MESH AND TIME-STEP INDEPENDENT COMPUTATIONAL FLUID DYNAMICS (CFD) SOLUTIONS

Justin J. Nijdam
University of Canterbury • Christchurch, New Zealand

For the past decade, the Chemical and Process Engineering (CAPE) Department of the University of Canterbury has offered an introductory course on computational fluid dynamics (CFD) to final-year undergraduate students. The popularity of this elective course, which is also open to final-year mechanical and civil engineering students, has increased, with student numbers rising from eight in 2001 to an average of 50 to 60 from 2009 onwards. This reflects the increased relevance of CFD as an engineering design tool, driven by improvements in the graphical user interface of commercial CFD packages, advances in mathematical models, and increases in computer processing power. The user-friendly nature of commercial CFD packages and the speed and reliability of their solutions make problems relevant to engineering industry more amenable to CFD analysis.

Since practicing engineers are likely to use commercially available CFD software as a design tool, a hands-on approach with a commercial CFD code is appropriate when teaching students CFD.[1-7] It is important that the CFD solver not be treated as a black box. Key solver concepts that need to be covered include the stability and accuracy of discretization schemes and the importance of gaining mesh- and (for transient problems) time-step-independent numerical solutions. We have found that an exercise demonstrating the links between discretization and the accuracy of the numerical solutions helps to demystify the black box of a commercial CFD solver.

In the CAPE CFD course, a homework assignment is given to students to solve the one-dimensional transient diffusion problem. The key learning objectives of this assignment are to teach students the importance of gaining mesh- and time-step-independent numerical solutions in CFD and to demonstrate that these predictions can be verified by comparison with an analytical solution. This paper describes two examples of the one-dimensional transient diffusion problem, which were set as homework assignments in 2007 and 2010. The first case is the Couette flow problem for transient development of the velocity profile between two parallel plates after the lower plate, initially at rest, instantaneously moves horizontally at a constant velocity. The second case is mass diffusion in a porous medium, specifically looking at the moisture content profiles that develop within timber as it dries. A third case that could be used is transient diffusion in the form of heat conduction in a thin metal plate.[8] These three cases cover important physical phenomena of interest to engineers. The aim of this paper is to demonstrate that these homework assignments help students learn useful concepts about the methodology and numerical aspects of CFD in a hands-on manner using physically realistic, easy-to-understand problems. Student responses to a survey on the 2010 homework assignment are presented.

COURSE DESCRIPTION

The primary aim of the introductory CFD course is to teach students CFD methodology. The course is taught in one semester (12 weeks), building on courses taken previously by students in fluid mechanics and numerical methods. It is delivered in 12 two- hour lectures, as shown in Table 1 (next page), using a similar approach as described by Aung[9] and Kaushik et al.[7] Familiarity with spreadsheets, Matlab and/or other programming codes is assumed. The textbook is Versteeg and Malalasekera's *Introduction-to-CFD* book.[8] A key feature of the lectures is to provide simulation examples

***Justin Nijdam** earned a Ph.D. in 1998 from the Chemical and Process Engineering Department at Canterbury University in New Zealand. He is currently a senior lecturer at Canterbury University teaching classes in CFD, fluid mechanics, heat and mass transfer, design and analysis of experiments, and technical communication. His research interests include wood processing (drying, sterilization by Joule heating) and food processing (spray dryers, fluidized beds, filters, mixers).*

(spreadsheet calculations or flow visualizations), where appropriate, to demonstrate the principles involved. The CFD methodology is threaded throughout the lectures, covering 1) geometry generation and appropriate types of and locations for boundaries; 2) mesh generation with a focus on mesh quality and gaining mesh independent numerical solutions; 3) choice of physics and numerical schemes; 4) solution algorithms (coupled and uncoupled solvers and structured and unstructured meshes); 5) post-processing; and 6) validation. The lectures are supported by three homework assignments.

TABLE 1
Introduction to CFD course outline in 2010

WEEK 1	Introduction to CFD, review of vector algebra
WEEK 2	Basic physical laws, conservation of mass and momentum, the substantive derivative
	ISSUE: Assignment 1 (practical experience with ANSYS-CFX; the CFD methodology)
WEEK 3	Navier-Stokes equations, conservation of energy, the general transport equation, boundary conditions
WEEK 4	Finite-volume method, 1D diffusion problems
WEEK 5	1D convection-diffusion problems, discretization schemes (central and upwind)
	DUE: Assignment 1
WEEK 6	Discretization schemes continued (Hybrid and QUICK), 1D transient diffusion problems
	ISSUE: Assignment 2 (numerical solution of 1D transient diffusion problem)
-- MID SEMESTER BREAK --	
WEEK 7	Iterative solution of Navier-Stokes equations, underrelaxation and false timesteps
WEEK 8	Turbulence structure, RANS
	DUE: Assignment 2; ISSUE: Assignment 3 (turbulence modeling using ANSYS-CFX with validation)
WEEK 9	Turbulence modeling (k-ε), Practical CFD issues (boundary conditions, mesh quality, convergence)
WEEK 10	Turbulence modeling (k-ω, SST, Reynolds Stress), Practical CFD issues (the wall)
WEEK 11	Turbulence modeling (DNS, LES), solvers (segregated and coupled), meshing (staggered and co-located, structured and unstructured)
	DUE: Assignment 3
WEEK 12	Other physical models (heat and mass transfer, reactions, flow in porous medium, multi-phase flow, Lagrangian modeling of particle transport)
-- END OF LECTURES --	
	FINAL EXAMINATION FOR ENGR401

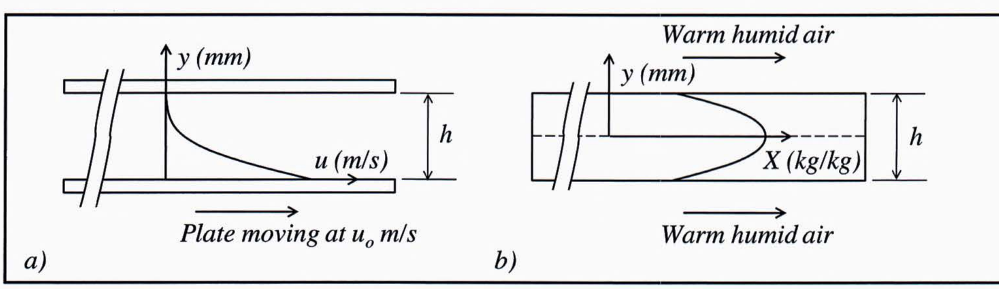

Figure 1. *Assignment 2. a) 2007: Couette-flow problem with a typical velocity profile overlaid; b) 2010: Timber-drying problem with a typical moisture-content profile overlaid.*

TRANSIENT DIFFUSION EXAMPLES, SOLUTION METHOD

Couette flow assignment

Two very large parallel plates, with a fluid in the space between them, are separated by a distance h (Figure 1a). The lower plate is suddenly accelerated from rest and moves at a constant velocity u_o while maintaining the same distance from the upper plate, which remains stationary. The following governing equation describes the development of the fluid velocity profile with time:

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial y^2} \tag{1}$$

where u is the fluid velocity (m/s) in the direction parallel to the plates, ν is the kinematic viscosity of the fluid (m^2/s), t is time (s), and y (m) is the distance in the direction perpendicular to the plates. The boundary and initial conditions are:

$$t \le 0: \ u = 0 \quad \text{for all } y \tag{2}$$

$$t > 0: \ u = u_o \quad \text{for } y = 0 \tag{3}$$

$$u = 0 \quad \text{for } y = h \tag{4}$$

The analytical solution of the governing equation, which satisfies these boundary and initial conditions, is[10]:

$$u(y,t) = \frac{u_o}{h}(h-y) - \frac{2u_o}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\sin\left(\frac{n\pi}{h}y\right)e^{-\left(\frac{n^2 t}{\lambda}\right)}$$
$$\text{where } \lambda = \frac{h^2}{\pi^2 \nu} \tag{5}$$

The distance between the plates is 10 mm, the velocity of the moving plate is 0.1 m/s, and the fluid is water with dynamic viscosity 1×10^{-3} kg/ms and density 1000 kg/m^3.

Mass diffusion in a porous medium assignment

A green timber board with an initial moisture content of 0.3 kg water per kg dry wood is dried by passing warm humid air over the top and bottom surfaces (Figure 1b). These surfaces equilibrate very quickly with the warm humid air to a moisture content of 0.12 kg/kg. The following governing equation describes the development of the moisture-content distribution within the timber board with time as it dries:

$$\frac{\partial X}{\partial t} = D\frac{\partial^2 X}{\partial y^2} \tag{6}$$

where X is the moisture content (kg/kg), D is the diffusion coefficient of water in the wood (m^2/s), t is time (s), and y (m) is the distance from the centerline of the timber board. The thickness of the timber board is h. The boundary and initial conditions can be written:

$$t < 0 : X = X_I \text{ for all } y \tag{7}$$

$$t \geq 0 : X = X_e \text{ for } y = -h/2 \tag{8}$$

$$X = X_e \text{ for } y = h/2 \tag{9}$$

where X_i is the initial moisture content of the timber board (0.3 kg/kg), and X_e is the equilibrium moisture content at the surfaces of the timber board (0.12 kg/kg). The analytical solution of the governing equation, which satisfies these boundary and initial conditions, is[11]:

$$\frac{X - X_e}{X_i - X_e} = \sum_{n=0}^{\infty}\left(\frac{2(-1)^n}{(n+1/2)\pi}\exp\left[-\left(\frac{(2n+1)\pi}{h}\right)^2 Dt\right]\cos\left[\frac{(2n+1)\pi y}{h}\right]\right) \tag{10}$$

The diffusion coefficient D of water in wood is assumed to be constant with a value of 1×10^{-10} m^2/s. The thickness of the timber board is 0.02 m.

Numerical solution using finite-volume method

The finite-volume method is commonly used in CFD for discretizing the governing equations.[8] For transient problems, the governing equations can be discretized using various schemes, with the focus in the homework assignment on the explicit and fully implicit schemes. For the sake of brevity, these mathematical discretizations are not shown in this paper, although they are available from the author on request for the Couette and timber-drying problems. An excellent description is given by Versteeg and Malalasekera[8] for the case of transient heat conduction in a thin metal plate. Students can solve the matrix equation that comes out using the fully implicit scheme using any convenient tool, whether it is Matlab or a spreadsheet such as Microsoft Excel. According to Guessous,[5] this enables students to focus on the important algorithmic and numerical aspects of CFD, rather than on tedious mathematical or file input/output tasks associated with matrix inversions and data formatting.

HOMEWORK 2 DESCRIPTION

Students conducted the homework assignment individually. First, they divided the flow domain into 10 equal-size finite volumes and discretized the governing equation at each control volume using the explicit discretization scheme. The set of equations was solved using a time step of 0.2 s for the Couette flow problem and 10000 s for the timber-drying problem to determine the development of the fluid velocity profile between the plates and moisture-content profile within the timber board, respectively, with time. Students then compared their numerical solution with the analytical solutions given by Eq. (5) and Eq. (10), and commented on any differences, providing percentage errors to back up their statements. In addition, students determined the condition that must be satisfied in order to achieve a stable solution and demonstrated graphically (using their numerical solver) what happens when this condition is not met. The condition for numerical stability of the explicit scheme is

$$\Delta t < \frac{(\Delta y)^2}{2\Gamma} \tag{11}$$

where Δt is the time step, Δy is the control volume height, and Γ is the diffusivity, here the kinematic viscosity ν in the Couette flow problem and the diffusion coefficient D in the timber-drying problem.

The fully implicit method was similarly explored, and in this case the students were required to recommend a mesh spacing and time step that produced a solution that was independent of these quantities. Students compared numerical solutions at different times for at least three different time steps and three different mesh spacings. In addition, students provided plots of error vs. time step and mesh spacing to illustrate the effect of reducing the time step and mesh spacing on the accuracy of the solution. Finally, students commented on which discretization scheme (explicit or fully implicit) is most appropriate to use when numerically solving the governing equation.

Calculations could be done using a spreadsheet or by writing a program in Matlab, and all spreadsheets and programs had to be documented (formulas shown in the case of spreadsheets, and programs commented) sufficiently well that the calculations could be understood from the hard copy alone. Students were required to provide the full method of discretization for both the explicit and fully implicit schemes for control volumes adjacent to the boundaries and an internal control volume, including tables summarizing the coefficients that appear in the resultant algebraic equations, as shown by Versteeg and Malalasekera[8] for heat conduction in a thin metal plate.

NUMERICAL SOLUTIONS

Not all of the results required by the students for the homework assignment are given here. These are available from the author on request, including spreadsheet calculations. A sub-set of the results is presented to highlight the principles covered.

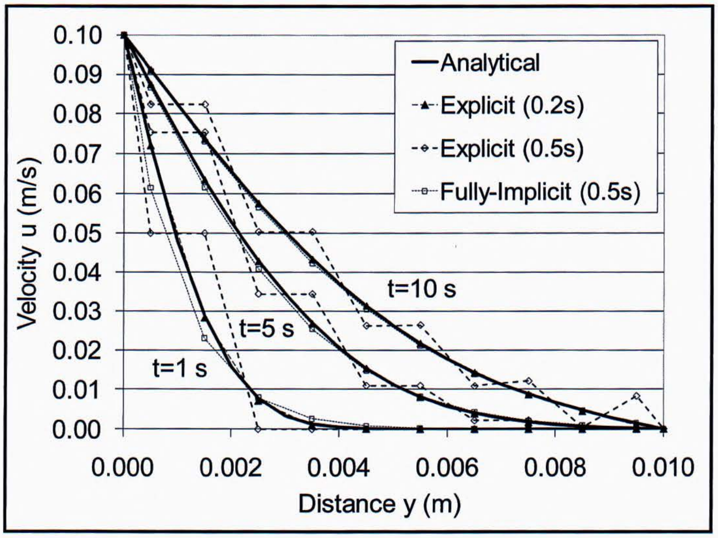

Figure 2. *Comparison of the analytical solution of the Couette-flow problem with the numerical solution based on the explicit discretization scheme at various times for 10 control volumes and two different time steps* Δt *of 0.2s and 0.5s. The numerical solution based on the fully implicit scheme with a time step* Δt *of 0.5s is included for comparison.*

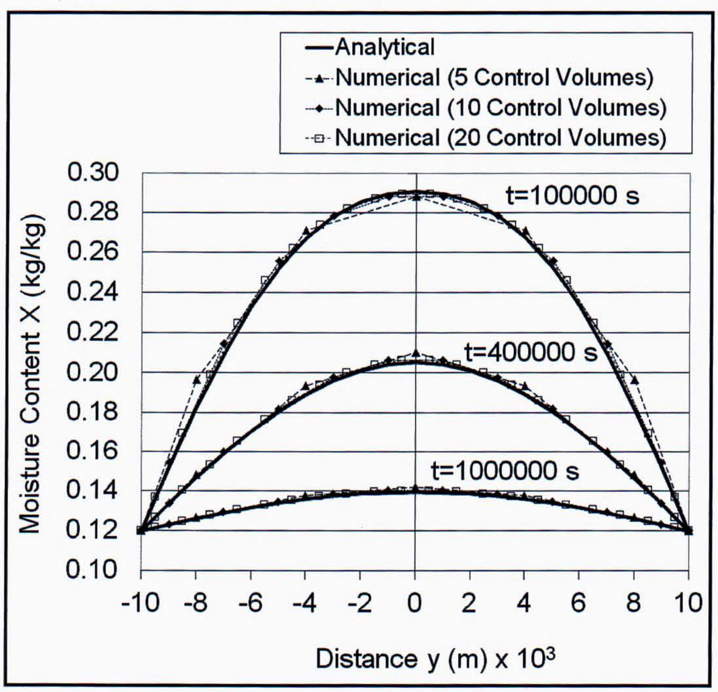

Figure 3. *Comparison of the analytical solution of the timber-drying problem with various numerical solutions based on the fully implicit discretization scheme at various times and for various numbers of control volumes and with a time-step* Δt *of 10000s.*

Figure 2 compares the numerical predictions based on the explicit discretization scheme with the analytical solution at three times t (1, 5, and 10 s) for two different time steps Δt (0.2s and 0.5 s) for the Couette flow problem. The larger time step was calculated from Eq. (11), which represents the stability criterion for the explicit discretization scheme. Any time step equal to or greater than this time step (in this case Δt=0.5 s) would result in an unstable and physically unrealistic numerical solution, as shown by the oscillations in Figure 2. This part of the exercise gives students practical experience in the stability of discretization schemes, and reinforces concepts learned in lectures on the numerical stability of discretization schemes for convection-diffusion problems, such as stability issues that arise when the central-differencing scheme is used. The smaller time step of 0.2 s results in a physically realistic numerical solution, which is in good agreement with the analytical solution. Students calculated the errors for the stable numerical solution, as demonstrated by Versteeg and Malalaseker.[8] This prepared them for a validation exercise in a subsequent homework assignment in which they compared CFD simulations of a simple turbulent flow with experimental data.

Figure 2 also compares the numerical predictions of the explicit and fully implicit discretization schemes for a time step Δt of 0.5s. This demonstrates that the fully implicit scheme, which is unconditionally stable, gives reasonable numerical solutions for time steps that the explicit scheme cannot handle. Through discussion in class, students come to appreciate the analogy to convection-diffusion problems, where upwind discretization is preferable to central-differencing for highly convective flows, due to the unconditional stability of the former. Students also appreciate that refining the mesh to gain a mesh-independent solution is not such a limitation for the fully implicit scheme as for the explicit scheme, for which mesh refining is often accompanied by a refinement in the time step so that the stability criterion given by Eq. (11) is met. This gives the fully implicit scheme advantages over the explicit scheme for use in CFD codes.

Students demonstrated the effect of refining the mesh and time step on the numerical accuracy of the solution. Here, they come to understand that the exact solution of the governing equations, given by the analytical solution, can only be approached numerically when a sufficiently fine mesh and a small enough time step are used. Figure 3 shows the improved accuracy that can be gained by using more control volumes for the timber drying problem. Smith[4] has used COMSOL Multi-physics, a commercial code with CFD functionality, to teach students the importance of proper mesh resolution for achieving numerically accurate CFD solutions. In the assignment presented here, students experience the numerical aspects of CFD more directly through the process of numerical discretization of the governing partial differential equation and solution of the resultant algebraic equations. In this way, students gain an appreciation of how the mesh and the underlying numerical approximations of gradients are linked. This concept is reinforced in class, where it is demonstrated that, in CFD problems, the mesh should be concentrated in areas of high gradients, which improves the numerical approximations of these gradients.

Figure 4 shows that the numerical error reduces as the flow domain is discretized with more control volumes (or in other words when the mesh spacing is reduced) and smaller time steps are used. In Figure 4, the error is calculated by taking the absolute difference between the analytical and numerical solution for each control volume at three times (t=1 s, 5 s, and 10 s) and averaging these. Thus, in this homework assignment, students gained experience in comparing their numerical solutions with "independent data" in an analogy to validating CFD models using experimental data. This experience came in handy when the students validated CFD simulations using experimental data in a subsequent homework assignment.

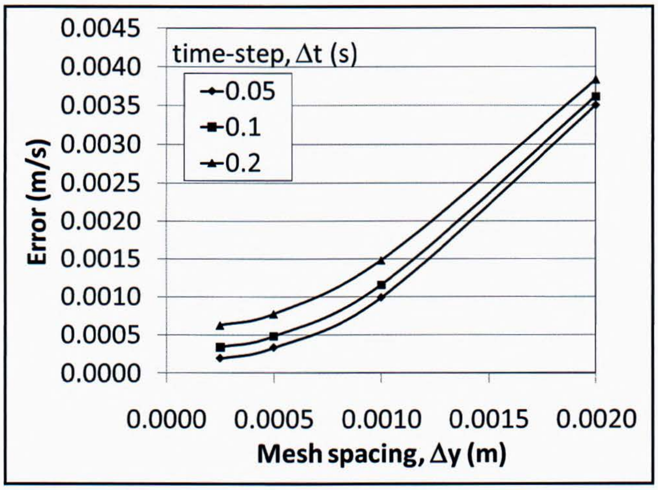

Figure 4. *The average error between the numerical and analytical predictions for various mesh spacings and time steps used in the solution of the Couette flow problem employing the fully implicit scheme. A combined error is calculated using solutions at times 1s, 5s, and 10s after the plate begins to move.*

STUDENT SURVEY

The students in the class of 2010 were given a survey to ascertain the value of the homework assignment. The class had 52 students and there was approximately 80% attendance at the lecture in which the survey was conducted. The students were asked to rate the given statements according to the following categories: 1 = strongly disagree; 2 = disagree; 3 = neutral; 4 = agree; 5 = strongly agree. The survey results are shown in Table 2.

Table 2
Student survey to asssess the value of the homework assignment

	Mean	Standard Deviation
The homework assignment has contributed to my understanding of how CFD works (concepts and methodology).	4.1	0.7
The homework assignment has given me a basic understanding of how partial differential equations are discretized using the finite-volume method.	4.2	0.6
The hands-on aspect of the homework assignment has helped me to understand the theory of numerical methods presented in the class.	4.3	0.7
The homework assignment was interesting and challenging.	3.8	0.6
The homework assignment was a worthwhile exercise.	4.1	0.6
Estimate how many hours it took you to complete the homework assignment.	23 hours	8 hours
Did you use Matlab, Excel, or another code (specify) to do the homework assignment?	Matlab 60%	Excel 40%

On average, the students agreed that this homework assignment contributed to their understanding of the CFD methodology and the finite-volume method of discretization. The students also appreciated the hands-on aspect of the homework assignment in reinforcing their understanding of numerical methods learned in the class. Overall, they found the homework assignment to be a worthwhile exercise although it rated slightly lower (although still well) for interest and challenge. The homework assignment took on average 23 hours to complete, in alignment with its 20% weighting for the course, which has been nominally allocated 120 hours work in total, covering lectures, self-study, exam preparation, and assignments. The high standard deviation of 8 hrs reflects the variation in student ability, as well as the amount of work students put into the assignment, with some able students putting in significantly more time to do a thorough job on the mesh and time step independence studies. Sixty percent of the students chose to conduct the calculations using Matlab, and the remaining 40 percent chose Microsoft Excel.

TEACHER PERSPECTIVE

Over the years, all students correctly carried out the numerical discretization, mainly due to the availability of the analytical solution, which provided a means of checking for errors. Depcik and Assanis[12] have pointed out that verifying a numerical method against an analytical solution is a useful way of increasing one's confidence in a correctly implemented numerical method. One common student issue is choosing an appropriate range of control-volume numbers for testing mesh independence. Each year, a small number of students choose meshes covering an inappropriately narrow range of control volumes, for example 5, 7, and 9 control volumes. The point is made in class that using at least three meshes with a doubling of the control-volume number between successive meshes will provide a satisfactory test for mesh independence. Students are not always clear on when to stop refining the mesh (or when to stop reducing the time step). It is explained that, for a validation exercise in which CFD simulations are compared with experimental data, refinement might continue until the difference in solution between successive refinements is smaller than the experimental uncertainty, since there is little advantage in gaining further numerical accuracy beyond this point. In addition, the gains in accuracy achieved by further refinement must be weighed against the additional computational effort required.

FINAL REMARKS

An undergraduate CFD course that teaches a commercial CFD package does not necessarily provide students with a firm grasp of underlying numerical concepts, and may give them the impression that the solver is a black box, which Coronell and Hariri[13] point out is valid for many types of numerical solvers available commercially. There are good lessons on the application of numerical methods and stability that can be learned from code development, which would be useful to students for understanding how converged and accurate CFD solutions are obtained. It is difficult, however, to see how code development could be fitted into the one-semester introductory CFD course taught at CAPE, whose focus is on teaching undergraduate students the CFD methodology so that they have a solid basis for when they apply CFD in industry. The CFD course at CAPE makes a compromise between a course with a focus on code development and a course that teaches students how to use commercial CFD software. A homework assignment is given in which discretization and numerical stability and accuracy are demonstrated in a hands-on manner using easy-to-understand, physically realistic problems of practical interest to engineers. Matlab and Microsoft Excel are used to bypass tedious calculations associated with code development such as data formatting and matrix inversions, while not taking away from the key concepts of discretization and numerical stability and accuracy. Through this homework assignment, student understanding of the CFD methodology is promoted because the process of solving the problem is analogous to conducting a typical CFD analysis, including laying out the geometry, generating the mesh, defining the physics and boundary conditions, solving the governing equations, and visualizing the solution. This connection is emphasized in class with the presentation of Versteeg and Malalasekera's[8] numerical solution of transient heat conduction in a thin metal plate. In the homework assignment, an analytical solution provides a means of verifying the numerical solutions, in a similar fashion to how mathematical models are validated by comparison with experimental data.

In summary, the homework assignment has proven to be an effective tool to help students learn the CFD methodology and understand how a commercial CFD solver works. The homework assignment helps students overcome the steep learning curve of CFD by giving them hands-on experience with the principles and methodologies first demonstrated in class. A balance is struck by teaching students numerical aspects to demystify the black box of a commercial CFD solver and showing them how this knowledge can be used to gain accurate, stable numerical solutions, while avoiding some of the more tedious calculations associated with code development.

ACKNOWLEDGMENTS

The author thanks Dr. Henk Versteeg (University of Loughborough, UK) for his helpful suggestions during the preparation of this paper.

REFERENCES

1. Stern, F., T. Xing, D.B. Yarbrough, A. Rothmayer, G. Rajagopalan, S.P. Otta, D. Caughey, R. Bhaskaran, S. Sonya, B. Hutchings, and S. Moeykens, "Hands-on CFD educational interface for engineering courses and laboratories," *J. Eng. Ed.*, **95**(1), 63 (2006)
2. Fraser, D.M., R. Pillay, L. Tjatindi, and J.M. Case, "Enhancing the learning of fluid mechanics using computer simulations," *J. Eng. Ed.*, **96**(4), 381 (2007)
3. Hailey, C.E., and R.E. Spall, "An introduction of CFD into the undergraduate engineering program," ASEE Annual Conference and Exposition, <http://www.asee.org/acPapers/20368.pdf> (2000)
4. Smith, M.K., "Computational fluid exploration as an engineering teaching tool," *Int. J. Eng. Ed.*, **25**(6), 1129 (2009)
5. Guessous, L., "Incorporating Matlab and FLUENT in an Introductory Computational Fluid Dynamics course," *Computers in Ed. J.*, **14**(1), 82 (2004)
6. Lawrence, B.J., J.D. Beene., S.V. Madihally, and R.S. Lewis, "Incorporating non-ideal reactors in a junior-level course using computational fluid dynamics (CFD)," *Chem. Eng. Ed.*, **38**(2), 136 (2004)
7. Kaushik, V.V.R., S. Ghosh, G. Das, and P.K. Das, "CFD modeling of water flow through sudden contraction and expansion in a horizontal pipe," *Chem. Eng. Ed.*, **45**(1), 30 (2011)
8. Versteeg, H.K., and W. Malalasekera, *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*, 2nd Ed., Pearson Education Limited, New York (2007)
9. Aung, K., "Design and implementation of an undergraduate computational fluid dynamics (CFD) course," ASEE Annual Conference and Exposition, <http://www.asee.org/acPapers/2003-24_Final.pdf> (2003)
10. Papanastasiou, T.C., G.C. Georgiou, and A.N. Alexandrou, *Viscous Fluid Flow*, CRC Press (1999)
11. Mills, A.F., *Basic Heat and Mass Transfer*, 2nd Ed., Prentice Hall Inc., Upper Saddle River, NJ (1999)
12. Depcik, C., and D. Assanis, "Merging undergraduate and graduate mechanics through the use of the SIMPLE method for the incompressible Navier-Stokes Equations," *Int. J. Eng. Ed.*, **23**(4), 816 (2007)
13. Coronell, D.G., and M.H. Hariri, "The chemical engineer's toolbox: a glass-box approach to numerical problem solving," *Chem. Eng. Ed.*, **43**(2), 143 (2009) ❐