

## Chapter 2

# An Introduction to Computational Fluid Dynamics and Its Application in Microfluidics

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### **ABSTRACT**

*The chapter aims to introduce the computational fluid dynamics (CFD). A review was provided, outlining its development and applications on chemical engineering and microfluidics. The fundamental points of the CFD, listing the advantages and precautions of this numerical technique were provided. The description of CFD methodology including the three essential stages (pre-processing, solving, and post-processing) was made. The fundamental transport equations—total mass (continuity), momentum, energy, and species mass balances—and the usual boundary conditions used in CFD were explained. The main approaches used in multicomponent single-phase flows, single-phase flow in porous media, and multiphase flows in microscale were detailed, as well as the numerical mesh types and its quality parameters. A brief introduction of finite volume method (FVM) used by most of the available CFD codes was also performed, describing the main numerical solution features. Finally, the conclusions and future prospects of CFD applications are exposed.*

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## **INTRODUCTION**

The Computational Fluid Dynamics or CFD is the numerical technique used in the analysis of flowing systems and other associated phenomena. CFD studies also include mass and heat transfer and chemical reactions (Versteeg & Malalasekera, 2007). The CFD could be understood as the combination of physics, mathematics and computational sciences aiming the fluid flow behavior description (Blazek, 2001).

With the advancement of computational processing power, CFD has become an essential design and optimization tool for engineers, including products and processes development, as well a substantial research tool in physical sciences (Blazek, 2001; Versteeg & Malalasekera, 2007). Engineering applications include reactor development, mixer and agitator design, contaminant dispersion studies, biomedical studies, among others.

In general, CFD solves numerically the transport equations for the case-relevant variables, necessarily including mass conservation (continuity) and momentum balance. From the classical continuum hypothesis, the fluid flow and heat and mass transport phenomena can be described by partial differential equations (PDE) in the most of engineer interest cases. Analytical solutions are possible only for a few simple special cases, as for example, the Hagen-Poiseuille flow.

Cases of industrial and academic interest are often more complex, involving other phenomena simultaneously with momentum transfer, as for example, chemical species mass transfer. For these cases, approximated numerical solution can be obtained from CFD simulations. Initially, the PDE are discretized, resulting in a system of algebraic equations, which can be computationally solved. The discretization procedure results in space and/or time (transient cases) approximations. Therefore, the numerical prediction accuracy depends on the discretization quality (Ferziger & Peric, 2002).

In this context, the CFD versatility can be highlighted, however, some precautions must be considered regarding the predicted results, keeping physical consistency. Wilcox (1994) highlighted three key-factors for a successful CFD modeling: numerical mesh generation, solution algorithm and turbulence modeling. In Microfluidics, interfacial and surface phenomena can play a key role, depending on the specific case. The first two points listed by Wilcox (1994) are discussed forward. Turbulence is difficult to be generated in microstructured devices unless the pressure head is high enough (Kirby, 2010; Tabeling, 2010), or the microflow experience of additional field forces, e.g. electrokinetic force, as demonstrated by Wang et al. (2014). Since generally the microfluidic devices operate under laminar flow regime, turbulence modeling is out of the scope of this Chapter, however it can be found in Versteeg and Malalasekera (2007), Ferziger and Peric (2002) and Wilcox (1994), which

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