# CFD Applications in Energy Engineering Research and Simulation: An Introduction to Published Reviews


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*Keywords:* thermal radiation, heat transfer, combustion, turbulence, Renewable and Sustainable Energy, Simulation, Modelling, energy engineering, Computational Fluid Dynamics



*Abstract:*

Computational Fluid Dynamics (CFD) has been firmly established as a fundamental discipline to advancing research on energy engineering. The major progresses achieved during the last two decades both on software modelling capabilities and hardware computing power have resulted in considerable and widespread CFD interest among scientist and engineers. Numerical modelling and simulation developments are increasingly contributing to the current state of the art in many energy engineering aspects, such as power generation, combustion, wind energy, concentrated solar power, hydro power, gas and steam turbines, fuel cells, and many others. This review intends to provide an overview of the CFD applications in energy and thermal engineering, as a presentation and background for the Special Issue “CFD Applications in Energy Engineering Research and Simulation” published by Processes in 2020. A brief introduction to the most significant reviews that have been published on the particular topics is provided. The objective is to provide an overview of the CFD applications in energy and thermal engineering, highlighting the review papers published on the different topics, so that readers can refer to the different review papers for a thorough revision of the state of the art and contributions into the particular field of interest.





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*Perspective*

# CFD Applications in Energy Engineering Research and Simulation: An Introduction to Published Reviews

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**Abstract:** Computational Fluid Dynamics (CFD) has been firmly established as a fundamental discipline to advancing research on energy engineering. The major progresses achieved during the last two decades both on software modelling capabilities and hardware computing power have resulted in considerable and widespread CFD interest among scientist and engineers. Numerical modelling and simulation developments are increasingly contributing to the current state of the art in many energy engineering aspects, such as power generation, combustion, wind energy, concentrated solar power, hydro power, gas and steam turbines, fuel cells, and many others. This review intends to provide an overview of the CFD applications in energy and thermal engineering, as a presentation and background for the Special Issue "CFD Applications in Energy Engineering Research and Simulation" published by Processes in 2020. A brief introduction to the most significant reviews that have been published on the particular topics is provided. The objective is to provide an overview of the CFD applications in energy and thermal engineering, highlighting the review papers published on the different topics, so that readers can refer to the different review papers for a thorough revision of the state of the art and contributions into the particular field of interest.

**Keywords:** computational fluid dynamics; energy engineering; modelling; simulation; renewable energy; combustion; turbulence; heat transfer; thermal radiation

## 1. Introduction

Since the early contributions from D.B. Spalding and co-workers at Imperial College London and CHAM (Concentration Heat and Momentum) [1–3], Computational Fluid Dynamics has become a powerful tool for engineers and researchers of a wide range of applications. With the increasing computing power and development of both physical models and numerical and discretization techniques, CFD is nowadays considered to be a highly valuable must-have tool in the investigation of fluid flow. The main reasons are that CFD allows for the systematic analysis and optimization of the fluid flow field without the need for interfering with the flow itself, which is not always possible with conventional experimental techniques. CFD also allows the (virtual) observation of flow variables at locations that may not be accessible to measuring instruments.

Computational Fluid Dynamics has a wide variety of applications in energy engineering and research, namely the modelling of combustion, heat transfer, and multiphase flow, and in the simulation of gas and steam turbines, wind turbines, or tidal and wave devices. A very significant widespread of CFD has been observed during the last two decades in terms of users and number of applications, and indeed the CFD business reached a value of $1.0 billion in 2013, with around a 10% annual growth rate in industry.

However, CFD is not yet at the level where it can be used by designers or analysts without a working knowledge of the numerical algorithms involved, and despite the increasing computational resources, CFD has not yet evolved to a level where it can be straightforward to use. Numerical analyses still require significant effort to be set up, run, and analyzed. Therefore, CFD is in fact an aid to other analysis and experimental tools and must be used in conjunction with them.

## 2. Computational Fluid Dynamics (CFD)

Computational fluid dynamics, commonly known as CFD, consists of the resolution of the fluid flow governing equations by using numerical techniques implemented in a computer code. The domain of interest is divided into small volumes using a mesh, where the set of partial differential equations are discretized into algebraic equations and then solved in an iterative fashion. The basic fluid flow simulation involves the Navier–Stokes equations for the transport and conservation of mass and momentum. Additional physical and chemical phenomena can be included in the model by adding the correspondent transport equations: Chemical species conservation, heat transfer, and other coupled phenomena such as electrochemistry, magneto-hydrodynamics, and others.

The methodology for a CFD analysis comprises a pre-processing stage, a solver stage, and a post-processing stage. During pre-processing, the geometry for the domain of interest is generated. The corresponding fluid volume is divided into discrete cells in the mesh generation process. The physical model is then setup by defining fluid properties, physical models, and boundary conditions. For transient problems, the initial conditions are defined, and the time continuum is discretized into time steps. The equations are solved iteratively using appropriate discretization and numerical algorithms, and finally during the post-processing stage, the results analysis and flow visualization is performed.

The Navier–Stokes equations, also known as conservation or transport equations, which govern the fluid flow motion, can be written in its general form as:

$$\frac{\partial}{\partial t}\int_{V} \rho\varnothing dV + \oint_{A} \rho\varnothing V\cdot dA = \oint_{A} \Gamma\nabla\varnothing\cdot dA + \int_{V} S_{\varnothing} dV \quad (1)$$

where $\emptyset$ is the transported quantity, t is the time, A the superficial area, V the volume, $\Gamma$ is transported quantity diffusivity, and $S_{\varnothing}$ is the source of $\emptyset$. The first term in the equation corresponds to the transient transport of $\emptyset$, the second term to the transport by convection mechanism, the third term represents the transport of $\emptyset$ by diffusion, and the fourth term represents the source (or sink) of $\emptyset$. The different transport equations are assembled by using the appropriate variables, as shown in Table 1.

**Table 1.** Main transport equations used in Computational Fluid Dynamics (CFD) analysis.

| Equation | Variable $\emptyset$ |
|---|---|
| Continuity | 1 |
| x-momentum | u (velocity in x-direction) |
| y-momentum | v (velocity in y-direction) |
| z-momentum | w (velocity in z-direction) |
| Energy | h (enthalpy) |
| Chemical specie i | yi (mass fraction of i) |

## 3. CFD Applications in Energy Engineering Research and Simulation

This section will cover the main CFD applications in energy and thermal engineering. A thorough review of such a wide variety of different applications is however not feasible within one single publication. Instead, a brief introduction to the most significant reviews that have been published on the particular topics related to CFD in energy and thermal engineering is provided. The objective of the review is thus to provide an overview of the CFD applications in energy and thermal engineering, highlighting the review papers published on the different topics, so that readers can refer to the different review papers for a thorough revision of the state of the art and contributions into the particular field of interest. The applications covered are depicted in Figure 1.

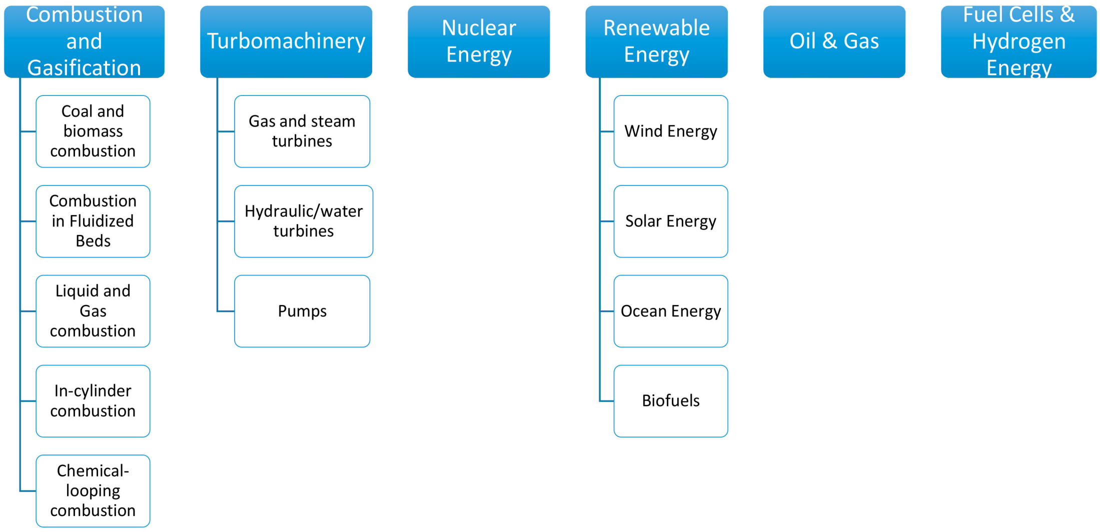


**Figure 1.** CFD applications related to energy and thermal engineering covered in this review.

To date, there has been a significant scientific production regarding CFD application in the areas indicated in Figure 1. The number of publications identified for each particular field are presented in Figure 2.

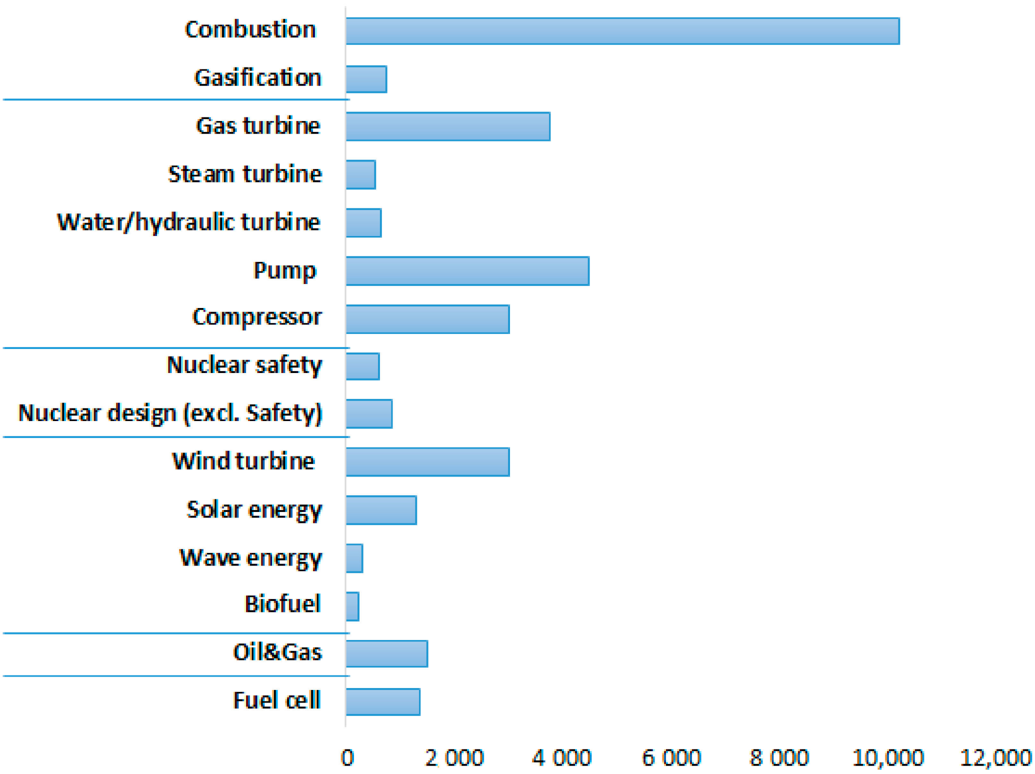


**Figure 2.** Bibliometric study: Number of scientific publications in the areas indicated in Figure 1.

### *3.1. Combustion and Gasification*

Combustion is one of the major fields of application of CFD, where the wide variety of combustion types have been deeply explored (coal and biomass, liquids, gas, oxy-combustion, and others). The basic models for turbulent combustion initially developed for very high or very low Damköhler numbers (reaction rate limited by reactants mixing or by chemical kinetics) were the eddy break up (EBU, also known as eddy dissipation model—EDM) and the finite rate chemistry (FRC) model. Both basic models were further developed and refined, and additional models have been progressively developed, such as the flamelet model for non-premixed combustion describing the interaction of chemistry with turbulence.

#### 3.1.1. Coal and Biomass Combustion

CFD simulation of coal combustion in boilers has attracted much attention during the last decades as it has been typically one of the main technologies for power generation. Coal combustion involves many different modelling issues such as multiphase modelling, chemical reactions, heat transfer, and radiation or emissions modelling (Figure 3). Pulverized coal particles tracked within a Lagrangian integration framework is the most typical simulation method to compute the multiphase flow, that must be coupled to heat and mass transfer models to account for devolatilization.

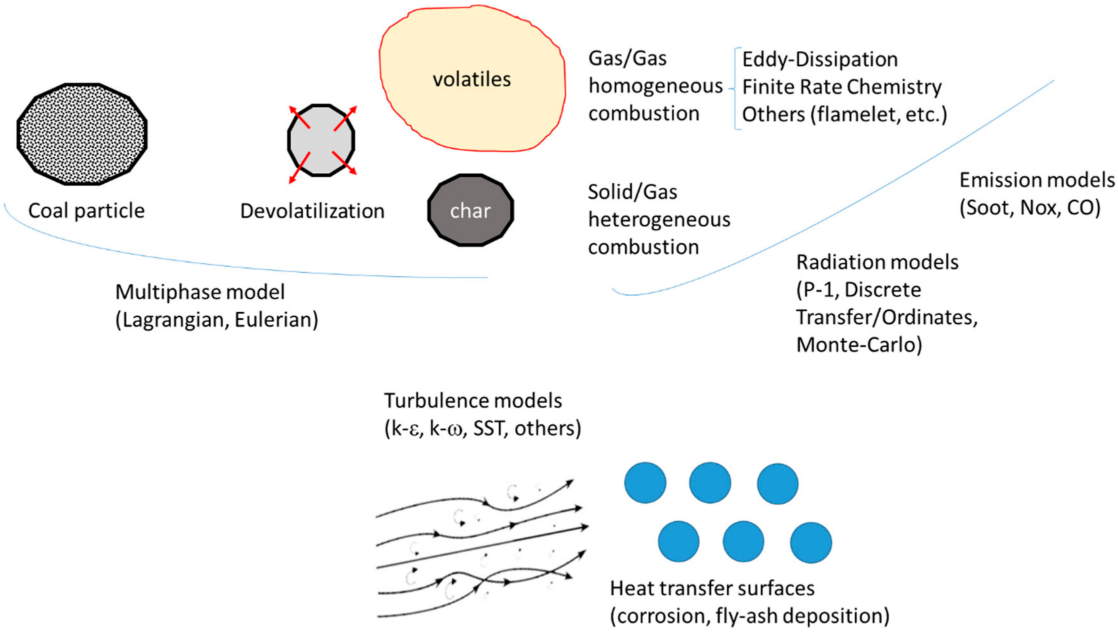


**Figure 3.** Main processes and models involved in coal combustion.

One of the first reviews on the topic was published by Phil Stopford [4] in 2002, when AEA Technology was owner of the CFX-4 code. The review focuses on coal-fired low-NOx burner design, furnace optimization, over-fire air, gas re-burn, and laminar flames. CFD modelling of pulverized coal boilers has been also reviewed by Díez et al. [5] and Sankar et al. [6], as well as by Kurose et al. [7]. Other applications such as pulverized coal in blast furnaces were reviewed by Shen et al. [8]. A particular focus on modelling of poly-dispersed particles in reactive flows by population balance models (PBM) was done by Rigopoulos [9] with applications not only on coal combustion, but also many others such as soot formation or spray combustion. Finally, the coupling of CFD simulation of equipment with process simulation codes have been reviewed by Zitney [10]. Overall, the major challenges in pulverized coal combustion are the modelling of chemical kinetics (both devolatilization and char combustion), radiation, and the overall furnace modelling. The current trends in devolatilization generally involve multi-step kinetic models [6]. In any case, it is crucial that an appropriate coal characterization is carried out. Regarding radiation, not only the adequate radiation model must be selected (that will depend on the optical thickness, where the effect of flying-ash should be considered), but also the gas radiation properties model.

Although most of the considerations above are applicable to biomass combustion, such a process presents particular modelling issues, and modelling approaches were reviewed by Dernbecher et al. [11] or Haberle et al. [12] and Chaney et al. [13] for small-scale grate furnaces and boilers. A particular focus on CFD modelling of biomass gasification was reviewed by Mazaheri et al. [14]. Gasification is a particularly complex process involving chemical kinetics, heat and mass transfer, and thermochemical equilibrium, that in addition can take place in a wide range of gasifier designs currently being investigated [14], and with very different types of biomass feedstock. All this complexity makes biomass gasification particularly challenging for CFD modelling, and it is generally recognized that there is still a lack of accurate gasification models and procedures for assessing the different types of gasifiers [14].

Co-firing of coal and biomass in industrial boilers and furnaces has been the covered in recent reviews by Tabet et al. [15] or Bhuiyan et al. [16], focusing as well on slagging issues when co-firing is used.

Oxy-fuel combustion of pulverized coal is also a topic of major interest (as a promising technology for CO2 capture) and its CFD modelling has been specifically addressed by Chen et al. [17], Yin et al. [18], or Edge et al. [19]. CFD is expected to play a vital role for the oxy-fuel combustion technology development as it played for conventional combustion processes. Research efforts are particularly put on modelling how oxy-fuel conditions are affecting combustion physics and chemistry such as turbulent gas–solid flow, heat and mass transfer, pyrolysis, or char reactions [19].

Finally, there are specific issues and challenges associated to coal combustion and its CFD modelling, such as slagging [20] or erosion modelling [21].

### 3.1.2. Combustion in Fluidized Beds

Fluidized beds (FBs) are widely used in the chemical and process industry and are also used for the combustion of solids and gasification. Simulations (Figure 4) are involving transient multiphase flows with particular treatments for very dense particulate flows (mostly based on the kinetic theory of gases) and, in general, small time-step sizes are required to achieve convergence. This makes CFD unsuitable to address large 3D industrial cases within the commonly available computing power.

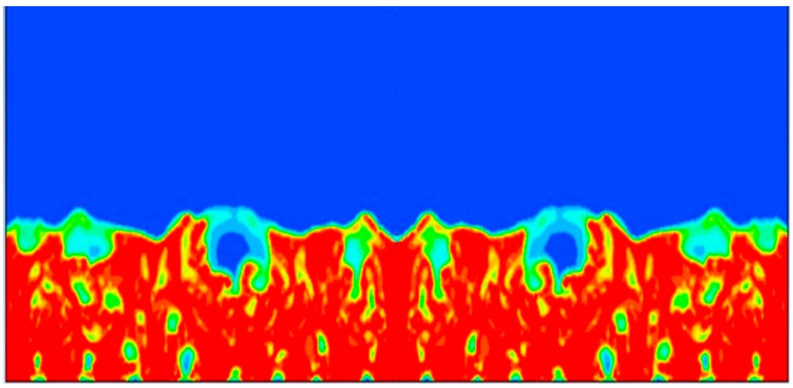

**Figure 4.** Time snapshot of a CFD simulation of fluidized bed (gas volume fraction in blue, sand particles volume fraction in red).

CFD modelling of fluidized bed combustion for biomass and co-firing was reviewed by Kumar et al. [22], Kuffa [23], and Singh [24], whereas the particular application of CFD simulation of FBs in waste-to-energy plants was discussed by Ravelli et al. [25]. The reviews demonstrate that CFD has been extensively used to analyze the distributions of chemical species, temperature and heat fluxes, ash deposition, and pollutants concentrations in both combustion and gasification in fluidized beds [24]. It is, however, clear that simulation models are still approximations and many assumptions are required, such as when considering Eulerian–Eulerian approaches with variation in particle sizes.

#### 3.1.3. Liquid and Gas Combustion

Roslyakov et al. [26] very recently published a review on CFD modelling of liquid and gaseous fuel combustion in power generation installations. An in-depth review on the modelling of turbulent burning rates for gaseous fuels was published by Bradley [27]. The atomization and transport of liquid fuel droplets during the evaporation process is of particular importance when modelling burners and combustion of liquid fuels, whereas the subsequent combustion in gas phase is typically modelled with the eddy break up model (EBU, also known as eddy dissipation model—EDM).

#### 3.1.4. In-Cylinder Combustion

Combustion in engines has been of major importance for the automotive industry and for other propulsion systems, aiming at developing low-fuel-consumption and low-emissions internal combustion engines. Review papers were published already in the 1990s such as by Reitz and Rutland [28] on diesel engines or Gosman [29]. CFD modelling of diesel combustion engines was reviewed by Barths et al. [30], and dual fuel diesel-CNG (Compressed Natural Gas) engines by Shah et al. [31]. A focus on turbulence modelling able to represent different combustion regimes and detailed chemical kinetics was carried out in the review of Haworth [32], while the application of Large-Eddy Simulation (LES) models represents a significant contribution to the topic [33]. The Engine Combustion Network (ECN) provided a review on the methodology to properly characterize and control ambient and fuel-injector boundary conditions [34], which is of major importance for accurate results. CFD combustion modelling in engines is a mature application, but there is a need for model improvements in some areas such as spray modelling (break-up, atomization) and other related phenomena such as wall films and wall heat transfer in such conditions. Some of the problems requiring a particular accuracy on flow unsteadiness such as cyclic variation and design sensitivity can be probably better studied with LES [33], but appropriate submodels must be carefully used.

#### 3.1.5. Chemical-Looping Combustion

Chemical-looping combustion (CLC) consists of a two-step process interconnecting two fluidized beds reactors (circulating fluidized bed for air reactor and bubbling fluidized bed for fuel reactor). Oxygen is carried from air to fuel by means of a carrier (a highly reactive metal particle) thus avoiding direct contact between air and fuel and resulting in a flameless combustion with pure CO2 exhaust stream suitable for sequestration. Multiphase modelling is one of the fundamental issues in chemical-looping combustion (apart to reacting flow), and thus different drag models to account for the solid–gas interaction can be found in the review by Banerjee and Agarwal [35] or Jung and Gamwo [36]. A better knowledge of the multiphase reactive gas–solid flow is fundamental for the simulation of CLC combustors.

### *3.2. Turbomachinery*

CFD is playing a major role in the aerodynamic design of turbomachines, and currently all modern designs are being aided by the use of CFD, with clear reductions in the costs and design cycles. Denton and Dawes [37] published one of the earliest reviews devoted to computational fluid dynamics for turbomachinery design in 1999, while Moore and Moore [38] reviewed methods and models related to in two-equation turbulence models applied to compressors and turbine cascades. The state of the art of the use of open-source CFD software was analyzed by Casartelli and Mangani [39], and Pinto et al. [40] reviewed the work carried out in the CFD analysis for turbines, compressors, and centrifugal pumps, also discussing parallelization issues and strategies.

#### 3.2.1. Gas and Steam Turbines

Predicting flow field and heat transfer in the cooling passages and cavities of gas turbines and jet engines is of major importance for the design of more efficient and robust machines. Flow is strongly turbulent along the intricate passages, with the aim to achieve higher heat transfer coefficients. Flow separation, rotation and curvature, and impingement, are some of the challenges to the advanced turbulence modelling currently being applied. For the particular application of blade cooling in gas turbines, Iacovides and Launder [41] published a review in 1995 and have later also been addressed together with additional modelling issues such as hot gas path modelling by Dawes [42] and Horlock and Denton [43]. Steam turbines were particularly addressed by Tominaga and Tanuma [44]. Multistage and unsteady predictions have become common practice in the last decade as the increased computer power has enable such simulations. Among the significance of unsteady calculations, it is relevant to mention the simulation of two-way fluid–structure interaction (FSI) for investigations such as unsteady blade loading and the assessment of mechanical aspects in the turbine blades. The consequences of unsteady flows on the loss generation are also being explored. Secondary gas paths are also significantly being analyzed, such as leakage flows, cooling flows, and cavity flows (as in shroud leakage flows in turbines). Such flows are highly turbulent and, thus, their simulation is very reliant on the turbulence modelling capabilities [43], where Scale Adaptive Simulation (SAS) has been applied with success.

#### 3.2.2. Hydraulic/Water Turbines

CFD modelling and simulation of hydraulic turbomachines has been the objective of review articles such as in Sick and Wilson [45], Keck and Sick [46], or Trivedi et al. [47]. A particular focus was put on horizontal axis turbines by Laín et al. [48], while the state of the art in CFD modelling of Pelton turbines was discussed by Židonis and Aggidis [49]. Both steady-state and transient simulation of hydraulic turbines are widely carried out, where steady-state conditions include the calculation of the best efficiency point, high load, and part load conditions. Transient simulations focus on load variation, startup, shutdown, and total load rejection [47]. Such simulations are challenging due to the time-dependent movement of the guide vanes, requiring dynamic/moving meshes (or overset or "chimera" meshes). Off-design conditions are also challenging as the flow field is usually unstable.

The simulation domain considered ranges from component modelling (which is the most common for example in Francis and Kaplan turbines), to the complete turbine modelling and passage modelling. When simulating a turbine component, accurate boundary conditions are crucial for ensuring reliable results [47]. Two-way FSI is also being applied to water turbines to analyze the mechanical behavior of the turbine components.

#### 3.2.3. Pumps

CFD is commonly applied to the investigation and design of centrifugal pumps, typically for the performance prediction at design and off-design conditions, cavitation analysis, diffuser design, parametric studies, or pump performance when running in turbine mode. Besides diffuser and impeller flows, the analysis of volute flow and the impeller-volute interaction is also being investigated for further improvement of the pump performance. Centrifugal pumps have been addressed by Shah et al. [50], and Niedzwiedzka et al. [51] reviewed the specific topic of CFD modelling of cavitating flows. The particular applications in pumps that can be likewise used as turbines (reverse running pumps) were discussed by Nautiyal et al. [52]. Some active research fields are two phase flow in pumps, fluid–structure interaction, and non-Newtonian fluids [50].

### *3.3. Nuclear*

The use of CFD in nuclear power generation has been traditionally focused on safety analysis, for modelling different scenarios such as loss-of-coolant, and the related safety measures. The results and progresses of the benchmark case proposed by the Organization for Economic Co-operation and

Development (OECD)/Nuclear Energy Agency to assess the predictive capabilities of (CFD) codes were reported by Kelm et al. [53]. The Korea Institute of Nuclear Safety (KINS) is auditing calculation activities on the applicability of CFD software to nuclear safety problems and discussed checking whether valid CFD software is used for nuclear safety problems [54]. Many other works investigate multiphase flow and boiling, involving critical heat flux (CHF) simulations [55–58]. Indeed, the thermal hydraulics of the reactor core is one of the key issues for safety. The complex geometry and non-uniform heating make thermal-hydraulics and CHF predictions in light water reactors (LWR) particularly challenging. Abrupt transients caused by sudden flow regime transition and their implications in CHF events have also been analyzed [57]. CFD modelling include additional challenges such as coupling of single and two-phase turbulent flow over a wide range of thermal-hydraulic conditions, and flow boiling, for both natural and forced convection [57].

Fuel bundle analysis and thermo-hydraulic design (spacers, etc.) have also been modelled, and reviews were published by Moorthi et al. [59] or Verman et al. [60]. The developments of AREVA S.A. on predicting flow field and thermal mixing within fuel bundles and fuel assembly components were discussed in [61], focusing as well on validation.

### *3.4. Renewable Energies*

#### 3.4.1. Wind

Wind energy is progressively increasing its share in electricity production worldwide, and major research efforts have been made for enhancing turbine blade aerodynamics [62–66]. Hybrid methods combining CFD with BEM (blade element momentum) have some advantages such as reducing the computational time required for the aerodynamic load analysis of turbine blades [63]. In addition, optimization methods such as GA (genetic algorithms) have been widely applied in the optimization of wind turbines [63]. It is fully recognized that CFD is enabling the achievement of better aerodynamic designs and larger turbine efficiencies [64], where CFD is primarily focused not only on blade optimization, but also on micro-siting, wind modelling and prediction, or noise prediction.

Flow aerodynamics around turbine blades is complex and challenging, and typically two approaches are used to account for the blades rotation: One being the multiple frames of reference (where steady-state simulations are possible), the second being the use of dynamic meshes where a transient simulation is defined to accurately capture the flow around the rotating blade (with obviously a much higher computational effort). CFD and blade aero-elasticity was discussed by Hansen et al. [67]. CFD for the particular design of horizontal-axis wind turbines (HAWT) has been discussed together with experimental approaches [68] transition modelling [69], and review of CFD, FE codes, and experimental practices [70]. It can be determined that the accuracy of the simulations is, overall, determined by the turbulence model, where for turbine wake modelling, LES is generally applied [68].

Darrieus vertical axis wind turbines were reviewed by Ghasemian et al. [71]. Similarly, wind farm aerodynamics is a significant contribution to CFD to wind energy [72], and wind flow around buildings for urban wind energy exploitation has also been recently reviewed by Toja-Silva et al. [73]. Some relevant physics such as wake meandering, effect of atmospheric stratification on wake development, or the response of the turbine to partial wake interaction can only be addressed currently by CFD [72]. Wind farms are also modelled with LES, and particularly with advanced SGS models. The correct modelling of the atmospheric boundary layer and its interaction with turbines is crucial for guaranteeing accurate results.

Further developments in CFD modelling for wind energy will be covering topics such as advanced atmospheric boundary layer simulation in complex terrains such as cliffs or wake–wake interactions [64].

#### 3.4.2. Solar

CFD has been widely and successfully used for optimizing the heat transfer in solar collectors and for components design, enhancing the efficiency of the collectors and receivers. Solar air heaters have been thoroughly investigated with aid of CFD modelling and simulations [74–78] for heat transfer enhancement. The thermal performance of solar air heaters has been extensively investigated, and optimum values of relative roughness pitch (P/e) and relative roughness height (e/D) in roughened solar air heater duct obtained by different researchers are summarized and tabulated in the review work by Manjunath et al. [75].

Solar drying systems [79] and solar receivers in central receiver systems have been reviewed recently [80]. Heliostats are an additional field of CFD work in order to assess aerodynamic wind loads for a suitable design of the related mechanical and tracking systems [81].

#### 3.4.3. Ocean Energy

Wave energy converters (WECs) are attracting a significant attention with progresses achieved within several development programs. Numerical tools such as CFD of numerical wave tanks (NWTs) provide an excellent and cost-effective tool. A comprehensive review on NWTs based on CFD approaches was published by Windt et al. [82] including best practice guidelines for CFD in the field of wave energy. CFD studies on axial flow turbines for WECs were reviewed by Cui et al. [83], whereas the particular case of numerical modelling of tidal stream turbines was discussed by Masters et al. [84]. CFD work on WECs started on 2004 [82] and has shown a clear progression in model fidelity and capabilities, although there are known shortcomings to be tackled, such as the accurate modelling of the power take-off (PTO) system dynamics for a better analysis of WEC performance, loading, or control strategies [82].

#### 3.4.4. Biofuels

Although biofuels production is not one of the most extensive application of CFD, many works can be found in the literature both for liquid biofuels (bioethanol, biodiesel, green diesel) [85] and biogas [86]. Thermochemical conversion of biomass to provide gaseous, liquid, and solid fuels was reviewed by Wang et al. [87]. It can be determined that biodiesel production has attracted much of the CFD activities in biofuel production simulation, while others (biogasoline or aviation biojet fuels) are not currently found in the literature [85]. Moreover, there is a significant potential for further refining the modelling of the chemical reactions involved, together with a need for the use of multi-physics modelling involving also heat and mass transfer and development of more accurate interfacial mass transfer for equipment involving multi-phase reactions [85].

### *3.5. Oil & Gas*

The oil and gas industry represents one of the major contributors to energy engineering (and it is slowly re-orienting some of its activities in order to increasingly become global players in the renewable energy industry in the medium term). Oil and gas and has extensively been applying CFD during the last decades [88], including liquid loading phenomena in gas wells [89] and piping systems [90]. Liquefied natural gas production has become likewise a relevant technology and CFD applications for heat exchangers have been discussed by Samokhvalov et al. [91]. Overall, a very large number of different applications are increasingly being simulated in oil and gas, involving different flow configurations, single-phase, or gas–liquid, gas–solid, and also gas–liquid–solid. The coupling of multi-phase flow with mass and heat transfer and with chemical reactions is one of the major challenges in CFD modelling in such applications [88]. Future developments are required in order to develop more accurate interaction laws between phases (involving momentum transfer and heat and mass transfer), particularly for the complex flows commonly found in oil and gas.

### *3.6. Fuel Cells and Hydrogen Energy*

In fuel cells, not only fluid flow and heat and mass transfer must be modelled, but also additional phenomena such as electrochemistry, in order to compute the reactants oxidation and reduction rates. The overpotential or difference between the solid and electrolyte/membrane potential is the driving force for the reactions, and therefore, potential equations are solved in these models (one equation describing the electron transport inside the solid materials such as current collectors, and a second potential equation representing the ionic transport inside the electrolyte). A comprehensive review on the fundamental models for fuel cells was published by Wang [92], including discussion for validation requirements, with additional reviews published afterwards [93–97]. Aman et al. [98] addressed the particular case of solid-oxide fuel cells. The numerical models for PEM (Polymer Electrolyte Membrane) fuel cell cold start were reviewed by Guo et al. [99]. Apart from the investigation of reactants distributions in bipolar plates and electrodes (Figure 5), it is well known that liquid water management is a fundamental research field in PEM-type fuel cells, and its CFD modelling has been the focus of several reviews [100–105]. Future developments in Fuel Cell CFD modelling will surely be devoted to the challenging water transport and multi-phase physics involved in the different cell components: Dissolved water for membrane hydration, phase change (evaporation, condensation), water transport in the porous media of both the catalyst and gas diffusion layers, and the different gas–liquid flows regimes occurring in the bipolar plate channels, also influenced by surface tension and wall adhesion, as well as further refinements of electrode models (cathode particle or agglomerate models).

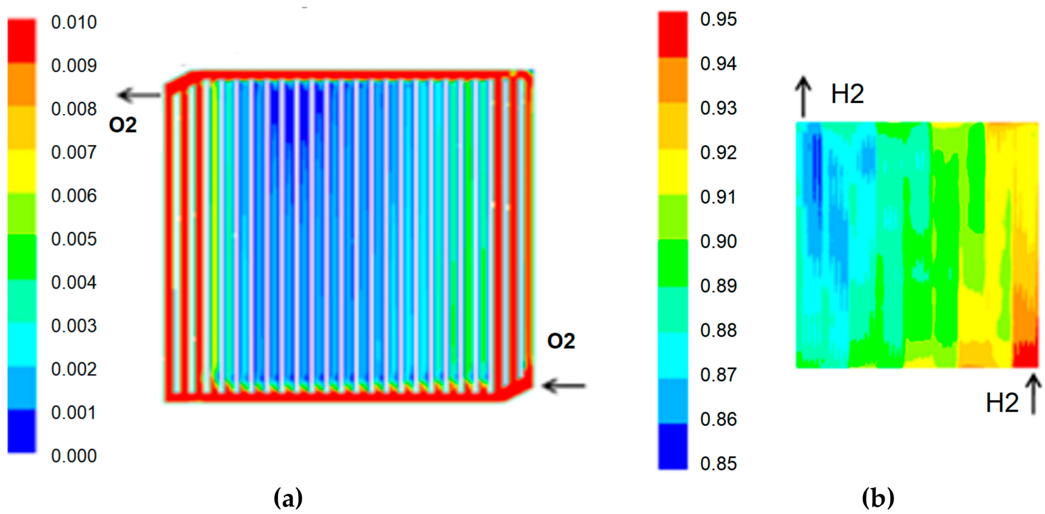


**Figure 5.** PEM fuel cell CFD simulation showing (**a**) velocity distribution in the cathode channels of a parallel bipolar plate; (**b**) hydrogen distribution over the anode electrode with a serpentine bipolar plate.

Regarding hydrogen production, Tapia et al. [106,107] reviewed a general CFD methodology for the design and analysis of solar reactors based on thermochemical cycles. The modelling of solar reactors requires the use of a radiation model, where, in general, surface-to-surface radiation is modelled as volumetric absorption in the media and can be neglected. However, in case the radiation direction is important (such as concentrated radiation coming from a heliostat field), the Monte-Carlo model is recommended in order to achieve a correct representation of the incoming radiation (Figure 6).

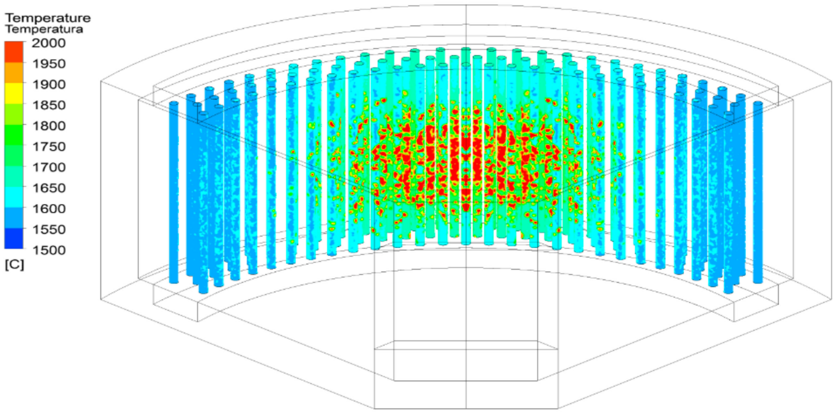


**Figure 6.** Temperature distribution over a multi-tubular solar reactor for hydrogen production.

### 3.7. Heat Transfer Processes and Other Applications

Other additional applications of CFD in energy engineering that have been thoroughly discussed are thermal energy storage, both for latent [108] and phase change materials [109]. Electronics cooling is also a field with a significant growth [110]. CFD analysis of heat exchangers was addressed by Aslam Bhutta et al. [111], and applications of for the design of thermal processes in the food industry by Norton et al. [112] and Zhao et al. [113].

## 4. Software Tools

There is currently a broad choice of CFD solvers, mesh generation software, and visualization tools. Both commercial and free or open source software is available, where the most common software tools currently being used are indicated in Table 2.

**Table 2.** Main software tools used in CFD analysis on energy engineering.

| Software Vendor | Software Name | Purpose |
|---|---|---|
| ANSYS Inc | ANSYS-FLUENT<br>ANSYS-CFX | Meshing/Solver/Visualization |
| Siemens Industry Software Inc. | STAR-CCM+ | Meshing/Solver/Visualization |
| COMSOL Group | COMSOL Multiphysics | Meshing/ Solver/Visualization |
| AVL List GmbH | AVL Fire | Meshing/ Solver/Visualization |
| NUMECA International | AutoMesh / FINE | Meshing/ Solver/Visualization |
| ESI Group | OpenFOAM [1,2] | Meshing/ Solver/Visualization |
| CHAM Ltd. | PHOENICS [3] | Meshing/ Solver/Visualization |
| Mentor Graphics (Siemens PLM) | FloTHERM / FloEFD | Meshing/ Solver/Visualization |
| Pointwise Inc. | Pointwise | Meshing |
| ANSYS Inc. | ANSYS-ICEM CFD | Meshing |
| Tecplot Inc | Tecplot | Visualization |
| ANSYS Inc. | Ensight | Visualization |

[1] freeware/shareware; [2] open source; [3] older versions available as shareware.

Most solvers are general-purpose CFD codes, whereas others are focused on particular applications (such as AVL Fire, focused on internal combustion engines, or FloTHERM, focused on electronics cooling). PHOENICS was the very first commercially available CFD code (released in 1981), but currently ANSYS is the most widely used CFD software nowadays (over 40% market share), with both major codes CFX (acquired in 2003) and FLUENT (acquired in 2006). Among the open source CFD software, OpenFOAM from ESI Group is the most widely used.

## 5. Conclusions

This brief review has covered the main CFD applications in energy and thermal engineering. A brief introduction to the most significant reviews that have been published on the particular topics related to CFD in energy and thermal engineering has been provided, so that readers can refer to the different review papers for a thorough revision of the state of the art and contributions into the particular field of interest. This has been intended as a presentation and background for the Special Issue "CFD Applications in Energy Engineering Research and Simulation" published by Processes in 2020. Overall, it has been shown that CFD is covering all major processes and equipment involved in energy engineering, with applications increasingly achieving more complex phenomena and simulations. The increase in the available computing power is allowing simulations with larger mesh sizes and increasing resolution. Nevertheless, regarding turbulence modelling, RANS modelling is currently still much more present than LES for most applications. It has been shown that CFD use in industry and academia continues to grow with a yearly rate of around 10%, with North America and Asia as major users. The strong competition among CFD software vendors will ensure further efforts on model developments to enhance accuracy and even cover new applications and novel technologies. Industry will continue to increase its reliance and trust on CFD to improve their product designs and reduce design cycles and associated costs. The expected transition towards an energy system mostly based on renewable energies that will (sooner or later) take place, will require major efforts in technology development that will surely be supported by CFD in energy engineering research. Based on the above, it can be thus ensured that CFD will continue to grow and expand, and it will be necessary to ensure that quality and trust is maintained among users, by further developing, refining, and using CFD best practice guidelines.

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