

# Practical teaching and learning evaluation of computational fluid dynamics based on traditional chemical engineering curriculum

Junjie Chen\*

School of Mechanical and Power Engineering, Henan Polytechnic University, Jiaozuo, Henan, China

\*E-mail address: comcjj@163.com, comcjj@yahoo.com

## ABSTRACT

Practical teaching and learning evaluation of computational fluid dynamics (CFD) have been incorporated into a chemical engineering curriculum at the intermediate undergraduate level. CFD has now become a component of professional life in engineering practice and to prepare students properly, they must get exposure to all aspects of their chosen profession. Issues of concern arise when mathematical modelling is being introduced into a curriculum. For example, at the practical level, it must be considered whether or not an appropriate platform has been developed to allow the students to use the software efficiently and importantly without frustration. Also it is important that students have been taught sufficient skills for the student to continue with simulations in a systematic and methodical manner. The incorporation of the CFD package into a traditional chemical engineering curriculum is described here, and evaluation results based on pre-post knowledge and skill experiments, and student survey results document successful learning outcomes and effectiveness of the approach.

**Keywords:** theoretical teaching; practical teaching; learning evaluation; computational fluid dynamics; finite-volume method; transport and reaction; mathematical modelling; engineering practice

## 1. INTRODUCTION

The development, implementation and evaluation of a suitable curriculum for students to use computational fluid dynamics (CFD) as an extension of their chemical engineering knowledge and skills at intermediate undergraduate level are described [1]. CFD is the simulation of transport phenomena, reacting systems, etc. using modelling, i.e. mathematical physical problem formulation and numerical methods, which include discretization methods, solvers, numerical parameters, and grid generation. Traditionally, in chemical engineering, formulation of mathematical models involves the solution of ordinary or partial differential equations to describe transport phenomena and reacting systems by incorporating analytical methods such as Laplace transforms or Fourier series expansions in Eigen functions [2]. Such methods are however restrictive, in that they usually require simple geometries and linear problems, whereas real chemical engineering problems can have very complex geometry and non-linear phenomena.

The use of mathematical modelling can now be found in many areas of engineering education, for example, for chemical reactions, for diesel engine simulation and in fluid

mechanics and heat transfer [3]. Some work has also been carried out in developing educational user-friendly CFD interfaces where the general aspects and simplification of the three main processes of CFD, the pre-processor, the solver and the post-processor were carefully considered [4]. However, although the educational benefits associated with integrating computer-assisted learning and simulation technology into undergraduate engineering courses are great, and computational fluid dynamics has revolutionized research and design, its incorporation into the teaching of undergraduate transport phenomena has been limited. This lack of penetration of CFD into the undergraduate curriculum is probably primarily due to a deficiency of faculty with training in CFD, the lack of knowledge by faculty of educational CFD tools available and the start-up time associated with developing educational CFD materials.

Why should CFD be included in an undergraduate chemical engineering curriculum? The answer is that CFD is now to a lesser or greater degree part of the professional lives of many chemical engineers and so, to prepare future engineers properly, they must get exposure to all aspects of their chosen profession [5]. In the areas of analysis and design, simulation based design is commonly used instead of the traditional “build and test”, as it is much more cost effective and a substantial database is provided for diagnosing the adjacent flow field. Simulations can readily be done of physical flow phenomena that are difficult to measure, for example, full scale situations, and environmental effects and importantly in chemical engineering hazards. Problem solving with modern engineering tools, such as found in CFD, can be applied to realistic problems [6].

Issues of concern arise when simulation is being introduced into a curriculum. These include learning vs. research objectives, usability vs. predetermined objectives and student demographics. A proper balance should be sought between these competing objectives, for example, it is just as important that a student be taught the practical and systematic ways of using a CFD package in a general sense, as well as achieving a specific result [7]. There is much evidence from previous studies that: the use of simulation enhances the curriculum; there is increased learning efficiency and understanding; there is effectiveness of new and hands-on learning methods; and it is effective to use a combination of physical and simulation laboratories [8].

Practical concerns concerning the introduction of CFD are for example, when to introduce, how much to introduce and how much CFD background is necessary. There is no doubt that when a student first uses CFD, a lot of new knowledge and required skills descend on them from many directions hence rendering a steep learning curve. Without careful planning this course can become overwhelming. Also, importantly, it is essential that students do not lose “feelings” for physical and chemical phenomena, needed assumptions used in mathematical modelling, nor the need to verify and validate the computational methods applied to a problem. This is a common concern when introducing mathematical modelling, for example process simulation software. Successful implementation of CFD usually requires a re-focus of course objectives and skills taught and a re-structuring of the course curriculum. An important concern is that students adapt a healthy skepticism as to the results they get and a willingness to be critical of the results should be instilled into them.

In the rest of this paper how computational fluid dynamics is implemented into the chemical engineering curriculum is first described. The next section presents evaluation design, results and discussion, in the form of three investigations, one an experiment comparing the students’ knowledge of chemical engineering before and after their CFD course, one measuring the student learned knowledge and skills regarding the CFD interface

and one eliciting student views on using CFD by questionnaire. The paper finishes with conclusions drawn and possible work for the future.

## 2. TEACHING IMPLEMENTATION

Computational fluid dynamics was introduced to students of chemical engineering in the form of necessary back-ground theory lectures, tutorials and hands-on laboratories. The course was held over a 4-week period, with the theory taught intensively during the first week of the course and as required during the last 3 weeks. Hands-on laboratory sessions were conducted throughout the final 3 weeks with students given short demonstrations where they watched the instructor building simple simulations while doing the same on their own computer, completing simulations using highly detailed instruction sheets fully supplied by faculty and teaching assistants, and finally solving problems without instructions and only occasional help from support staff [9].

The students had already successfully completed courses on matrix algebra, vector calculus, ordinary differential equations and partial differential equations, with the latter being solved using a variety of numerical methods [10]. They had also been exposed to courses on fluid mechanics, thermodynamics and chemical processes.

The main learning outcomes are to understand the equations that govern fluid flow (conservation of mass, momentum, species, and energy) and be able to apply them to a range of practical problems in the areas of fluid flow, heat transfer and chemically reacting flows. Two seminars were held before the course, to discuss expectations regarding CFD laboratory practice and reporting. During these seminars, the students were introduced to the idea that theoretical chemical engineering, experimental chemical engineering and computational fluid dynamics are complementary in modern engineering practice. Students were then introduced to CFD general methodology and procedures. The students learned as to when and why CFD is used, and the breakdown of CFD into three processes namely the pre-processor, the solver and the post-processor. The student group was then initiated to CFD with an intensive 1-week course outlining theory and good practice. The course followed the headings of,

- Getting started
- CFD notation;
- CFD equations (continuity, momentum, energy, concentration of species);
- Finite differencing;
- The finite volume method;
- Boundary conditions;
- Accounting for the pressure term;
- Mass averaged equations;
- Time-stepping techniques; and
- Properties of numerical methods.

The theory course also included good practice and showed students the need for CFD methodology to be systematic and rigorous. It was pointed out that the complete process, at this level of CFD can, if so desired, be completely automated with the students going through a step-by-step process seamlessly from the set-up of the problem, through the solving to the display of the results without much thought. Importantly then, the students were taught to be critical of their results and how to examine if what they were getting is what they might have expected.

The general process of solving using CFD techniques, which the students were encouraged to strictly adhere to in this early stage of their CFD studies.

As mentioned above, the laboratory part of the course started with a series of demonstrations with full facilities for students to have ‘hands-on’ experience as the demonstration proceeds. Several simple three-dimensional flows are used as exemplars to give an overall view of the CFD process. A period of time was always given so students could go back to different stages of the process to experiment either by themselves or with suggestions from the faculty and teaching assistants. Gradually students moved on to working by themselves, first with provided detailed instructions, then to semi-detailed instructions and finally only to specifications of the problem to be solved.

A brief description of the course material used during the ‘hands-on’ section of the course is now given. Three relatively easy exemplars were first used, namely, an introduction to setting-up flow problems, adding heat transfer to the calculation domain and, refining the computational grid in the flow domain. These were slowly and carefully demonstrated with the students processing each described step on their individual computers. This was followed by six major simulations, namely,

- Importing geometry into the calculation domain

It is important that students are comfortable importing geometry generated elsewhere into the calculation domain. This geometry could be initially built using any computer-aided drawing (CAD) package or an in-house computer program. In this exercise a NACA 4-digit 2D aerofoil was generated and imported.

- Flow and heat transfer in a mixing elbow

In this, students set-up and solved a three-dimensional turbulent flow and heat transfer problem in a mixing elbow. The mixing elbow configuration is used in piping systems in the process industry and it is often important to correctly predict the flow and temperature fields in the mixing region.

- Modelling species transport and gaseous combustion

The mixing of chemical species and the combustion of a gaseous fuel is examined here. A cylindrical combustor burning methane ( $\text{CH}_4$ ) in air is studied using the eddy-dissipation model. The exercise will allow for the prediction of the thermal field and for the production of  $\text{NO}_x$ .

- Using the non-premixed combustion model

Here, a natural gas combustion problem is set and solved using the non-premixed combustion model for the reaction chemistry. The non-mixed combustion model uses a modelling approach which solves transport equations for one or two conserved scalars and the mixture fraction. Property data for the species are accessed through a chemical database and turbulence-chemistry interaction is modelled using a probability density function mixture fraction model.

- Modelling surface chemistry

In chemically reacting laminar flows, such as those encountered in chemical vapour deposition (CVD) applications, accurate modelling of time-dependent hydrodynamics, heat and mass transfer and chemical reactions, including wall surface reactions, is important.

- Modelling evaporating liquid spray

An air-blast atomizer model is used to predict the behaviour of an evaporating methanol spray. Initially, the air flow is modelled without droplets. To predict the behaviour of the spray, several other discrete-phase models, including collision and breakup are used.

### 3. TEACHING AND LEARNING EVALUATION

The CFD course was taught in the fourth semester of a chemical engineering undergraduate degree course with the number of students in the group. The evaluation process was subdivided into three investigations, one in the form of an experiment comparing the knowledge of the group concerning chemical engineering and related mathematics before and after their CFD course, the second measuring student knowledge and skill outcomes for the CFD interface, again before and after their CFD course, and, the third in the form of an online questionnaire eliciting the views of students on using CFD.

#### 3.1. Effectiveness of using CFD for chemical engineering teaching and learning

To investigate the effectiveness of introducing CFD into the chemical engineering course, an experiment applying a pre-test post-test design was conducted to test if the students' knowledge and skills outcomes in the form of their post-test scores were significantly higher than their pre-test scores. Implementing this summative evaluation required an objective measure of student outcomes in at least one curricular area of chemical engineering with the areas chosen here being heat and mass transfer and chemically reacting flows. A pool of assessment questions covering these two areas was assembled and then paired for equivalency following a Table of Specification by the instructional staff [11]. The dependent variables are constructs used to capture aspects of learning provided by the courses and each was measured using three or more questions.

One concern was that students simply remembered the topics tested during the pre-test and concentrated on learning those better during the CFD course and thus did better over the same topics even though they may not have learned the outcomes properly. So, topics in each pair were randomly assigned to either an A or B version of the pre-test and at the same time students were randomly assigned to either the A or B version of the pre-test which they completed. For the post-test the students completed both the A and B versions. To be clear, all students completed only an A or B version for the pre-test, but took both the A and the B for the post-test.

#### 3.2. Student knowledge and skill outcomes for the CFD interface

An objective measure of student knowledge and skill outcomes for the CFD interface as applied to the chemical engineering curriculum was devised. This test was again run on a pre/post CFD studies basis, i.e. during the first week of the course students completed the pre-test and later in the semester, and after completing the CFD studies, the students completed the post-test. The most intuitive test of students' knowledge and skill outcomes is whether the post-test scores were significantly higher than those of the pre-test scores. It can be seen that the effect is substantial between pre- and post-tests and therefore represents significant improvement in outcomes of the students' knowledge and skills of CFD knowledge and skills [12]. The students, after a relatively brief exposure to and with limited practice of CFD have shown considerable growth in their understanding of CFD concepts, principles and applied problems.



### 3.3. On-line questionnaire

An anonymous online survey was conducted after students obtained their grades for the laboratory reports to aid formative evaluation of the introduction of CFD. The survey was in two parts, with one part the students' feeling regarding how well they were prepared for the introduction of CFD into their curriculum and the other exploring their opinions on the skills and knowledge acquired when using the actual computer package [13]. Students were requested to respond to each item in the questionnaire using a five-point scale: strongly agree, agree, neutral, disagree and strongly disagree plus a column for no opinion. An opportunity was also provided for students to comment on their experience at the end of the questionnaire to collect qualitative feedback on their experience so far with CFD. Students felt that they had been reasonably prepared for and benefited from their exposure to CFD. In addition, comments from most of the students expressed the view that the amount of material introduced was correct, although some felt that the exercises took a long time to complete correctly. Students were particularly appreciative that they could easily visualize flow using contour and vector plots and generally agreed that the combination of theory, experimental and CFD led to better understanding of fluid mechanics [14]. Students also showed enthusiasm for learning more about CFD.

The students indicated that their previously gained knowledge and skills of matrix algebra and vector/tensor calculus was sufficient and that their existing knowledge of PDEs was adequate. However, for PDEs comments were made that they did need to revise their previous course in that some details had been forgotten. More problematic was the responses given by the students regarding the theory needed for discretization of the equations. Basically the thought was that the background material, though reasonably interesting did not contribute to the use of the CFD package. Most students felt that more worked examples would be a good innovation. Therefore, more development will be necessary to bridge the obvious gap between the theory and practice of CFD. Generally the students were of the opinion that they were now well acquainted with some of the important aspects of CFD practice, that is using turbulence modeling, implementing suitable boundary and initial conditions and the important mathematical aspects of grid independence and when and how to implement under-relaxation.

It was noted that the students liked the hands-on and self-discovery approach, although at times some frustration was also noted. Once a demonstration was given there was only an interest to learn by themselves, backed up when required by a teaching assistant's advice [15]. The traditional view of CFD is that it has a steep learning curve, but with a structured CFD interface and, with limited depth imposed, it has been demonstrated that the gradient of the curve can be brought to an acceptable level.

During the skills training at this level, no real mention was made of code development, as the purpose was to develop users of the code only. This can be remedied by a later course which involves the student as a user and starts showing ways of writing new codes for special conditions.

### 3.4. Instructor views

The following is a brief summary of views of instructors concerning introducing computational fluid dynamics into a chemical engineering curriculum. One concern was to ensure proper underpinning understanding of the mathematical aspects of computational fluid dynamics, which involved an intensive course, mainly centered primarily on

mathematical numerical methods. It should be recognized that for some chemical engineering students such a course is quite challenging and perhaps a longer, more leisurely course may be better for learning [16]. Some topics introduced are by necessity advanced, for example “accounting for the pressure term”. The course should also be very systematic without many assumptions being made of student prior knowledge and delivered with much interaction and feed-back from the students. However, it is thought that although having hurdles to overcome, it is thought that the best approach for intermediate level undergraduate students is to teach a reasonably deep and broad range of numerical methods leading to CFD theory so giving a sound basis for the later methodology and procedures.

While lectures and laboratory course teaching seemed to work here, there is a case, towards the end of the course some studio and/or multi-media may need to be developed that students can think and work at their own pace and alone, with only occasional help from written instructions and instructing staff [17]. This has the benefits of reducing the sometimes considerable work-load imposed on the instructing staff and also increasing the students’ confidence and willingness to experiment [18].

There can be a steep learning curve associated with CFD interfaces. It is important that time is taken to carefully allow the students to become familiar with, sometimes quite hidden, interface windows necessary for setting calculations up correctly [19]. Much practice and experimentation by the students is worthwhile, so generating confidence and reducing student frustration. A problem instructors should be aware of, is that all students do not come with the same background knowledge and skills regarding the use of modern interfaces. If necessary, a separate hands-on course should be offered in this area [20].

Traditionally a CFD curriculum has focused on code development while not training component users, as is the purpose in this work. In traditional approaches, students are asked to either partly or completely develop their own research code using CFD theory learned. It is thought that this is not necessary at this stage of CFD user training but a subject for post-graduate studies.

It is the view of the instructing staff that the use of computational fluid dynamics to simulate various chemical engineering scenarios allowed the students to more easily explore and understand some basic concepts taught in the traditional course. The use of colour in the graphical representations allows for easy visualization of the phenomena, which can significantly facilitate and enhance the learning process. Also, the students can more easily explore the effects of changing the simulation conditions without requiring additional physical laboratory experiments. In addition to varying the chemistry, geometry dimensions or configurations can be relatively easily varied.

#### 4. CONCLUSION

This paper has described the use and efficacy of incorporating computational fluid dynamics into a traditional chemical engineering curriculum. The experiment has shown that the inclusion of CFD gave students a better appreciation of chemical engineering in general and the students gained better knowledge of simple concepts. It was found from the study of student knowledge and skill outcomes for the CFD interface that the students could cope with CFD reasonably well, provided the subject is introduced with care. One of the main reasons for the inclusion of CFD was to contribute to the teaching of professional practice skills to intermediate level undergraduate students. It was found that the interface design does provide students with hands-on experience, gained through an interactive and user-friendly

environment, and encourages student self-learning. It was noted from the survey that the students liked the hands-on and self-discovery approach, although at times some frustration was also noted.

The success of the present work encourages future development in this area of the curriculum with inclusion of more examples found in chemical engineering. There was evidence that more time should be spent on the theory underlying CFD, especially in the area of finite differencing of equations, as well as emphasis should be placed on, and more opportunity provided, for students to verify and validate their results. The assembly of a strong centralized database for comparison would be desirable. Again the idea of obtaining a grid independent solution should be reinforced.

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