

Preface

Computational fluid dynamics (CFD) has become an indispensable tool for engineers. CFD simulations provide insight into the details of how products and processes work, and allow new products to be evaluated in the computer, even before prototypes have been built. It is also successfully used for problem shooting and optimization. The turnover time for a CFD analysis is continuously being reduced since computers are becoming ever more powerful and software uses ever more efficient algorithms. Low cost, satisfactory accuracy and short lead times allow CFD to compete with building physical prototypes, i.e. ‘virtual prototyping’.

There are many commercial programs available, which have become easy to use, and with many default settings, so that even an inexperienced user can obtain reliable results for simple problems. However, most applications require a deeper understanding of fluid dynamics, numerics and modelling. Since no models are universal, CFD engineers have to determine which models are most appropriate to the particular case. Furthermore, this deeper knowledge is required since it gives the skilled engineer the capability to judge the potential lack of accuracy in a CFD analysis. This is important since the analysis results are often used to make decisions about what prototypes and processes to build.

Our ambition is that this book will provide sufficient background for CFD engineers to solve more advanced problems involving advanced turbulence modelling, mixing, reaction/combustion and multiphase flows. This book presents the equations that are to be solved, *but, more importantly*, the essential physics in the models is described, and the limitations of the models are discussed. In our experience, the most difficult part for a CFD engineer is not to select the best numerical schemes but to understand the fluid dynamics and select the appropriate models. This approach makes the book useful as an introduction to CFD irrespective of the CFD code that is used, e.g. finite-volume, finite-element, lattice Boltzmann etc.

This book requires a prior knowledge of transport phenomena and some understanding of computer programming. The book (and the tutorials/project) is primarily intended for engineering students. The objective is to teach the students how to do CFD analysis correctly but not to write their own CFD code. Beyond this, the book will give an understanding of the strengths and weakness of CFD simulations. The book is also useful for experienced and practicing engineers who want to start using CFD themselves or, as project managers, purchase these services from consulting firms.

We have added several questions of reflective character throughout the book; it is recommended that you read these to confirm that the most important parts have

been understood. However, the book intentionally contains few simulation results and worked-through examples. Instead we have developed three tutorials and one larger project that give students the required hands-on experience. The tutorials take 6–8 hours each to run; the project takes 30 hours to run and write a report. These tutorials and the project are available from the authors. We have chosen to use a commercial code (ANSYS/Fluent) in our course, but the problem formulations are written very generally and any commercial program could be used. Our experience is that commercial CFD programs can be obtained for teaching purposes at very low cost or even free. An alternative is to use an open-source program, e.g. OpenFoam. Unfortunately, the user interface in OpenFoam is not as well developed as are those in the commercial programs, so students will have additional problems in getting their programs working.

This book has successfully been used in a CFD course at Chalmers University since 2004. Every year approximately 60 chemical and mechanical engineering students take the course. Over the years this book has also been used for PhD courses and courses in the industry. The text has been rewritten every year to correct errors and in response to very valuable suggestions from the students. PowerPoint lecture notes are also available from the authors.

Scope

Chapter 1 provides an introduction to what can be solved with a CFD program and what inputs are required from the user. It also gives an insight into what kind of problems are easy or difficult to solve and how to obtain reliable results.

Chapter 2 contains the equations that are solved by the CFD software. The student should know these equations from their prior courses in transport phenomena, but we have included them because they are the basis for CFD and an up-to-date knowledge of them is essential.

In *Chapter 3* the most common numerical methods are presented and the importance of boundedness, stability, accuracy and convergence is discussed. We focus on the finite volumes on which most commercial software is based and only a short comparison with the finite-element method is included. There is no best method available for all simulations since the balance among stability, accuracy and speed depends on the specific task.

Chapter 4 gives a solid introduction to turbulence and turbulence modelling. Since simulation of turbulent flows is the most common application for engineers, we have set aside a large part of the chapter to describe the physics of turbulence. With this background it is easier to present turbulence modelling, e.g. why sources and sinks for turbulence are important. The k – ε model family, k – ω , Reynolds stress and large-eddy models are presented and boundary conditions are discussed in detailed.

Chapter 5 carefully analyses turbulent mixing, reaction and combustion. The physics of mixing is presented and the consequence of large fluctuations in concentration is discussed. A probability distribution method is presented and methods to solve instantaneous, fast and slow kinetics are formulated. A simple eddy-dissipation model is also presented.

In *Chapter 6* multiphase models are presented. First various tools with which to characterize multiphase flow and forces acting on particles are presented. Eulerian–Lagrangian, Euler–Euler, mixture (algebraic slip), volume-of-fluid and porous-bed models are presented and various closures for drag, viscosity etc. are formulated. Simple models for mass and heat transfer between the phases are also presented.

Finally, *Chapter 7* contains a best-practice guideline. It is based on the guidelines presented by the European Research Community on Flow Turbulence and Combustion, ERCOFTAC, in 2000 and 2009 for single-phase and multiphase systems, respectively.

In *Tutorial 1* reactions inside a spherical porous catalyst particle are studied. The reaction is exothermic and flow, heat and species must be modelled. The student will learn how to draw and mesh a two-dimensional (2D) geometry. They will also specify boundary conditions and select the models to solve. The kinetics is written as a user-defined function (UDF) and the student will learn how to implement a UDF in a CFD simulation. Convergence is a problem, and the student will learn about physical reaction instability, numerical instabilities, under-relaxation and numerical diffusion. In the report the student is required to show that their simulations fulfil the criteria given in the best practice guidelines.

In *Tutorial 2* turbulent mixing and combustion in a bluff-body stabilized non-premixed turbulent flame is studied. An instantaneous adiabatic equilibrium reaction, i.e. combustion of methane in air, is simulated. The student should select an appropriate turbulence model and solve for flow, turbulence, mean mixture fraction, mixture fraction variance, species and heat with appropriate boundary conditions, e.g. wall functions. Mesh adaptation to obtain the proper y^+ for the wall functions is introduced. The students should analyse whether jets and recirculations exist in the flow and whether the reaction is fast compared with turbulent mixing.

In *Tutorial 3* a spray is modelled using an Eulerian–Lagrangian multiphase model. Continuous phase and spray velocity combined with heat transfer and evaporation are modelled. The student should analyse the fluid–spray interaction and choose what forces should be included in the model.

The *Project* is dedicated to the design of an industrial-scale selective catalytic reduction (SCR) process. The student generates a three-dimensional (3D) computer-aided design (CAD) model and mesh, analyses the performance, and suggests and evaluates design improvements of the SCR reactor.

Acknowledgements

We are very grateful to the students who have given us very valuable feedback and thus helped us to improve the book. We would also like to thank Mrs Linda Hellström, who did the graphics, and Mr Justin Kamp, who corrected most of our mistakes in the English language.

Bengt Andersson

