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Building on a traditional chemical engineering curriculum using computational fluid dynamics

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ABSTRACT

Computational fluid dynamics (CFD) has 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: Computational fluid dynamics; Finite-volume method; Transport and reaction

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. 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 eigenfunctions. 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 (Qian and Tinker, 2006), for diesel engine simulation (Assanis and Heywood, 1986) and in fluid mechanics and heat transfer (Devenport and Schetz, 1998; Zheng and Keith, 2003; Rozza et al., 2009). Some work has also been carried out in developing educational user-friendly CFD interfaces (Pieritz et al., 2004; Stern et al., 2006) 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. However, although the educational benefits associated with integrating computer-assisted learning and simulation technology into undergraduate engineering courses are great (Curtis, 2008), and computational

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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. 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, 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.

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 (Stern et al., 2006). 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. There is much evidence from previous studies that: the use of simulation enhances the curriculum (Rozza et al., 2009); there is increased learning efficiency and understanding (Keller et al., 2007; Jaeger and Adair, 2010, 2012; Kelsey, 2001; LaRoche et al., 2002); there is effectiveness of new and hands-on learning methods (Patil et al., 2009); and, it is effective to use a combination of physical and simulation laboratories (Stern et al., 2006).

Practical concerns concerning the introduction of CFD are for example, when to introduce, how much to introduce and how much CFD background is necessary (Edgar, 2006). 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 curve can become overwhelming. Also, importantly, it is essential that students do not lose 'feeling' for physical and chemical phenomena, needed assumptions used in mathematical modelling, nor the need to verify and validate the computational methods applied to the problem (Parulekar, 2006). This is a common concern when introducing mathematical modelling, for example process simulation software (Dahm et al., 2002). Successful implementation of CFD usually requires a re-focus of course objectives and skills taught and a re-structuring of the course curriculum (Rockstraw, 2005). An important concern is that students adapt a healthy scepticism as to the results they get and a willingness to be critical of the results should be instilled into them (Finlayson and Rosendall, 2000).

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. Computational fluid dynamics implementation

Computational fluid dynamics was introduced to students of chemical engineering in the form of necessary background 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 supported by faculty and teaching assistants, and finally solving problems without instructions and only occasional help from support staff (Rockstraw, 2005).

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. Required reading for the course included LeVeque (2007) and Ferziger and Peric (1996). 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;
- Closure of 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