'$

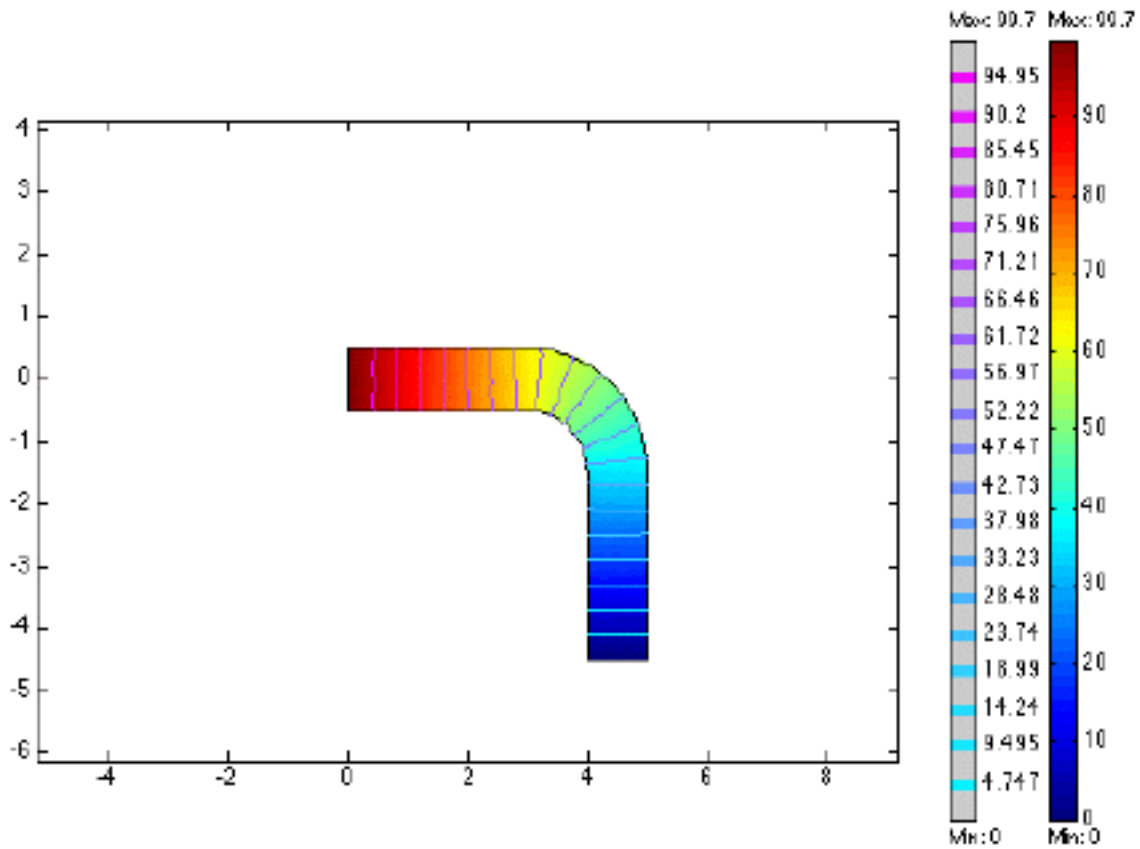
choose  $p_s = \mu u_s / x_s$  :  $\Delta P' = K \langle u \rangle'$

Figure 8. Definition of Pressure Coefficient



**Slow Flow Correlation      Fast Flow Correlation**

**Figure 9. Two correlations of the same pressure drop**



**Figure 10. Pressure Contours in Rounded Corner (due to Suwimol Kunaridtipol)**



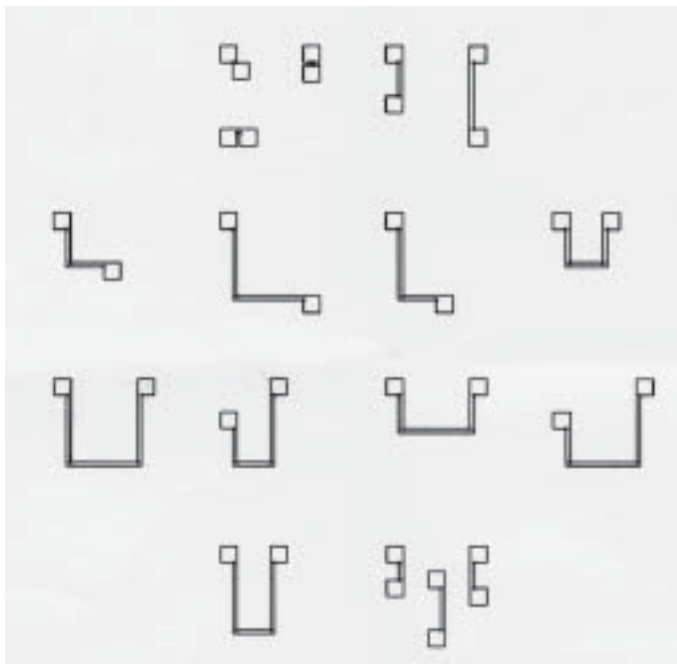
$$\begin{aligned}
 \Delta p' &= \Delta p'(\text{total}) - \Delta p'(\text{entry}) - \Delta p'(\text{exit}) \\
 &= 99.7 - 36 - 36 \\
 &= 27.7
 \end{aligned}$$

$$\Delta p' = K \langle u \rangle', \langle u \rangle' = 1$$

$$K = 27.7$$

**Figure 11. Pressure Coefficient of Rounded Corner (due to Suwimol Kunaridtipol)**

2D problems that contain the essence of the problem. Once one is 'certified', 3D problems can be solved. Shown in Figure 12 are some geometries that were studied in conjunction with a small, local start-up company. The flow came up from the bottom, went down a square channel, and exited up or down. To determine the pressure drop in each device, the flow elements shown in Figure 13 suffice. One example calculation is shown in Figure 14.



**Figure 12. Flow Geometries**

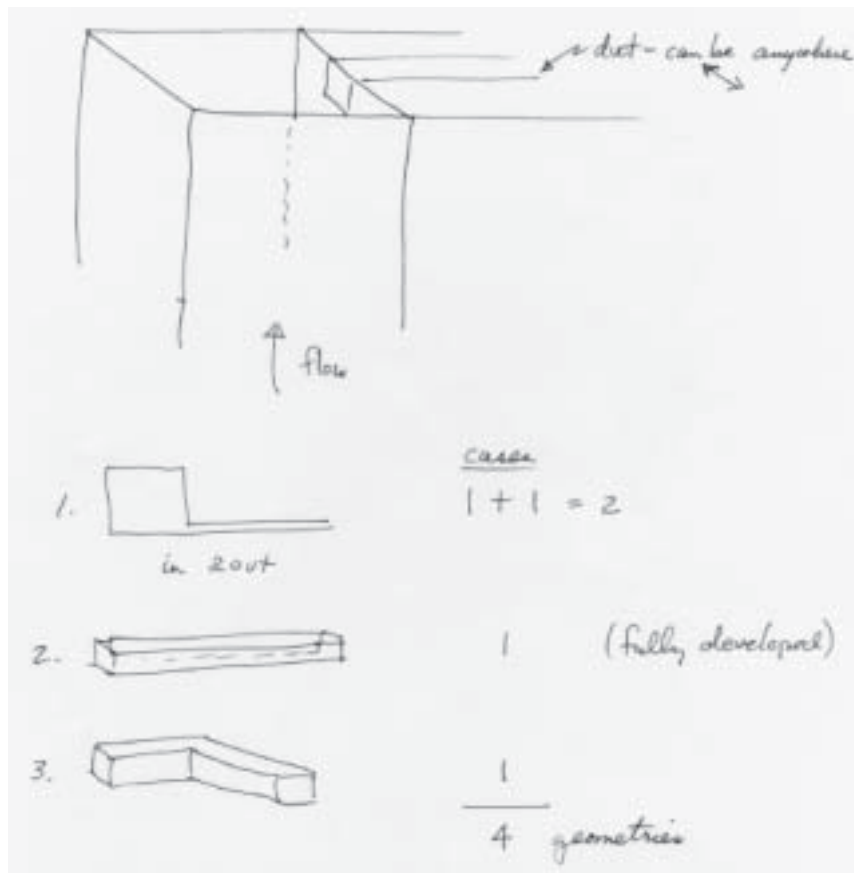


Figure 13. Flow Elements for Pressure Drop Calculations

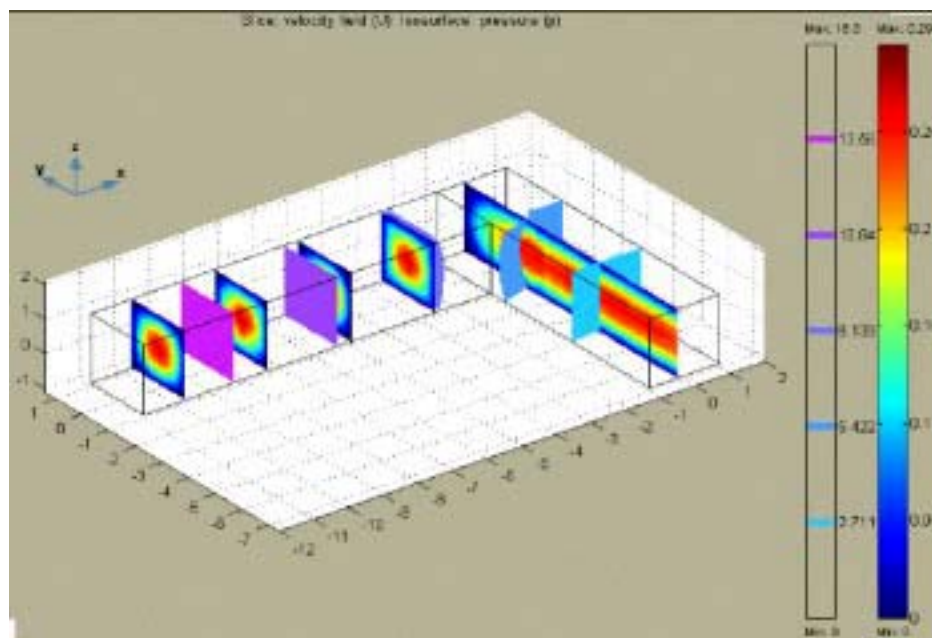
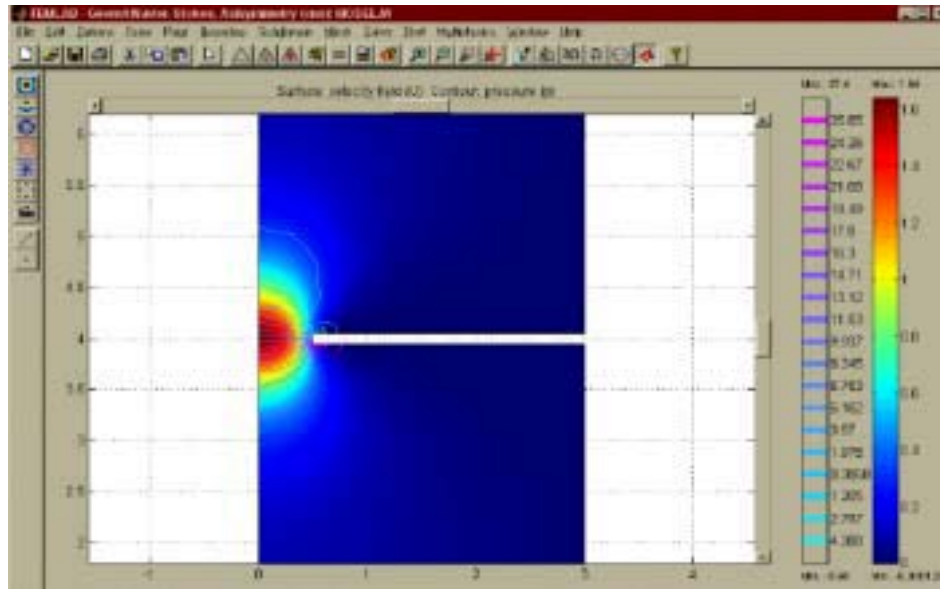


Figure 14. Flow in 90 degree corner, square channel (due to Marlina Lukman)



**Figure 15. Pressure contours in Flow through Orifice (due to Febe Kusamanto)**

The next case is flow through an orifice when the thickness of the orifice is appreciable. Figure 15 shows the pressure profile from one simulation. An exact solution exists for slow flow, as shown in Figure 16. Essentially, the exact solution gives the value of  $K_1$  in the correlation above it. The exact solution shows that the thickness of the orifice matters, even in slow flow. A comparison of calculated results with experimental ones is shown in Figure 17, and clearly the curve depends upon the thickness,  $L$ , in both the calculations and experiment. The experimental data [2] found that the pressure drop depended on the thickness, but misinterpreted the theory [3] at slow flow. Hasagawa, *et al.* reported the theory had no dependence on thickness. They also did calculations with another CFD program, FIDAP, and found no dependence on thickness either. Both results contradicted their data, and this discrepancy is widely reported to indicate that the Navier-Stokes equations are not valid when the capillary is small, with a diameter in the range of a few microns. The calculations reported here, which agree quite nicely with the experiments and theory [3], refute that contention. Being able to make the equations nondimensional and interpret the computer results is obviously an important skill.

$$\frac{2 \Delta p}{\rho U^2} = K_2 + \frac{K_1}{Re}$$

$$\frac{2 \Delta p}{\rho U^2} = \frac{64 L}{Re D} + \frac{12 \pi}{Re}$$

Figure 16. Exact Solution for Pressure Drop for Flow Through an Orifice

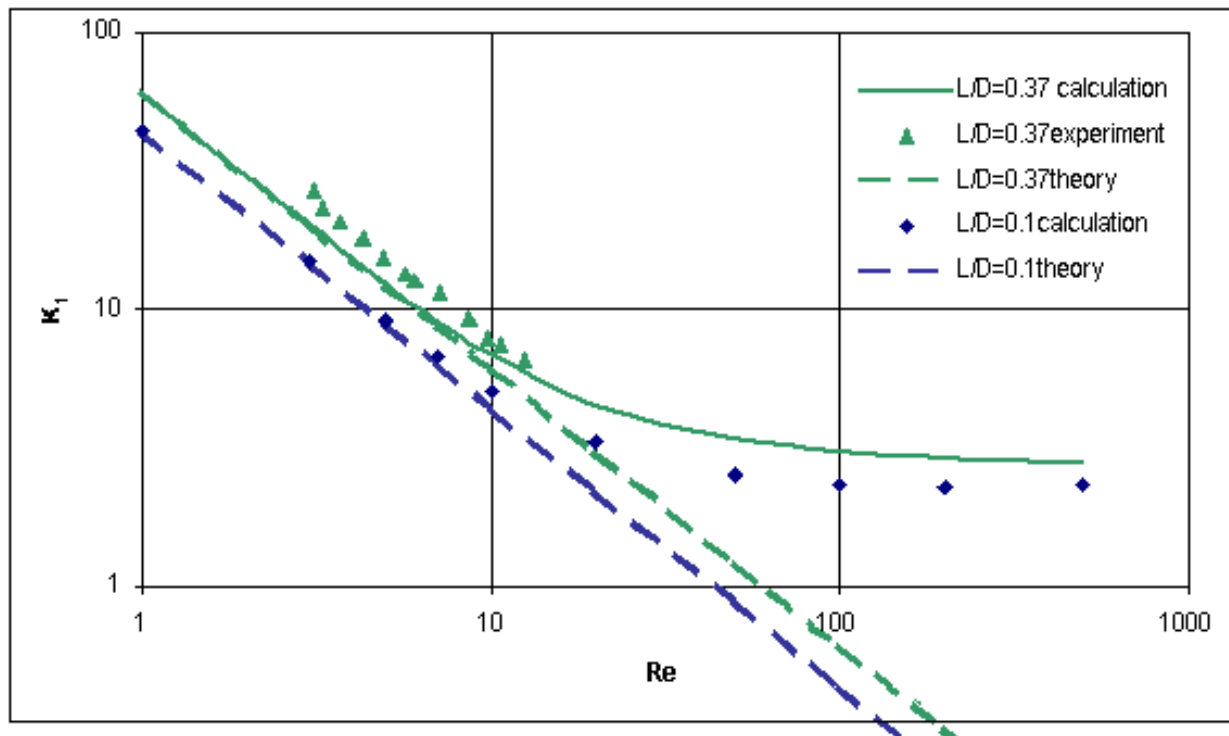
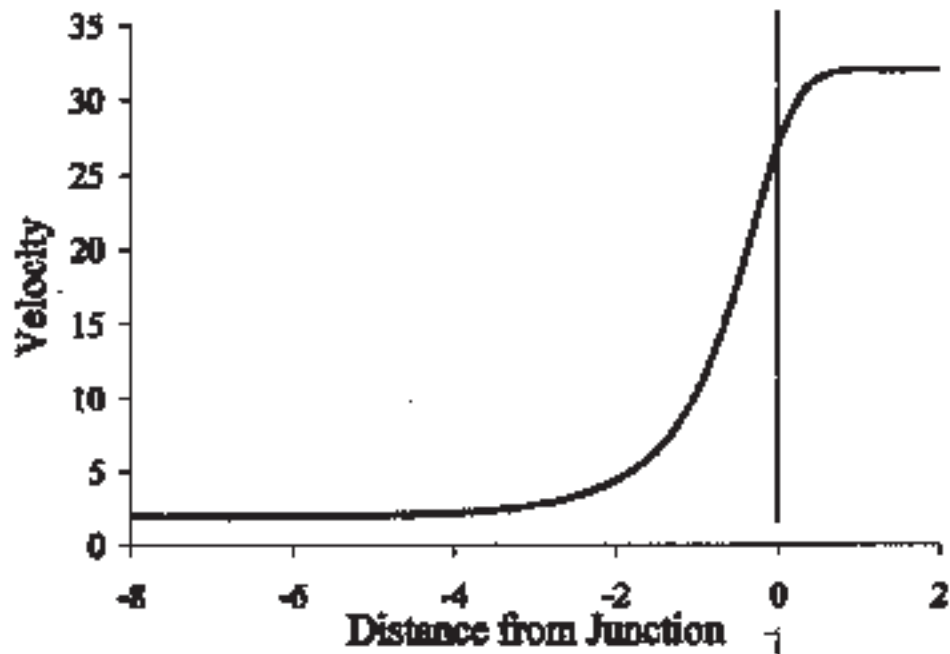


Figure 17. Pressure Coefficient for Orifice Flow (due to Febe Kusamanto)



**Figure 2. Centerline Velocity versus Distance from the Junction in a 4:1C Contraction**

**Figure 18. Centerline Velocity for 4:1 Contraction in Cylinder (due to Trevor Plaisted)**

The next example is one for entry length in a 4:1 cylindrical contraction. The velocity starts to rearrange upstream, as shown in Figure 18, and this rearrangement occurs further upstream at low Reynolds number. Thus, it is important to correlate that ‘approach length’. Then if one looks at the contraction, the flow has partially rearranged as it enters the small section. Thus, it makes no sense to use an entry length correlation obtained by assuming the velocity profile is flat at entrance to the small pipe. The correlation is of the same form, with different constants.

$$\frac{X_e}{D} = 0.278 + 0.0968 \text{ Re}$$

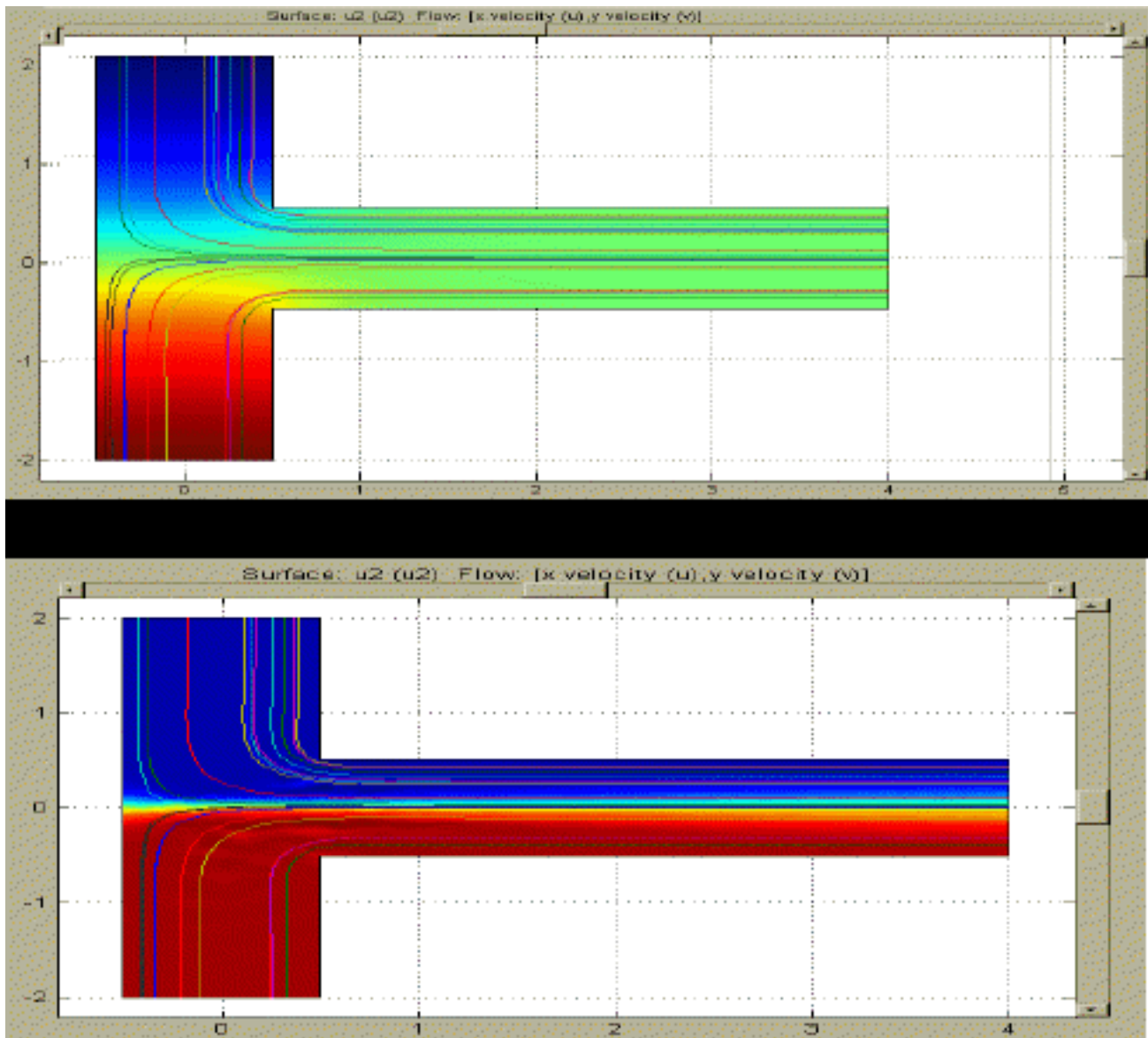
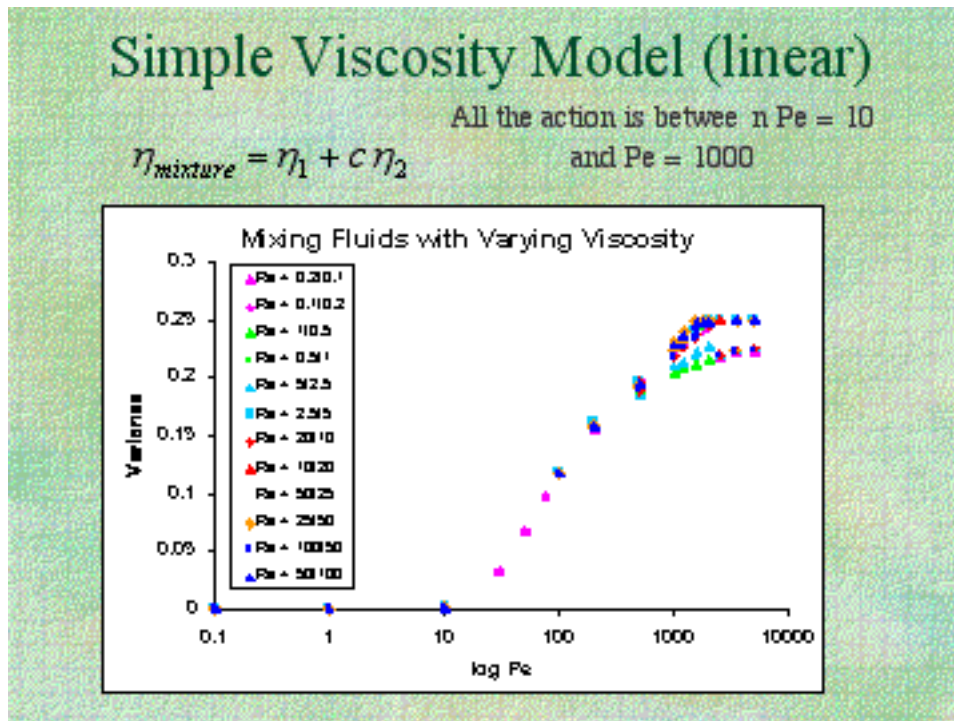


Figure 19. Diffusion as a Function of Peclet Number (due to Marlina Lukman)

$$\bar{c} = \frac{\int_{-H}^H c u \, dy}{\int_{-H}^H u \, dy}, \quad \sigma^2 = \frac{\int_{-H}^H (c - \bar{c})^2 u \, dy}{\int_{-H}^H u \, dy}$$

$\sigma^2 = 0$  is good mixing,  $\sigma^2 = 0.25$  is bad mixing

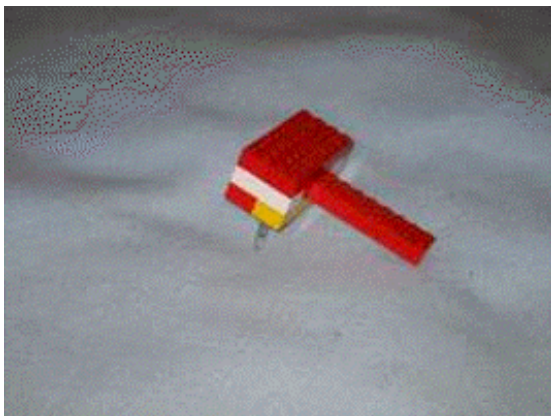
The final example is one involving diffusion and mixing. The question was posed: what happens when two miscible liquids come together. How is the diffusion and mixing affected when the viscosity depends upon concentration? Typical cases are shown in Figure 19 and show the effect of Peclet number. In order to quantify the mixing, we used the following definitions. The results are shown in Figure 20. Notice that the viscosity depends upon the concentration, and this is easy to achieve in FEMLAB. One merely types the formula shown in a GUI box. It was surprising to us that the variance was so similar under different conditions.



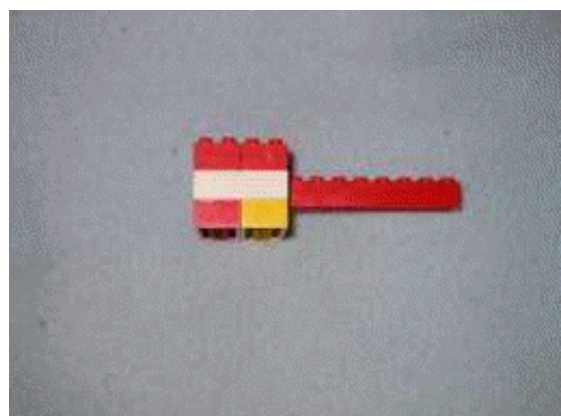
**Figure 20. Variance for Mixing of Miscible Liquids (due to Marlina Lukman)**

### Beginning Graduate Fluid Mechanics

The learning curve is the same for graduate students, but it is traversed more rapidly with less detailed help. Here we describe the experience using a CFD program in a beginning fluid mechanics class. The goal was to expand the students' horizons beyond the simple cases described in their textbook, which were solved analytically. Thus, two projects were assigned. The first project used the geometry shown as a prop. (Figure 21 and 22) The problem was reduced to a two-dimensional problem so that the student groups could work efficiently using the old, slow PCs provided by the



**Figure 21. Three D View of Object**



**Figure 22. Side View of Object**



University of Washington. The project assignment is described in Figure 23.

**Figure 23. Ch.E. 530 - Fluid Mechanics and Transport - Projects - Winter, 2002**

Text: *Analysis of Transport Phenomena*, William M. Deen, Oxford Univ. Press, 1998; required.

Course Web Page: <http://courses.washington.edu/che530/>

Course List Process (send a message to entire class) [chem\\_e530a\\_wi02@u.washington.edu](mailto:chem_e530a_wi02@u.washington.edu)

Project One. Your team is to analyze the fluid flow in the device shown. Your final report and presentation should include quantitative estimates (before you do the finite element calculations) of:

entry length in region A

entry length in region B

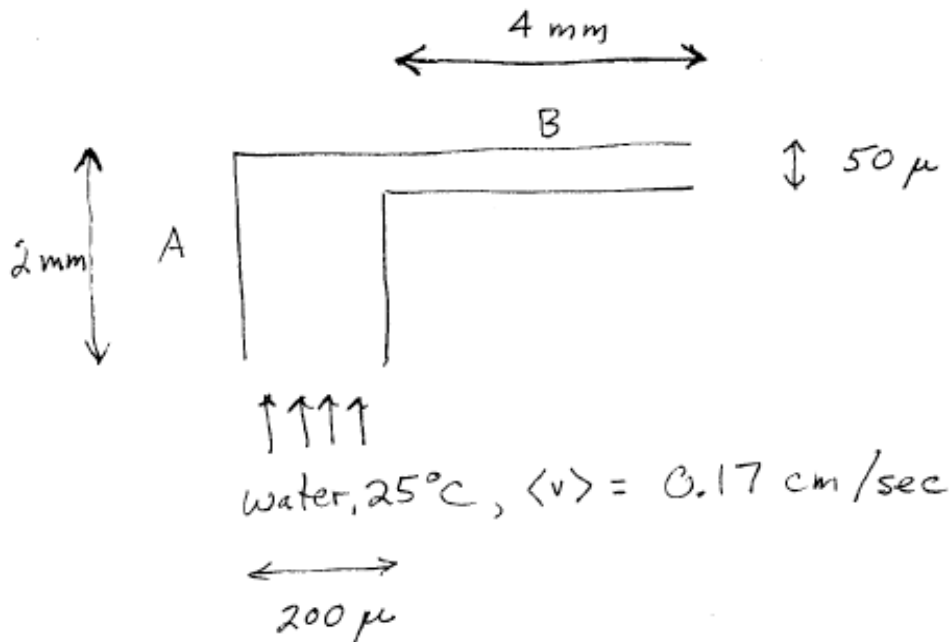
temperature rise if the device is adiabatic

how long it takes to reach steady state after a disturbance or change of conditions

pressure drop from inlet to exit

If half of the inlet is red (left half,  $c = 0$ ) and half is yellow (right half,  $c = 1$ ), what will be the concentration distribution coming out? Use a diffusivity of  $3.4 \times 10^{-6} \text{ cm}^2/\text{sec}$ .

After making these quantitative estimates, solve the problem(s) in FEMLAB and compare the quantitative predictions with the calculations. Do the same thing without making the no-slip assumption on the solid walls. How do the solutions differ?





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The students estimated these phenomena using the classical, analytic solutions for simple cases, and then the full 2D situations were calculated including all the phenomena to test their ability to estimate or bound the effects. After mistakes were corrected, the students found that they could in fact estimate the importance of all these phenomena. This is a useful skill for their graduate work, since it shows them that they do not have to model everything and can focus on what matters most, and sometimes they can eliminate certain phenomena using simple, analytical cases. FEMLAB™ has the convenient feature of being able to integrate algebraic formula over the domain or boundaries; what is especially nice is the ability to just type in the formula and get the result immediately. Thus, the viscous dissipation can be integrated over the domain provided they can copy the formula from their book to the computer. In fact, any expression can be integrated over the domain or a boundary.

Once the student teams understood what was possible with CFD, the second project was assigned: model an aspect of a patent in the microfluidic field. In this project, students looked at diffusion and mixing (including Taylor-Aris diffusion), did transient problems, and prepared movies of the transient problems. The second project assignment is in Figure 24.

**Figure 24. Project Two. For the patent you were assigned, design a flow problem illustrating some aspect of the patent.**

Schedule for projects:

March 1: present a written and oral report on Project One, given above.

Feb. 26: propose the problem for Project Two.

Mar. 13, 15: oral presentations of Project Two; written report due Mar. 15.

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Typical patents are shown in Figures 25-28. The students were asked to read the patent and suggest a problem to solve; this was discussed with the instructor to insure a reasonable problem that could be solved in the time available.

Figure 25

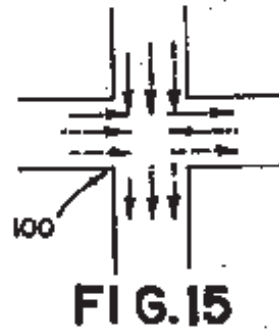
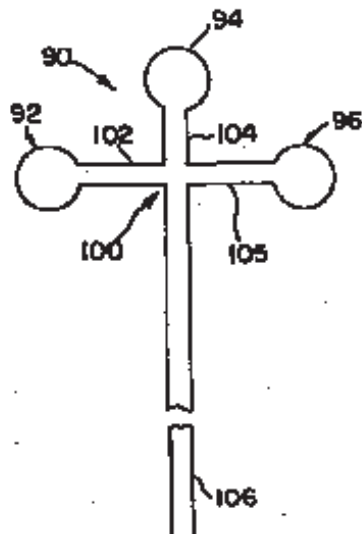


Figure 25

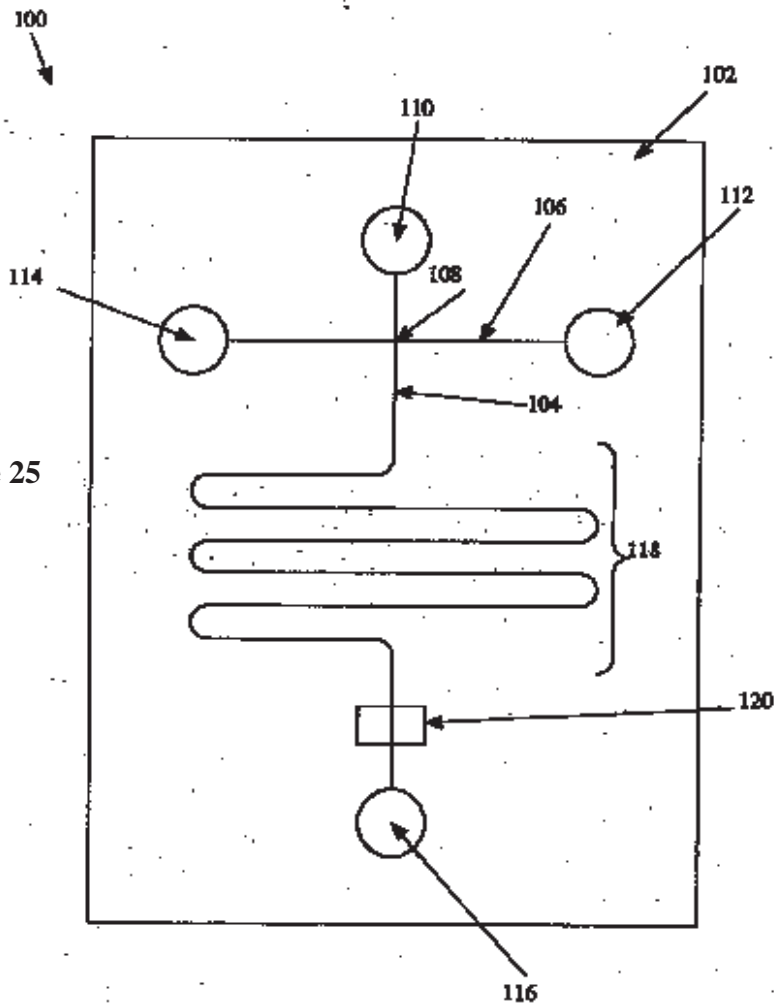


Figure 26

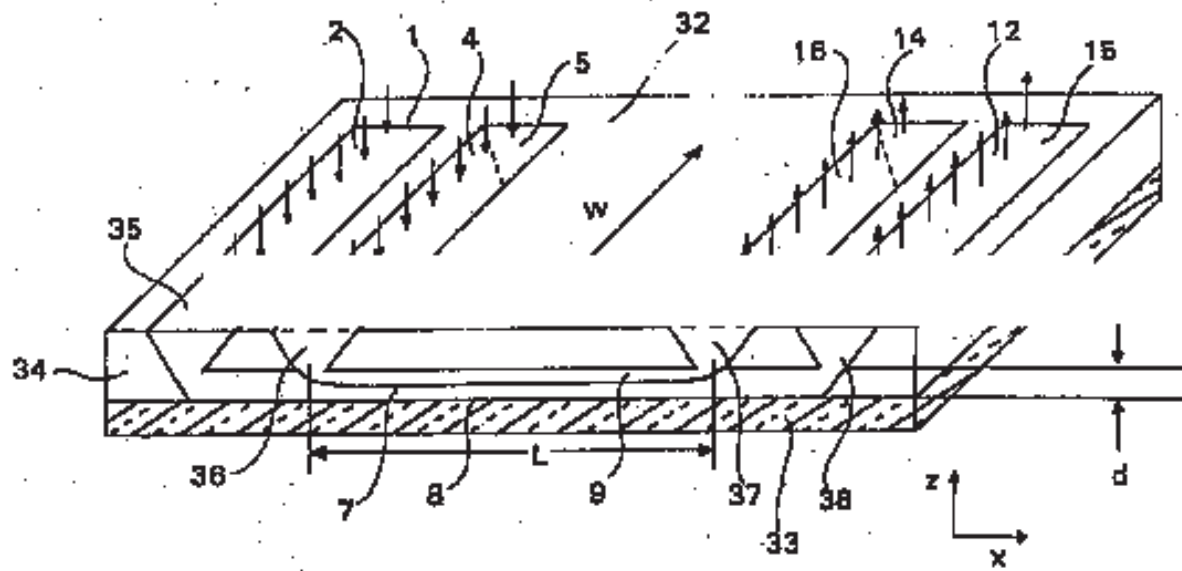


FIGURE 5

Figure 27

U.S. PATENT OFFICE  
AUG 3 1999  
5,932,100

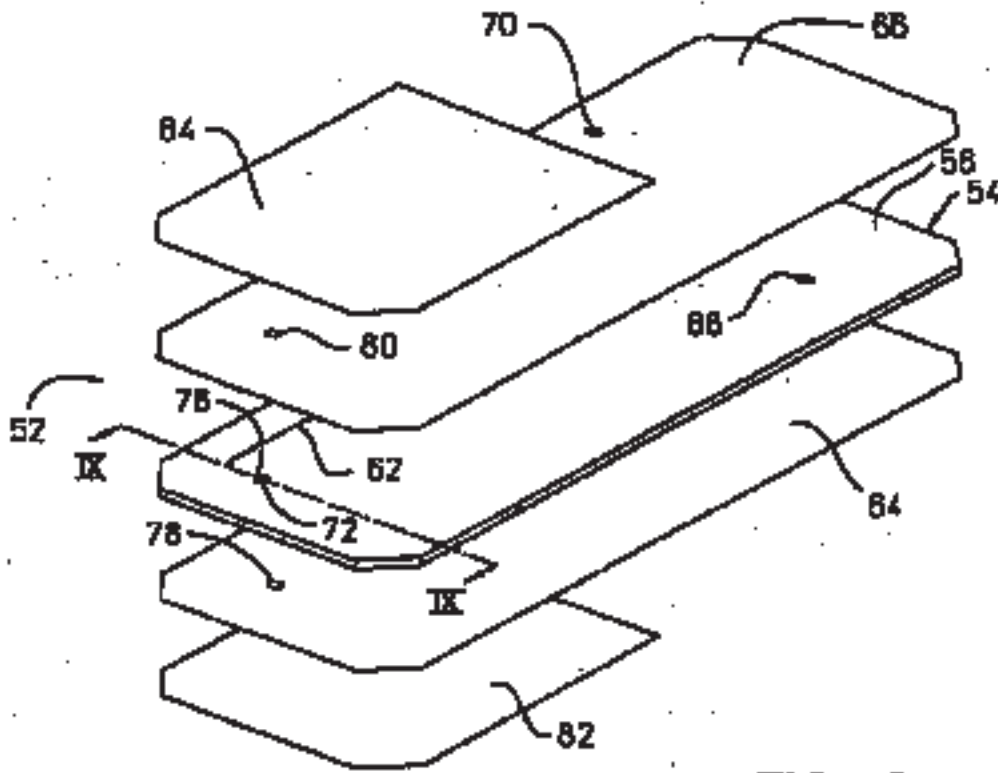


FIG. 8

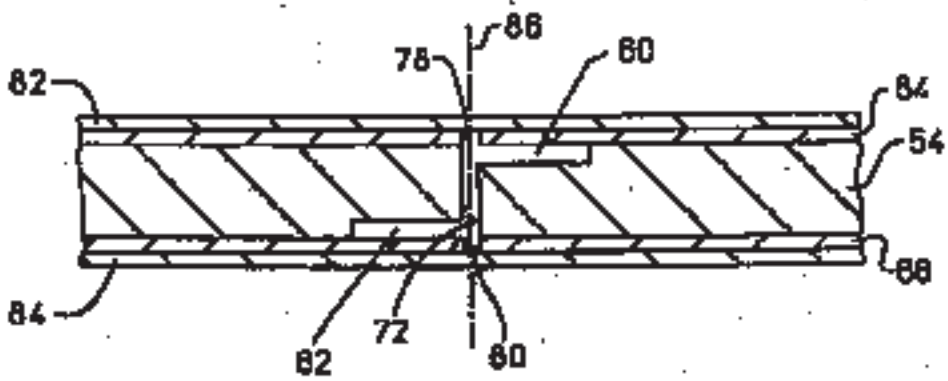
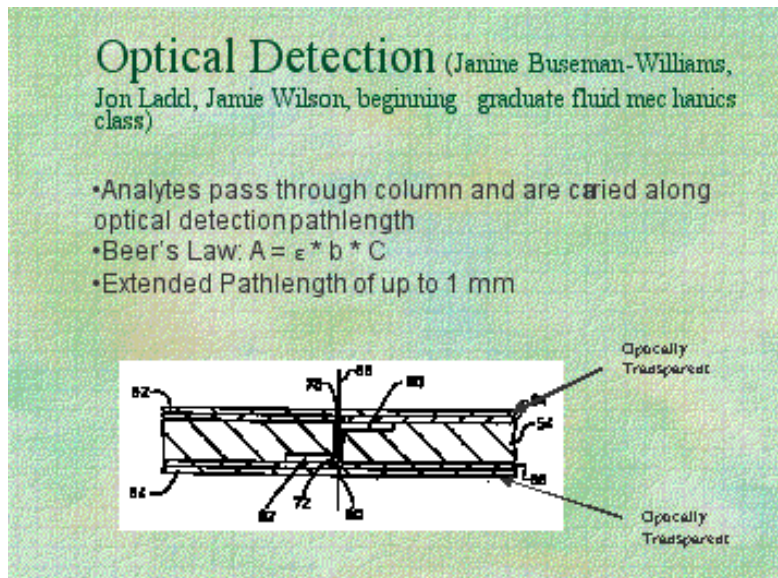
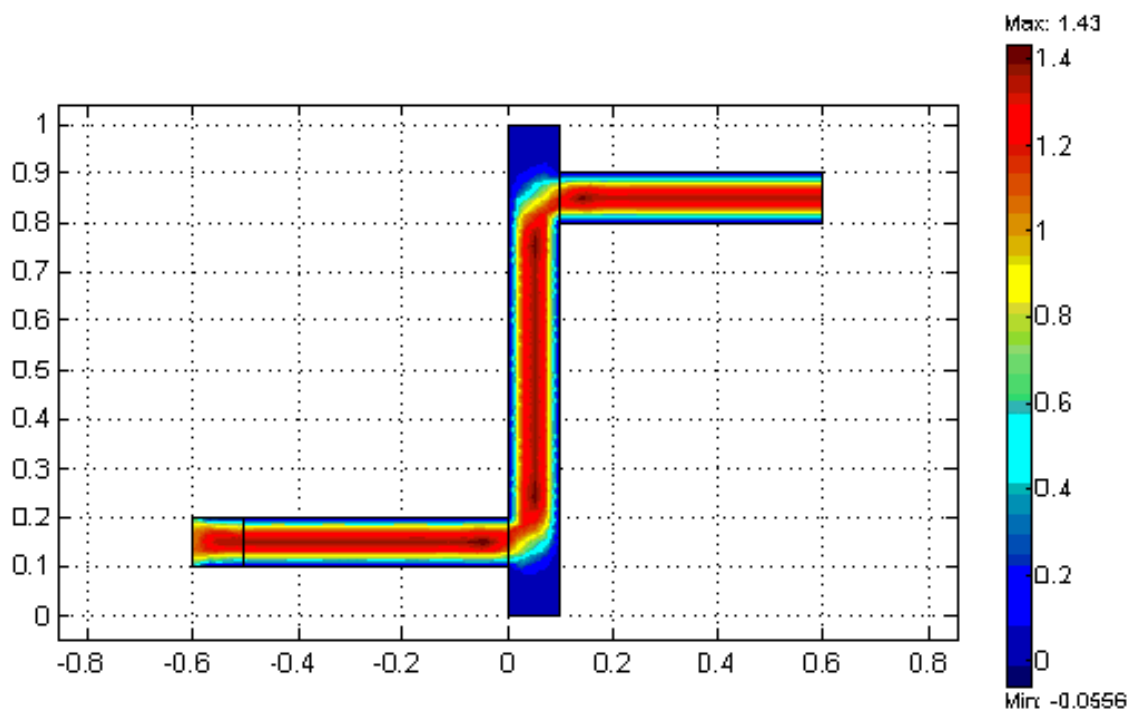


FIG. 9

Figure 28



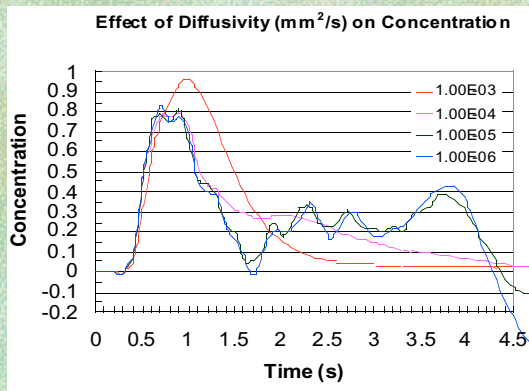
**Figure 29. Optical Detection Device**



**Figure 30. Flow Profile in Optical Detection Device**

A sample problem statement and results are shown in Figure 29 and 30. Whenever students are asked to use CFD, they are always cautioned to look carefully at their results to insure that there aren't any artifacts (in addition to doing mesh refinement). This group noticed something unusual. Figure 31 shows three concentration plots. The students noticed that when the diffusivity became smaller, the concentration plots became highly irregular (the color imitates a flower!). At this point the instructor could teach them (and the class) about numerical dispersion, the need for mesh refinement, and the criterion for eliminating the bogus oscillations when no numerical dispersion is added, and when some is added. The group did get high marks for noticing the effect, even if they didn't initially know what to do. They then looked at design questions, like varying the pathlength, as illustrated in Figure 32.

# FEMLAB Choices: Diffusivity



•Mesh: Unrefined

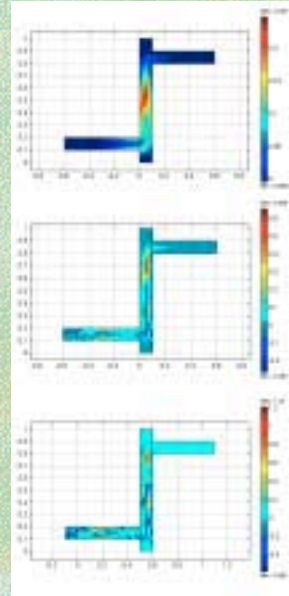


Figure 31. Concentration Solutions for Different Diffusivities

# Varying Pathlength

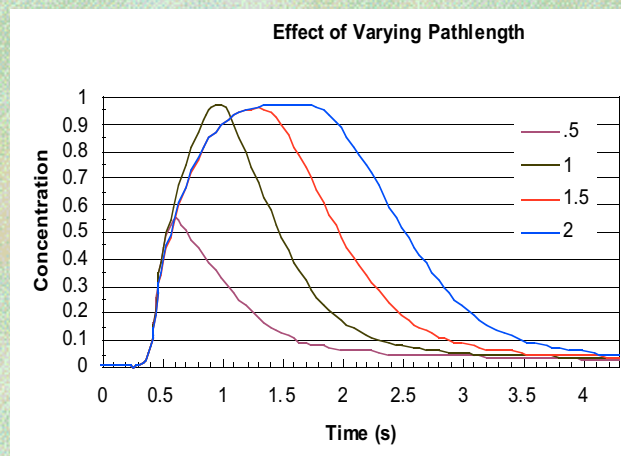
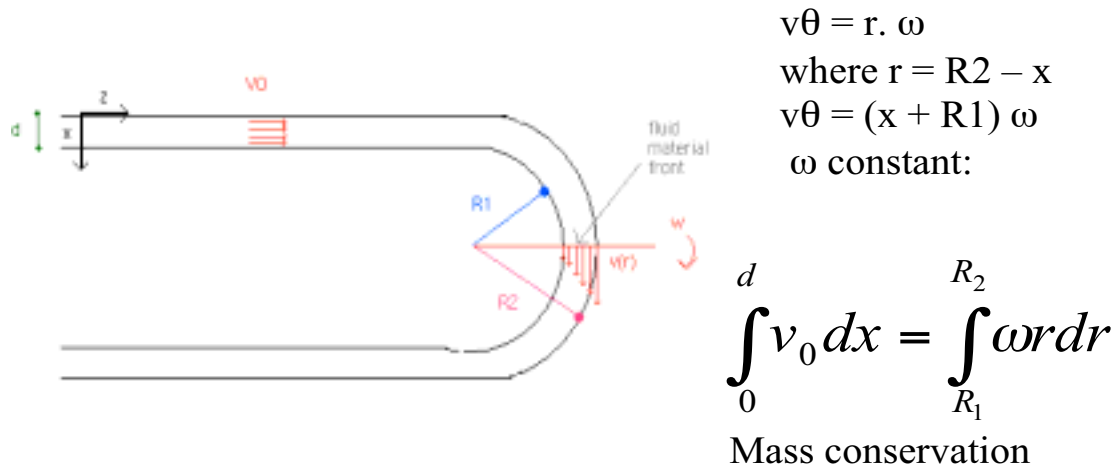


Figure 32. Signal for Different Pathlengths

# Part 1-Theoretical model no diffusion, full-slip, steady state



**Figure 33. Due to Kevin Dornfeld, Alex Holland, Daniel Ramrus, Sylvie Theas**

Another group modeled flow in a serpentine. In order to approximate some aspects of electro-osmotic flow, we assumed that perfect slip occurred at the boundary. The program FEMLAB allowed the students to specify that the normal velocity on a boundary was zero. This group also noticed an anomaly. At the exact corner, there seemed to be fluid leaving the device (see Figure 33). The instructor named this a pin-hole leak. After some consternation, and consultation with the support personnel, we discovered the reason: when the finite element method is used on a curved surface in some formulations, the normal to the surface is calculated at Gauss points, but not in between. The end result is that small errors in the normal to a curved surface can lead to small velocities ‘through the surface’. This group also got high marks for noticing an anomaly.

Naturally, the students were interested in seeing what happened to a slug of material going through their device, and they did transient simulations as well.

## Student Interest and Benefits

Students showed great interest in using CFD. The color pictures are great motivators, and successful completion of the projects give students a real sense of accomplishment. The importance of validation was emphasized over and over so that they leave with that important lesson. The most important lesson required the continuing reinforcement of the necessity to solve the right problem with known accuracy, and to convince their instructor of that accuracy.

## References

1. Bird, R. B., Stewart, W. E., and Lightfoot, E. N., *Transport Phenomena*, Wiley (1960).
2. Hasagawa, T., Suganuma, M., Watanabe, H., “Anomaly of excess pressure drops of the flow through very small orifices,” *Phys. Fluids* **9** 1-3 (1997).
3. Dagan, Z., Weinbaum, S. and Pfeffer, R., “An infinite-series solution for the creeping motion through an orifice of finite length,” *J. Fluid Mech.* **115** 505-523 (1982).



# Survey of Computing in Industry and Academia

*Thomas F. Edgar – University of Texas*

The CACHE Corporation in cooperation with a number of chemical engineering departments is performing a survey of computing in industry and academia. The purpose of this survey is to generate data on how recent chemical engineering graduates in industry are using computers. Additionally, the survey is intended to provide a perspective on how computing should be taught to chemical engineers. Universities may be interested in using the survey results to guide changes in degree requirements and the content of computing-related courses. Also it may be helpful as part of an ABET accreditation continuous improvement process. This survey is being sent to recent graduates from several selected universities, although there is interest in having other universities participate. Contact Tom Edgar ([edgar@che.utexas.edu](mailto:edgar@che.utexas.edu)) if you are interested.

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## Perspectives on Computing - A CACHE Survey

### Section I - General Questions

1. **What is your primary job function?**
  - a. Administration
  - b. Technical Management
  - c. Technical
  - d. Sales/Marketing
  - e. Academic
  - f. Other (\_\_\_\_\_)
  
2. **What is your highest technical degree?**
  - a. B.S.
  - b. M.Eng.
  - c. M.S.
  - d. Ph.D.
  - e. Other (\_\_\_\_\_)
  
3. **Years of professional experience**
  - a. None
  - b. Less than 5

- c. 5 - 10
- d. 11 - 15
- e. More than 15

4. **Do you have an MBA (or are studying for one)?**

- a. Yes
- b. No

5. **Optional: From which university did you get your B.S. degree?**

\_\_\_\_\_

6. **Optional: Who is your employer?**

\_\_\_\_\_

## **Section II: Computing in Industry**

1. **What type of work do you do? Please rank in order with 1 as the most important.**

- \_\_\_ Process Design/Analysis
- \_\_\_ Research and Development
- \_\_\_ Process Control
- \_\_\_ Administrative
- \_\_\_ Plant/Process Support
- \_\_\_ Systems
- \_\_\_ Other (Specify) \_\_\_\_\_
- \_\_\_ Don't Know

2. **What fraction of the day do you spend at the computer:**

- a. None
- b. 0 to  $\frac{1}{4}$
- c.  $\frac{1}{4}$  to  $\frac{1}{2}$
- d.  $\frac{1}{2}$  to  $\frac{3}{4}$
- e.  $\frac{3}{4}$  to 1
- f. All
- g. No idea

3. **Do you use the computer for office tasks? Examples: E-mail, word processing, calendars, and worldwide web.**

- a. Yes
- b. No

4. **Do you use spreadsheet programs? Examples: Lotus 1-2-3, Quattro Pro, Excel.**
- Yes
  - If yes, specify \_\_\_\_\_
  - No
5. **For what purpose do you use spreadsheet programs? Circle at most two letters.**
- Economic Studies
  - Data Analysis
  - Numerical Analysis
  - Material Balances
  - Other (specify): \_\_\_\_\_
  - Don't Know
6. **Do you use presentation graphics software? Examples: Powerpoint, Corel Draw, Micrographx Designer.**
- Yes
  - If yes, specify \_\_\_\_\_
  - No
7. **Do you use scientific or engineering data visualization software? Examples: Tecplot, Spyglass, CADKEY.**
- Yes
  - If yes, specify \_\_\_\_\_
  - No
8. **Do you use dedicated statistical software packages? Examples: SAS, Statistica, JMP.**
- Yes
  - If yes, specify \_\_\_\_\_
  - No
9. **Do you use numerical analysis software? Examples: MathCAD, MATLAB, Octave.**
- Yes
  - If yes, specify \_\_\_\_\_
  - No
10. **Do you use symbolic and mathematical manipulation packages? Examples: Mathematica, Maple, Macsyma, Reduce, Derive.**
- Yes
  - If yes, specify \_\_\_\_\_
  - No

11. **Do you use numerical methods libraries?**  
**Examples: IMSL, DASSL, LAPACK.** Note - software in this category must be linked with other programs, often written by the user in languages such as Fortran or C.
- Yes
  - If yes, specify \_\_\_\_\_
  - No
12. **Do you use database management systems for project information, general engineering data, process information, etc.?**  
**Examples: Access, Paradox, Oracle.**
- Yes
  - If yes, specify \_\_\_\_\_
  - No
13. **What chemical process simulation programs (flowsheeting systems) are used in your organization? Mark all that apply.**
- None
  - Aspen+
  - Hysys
  - ChemCAD
  - SIMSCI Pro II
  - WINSIM (Design II)
  - gPROMS
  - Other (Specify \_\_\_\_\_)

### Section III - Training

1. **How much time did you need initially to learn the computer skills for your job function?**
- Less than 1 month
  - 1 - 3 months
  - 3 - 6 months
  - More than 6 months
  - Don't Know
2. **From where did you receive training in the use of new computer tools? Estimate the fraction that should be assigned to each of the following:**
- \_\_\_ From the organization itself
  - \_\_\_ Self
  - \_\_\_ Company colleagues
  - \_\_\_ Outside training companies
  - \_\_\_ The computer tool vendor
  - \_\_\_ Other (\_\_\_\_\_)

**Were you adequately trained at your university to use and to understand chemical process simulation programs? (See question 13 of the Section II for examples).**

- a. Yes
- b. No
- c. No opinion

## **Section IV - Computer Programming**

1. **Does your work utilize your ability to write computer programs in Visual Basic, Fortran, C, Pascal, or other high-level language in order to do your work?**
  - a. Yes
  - b. If yes, specify \_\_\_\_\_
  - c. No
  
2. **Should computer programming in at least one programming language (see the next question for examples) be a required part of the undergraduate curriculum for chemical engineers?**
  - a. Yes, it is important (answer next 2 questions)
  - b. No, it is not necessary (go to question 5)
  - c. No opinion (go to question 5)
  
3. **If you answered yes to the previous question, what language should be taught to undergraduate chemical engineering students? Mark only one item.**
  - a. Fortran 77
  - b. Fortran 90
  - c. C
  - d. C++
  - e. Pascal
  - f. Visual Basic
  - g. Java
  - h. Other: (Specify \_\_\_\_\_)
  - i. Does not matter as long as one is taught
  
4. **Should additional programming language(s) be part of the undergraduate curriculum for chemical engineers?**
  - a. None
  - b. Fortran 77
  - c. Fortran 90
  - d. C
  - e. C++
  - f. Pascal
  - g. Basic

- h. Other: (Specify \_\_\_\_\_)
- i. Does not matter which

**5. Are you expected by your employer to be competent in a computer programming language?**

- a. Yes
- b. No

**6. Are you expected to be literate in different computer languages?**

- a. Yes
- b. No

## **Section V - The Value of Computing**

**1. Do you feel that your exposure to computer tools is sufficient for solving a wide range of industrial problems?**

- a. Not enough
- b. About right
- c. More than enough
- d. Don't Know

**2. Has exposure to computers enhanced or hindered your ability to formulate or define problems conceptually and mathematically?**

- a. Significant enhancement
- b. Modest enhancement
- c. No effect
- d. Modest hindrance
- e. Significant hindrance
- f. Don't Know

**3. Do you feel there is a relationship between computer skills and problem solving skills?**

- a. Yes, strong positive correlation
- b. Yes, weak positive correlation
- c. No correlation
- d. Yes, weak negative correlation
- e. Yes, strong negative correlation
- f. Don't Know

**4. Do you believe undergraduate engineers would benefit from experience with more than one computer operating system? Examples: UNIX, Windows, Windows NT, LINUX**

- a. Highly desirable, should be required

- b. Desirable, but should not be required
  - b. Not necessary
  - c. Unimportant
5. **Do you think new graduates are able to use process simulation software to model entire processes rather than single unit operations?**
- a. Yes
  - b. No
  - c. Don't know
6. **Have you noticed any difference in use of computers during the past several years?**
- a. Yes, significant changes
  - b. If yes, specify \_\_\_\_\_
  - c. No
  - d. Unaware of any differences

**Please elaborate if you answered yes to this question.**

## **Section VI. - Additional Comments (Optional)**

# Learning FEMLAB/Matlab for Chemical Engineering – Unsteady State Heat Conduction In A One-Dimensional Slab

*Edward M. Rosen - EMR Technology Group*

## Discussion and Conclusions

Equations (1) has been solved using (a) finite differences in a spreadsheet using Excel (3), (b) the method of lines (4, 5) and (c) exactly (6). Table 1 compares the solutions at  $t = 0.12$  and at various values of  $\eta$ . The FEMLAB solution was tabulated by reading point values on a graph of the solution curve. FEMLAB allows the user an ability to solve PDEs with an accuracy similar to other methods. Most important, FEMLAB has considerable capabilities to solve much more difficult problems.

## The Model System

The parabolic differential equation

$$\frac{\partial q}{\partial t} = \frac{\partial^2 q}{\partial h^2} \quad (1)$$

where

$$q = \frac{T_1 - T}{T_1 - T_0}, \quad h = \frac{x}{b}, \quad t = \frac{at}{b^2}$$

and

- x = distance from center to a point in slab in m
- b = distance from boundary to center of the slab in m
- a = thermal diffusivity in  $m^2/s$  ( $k/ \rho C_p$ )
- t = time in s
- $T_1$  = temperature at boundary
- $T_0$  = temperature in slab at  $t = 0$
- T = temperature in slab at time t

with boundary conditions

- At  $t = 0$ ,  $T = T_0$  at all x
- At  $t \geq 0$ ,  $T = T_1$  at  $x = \pm b$

has been solved both analytically and numerically in a number of ways. If  $T_1 < T_0$  then cooling takes place. If  $T_1 > T_0$  then heating takes place (Fig. 1)



## The FEMLAB Solution (1)

FEMLAB is a windows-based system built on Matlab (2) and is designed to numerically solve partial differential equations (PDE's) utilizing a finite element approach. It has a large number of built in equations that can be modified by the user. Applications in chemical engineering include momentum transport, energy transport and mass transport. Significantly, FEMLAB can solve the applicable equations simultaneously. A drawing facility allows the user to specify arbitrary geometries. Its output is generally graphical although numerical output is also available.

The following steps in FEMLAB are used in setting up and solving the above PDE for cooling ( $T_0 = 100$ ,  $T_1 = 0$ )

Select:

1D (one dimensional)  
Chemical Engineering Module  
Cartesian Coordinates  
Energy Balance  
Heat Transfer  
Time Dependent

*Draw Mode*

The simple geometry indicated Fig (1) is entered with  $b = \pm 1$

*Boundary Mode*

The temperature at the boundaries is entered,  $T_1 = 0$  and the physical properties for  $r$ ,  $C_p$  and  $k$ .

*Subdomain Mode*

The initial value  $T_0 = 100$  is entered.

*Mesh Mode*

The mesh desired for the finite elements is specified. After the initial mesh is set, the mesh is refined twice.

*Solve Mode*

The values of  $t$  at which the solution is desired are entered, from 0 to 1 in increments of 0.01.

*Post Mode*

The temperature profile at  $t = 0.12$  is selected. The profile can be zoomed in to get a better reading which may be done by pointing the mouse and clicking on the profile. The temperature is displayed in the lower left window.

An animation of the solution (temperature profiles at various values of  $t$ ) can also be specified.

FEMLAB screens used in the problem can be found at the end of this document.

## **References**

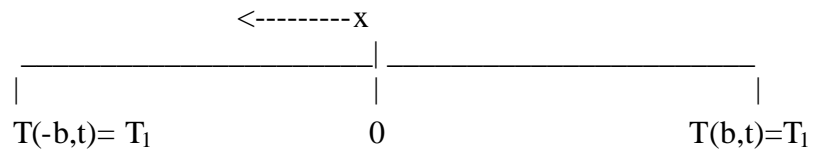
1. FEMLAB Chemical Engineering Module, COMSOL AB Version 2.3  
<http://www.comsol.com>
2. The MathWorks, Inc Natick, MA <http://www.mathworks.com>
3. Rosen, E. M., "Reprise: Solving Partial Differential Equations Using Excel 2000"  
*CACHE News*, No 51 Fall 2000
4. Cutlip, M. B. and M. Shacham, "The Numerical Method of Lines for Partial Differential Equations", *CACHE News*, Fall 1998 p 18
5. Taylor, R. , Engineering Computing with maple: Solution of PDEs via the Method of Lines, *CACHE News*, No 49 Fall 1999 p. 5
6. Boelter, L.M. K., Cherry, V. H., Johnson, H. A. and Marteinelli, R. C., Heat Transfer Notes, University of California Press, Berkeley (1948) p V-12-b

## **Acknowledgements**

This work was done during a trial period for FEMLAB/Matlab. The author would like to thank The MathWorks, Inc. and Comsol, Inc.

Peter R. Rony's comments have been incorporated into this paper. He supplied the Power Point copies of the FEMLAB screens as well.

**Figure 1.** One Dimensional Slab

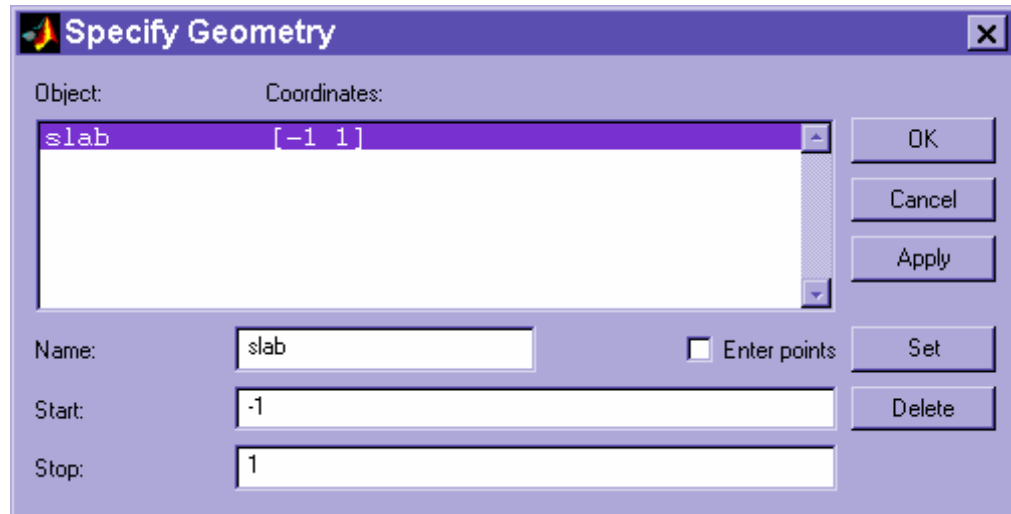


**Table 1.**

Comparison of Methods at  $t = 0.12$  (Time = 6000 sec.,  $a = 0.00002$ ,  $b = 1$ )  
 $T_0 = 100$ ,  $T_1 = 0$

$h$	Finite Differences (3)	Method of Lines(4)	FEMLAB Finite Elements (1)	Exact (6)
0	91.72	91.73	91.84	91.75
0.2	88.29	88.31	88.36	88.32
0.4	77.49	77.50	77.47	77.51
0.6	58.47	58.47	58.35	58.47
0.8	31.68	31.67	31.62	31.67
1.0	0.	0.	0.	0.

## Draw Mode



The image shows a software dialog box titled "Specify Geometry". It has a purple title bar with a close button (X) in the top right corner. The dialog is divided into several sections:

- Object/Coordinates Table:** A table with two columns, "Object" and "Coordinates". The first row contains the text "slab" and the coordinates "[-1 1]".
- Name:** A text input field containing the word "slab".
- Start:** A text input field containing the value "-1".
- Stop:** A text input field containing the value "1".
- Buttons:** On the right side, there are five buttons: "OK", "Cancel", "Apply", "Set", and "Delete".
- Enter points:** A checkbox labeled "Enter points" is located to the right of the "Name" field and is currently unchecked.

# Boundary Mode

Boundary Settings/ht

Equation:  $T = T_0$

Domain selection

1  
2

Name: 1

Select by group  
 Enable borders

Boundary coefficients  Unlock

Quantity	Value	Description
<input type="radio"/> q	0	Inward heat flux
<input type="radio"/> h	0	Heat transfer coefficient
<input type="radio"/> $T_{inf}$	0	External temperature
<input type="radio"/> Const	0	Problem-dependent constant
<input type="radio"/> $T_{amb}$	0	Ambient temperature
<input type="radio"/> $n \cdot (k \cdot \text{grad}T) = 0$		Insulation/symmetry
<input checked="" type="radio"/> T	0	Temperature
<input type="radio"/> T=0		Zero temperature

On top    OK    Cancel    Apply

# Boundary Mode – Physical Properties

**Subdomain Settings/ht**

Equation:  $\rho \cdot C \cdot T' \cdot \nabla \cdot (k \nabla T) = Q + h_{\text{trans}} \cdot (T_{\text{ext}} - T) + C_{\text{trans}} \cdot (T_{\text{ambtrans}}^4 - T^4)$ , T = temperature

Coefficients | Init | Element

Domain selection

1

Name: 1

Select by group

Active in this domain

PDE coefficients  Unlock

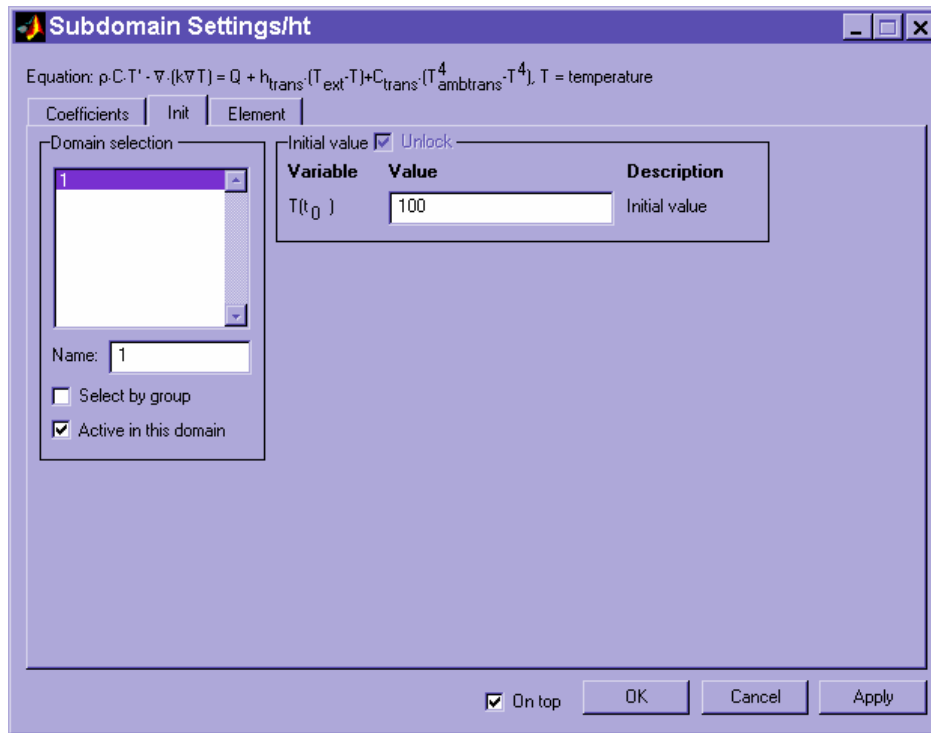
Use defined material

Coefficient	Value	Description
$\rho$	1	Density
C	1	Heat capacity
k	1	Thermal conductivity
Q	0	Heat source
$h_{\text{trans}}$	0	Convect. heat transf. coeff.
$T_{\text{ext}}$	0	External temperature
$C_{\text{trans}}$	0	User-defined constant
$T_{\text{ambtrans}}$	0	Ambient temperature

Add Material Update Material Add/Edit Material...

On top OK Cancel Apply

# Boundary Mode – Initial Value



# Solve Mode

**Solver Parameters**

General | Adaption | Nonlinear | **Timestepping** | Eigenvalue | Parametric | Iterative | Multigrid | Multiphysics

Output times: 0:0.01:1.0

ODE/DAE solver

Timestepping algorithm: ode15s

Relative tolerance: 0.01

Absolute tolerance: 0.001

Advanced...

Mass matrix

Lumped  Full

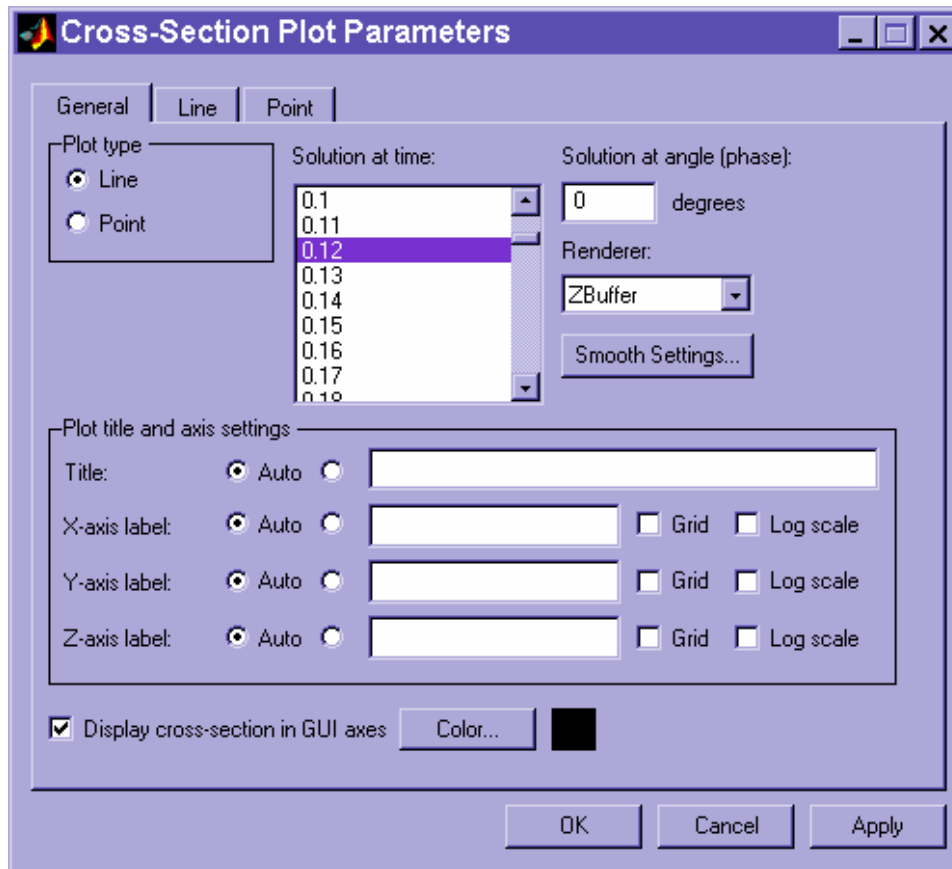
Manual control of reassembly

<input type="checkbox"/> Mass constant	<input type="checkbox"/> Mass independent of u
<input type="checkbox"/> Load constant	<input type="checkbox"/> Jacobian constant
<input type="checkbox"/> Constraint constant	<input type="checkbox"/> Constraint Jacobian constant

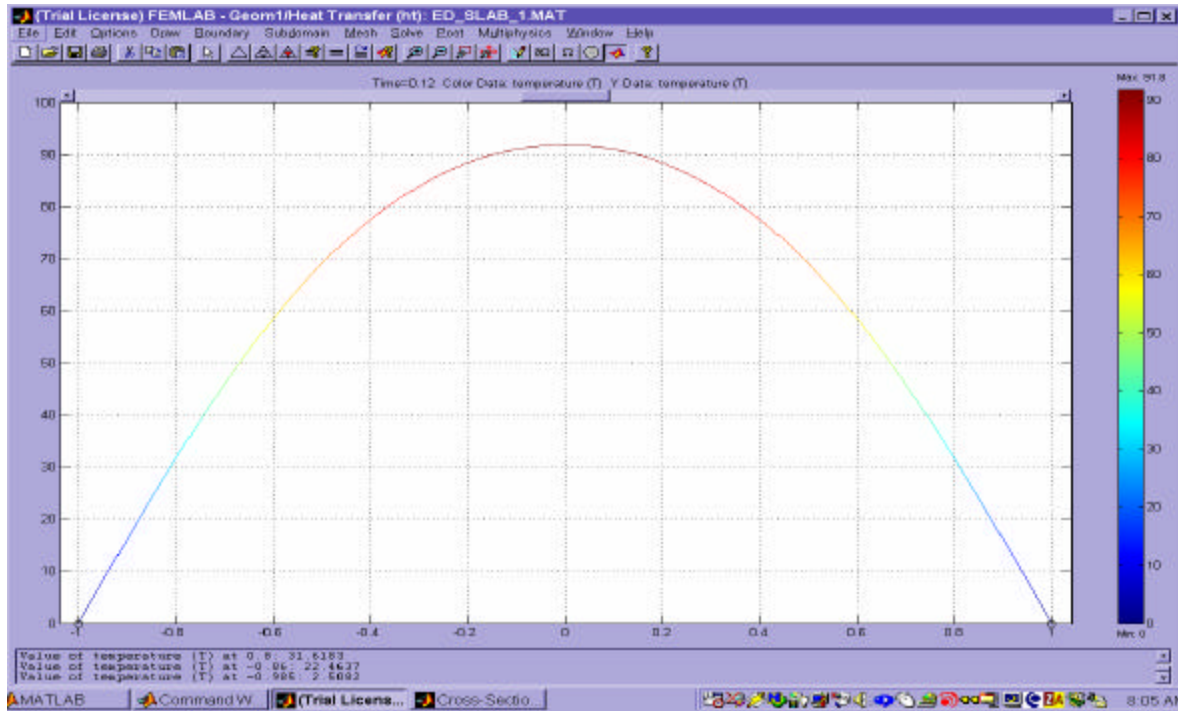
Solve OK Cancel Apply



## Post Mode – Selection of Tau



# Solution at Tau = 0.12



## New CACHE Trustee

**Chau-Chyun Chen** is a Technology Fellow at Aspen Technology, Inc. He is currently responsible for AspenTech's applied physical properties and chemistries business and technology. He received ScD and MS degrees in chemical engineering from the Massachusetts Institute of Technology in 1980 and in 1977, and a BS degree in chemistry from the National Taiwan University in 1973. Before joining AspenTech as a co-founder in 1981, he was a researcher on the Aspen Project at MIT. Dr. Chen's research interests are in applied thermodynamics, reaction engineering, process modeling and simulation, and their industrial applications. At AspenTech, he contributed to various research and development and business management activities to



extend applications of first principles-based process modeling technologies. He is the inventor and architect of the electrolyte modeling and polymer modeling capabilities in AspenTech's process modeling tools, which are widely used to model industrial processes involving complex chemical systems with electrolytes and with polymers. More recently, his research activities have extended to pharmaceutical and biological product and process modeling.

Dr. Chen is the recipient of the 2001 Computing Practice Award, Computing and Systems Technology (CAST) Division of the American Institute of Chemical Engineers (AIChE), and the 1984 Ted Peterson Student Paper Award also from CAST Division of AIChE. He serves in the editorial board of the International Journal of Fluid Phase Equilibria. Dr. Chen is a member of the American Chemical Society, the American Institute of Chemical Engineers, and the American Association for the Advancement of Science, and the Chinese American Chemical Society.

GAMS Newsletter Number 11  
Bruce McCarl

## **Documentation**

The McCarl GAMS Users Guide 2003 is ready. I wrote it with GAMS Corporation support and cooperation. It covers all user oriented GAMS features for releases up until 20.7 (the current release) excepting those in the MPSGE processor. The document is described in [http://www.gams.com/dd/docs/bigdocs/gams2002/mcc\\_introduction.pdf](http://www.gams.com/dd/docs/bigdocs/gams2002/mcc_introduction.pdf). Note that the User Guide is not totally consistent with 20.7 (GDXXRW and the GAMSIDE in particular) and installation of the patches below is required for consistency. Also until the next GAMS release the User Guide needs to be downloaded following <http://www.gams.com/dd/docs/bigdocs/gams2002/update.htm>.

Take a look, the document covers many features that have either not been documented or collected under one roof. Prior downloaders should get the latest version as we fixed a capitalization issue that caused trouble on UNIX/LINUX machines and added [mccguide.htm](#).

## **Solver Documents**

GAMS has revised and added to the solver documents. If you want these before the next release go to <http://www.gams.com/docs/document.htm> or download the patch below.

## **Patches to use documentation**

The documentation covers some features of the next GAMS release. To make the documentation consistent with your software on a PC system you need to install a patch that includes a new GAMSIDE, GDXXRW, new Solver Documents and repairs for GAMSBAS and GAMSCHK. Download the patch from <http://www.gams.com/update/mccupdate.zip> into the GAMS system directory nominally `c:\program files\gams20.7`. In turn to install

1. Close the GAMSIDE
2. Insure `mccupdate.zip` is in the GAMS system directory and do one of the following:
  - a. open a DOS box, `cd` into the GAMS system directory and run `"gamsinst -a"`
  - b. unzip the file then run the IDE and go into the File -> Options -> Execute dialogue and press update.

## **A new release on the horizon**

GAMS will soon release a major new update with the documentation fully integrated, several new language elements, 3 or so new solvers and faster internal code plus some bug repairs. Currently it is in testing. A newsletter will follow its release describing the new features.

## **Courses offered**

I will teach Basic GAMS in College Station, TX May 19-22, 2003. Offerings of Advanced GAMS will be in Hamburg Germany, June 10-13, 2003 and in Texas January 12-15, 2004. Further information and other courses are listed on <http://www.gams.com/courses.htm>.

February 24, 2003

# **FOCAPO 2003**

**"A View to the Future Integration of R&D,  
Manufacturing and the Global Supply Chain"**

**Conference took place on January 12-15, 2003**

**Coral Springs Marriott at Heron Bay  
Coral Springs, Florida**

<http://www.cheme.cmu.edu/focapo>

FOCAPO 2003 (Foundations of Computer-Aided Process Operations) convened a group of international experts from industry, academia, vendors, and consulting companies to discuss new directions and challenges in process operations.

Participants discussed challenges and needs for process oriented industries such as chemicals, energy, food and beverage, pharmaceuticals, and metals.

Conference sessions included topics such as supply chain optimization, integration of R&D and new product development with manufacturing and operations, strategies for handling uncertainty, modeling for process operations, control in operations, product quality, safety & sustainability, bioprocessing and electronics manufacturing, impact of information technology on process operations, web-enabled enterprise, and advances in data handling (e.g. data mining, statistics).

# **FOMMS 2003**

## Foundations of Molecular Modeling and Simulation

**July 6 – 11, 2003**

Keystone Resort, Colorado

This is the second international conference dealing with applications and theory of computational quantum chemistry and molecular simulation. The motivation for this conference is the need for precise control of product properties and the development of a microscopic and mesoscopic understanding that allows creation and design of new products to meet specific marketplace demands. During the past fifteen years, theoretical and algorithmic advances along with the revolution in computing technology have made it possible for design questions of practical importance to be addressed by these methods. The advances offered by these methods will continue to make inroads in the chemical and related industries in the coming decade.

### **Format and Topics for the Conference**

The content of the meeting will be balanced between molecular simulation and computational chemistry. The format will follow the highly successful FOMMS 2000 conference. All talks will be invited. Two poster sessions will provide opportunities for attendees to present their work. One afternoon will be devoted to a software/hardware demonstration session for providers to showcase their products and services. There will be large blocks of time available for informal discussions. Receptions will be held to facilitate interaction between conference participants. Each invited talk will represent a state-of-the-art review and will be rigorously reviewed and edited. Accepted papers (both poster and invited) will be published in an archival medium.

Topics of special interest include the following:

- Nanotechnology
- Molecular Materials Design
- Conceptual Chemical Process Design
- Molecular Scale Reaction Engineering
- Molecular Rheology
- Multiple Time Scale and Mesoscopic Simulation Techniques
- Future Trends in Molecular Modeling, Simulation and Design

The meeting will be informal and the dress code will be casual.

The conference is presented by the non-profit educational CACHE Corporation (Computer Aids for Chemical Engineering) and by CoMSEF (Computational Molecular Science and Engineering Forum) of the American Institute of Chemical Engineers; local

arrangements will be coordinated by Alliance LLC. The conference chairs are Jim Ely of Colorado School of Mines and George Jackson of Imperial College. For more details on the conference or submitting a contributed paper see:

<http://www.mines.edu/Academic/chemeng/conferences/fomms/>



# **FOCAPD 2004**

Foundations of Computer Aided Process Design

**July 11-16, 2004**

The Friend Center  
Princeton University, New Jersey

<http://www.alliancellc.com/about.htm>

The major theme of FOCAPD 2004, Discovery Through Product and Process Design, reflects this remarkable shift in the industrial sector. Princeton University Professor Christodoulos A. Floudas and Dr. Rakesh Agrawal of Air Products and Chemicals, chair this conference with a goal to create an academic and industrial dialogue, a critical assessment of existing enabling technologies, a discussion on research, education, and industrial needs, and a forum of new directions, challenges and opportunities in product and process design.

FOCAPD 2004 will be held at the Friend Center at Princeton University, Princeton, New Jersey, July 11-16, 2004. This international conference will attract world-renowned experts from academia and industry, researchers and practitioners from government laboratories, product and processing industries, technology and consulting companies, and graduate students. Please check out the above website for more information.

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