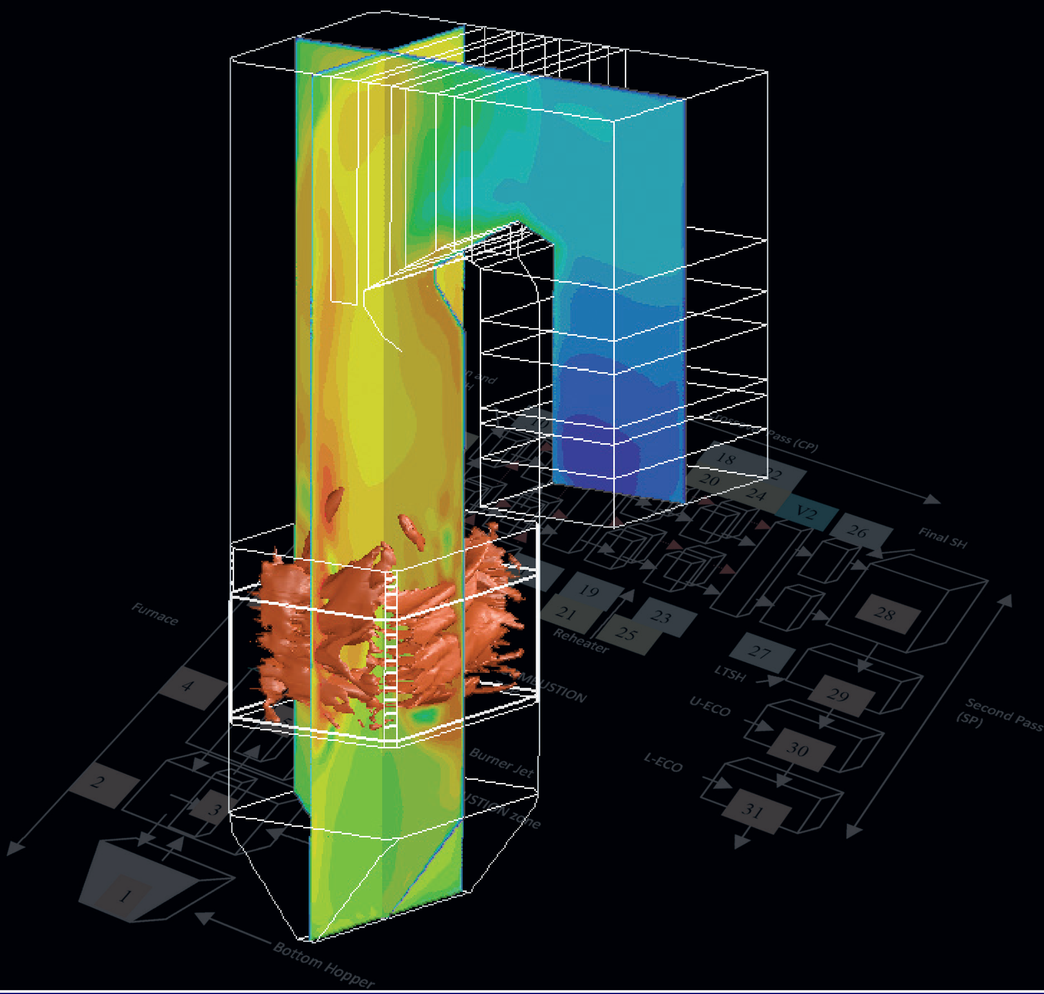
# Computational Modeling of Pulverized Coal Fired Boilers




Vivek V. Ranade
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# Preface

Pulverized coal fired boilers have been and will be the mainstay of coal-based power generation worldwide. Such pulverized coal boilers are complex chemical reactors comprising many processes such as gas-solid flows, combustion, heat transfer (conduction, convection, and radiation), and phase change simultaneously. Conventional pulverized coal fired boiler designs have been continuously improved upon and even today new combustion technologies are being developed. Improving the efficiency of pulverized coal (PC) fired boilers has been the focus of considerable efforts by the utility industry since it leads to several benefits (reduced emissions and consumption of coal per MWe). Typically, a one percent improvement in overall efficiency can result in a nearly three percent reduction in $CO_2$ emission.

Efficiency of these PC boilers depends on several issues such as flow and mixing, inter-phase and intra-particle heat and mass transfer, and homogeneous and heterogeneous reactions. Some specific issues are critical in determining overall efficiency of such boilers. These are coal composition (proximate and ultimate analysis), characteristics of pulverized coal particles (shape and size distributions), reactivity of coal (devolatalization and combustion kinetics of coal), boiler design and configuration (size and shape of combustion chamber, burner design, number and locations of burners), excess air used, mixing of air and coal, flow mal-distribution, generation of fly and bottom ash particles, radiative heat transfer, heat recovery, and so on. Any efforts in improving the effective operating efficiency of these boilers therefore rest on fundamental understanding and control of the underlying flow, mixing, heat transfer, and reactions.

Computational modeling offers an excellent way to develop such fundamental understanding and to develop an ability to optimize boiler performance. However, through our interactions with industry, we realized that there is insufficient help available to practicing engineers for harnessing state-of-the-art computational modeling tools for complex, industrial boiler-like applications. Many boiler engineers either consider the complexities of industrial PC boilers impossible to simulate or expect miracles from off-the-shelf, commercial modeling tools. These two diverse views arise because of inadequate understanding about the role, state of the art, and possible limitations of computational modeling.

This book is aimed at filling this gap and providing a detailed account of the methodology of computational modeling of pulverized coal boilers. The book attempts to develop and discuss an appropriate approach to model complex processes occurring in PC boilers in a tractable way. The scope is restricted to the combustion side of the boiler. The rest of the components of PC boilers are outside the scope. Even for the combustion side, the scope is restricted to the burner/excess air entry points to the exit of flue gases (and fly ash) from the heat recovery section. Milling and conveying of coal particles as well as further processing of flue gas beyond heat recovery sections (electro-static precipitators and so on) are beyond the scope of the present work. We have written this book with an intention to describe the individual aspects of combustion and heat recovery sections of PC boilers in a coherent fashion that may be useful to further improve design methodologies and optimize boiler performance. The intended users of this book are practicing engineers working in utility industries and in boiler design companies, as industrial consultants, in R & D laboratories, as well as engineering scientists/research students. Some prior background of reaction engineering and numerical techniques is assumed.

The information in the book is organized in mainly six chapters: the first chapter provides a general introduction. The second chapter discusses the overall approach and methodology. Kinetics of coal pyrolysis (devolatilization) and combustion and methods of its evaluation are discussed in Chapter 3. Computational flow modeling is discussed in Chapter 4. This chapter covers modeling aspects from the formulation of model equations to simulation methodology. Typical results obtained with computational flow models are also discussed in this chapter. Computational flow models provide a framework for developing a deeper understanding of the underlying processes in PC boilers. These models also provide a quantitative relationship between boiler hardware and operating protocols with boiler performance and efficiency. Phenomenological models or reactor network models are discussed in Chapter 5. These models require significantly less computational resources than computational flow models and therefore can be used for boiler optimization. A brief discussion on practical applications of computational modeling is included in Chapter 6. An attempt is made here to provide specific comments to connect modeling with real-life applications. Key points are summarized in the last chapter (Chapter 7) along with some comments about the path forward.

Though many of the examples are for the older generation 210 MWe boiler, we have made an attempt to evolve general guidelines that will be useful for solving practical problems related to current and future generations of PC boilers. The material presented here can be extended to model larger boilers based on conventional, super-critical, or ultra-super-critical technologies as well as based on oxy-fuel technologies. The material included in this book may be used in several ways: as a basic resource of methodologies or in making decisions about applications of computational modeling in practice. The content could be useful as a study material for an in-house course on pulverized coal boilers, for example, design and optimization or a companion book while solving practical boiler-related problems. We hope that this book will encourage chemical engineers to exploit the potential of computational models for better engineering of pulverized coal boilers.

We are grateful to many of our associates and collaborators with whom we worked on different industrial projects. Many of VVR's students have contributed to this book in different ways. Particularly, Ankit Jain, Akshay Singan, Ajinkya Pandit, Deepankar Sharma, and Dhananjay Mote read the early drafts of manuscript and provided useful suggestions from a student's perspective. Vinayak Ranade, Nanda Ranade, and Maya Gupta also read the early drafts and suggested ways to improve overall readability. The manuscript was improved wherever their suggestions were incorporated. Any remaining errors or shortcomings are, needless to say, the responsibility of the authors. We also wish to thank the editorial team at CRC Press, particularly Dr. Gagandeep Singh, for their patience and help during the process of writing this book.

Besides the professional associates, VVR would like to acknowledge his wife Nanda and daughter Vishakha, and DFG would like to acknowledge his wife Maya and daughters Suhani and Anjani for their understanding and enthusiastic support all along.

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**Devkumar F. Gupta** is currently a principal scientist at Thermax Limited, Pune, India. His research interest lies in converting solid fuels into high-value-added products using fluidized bed reactors. He has been actively involved and had an instrumental role in the design, computational modeling, and establishment of high-pressure gasification demonstration plants in India. He has worked jointly with utility industries to develop computational fluid dynamics (CFD) and reduced order numerical models for pulverized coal fired boilers. He has presented several research papers at international and national conferences on clean coal technology. He holds a PhD (2011) in chemical engineering from the University of Pune.

# 1

# *Introduction*

Pulverized coal (PC) fired boilers have been the mainstay of coal-based power generation worldwide for almost 100 years. This is not surprising as coal is the most abundant and widely distributed fossil fuel, with global reserves of about 1,000 billion tons (IEA, 2010a). Coal fuels more than 40% of the world's electricity. The percentage of coal-based electricity is much higher in some countries, such as South Africa (93%), Poland (92%), China (79%), Australia (78%), Kazakhstan (75%), and India (69%). The growing needs of developing countries are likely to ensure that coal remains a major source of electricity in the foreseeable future despite climate change policies (IEA, 2010 a, b).

Electricity generation from coal appears to be a rather simple process. In most coal-fired power plants, coal is first milled to a fine powder (pulverized coal). Fine particles of coal have more surface area and therefore burn more effectively. In these systems, called pulverized coal (PC) combustion systems, the powdered coal is fed to the combustion chamber of a boiler. Coal particles burn in this chamber and generate a fireball (high-temperature zone) and hot gases. The energy released in radiative and convective form is used to convert water (flowing through the tubes lining the boiler walls) into steam. The high-pressure steam is passed into a turbine, causing the turbine shaft to rotate at high speed. A generator is mounted at one end of the turbine shaft where electricity is generated (via rotating coils in a strong magnetic field). The steam exiting from the turbines condenses, and the condensed water is recycled to the boiler to be used once again. A schematic of a typical PC fired boiler is shown in Figure 1.1.

The PC fired systems were developed in the 1920s. This process brought advantages that included a higher combustion temperature, improved thermal efficiency, and a lower requirement of excess air for combustion. Improvements continue to be made in conventional PC fired power station design, and new combustion technologies are being developed. The focus of considerable efforts by the coal industry has been on improving the efficiency of PC fired power plants. Increasing the efficiency offers several benefits (Burnard and Bhattacharya, 2011):

- Lower coal consumption per megawatt (MW) (i.e., resource preservation)
- Reduced emission of pollutants (e.g., SOx [sulfur oxides], NOx [nitrogen oxides], etc.)

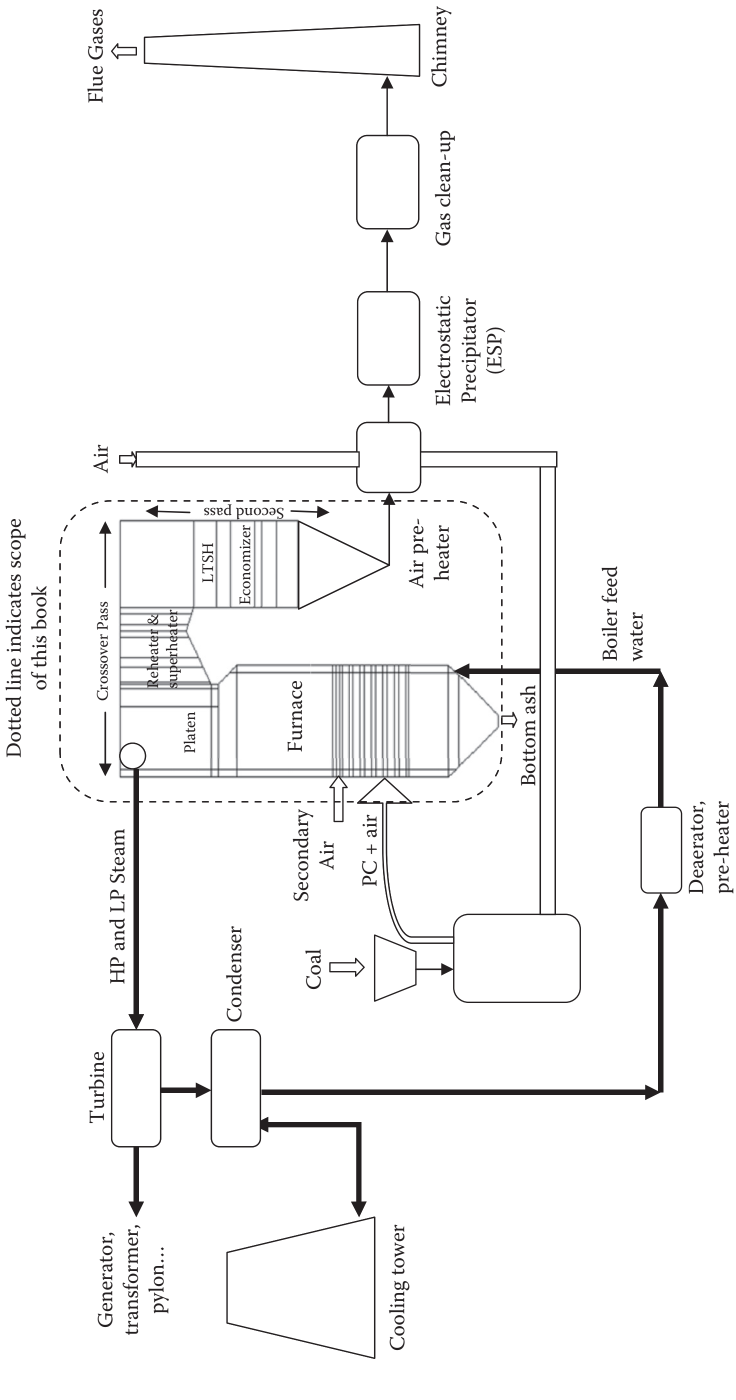



**FIGURE 1.1**
Schematic of typical pulverized coal fired power plant and scope of this book.

- Reduced $CO_2$ emission (greenhouse gas): a one percentage-point improvement in overall efficiency can result in ~3% reduction in $CO_2$ emissions
- Existing power plant efficiencies in developing countries are generally lower. The coal use in these countries for electricity generation is increasing. The improvements in efficiencies of PC fired boilers will therefore have a significant impact on resource conservation and reduction in emissions of $CO_2$ per megawatt (MW). There is a huge scope for achieving significant efficiency improvements as the existing fleet of power plants is replaced over the next 10 to 20 years.

In recent years, considerable progress has been made in the development of more efficient coal-based systems such as supercritical (SC) and ultra-supercritical (USC) steam cycles. These also include systems based on coal gasification (such as IGCC: integrated gasification combined cycle). However, while there are several proposals for further commercial demonstrations of IGCC and some are being constructed, PC combustion-based plants continue to dominate new plant orders. It may be possible that IGCC will penetrate the market on a large scale only where the co-production of power and chemicals can be economically demonstrated.

Considering the dominance of PC fired systems for electricity generation, several efforts have been made to enhance the overall efficiencies of these systems. The efficiency of a PC fired boiler depends on a variety of factors:

- Plant design (milling, burner, heat recovery systems, and so on)
- Operating conditions (pressure/steam conditions)
- Quality of coal
- Turbine efficiencies
- Ambient conditions
- Operating protocols
- Maintenance practices

In this book we restrict the scope of our discussions to the combustion side of the boiler. The components of the PC fired boiler other than the combustion side are outside the scope of this book. Even for the combustion side, the scope is restricted: from burner/excess air entry points to the exit of flue gases (and fly ash) from the heat recovery section. The milling and conveying of coal particles, as well as further processing of flue gas beyond the heat recovery section (electrostatic precipitators, etc.), are beyond the scope of the present work. The scope of this book is clearly marked over a schematic of a power plant shown in Figure 1.1. Therefore, in the context of this book, PC boiler and PC boiler efficiency essentially refer to the combustion chamber of the PC fired boiler and thermal efficiency, unless stated otherwise.

Several developments on higher-temperature (and -pressure) systems—namely, SC and USC pulverized coal fired boilers—have been realized in recent years (or are being realized). While sub-critical plants achieve overall efficiencies of 32% to 38% (on an LHV [lower heating value] basis), state-of-the-art USC boilers are expected to realize overall efficiencies of 42% to 45% (LHV basis). Single-unit capacities of these plants have reached 1,100 MWe (megawatt electrical). Parallel developments are also being made in oxy-fuel technologies to facilitate $CO_2$ capture. Efforts have been made to reduce other emissions, such as NOx, SOx, and particulates. Significant research is being done in areas such as new emission control technologies, state-of-the-art boiler designs, and low-temperature heat recovery systems for improved plant efficiencies; systems for improved ash disposability and reduced waste generation; and optimum system integration and plant controls. These research areas are still reinventing themselves.

Key components of efficiency improvement initiatives depend on a better understanding of the burning of coal and subsequent heat transfer for converting water into steam. The overall performance of the boiler critically depends on our understanding as well as our ability to manipulate the following key processes:

- Gas-solid flow (through ducts, burner nozzles, combustion chamber, heat recovery systems, electrostatic precipitators, etc.):
  - Gas: air/flue gas
  - Particles: coal/ash
- Combustion:
  - Volatile combustion
  - Char combustion
  - Pollutant formation and role of furnace aerodynamics
- Radiative and convective heat transfer

Technology advancements in PC fired boilers require a thorough and quantitative understanding of these aspects. Anyone interested in enhancing boiler performance will want to establish quantitative relationships among fuel (coal) characteristics, hardware design of boiler, and operating protocols with boiler efficiency. Such a quantitative relationship can then be used to optimize fuel mix and design as well as operating practices. Computational modeling, particularly computational flow modeling (CFM), plays a crucial role in developing such an understanding as does the ability to tailor the design and operating protocol to enhance overall performance.

Over the years, computational fluid dynamics (CFD) tools have evolved as powerful design and predictive tools to simulate complex equipment (Ranade, 2002). Computational fluid dynamics (CFD) is a body of knowledge and techniques to solve mathematical models (primarily based on conservation of mass, momentum, and energy) on digital computers. The development of high-performance computers, advances in the physics of fluids, and advances in numerical techniques and algorithms has made it increasingly possible to use CFD models for complex reacting systems such as PC fired boilers. It is, however, necessary to adapt CFD techniques and develop an appropriate CFM approach for meaningfully applying them to complex systems like PC fired boilers.

This book is written with the intention of assisting practicing engineers and researchers in developing such an approach. It describes the methodology to formulate a CFD model for simulating PC fired boilers. Although most of the results included here are for an old-generation 210-MWe unit, the methodology can be extended in a straightforward way to model advanced supercritical, ultra-supercritical, and oxy-fuel combustion systems.

CFD models/simulations of PC fired boilers are usually computationally expensive and time consuming. Therefore, even if these models/simulations provide extensive insight into processes occurring in PC fired boilers, they are not very suitable for real-time optimization (which requires much quicker response times). A complementary approach called reactor network modeling (RNM) is therefore developed and presented in this book. The RNMs are essentially lower-order computational models (typically with a few hundred variables, in contrast to a few million or more variables used in CFD models) that can be used for overall optimization and even for real-time process control. The methodology and process of developing an RNM based on data extracted from detailed CFD models of PC fired boilers are discussed here. Efforts are made to provide guidelines for

- Characterizing coal using a drop-tube furnace and a thermogravimetric analyzer (TGA)
- CFD modeling of a PC fired boiler
- Developing reactor network models (RNMs)
- Applying computational models to industrial practice

The presented results and discussion will also provide insight into the complex processes occurring in PC fired boilers. The basic information and key issues of coal fired boilers are discussed in Section 1.1. Key aspects of CFM with reference to potential application to coal fired boilers are then discussed in Section 1.2, and the organization of the book is briefly discussed in Section 1.3.

## 1.1 Coal Fired Boilers

Worldwide, coal fired generating capacity is expected to reach approximately 2,500 GW (gigawatt) by the end of 2020. This is an increase of nearly 60% since 2008, and more than 55% of the projected new generating capacity is expected to be in Asia (Mcllvaine, 2009). The capacity enhancement is based on the addition of advanced low-emission boiler systems. Continuing efforts are also being made on existing power plants to achieve higher efficiency, reliability, and availability with low maintenance, while complying with stringent emissions regulations for $CO_2$, SOx, NOx, and particulates. Coal fired boilers have undergone major innovations in order to satisfy both economics and increasing stringent environmental regulations. In principle, solid-fuel combustion technologies are divided into three categories:

1. Bed or grate combustion
2. Suspension or pulverized combustion
3. Fluidized bed combustion

The traveling grate stoker was the early coal combustion system for power generation. Traveling grate stokers are capable of burning coals over a wide range of coal rankings (from anthracite to lignite). The typical particle sizes are 1 to 5 cm (centimeter) with residence times of 3,000 to 5,000 s (second). The flame temperature is around 1,750K (Essenhigh, 1981). Stoker firing is not able to scale beyond 50-MWe unit capacities. The boiler efficiency gets suppressed by the high excess air (about 40%) that was required for acceptable coal burnout.

In 1946, Babcock and Wilcox introduced the cyclone furnace for use with slagging coal (i.e., coal that contains inorganic constituents that will form a liquid ash at temperatures of ~1,700K or lower); this was the most significant advance in coal firing since the introduction of pulverized coal firing (Miller, 2005). A cyclone furnace provides the benefits obtained with PC firing and also has the advantages of utilizing slagging coals and reducing costs due to less fuel preparation (i.e., fuel can be coarser and does not need to be pulverized). In slagging combustion, the boiler tubes in the lower part of the furnace are covered by a refractory to reduce heat extraction and to allow the combustion temperature to rise beyond the melting point of the ash. The temperature must be sufficiently high for the viscosity of the slag to be reduced to about 150 Poise, which is necessary for removal in liquid form. The most notable application of slagging combustion technology in the United States is the cyclone furnace, in which about 85% of the coal ash can be removed in molten form in a single pass without ash recirculation. Because of the high temperature and the oxidizing atmosphere, slagging furnaces produce very high NOx emissions and therefore fell into disfavor in the 1970s.

Fluidized bed boilers for utilizing coal were originally developed in the 1960s and 1970s; they offer several inherent advantages over conventional combustion systems, including the ability to burn coal cleanly by reducing $SO_x$ emissions during combustion (i.e., *in situ* sulfur capture) and generating lower emissions of $NO_x$. In addition, fluidized bed boilers provide fuel flexibility as a range of low-grade fuels can be burned efficiently. In fluidized bed combustion (FBC), crushed coal of 5 to 10 mm (millimeter) is burned in a hot fluidized bed of 0.5- to 3.0-mm-sized inert solids. The typical particle residence time is around 100 to 500 s (Essenhigh, 1981). Less than 2% of the bed material is coal; the rest is coal ash and limestone, or dolomite, which are added to capture sulfur during the course of combustion. The bed is cooled by steam-generating tubes immersed in the bed to a temperature in the range of 1,050K to 1,170K (Baranski, 2002). This prevents the softening of the coal ash and the decomposition of $CaSO_4$, which is the product of sulfur capture. The heated bed material, after coming into direct contact with the tubes (heating by conduction), helps improve the efficiency of heat transfer. Because this allows coal plants to burn at lower temperatures, less NOx is emitted. This technology, however, was limited to small industrial-sized fluidized boilers and was not useful for very large steam capacities like those of PC fired units unless use of high pressures.

Circulating fluidized bed (CFB) boilers were developed to enhance the flexibility of using a wider range of fuels. CFB boilers involve a circulating fluidized bed of inert material with a hot cyclone to recirculate solids particles. Usually, combustion in CFB boilers takes place at temperatures from 1,075K to 1,175K, resulting in reduced NOx formation compared with conventional PC fired boilers. Another advantage of CFB combustors is their ability to handle low calorific value fuels, *in situ* sulfur capture, no need to pulverize the fuel, and comparatively lower capital costs than PC boilers. The thermal efficiency of CFB boiler units is lower by 3 to 4 percentage points than that for equivalent-sized PC boilers (Western Governors' Association, 2008). CFB boilers represent the market for medium-scale units (typically < 300 MWe) in terms of utility requirements. They are used more extensively by industrial and commercial operators in small to medium range sizes (50 to 100 MWe), both for the production of process heat and for on-site power supply.

Pulverized coal (PC) combustion became a widely accepted combustion system for power generation in the period between 1900 and 1920. This was the major development in order to take advantage of the following:

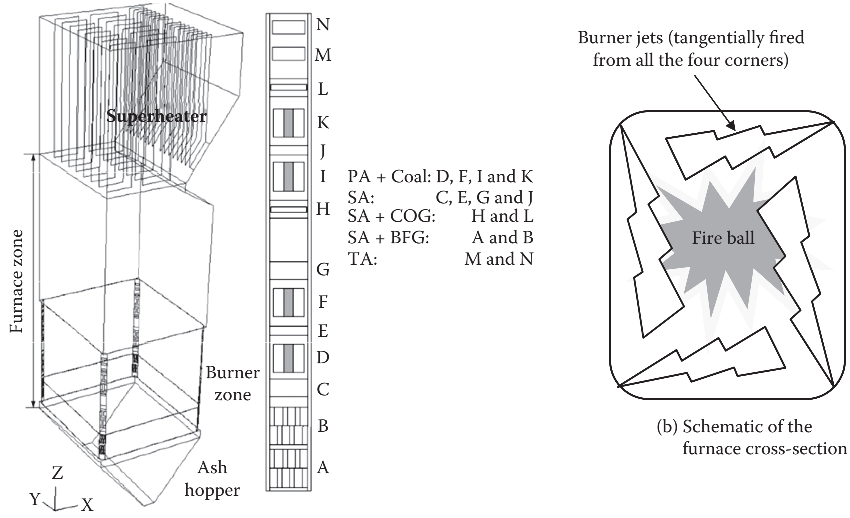
- Higher volumetric heat release rates of pulverized coal ($MW/m^3$)
- Increased system efficiencies using superheaters (heat-exchange surface to increase the steam temperature), economizer (heat-exchange surface to preheat the boiler feed water), and combustion air preheaters (heat-exchange surface to preheat combustion air)
- Improved material of construction, which will allow for higher pressures in the steam generator (>83 barg [bar gauge])

The development of the superheater, reheater, economizer, and air preheater played a significant role in improving overall system efficiency by absorbing most of the heat generated from burning the coal. The separation of steam from water and the use of super-heaters and reheaters allowed for higher boiler pressure and larger capacities. Hence, the pulverized coal combustion system became widespread due to increased boiler capacity, and improved combustion and boiler efficiencies over stoker-fired boilers. The PC fired boiler was found to be the most suitable for utility power plants and contributes to more than 50% of the world's electricity demand.

Advances in materials of construction, system design, and fuel firing have led to increased capacity and higher steam operating temperatures and pressures. There are two basic PC-fired water tube steam generators: (1) subcritical drum-type boilers with nominal operating pressures of either 131 or 179 barg, and (2) once-through supercritical units operating at 262 barg. These units typically range between 300 and 800 MW (i.e., produce steam in the range of 900 to 3,000 tons/hour). Ultra-supercritical units entered into service in 1988. These units operate at steam pressures of 310 barg and steam temperatures of 838K, with capacities as high as 1,300 MW. This book, as mentioned earlier, focuses on developing a better understanding of the various processes occurring in the most widely adopted PC fired boilers. Some aspects of these tangentially PC boilers are discussed here.

A typical tangentially fired PC boiler is shown in Figure 1.2(a). There are three major parts of the boiler: furnace, crossover pass, and second pass. In a tangentially fired furnace, the burners generate a rotational flow in the furnace by directing the jets tangent to an imaginary circle whose center is located at the center of the furnace. The resultant swirling and combusting flow generates a fireball at the center of the furnace, where the majority of combustion occurs (Figure 1.2(b)).

In PC combustion, the coal is dried and crushed into fine particles, and the powdered coal is pneumatically transported to the burners. Typical particle sizes used in PC boilers range from 10 to 100 μm (micrometer). The design of the combustion chamber must provide sufficient residence time for the coal particle to complete its combustion, and for the fly ash to cool down to below its "softening temperature" to prevent the build-up of ash deposits on heat exchanger surfaces. A typical residence time of particles in PC boilers is approximately 10 s (Essenhigh, 1981). The transport air that carries the coal from the mill to the burners must be maintained at around 373K to avoid ignition hazards. This transport air (also called fuel air [FA]) is about 40% to 50% of the total air injected into the boiler. The remaining air other than the FA enters the PC boiler via secondary air (SA) inlets and over fire air (OFA). The air entering through these other inlets is usually preheated to 550K.




(a) Schematic of tangentially fired PC boiler and details of burner nozzles

(b) Schematic of the furnace cross-section

**FIGURE 1.2**
Tangentially fired furnace of pulverized coal fired boiler. (Figure 1.2 (a) reprinted with permission from Fang, Q., Musa, A.A.B., Wei, Y., Luo, Z. and Zhou, H., Numerical simulation of multifuel combustion in a 200 MW tangentially fired utility boiler, *Energy & Fuels*, 26, 313–323. (2012); © 2012 American Chemical Society.)

The design of the furnace is influenced by the type of burner system adopted in the design, such as a wall-mounted circular type or a corner-fired rectangular shape. Circular burners are usually positioned perpendicular to the combustion chamber walls, while the vertical nozzle arrays are in the corners, firing tangentially to the circumference of an imaginary cylinder in the middle of the combustion chamber. Wall-mounted burners can also be designed to provide tangential entry to the coal and air, forming a rotating fireball in the center of the furnace. The majority of boilers in countries such as India are tangentially fired and use rectangular slotted burners. The pulverized coal, air mixture (primary air), and secondary air are injected from sixteen to twenty-four burners located in the four corners of the furnace (Figure 1.2(b)).

The heat generated due to the combustion reactions is radiated and transported to the water walls of the boiler to generate steam. This steam is further superheated in superheaters at the crossover pass by radiative and convective heat transfer. The last few percentages of residual carbon in the char burns in an environment of depleted oxygen concentration and reduced temperature before the fly ash leaves the combustion chamber and enters the pass of convective heat exchangers. In the majority of cases, most of the fly ash formed in PC combustion is removed from the flue gas in the form of dry

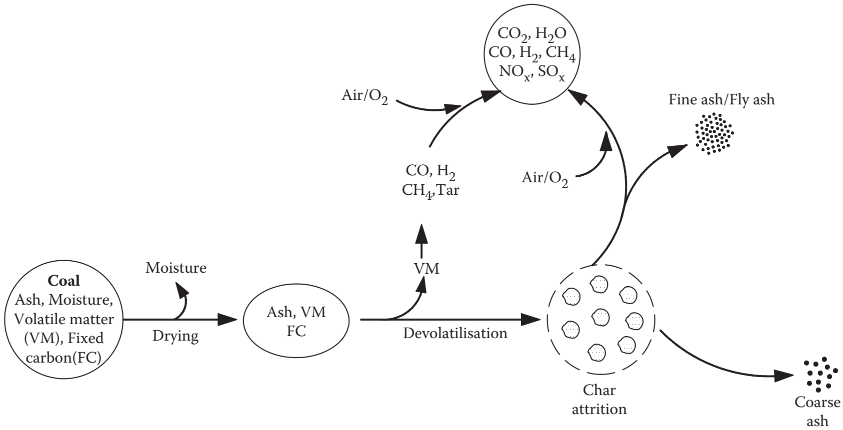



**FIGURE 1.3**
Particle-level processes during coal combustion.

particulate matter, with a small portion (about 10%) of the coal ash falling off the tube walls as semi-molten agglomerated ash, which is collected from the bottom hopper of the combustion chamber ("bottom ash"). Pulverized coal fired boilers offer high combustion intensities (~1 $MW/m^3$) and high heat transfer rates (~1 $MW/m^2$).

The coal particles injected in PC fired boilers get heated. Moisture and volatile materials are released during the drying and devolatilization stage. The char content of the particles eventually burns, and the remaining ash can exit the boiler in the form of fly ash (finer particles) or bottom ash (coarser particles). These processes are schematically shown in Figure 1.3. Pyrolysis or devolatilization results in a vast array of products such as CO, tar, $H_2$, $H_2O$, HCN, hydrocarbon and gases, etc. These products react with oxygen in the vicinity of the char particles, depleting oxygen and increasing the temperature. These complex reaction processes are very important in controlling the nitrogen oxides, formation of soot, stability of coal flames, and ignition of char. The char combustion may then occur along with the combustion of the volatile species in the gas phase. After the completion of char combustion, the inorganic constituents remain as ash. Typically, ash contains $SiO_2$, $Al_2O_3$, $Fe_2O_3$, $TiO_2$, CaO, MgO, $Na_2O$, $K_2O$, $SO_3$, and $P_2O_5$ (primarily the first 3 compounds). Ash composition varies with the rank of the coal. The ash material may further decompose to form slag at high temperatures (beyond the ash fusion temperature). Nitrogen is released from the coal and forms nitrogen oxides (NOx). The sulfur released during coal combustion forms sulfur oxides (SOx).

The process of char combustion is of central importance in industrial PC fired boiler applications. However, despite extensive investigations over the past half-century, the mechanism of the char/oxygen reaction is not completely understood because of a number of factors, including the reaction due to pore growth and mass transfer effects (Williams et al., 2001). It is further complicated by the influence of particle size distribution, char mineral content, and fragmentation of the char particle. The rate-limiting step in the combustion of a char particle can be chemical reactions, or the diffusion of gases into the particle, or a combination of these factors.

The furnace is a key part of the boiler where turbulent mixing, two-phase flow, exothermic reactions, and radiative heat transfer dominate. Preliminary calculations shows that combustion of a typical 70 μm coal particle require nearly 1 s at typical furnace temperatures. The industrial data, however, confirm the presence of unburned carbon in fly ash (~5%) as well as in bottom ash, which affects the thermal efficiency of the boiler and the salability (value) of the ash. Turbulent and recirculating flow affects the mixing of the fuel and oxidants, and thereby the rate of the combustion reaction. Understanding the behavior of coal fired boilers and translating this understanding into computational models for simulating such boilers is complicated by the existence of turbulent, multi-phase recirculating flows, coupled with chemical reactions and radiative heat transfer. The existence of a wide range of spatiotemporal scales (chemical reactions occurring on molecular scales to micron-size particles to tens of meters of boiler; reaction time scales on the order of microseconds to particle residence time on the order of a few

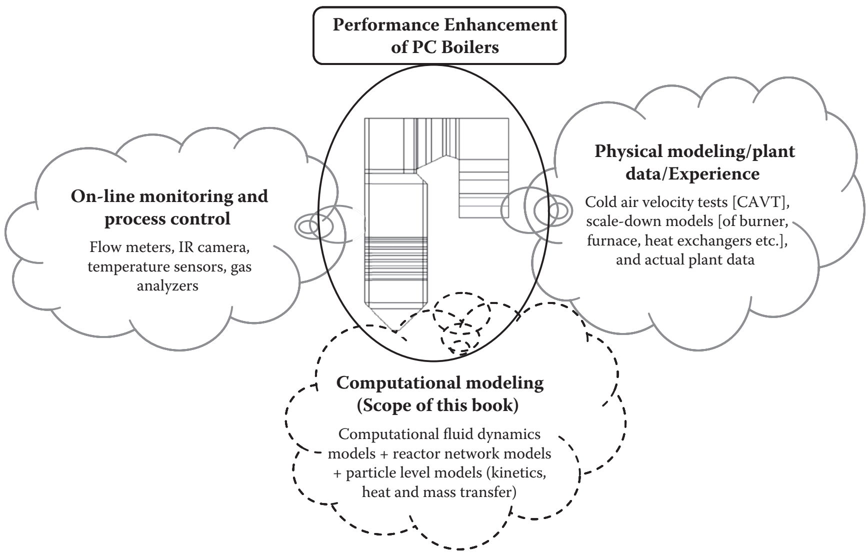



**FIGURE 1.4**
Approaches for performance enhancement of boilers.

seconds) often complicates the matter further. The thermo-fluid interaction processes between neighboring burners and between the burners and the furnace as a whole are complex and not yet well understood.

As mentioned earlier, significant efforts have been made and are still being made to enhance the performance of PC fired boilers. Possible ways of enhancing the performance of such boilers (see Figure 1.4) may be broadly grouped into two types:

1. On-line monitoring and process control. These methods are usually based on data-driven models and can be effectively used for optimizing the operation of a PC fired boiler over a narrow range of parameters.
2. Establishing the relationship between performance and hardware/operating protocols. These methods may be further classified into two subtypes:
   - Based on physical modeling, data and empirical correlations, experience, and heuristic relationships
   - Phenomenological modeling: representing the behavior of a PC fired boiler using conservation equations of mass, momentum, and energy

In this book we mainly restrict our scope to the discussion of phenomenological models. Considering the complexity of PC fired boilers, most phenomenological models of PC boilers require the help of a digital computer for their solution. The combined set of underlying phenomenological models, initial and boundary conditions, numerical methods, and their computer implementation is broadly called a "computational model." This book essentially deals with the development and application of such computational models for simulations and for performance enhancement of PC fired boilers.

The performance of PC fired boilers operating with high-ash coal (like Indian coal) faces some special challenges. These include problems of ash handling, slagging, ash deposition on heat exchanger surfaces, as well as unburned char in the fly ash. With emission norms becoming more stringent and increasing pressures on enhancing overall efficiency of PC fired boilers, it is essential to develop relationships among the availability, performance, and reliability of these boilers with factors such as burner design, operational protocols, coal quality, age of boiler, furnace hardware configuration, etc.

Computational modeling offers an excellent way to develop such relationships and to develop an ability to optimize boiler performance. Some aspects of computational flow modeling are discussed in Section 1.2.

## 1.2 Computational Modeling

Computational models attempt to represent processes occurring in PC fired boilers with the help of conservation equations of mass, momentum, and energy. A generic conservation equation for any conserved quantity $\phi$ can be represented as

$$\begin{array}{c} \text{accumulation of} \\ \text{component } \phi \end{array} = \begin{array}{c} \text{rate of change of} \\ \text{component } \phi \text{ due} \\ \text{to convection} \end{array} + \begin{array}{c} \text{rate of change of} \\ \text{component } \phi \text{ due} \\ \text{to dispersion} \end{array} + \begin{array}{c} \text{rate of change of} \\ \text{component } \phi \text{ due to} \\ \text{reaction / mass transfer} \end{array} \tag{1.1}$$

If there are any additional modes of transport for $\phi$, corresponding additional terms may appear on the right-hand side of Equation (1.1). This general balance equation can be mathematically represented in a variety of forms, depending on various underlying assumptions. One can use a classical chemical reaction engineering (CRE) approach and develop a RNM to represent the PC fired boiler. Alternatively, one can use a CFD-based framework to represent the PC fired boiler. The term "computational modeling" essentially covers the selection of a modeling approach, development of model equations and boundary conditions, development of numerical methods to solve model equations, mapping of numerical methods on digital computers to generate solutions of model equations, verification of developed computer implementation and validation of the underlying phenomenological model, carrying out simulations to gain a better understanding, and using that gained understanding to enhance performance in practice.

Computational modeling of PC fired boilers therefore requires broad-based expertise in the various aspects of PC combustion and an in-depth understanding of various aspects of computational modeling (CFD and CRE), along with a generous dose of creativity. Ranade (2002) has discussed the application of computational flow modeling for a variety of chemical reactors. The discussion is very relevant for modeling and simulating the PC fired boiler as well and is therefore recommended for further reading. Computational modeling requires relatively few restrictive assumptions, can handle complex configurations, and can incorporate a variety of processes simultaneously. Simulations based on such computational models often serve as a bridge between theory and reality. Computational models allow switching on and off the various interactions included in the model in order to understand the relative contributions of each individual process, which is extremely difficult—if not impossible—to achieve in experiments. These advantages of computational