Design of Advanced Industrial Furnaces
Using Numerical Modeling Method

Wei Dong

Doctoral Thesis

STOCKHOLM

March 2000

Heat and Furnace Technology
Department of Materials Science and Engineering
Royal Institute of Technology
S-10044 Stockholm
Sweden
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Keywords: air staging, bed model, boiler, burner, computational fluid dynamics (CFD), Ecotube, fuel staging, furnace, grate combustion, highly preheated and diluted air combustion (HPDAC), large eddy simulation (LES), mathematical modeling, nitrogen oxides (NOx), numerical simulation
Preface

In the April 1996, I joined the combustion research for advanced industrial furnace development in the Division of Heat and Furnace Technology, Royal Institute of Technology (KTH), Stockholm, Sweden. My first research topic was the mathematical modeling of grate combustion and NOx emission with a new supply Ecotube system. After two years, I received the KTH licentiate degree under the supervision of Associate Professor Wlodzimierz Blasiak, the head of the Division. I am greatly indebted him for giving me this opportunity to work on this exciting research field, and for his continuous encouragement and support during the thesis work. Since then, I continued working on the field of advanced industrial combustion/furnace technology under his guidance. It results in this doctoral thesis, in which the numerical simulations are extended to the topics of different advanced combustion technologies with the numerical modeling and design for advanced industrial furnaces. This doctoral thesis is mainly based on the following six papers:

Paper 1

Paper 2

Paper 3

Paper 4
Dong W. and Blasiak W. Study on Mathematical Modeling of Highly Preheated Air Combustion. In 2nd High Temperature Air Combustion Symposium, Taiwan, 1999

Paper 5

Paper 6
Dong W. and Blasiak W. Large Eddy Simulation (LES) of a Single Jet Flow in Highly Preheated and Diluted Air Combustion. Archivum combustionis, 2000 (submitted)

There are also author’s other papers and reports which may be referred in the thesis:

[5] Dong W. and Blasiak W. 3D numerical simulation for biomass combustion and NOx emission in a grate fired boiler, In 1st Energy from Waste'97, Ustron, Poland, 1997
I would like to thank my colleagues in our furnace research group:
Associate Professor Jiri Vaclavinek, Christer Helen, Jan Bång, Rasmus Friberg, Simon Lille, Reza Fakhrai and Hilmer Thunman for their helps and the pleasant working environment we have shared.

I am indebted to NUTEK (Swedish National Board for Technical Development), ÅFORSK, and Jernkontoret for the financial support of this thesis work.

Many thanks to my wife Ms. Yun Hou, she has accepted my work during numerous evenings and weekends even with some objections. Her understanding and patience along with our lovely son Xiuchuan make my life happy and hopeful.

Last, but not least, I cordially thank my old parents for they always encourage and support me to make progresses in my life.

Wei Dong
Stockholm, Sweden, March 2000
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Department of Materials Science and Engineering
Royal Institute of Technology (KTH)
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### Nomenclature

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<th>Units</th>
<th>Definition</th>
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<tr>
<td>$A$</td>
<td></td>
<td>pre-exponential factor</td>
</tr>
<tr>
<td>$Bo$</td>
<td>kJ/kg</td>
<td>Boltzmann number ($Bo = \frac{\rho u c_p}{\sigma T^3}$)</td>
</tr>
<tr>
<td>$C_p$</td>
<td>kJ/kg</td>
<td>specific heat at constant pressure</td>
</tr>
<tr>
<td>$C_s$</td>
<td></td>
<td>Smagorinsky model constant</td>
</tr>
<tr>
<td>$C_v$</td>
<td>kJ/kg</td>
<td>specific heat at constant volume</td>
</tr>
<tr>
<td>$D_{i,m}$</td>
<td>m$^2$/s</td>
<td>diffusion coefficient for species $i$ in the mixture</td>
</tr>
<tr>
<td>$E_k$</td>
<td>kJ/m$^3$s</td>
<td>activation energy for $k$th reaction</td>
</tr>
<tr>
<td>$f$</td>
<td></td>
<td>mixture fraction</td>
</tr>
<tr>
<td>$H$</td>
<td>kJ</td>
<td>heat of reaction</td>
</tr>
<tr>
<td>$h$</td>
<td>kJ/kg</td>
<td>enthalpy</td>
</tr>
<tr>
<td>$I$</td>
<td></td>
<td>radiation intensity</td>
</tr>
<tr>
<td>$k$</td>
<td>m$^2$/s$^2$</td>
<td>turbulence kinetic energy</td>
</tr>
<tr>
<td>$LHV$</td>
<td>kJ/kg</td>
<td>lower heating value</td>
</tr>
<tr>
<td>$Le$</td>
<td></td>
<td>Lewis number ($Le = \frac{Sc}{Pr}$)</td>
</tr>
<tr>
<td>$M$</td>
<td></td>
<td>Mach number</td>
</tr>
<tr>
<td>$m$</td>
<td></td>
<td>mixing factor</td>
</tr>
<tr>
<td>$m_i$</td>
<td>kg</td>
<td>mass of species $i$</td>
</tr>
<tr>
<td>$\dot{m}$</td>
<td>kg/s</td>
<td>mass flow rate</td>
</tr>
<tr>
<td>$p$</td>
<td>kg/m$^2$</td>
<td>pressure</td>
</tr>
<tr>
<td>$Pe$</td>
<td></td>
<td>Peclet number ($Pe = \frac{Re Sc}{Pr}$)</td>
</tr>
<tr>
<td>$Pr$</td>
<td></td>
<td>Prandtl number ($Pr = \frac{C_p \mu}{k}$)</td>
</tr>
<tr>
<td>$Q$</td>
<td>kJ/s</td>
<td>energy flux</td>
</tr>
<tr>
<td>$q$</td>
<td>kJ/s</td>
<td>radiation heat flux</td>
</tr>
<tr>
<td>$R_i$</td>
<td>mol/s</td>
<td>reaction rate of $i$th reaction</td>
</tr>
<tr>
<td>$Re$</td>
<td></td>
<td>Reynolds number ($Re = \frac{\rho u \ell}{\mu}$)</td>
</tr>
<tr>
<td>$S$</td>
<td></td>
<td>source term</td>
</tr>
<tr>
<td>$Sc$</td>
<td></td>
<td>Schmidt number ($Sc = \frac{\mu D}{\rho}$)</td>
</tr>
<tr>
<td>$T$</td>
<td>K</td>
<td>temperature</td>
</tr>
<tr>
<td>$t$</td>
<td>s</td>
<td>time</td>
</tr>
<tr>
<td>$V$</td>
<td>m$^3$</td>
<td>volume</td>
</tr>
<tr>
<td>$u$</td>
<td>m/s</td>
<td>velocity</td>
</tr>
<tr>
<td>$\alpha$</td>
<td></td>
<td>absorptivity or degree of non-mixing</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>m$^2$/s$^3$</td>
<td>turbulence dissipation rate</td>
</tr>
<tr>
<td>$\phi$</td>
<td></td>
<td>general physical variable</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td></td>
<td>diffusion coefficient</td>
</tr>
<tr>
<td>$\gamma$</td>
<td></td>
<td>the ratio of specific heats $C_p/C_v$</td>
</tr>
<tr>
<td>$\lambda$</td>
<td></td>
<td>excess air ratio</td>
</tr>
<tr>
<td>$\mu$</td>
<td>kg/ms</td>
<td>fluid viscosity</td>
</tr>
<tr>
<td>$\nu$</td>
<td>m$^2$/s</td>
<td>kinematic viscosity</td>
</tr>
<tr>
<td>$\nu_i$</td>
<td></td>
<td>exponent on the concentration of species $i$</td>
</tr>
<tr>
<td>$\rho$</td>
<td>kg/m$^3$</td>
<td>density</td>
</tr>
<tr>
<td>$\sigma$</td>
<td></td>
<td>Stefan-Boltzmann constant</td>
</tr>
<tr>
<td>$\tau_{ij}$</td>
<td></td>
<td>stress tensor</td>
</tr>
<tr>
<td>$\omega$</td>
<td></td>
<td>solid angle</td>
</tr>
<tr>
<td>$\xi$</td>
<td></td>
<td>degree of mixing</td>
</tr>
<tr>
<td>$\Omega$</td>
<td></td>
<td>hemispherical solid angle</td>
</tr>
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</table>
## Abbreviation

<table>
<thead>
<tr>
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<th>Description</th>
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<tbody>
<tr>
<td>AMG</td>
<td>algebraic multigrid method</td>
</tr>
<tr>
<td>BET</td>
<td>Brunauer-Emmett-Teller’s pore surface area</td>
</tr>
<tr>
<td>CAD</td>
<td>computer aid design</td>
</tr>
<tr>
<td>CFD</td>
<td>computational fluid dynamics</td>
</tr>
<tr>
<td>CFF</td>
<td>custom field function</td>
</tr>
<tr>
<td>CFL</td>
<td>Courant-Friedrichs-Lewy stable condition</td>
</tr>
<tr>
<td>DNS</td>
<td>direct numerical simulation</td>
</tr>
<tr>
<td>DO</td>
<td>discrete ordinates (radiation model)</td>
</tr>
<tr>
<td>DT</td>
<td>discrete transfer (radiation model)</td>
</tr>
<tr>
<td>EDC</td>
<td>eddy dissipation conception</td>
</tr>
<tr>
<td>FDI</td>
<td>fuel direct injection</td>
</tr>
<tr>
<td>FLOX</td>
<td>flameless oxidation</td>
</tr>
<tr>
<td>FRED</td>
<td>finite-rate / eddy-dissipation model</td>
</tr>
<tr>
<td>FVM</td>
<td>finite volume method</td>
</tr>
<tr>
<td>HPAC</td>
<td>highly preheated air combustion</td>
</tr>
<tr>
<td>HPDAC</td>
<td>highly preheated and diluted air combustion</td>
</tr>
<tr>
<td>LES</td>
<td>large eddy simulation</td>
</tr>
<tr>
<td>MG</td>
<td>multigrid method</td>
</tr>
<tr>
<td>MPDF</td>
<td>mixture fraction / PDF approach</td>
</tr>
<tr>
<td>MSW</td>
<td>municipal solid waste</td>
</tr>
<tr>
<td>OFA</td>
<td>over fire air</td>
</tr>
<tr>
<td>QUICK</td>
<td>quadratic upstream interpolation for convective kinetics</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds averaged Navier-Stokes equation</td>
</tr>
<tr>
<td>RNG</td>
<td>renormalized group</td>
</tr>
<tr>
<td>RSM</td>
<td>Reynolds stress model</td>
</tr>
<tr>
<td>RTE</td>
<td>radiation transport equation</td>
</tr>
<tr>
<td>PDE</td>
<td>partial differential equation</td>
</tr>
<tr>
<td>PDF</td>
<td>probability density function</td>
</tr>
<tr>
<td>RTD</td>
<td>residence time distribution</td>
</tr>
<tr>
<td>SGS</td>
<td>sub-grid scale</td>
</tr>
<tr>
<td>SIMPLE</td>
<td>semi-implicit method for pressure-linked equation</td>
</tr>
<tr>
<td>SIMPLEC</td>
<td>SIMPLE-consistent</td>
</tr>
<tr>
<td>SNCR</td>
<td>selective non-catalytic reduction</td>
</tr>
<tr>
<td>SOFA</td>
<td>secondary / over fire air</td>
</tr>
<tr>
<td>SRR</td>
<td>staging, reburning and recirculation</td>
</tr>
<tr>
<td>UDF</td>
<td>user defined function</td>
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Abstract

Nomenclature

Abbreviation

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- **Paper 2**: Design and Optimizing Ecotube Air System for Clean Combustion of Coal in a Grate Fired Boiler

- **Paper 3**: Modeling of Fluid-Flow and Mixing Patterns in an Entrained Boiler

- **Paper 4**: Study on Mathematical Modeling of Highly Preheated Air Combustion

- **Paper 5**: Numerical Modeling of Highly Preheated Air Combustion in a 589KW Testing Furnace at IFRF

- **Paper 6**: Large Eddy Simulation of a Single Jet Flow in Highly Preheated and Diluted Air Combustion
Chapter 1
Introduction

1.1 Motivation for the thesis

The development of advanced industrial burners, furnaces and boilers with the higher performance of higher efficiency and lower pollutant emissions is a major goal of combustion researchers, furnace designers and manufacturers. To realize the goal, on one hand, the new technical concepts and novelties for different combustion routes and processes have to be continuously developed. On the other hand, more efficient and economic tools, such as computer simulation by using computational fluid dynamics (CFD) technology, are also extremely important to be developed and applied for the design process and performance simulation of the new advanced furnaces.

In recent decade, compared with the traditionally experimental methods and physical modeling methods, the computer simulation with numerical methods is considered as a more attractive tool, since the modern computer can be manufactured much faster, bigger and cheaper. Furthermore, the models developed for turbulent reacting flows in homogeneous and heterogeneous combustion systems are so sophisticated that together with a large computational source ability, a comprehensive computer simulation with numerical methods becomes possible for very complicated applications in industry.

However, the numerical methods can lead to errors exceeding those arising from turbulent and reacting flow closure assumptions. In addition, the numerical schemes used in practical combustion flows with very complicated physico-chemical processes and complex geometry of computational domain of an utility furnace, may meet serious problems of numerical unstability and divergence, since there are lots of uncertainties and simplified assumptions in fundamental models. To overcome these limitations, various models are in developing and it needs to speed up technology transfer from research to practical applications.

1.2 Advanced industrial heat and furnace technologies related in the thesis

Since 1995, several new advanced industrial heat and furnace technologies have been studied in the Division of Heat and Furnace Technology at KTH. All these technologies emphasize mainly on energy savings, energy conversion and pollutant reduction.

1.2.1 Staging, reburning and recirculation principles

In order to save fuels and comply with more strict regulations for NOx emissions in a combustion system, various strategies and techniques have been developed. Basically, there are three new combustion principles used: air staging (two-staged combustion), fuel staging (reburnning, three-stage combustion), and hot flue gas recirculation. Shortly, they can be called Staging, Reburnning, and Recirculation (SRR) techniques.
Most of state-of-the-art low NOx and highly efficient burners and furnaces are designed based on one or more of these three techniques.

The principle of the air staging method is that part of the combustion air is introduced after the main combustion zone in order to reduce the level of available oxygen in zones where it is critical for NOx formation. It is a two-stage combustion process in which the primary combustion zone is operated fuel rich and the secondary air or over-fire-air (OFA) required to complete the combustion process is introduced downstream of the main firing zone. The possible NOx reduction by means of this air staging method is about 20~50% without negative impact on furnace efficiency (Chen 1982).

The principle of the fuel staging (reburnning) method is that a source of hydrocarbon radicals is introduced after the main combustion zone. It is a three-stage combustion process in which the nitrogen oxides are formed in a fuel lean primary combustion zone and then destroyed in a fuel rich secondary zone created by introducing a secondary fuel, and then additional air is added further downstream to obtain an overall fuel lean environment and complete combustion. The hydrocarbon radicals can react with NO to produce HCN intermediate, which initiates a path that favors N2 formation in a fuel rich environment. The possible NOx reduction by means of this reburnning method is about 50% without negative impact on furnace efficiency (Wendt 1991).

The principle of the hot flue gas recirculation is that a reheat cycle from hot flue gas to primary air in a furnace system is generated by using recuperators, regenerators or any other heat recycling devices. In this recirculation process, the exhaust hot flue gas is used to preheat the fresh air to a high temperature and at the same time to dilute the fresh air to a lower oxygen level. If a strong exhaust gas recirculation is reached and thus the primary air is highly preheated up to 1300K with a quite lower oxygen concentration (<5%), then the fuel or energy savings can be expected to be 50% with a dramatic low NOx emission level (Katsuki 1998). Most recently, this principle results in a wide range of research, demonstration and development of highly preheated and diluted air combustion (HPDAC) technology in industry.

Principle is in principle. In practical situation, there are a lot of uncertainties, so, the design of a furnace is always greatly dependent on a lot of factors as type of process, fuel, etc. There are therefore a lot of different designs, experimental tests, modeling and simulations, and demonstrations for industrial applications of these principles. This thesis also concerns the applications of SRR principles in practical furnaces and boilers.

1.2.2 Grate combustion of coal and biomass fuels

A furnace or a boiler applying grate combustion technology to coarse solid fuels can basically be divided into three subsystems. They are here termed as the over-bed system, the fuel bed system and the grate system. Over-bed system is defined as the flowing gas phase resulting from the off-bed gases from the burning fuel in the fuel bed system. Important phenomena in this section are the gas phase combustion reactions
and the fluid dynamics. The lower system boundary of the over-bed system is defined by the bed surface. The secondary/tertiary air jets or recirculated flue gas jets are also introduced in the over-bed section. Fuel bed system is a two-phase system comprising the solid fuel particles and the interstitial gas phase. Important phenomena occurring inside the fuel bed system is the thermochemical conversion of solid fuels. Grate system can be inclined or horizontal, and fixed or moving. As the solid fuel is heated on the grate, the moisture will be driven off and then the organic matter will decompose, evolving combustible volatile. The amount of volatile released depends on the material and the temperature range. Almost all the volatile may be expected to be released from 450 K to 800 K. The decomposition process can be exothermic or endothermic. However, the net heats involved for coal and presumably for other organic materials are so small that for practical purposes the decomposition process may be regarded as thermally neutral.

Since 1996, grate combustion boilers for biomass fuel and coal have been studied by using mathematical modeling method and physical modeling method in the division of heat and furnace technology at KTH. Especially, the air staging method together with a new air supply system — Ecotube, have been emphasized in research. In addition, a typical fixed-bed reactor with three-step conversion and combustion system model has been proposed to study the thermochemical processes of solid fuels (biomass, coal, MSW) in grate combustion (Friberg 2000). Furthermore, an experimental fixed-bed reactor was established for studying solid fuel gasification and combustion.

1.2.3 Ecotube system for clean combustion of coal and biomass fuels

The new air supply system used to retrofit an already existing boiler is called Ecotube (Hagström 1997). It aims to distribute the secondary air inside the boiler more evenly and to make mixing in the over-bed section more effectively. It also aims to reduce the emission of pollutants from the furnace chamber by using Ecotube as means of reburning fuel supply system. As shown in Figure 1.1, the Ecotube system

![Figure 1.1. Scheme of Ecotube system for secondary air supply](image)

in the boiler consists of a few (e.g. two) air tubes that are mounted parallel to each other in the over-bed section. Each tube has a set of small air nozzles distributed on two
opposite sides and pointing in suitable directions. Using this arrangement, it is expected that the secondary air will mix more efficiently with the off-bed gases. The first combustion zone where the Ecotube system is placed may then be considered as a well stirred reactor while the section above through the boiler can be treated as a plug flow reactor.

1.2.4 Highly preheated and diluted air combustion technology

It has long been recognized that fuel savings, or say, CO₂ reduction, can be obtained when a combustion system is equipped with a heat recovery system. At British Gas and later at Dyson Hotwork company, UK, throughout the 1970s and 1980s, substantial resources were allocated to the development of both recuperative and regenerative burners (Masters 1979). However, because of material problems, the previous recuperative and regenerative burners could offer only modest fuel savings since the combustion air could not be preheated to high temperatures larger than 873K. Recent developments on new honeycomb type regenerators at Nippon Furnace Kogyo (NFK), made it possible to preheat the combustion air up to temperatures higher than 1300K by recirculating the hot exhaust gas and, thus, fuel savings up to 50%, as well as significant decreasing of NOₓ emissions. The important constraint of state-of-the-art recuperative/regenerative burner technology is the conflict between technologies designed to reduce emissions and those focusing on energy efficiency. Due to the high air preheat conventional flames have high peak temperature which especially leads to strongly increasing NOₓ emissions. Compared to this state-of-the-art technique, the main feature of the present HPDAC technique is a novel combustion mode with extremely homogeneous flame temperature (without the temperature peaks of a conventional flame) in a substantially extended combustion zone. It was possible to achieve using concept of separated (or direct) fuel injection into the furnace also numerically studied in this work.

![Diagram of heat recirculating furnace with switching regenerative burners](image-url)
Most classical example of this new combustion technique practical realization is based on two regenerative burners working as a high frequency switching (every 10-30 seconds) pair of regenerative burners developed mostly by NFK. This type of solution is shown schematically in Figure 1.2. Another technical solution based on one integrated regenerative burner known under trade mark FLOX (flameless oxidation) was developed by company WS, WärmeProcesstechnik, (Wunning 1991, 1997) and is shown in Figure 1.3. It is primarily based on the dilution of the unburnt gases as a very effective method to lower peak flame temperatures, resulting in lower NOx emissions.

![Figure 1.3 Schematic structure of the FLOX burner](image)

In FLOX process, the exhaust gases are recirculated internally in three stages. Mixing of air and exhaust gases is followed by addition of fuel to the diluted air. Finally, a non-burner-stabilized combustion, referred to as flameless oxidation, takes place, in which exhaust gases are internally recirculated again. The big difference between honeycomb typed HPADC and FLOX is in that the preheating of air is not a necessary requirement for FLOX due to exhaust gas recirculation dominates the process of heating up unburnt gases. Furthermore, in FLOX, there is no combustion noise and no visible reaction.

Using these kinds of technical solutions (separated and integrated) air and fuel are injected "together" via a burner. However it is possible to use the heat regenerator concept only to preheat combustion air and/or fuel. Fuel and air can be next injected to the furnace by means of high velocity separated nozzles through the furnace walls. In this case fuel and air can be injected to furnace in a free way not dependent on regenerative burner design.

### 1.3 Numerical methods and CFD technology for industrial furnaces

Design requirements of high-performance boilers are usually summarized as the achievement of time, temperature, and turbulence, commonly called 3Ts. Mathematical modeling has been very widely used tools for the design of a complicated boiler since 80s. In 1988, a special issue of Combustion Science and Technology collected fourteen papers concerned with numerical methods for practical combusting flows and first
formally illustrated their ability to contribute to the design process of industrial combustion equipment. Since then, both the digital computer technology and the numerical software have got very fast developed and are still growing quickly. Recently the computational fluid dynamic (CFD) tools, such as FLUENT and STAR-CD, etc., have been successfully used for comprehensive simulations of different types of furnaces and boilers.

CFD technology mainly consists of three parts. The first part is the physical models which are a set of conservation equations of mass, momentum, energy, state equation, turbulent equations, chemical reaction source term equations, etc. The second part is a series of solution approaches for solving these physical models, and the third part is the preprocessor of discretization of computational domain and the postprocessor of visualization of numerical results. The early versions of commercial CFD codes usually applied the structured grid, which made the codes very difficult to deal with the industrial furnaces that may have very complicated geometry. Recently the new generation CFD codes, such as FLUENT/UNS, are based on the unstructured grid configurations, which make it possible to handle flexibly the very complicated geometry of an industrial furnace or boiler.

1.4 Objectives of the thesis

This thesis aims to use CFD technology to simulate and evaluate some new combustion processes and technologies for advanced industrial furnaces and boilers, such as moving grate bed furnace with a new air supply ECOTUBE system, pulverized fuel boiler, and highly preheated and diluted air combustion. To do so, a series of research of mathematical modeling have been carried out including the fluid flow, the grate bed process, the gas phase combustion, turbulent reacting flow and the NOx emissions in these different combustion systems. A new computational environment of Fluent/UNS, which is one of the largest commercial CFD codes based on unstructured grid, is employed to solve the numerical problems with the complicated geometry of industrial furnaces and boilers.

The technical objectives of this work include:

- Evaluation of air staging combustion technology applied to grate fired boilers,
- Evaluation of the performance of the Ecotube system for aerodynamic design for the grate fired boiler;
- Grate bed model;
- Comprehensive 3D numerical simulations for combustion and NOx emission in typical grate fired boilers;
- Simulation of aerodynamic performance of a pulverized coal and biomass co-firing boiler;
- Modeling of single jet highly preheated and diluted air combustion;
- Modeling of highly preheated and diluted air combustion furnace with a pair of regenerative burners.
1.5 Work environment

This thesis work is carried out using the computational fluid dynamics software Fluent/UNS code which is licensed by Fluent Inc. (Fluent Incorporated 1996, 1997, 1998, 1999). Fluent/UNS is a state-of-the art computer program for the modeling of fluid flow and heat transfer in complex geometry. It provides a complete mesh flexibility, as it solves fluid flow problems using unstructured grid that can be generated for complex geometry with relative ease. GeoMesh and TGrid from Fluent Inc., are also used for the geometry set-up and mesh generation. GeoMesh is a pre-processor for geometry modeling, block-structured mesh generation and unstructured triangular surface mesh generation in two and three dimensions. TGrid is a 2D triangular and 3D tetrahedral mesh generator that is used to generate 3D grid cases in this thesis work.

All the simulations are performed on an IBM Risc 6000/591 work station with 512 MB main memory running under the AIX version 4.1 Base Operating System. The workstation has two terminals and a color jet printer.
Chapter 2
Homogenous Turbulent Combustion Modeling

Basically, for a homogenous Newtonian fluid flow, the mathematical modeling is based on a set of coupled conservation equations of mass, momentum, energy, and chemical species transport and reactions, and the state equations of the fluid system. Furthermore, since most practical flows are turbulent, thus these conservation equations should be treated into the time-averaged or spatial filtered forms, which need to be closed by using additional turbulent models.

2.1 Basic governing equations

2.1.1 Conservation equations

The conservation equations of mass can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = S_i$$  \hspace{1cm} (2-1)

where $S_i$ is the mass source in the system.

For a multi-component system, the mass balance can be expressed as

$$\frac{\partial (\rho m_i)}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i m_i) = -\frac{\partial}{\partial x_i} J_{i,j} + R_i + S_i$$  \hspace{1cm} (2-2)

where $m_i$ is the local mass fraction of each species in the system.
$J_{i,j}$ is the diffusion flux of species $i'$, which arises due to concentration gradients.
$R_i$ is the mass rate of creation or depletion by chemical reaction.
$S_i$ is the mass rate of any other sources.

For laminar flows of dilute gas system, the diffusion flux meets the Fick’s law as

$$J_{i,j} = -\rho D_{i,m} \frac{\partial m_i}{\partial x_j}$$  \hspace{1cm} (2-3)

where $D_{i,m}$ is the diffusion coefficient for species $i'$ in the mixture.

The conservation equations of momentum can be described as Navier-Stokes equations as

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \tau_{ij} + S_{mi}$$  \hspace{1cm} (2-4)

where $p$ is the static pressure. $\tau_{ij}$ is the stress tensor. $S_{mi}$ is the momentum source in $i$ direction. The stress tensor $\tau_{ij}$ is given by

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_i}{\partial x_i} \delta_{ij}$$  \hspace{1cm} (2-5)
where $\mu$ is the molecular viscosity.

The conservation equations of energy can be written as

$$
\frac{\partial (\rho h)}{\partial t} + \frac{\partial (\rho hu_i)}{\partial x_i} = \frac{\partial p}{\partial x_i} + u_i \frac{\partial p}{\partial x_i} - \frac{\partial (k \frac{\partial T}{\partial x_i})}{\partial x_i} - \frac{\partial}{\partial x_i} h_j J_{ij} + \tau_{ik} \frac{\partial u_i}{\partial x_k} + S_h
$$

(2-6)

where

$$
h = \sum_j m_j h_j
$$

(2-7)

$$
h_j' = \tau_{i,j} c_{p,j} dT
$$

(2-8)

The energy source due to chemical reactions can be expressed as

$$
S_{h,\text{reaction}} = \sum_j \left[ \frac{h_j^0}{M_j} + \frac{\tau_{i,j} c_{p,j}}{\rho \rho} \right] R_j
$$

(2-9)

and the energy source due to radiation will be calculated in radiation models.

### 2.1.2 General transport equation

For a general variable $\phi$ of the fluid, such as mass or species, momentum, energy, the above conservation equations can be summarized into a general transport equation of $\phi$ as

$$
\frac{\partial (\rho \phi)}{\partial t} + \frac{\partial (\rho \phi u_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \Gamma_\phi \frac{\partial \phi}{\partial x_i} \right) + S_\phi
$$

(2-10)

where $\Gamma_\phi$ is the transport coefficient of the general variable $\phi$.

### 2.1.3 The state equation of system

For a perfect gas system, the state equations can be written as

$$
p = \rho RT = \rho RT \sum_{i=1}^{N} \frac{m_i}{M_i}
$$

(2-11)

where $m_i$ and $M_i$ are the mass fraction and the molecular weight of the $i$th species, respectively.

### 2.2 Turbulence models

The above basic governing equations for a homogenous Newtonian fluid flow form a closed set of partial differential equations (PDE). This situation is only suitable to solve numerically a laminar flow. For turbulence, it can be characterized as a three dimensional, time-dependent, chaotic, random and dissipative flow. In a turbulent flow, there exists an energy cascade corresponding to a wide range of length scales from
largest eddies (anisotropic integral length scales) to smallest eddies (isotropic Kolmogorov length scales) (Tennekes and Lumley 1972). By using dimensional analysis, it is known that in order to capture all length scales it needs a computational mesh with spatial grids in order of $O(Re^{3/4})$ and time steps in order of $O(Re^{3/4})$. Therefore, the direct numerical simulation (DNS) of a turbulent flow with a high Reynolds number in a complicated modern furnace or boiler is practically impossible to today’s computer capacity.

For most engineering applications, the time-averaged or spatial filtered properties of the flow are interested, thus the time-averaged transport equations, such as the Reynolds-averaged Navier-Stokes (RANS) equations, are established. However, time-averaged equations are unfortunately not closed and thus additional closure methods corresponding to different turbulence models have to be developed.

### 2.2.1 Time-averaged transport equations

By using Reynolds decomposition approach, an instantaneous flow variable $\phi$ can be decomposed as the mean variable $\bar{\phi}$ and the fluctuation variable $'\phi'$. For the sake of convenience, let $\phi$ denotes the mean variable $\bar{\phi}$ for the time-averaged transport equations. Thus, the time-averaged continuity equations can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = S_i$$  \hspace{1cm} (2-12)

where $\rho$, $u_i$, and $S_i$ are mean variables.

Reynolds-averaged Navier-Stokes (RANS) equations can be written as

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = \frac{\partial}{\partial x_j} \left( \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial \bar{u}_i}{\partial x_i} \right) - \frac{\partial \rho}{\partial x_j} + \frac{\partial}{\partial x_j} (-\bar{\rho} u_i u_j) + S_i$$  \hspace{1cm} (2-13)

where $-\bar{\rho} u_i u_j$ are Reynolds stresses ($\tau_{ij}$) and can be modeled using Boussinesq hypothesis as

$$-\bar{\rho} u_i u_j = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \left( \rho k + \mu \frac{\partial \bar{u}_i}{\partial x_i} \right) \delta_{ij}$$  \hspace{1cm} (2-14)

where $\mu$ is the turbulent viscosity.

Time-averaged transport equations can be written as

$$\frac{\partial (\rho \phi)}{\partial t} + \frac{\partial}{\partial x_i} (\rho \phi u_i) = \frac{\partial}{\partial x_j} \left( \Gamma \frac{\partial \phi}{\partial x_j} \right) + \frac{\partial}{\partial x_j} (-\bar{\rho} u_i '\phi') + S_{\phi}$$  \hspace{1cm} (2-15)

where the turbulent term $-\bar{\rho} u_i '\phi'$ can be taken to be proportional to the gradient of the mean variable $\phi$ as
\[ - \rho u'_i \phi = \Gamma \frac{\partial \phi}{\partial x_j} \tag{2-16} \]

where \( \Gamma \) is the turbulent transport coefficient of the mean variable \( \phi \).

It is obvious that in the time-averaged transport equations the turbulent transport coefficient, such as turbulent viscosity \( \mu_t \) in RANS, needs to be modeled.

### 2.2.2 The standard \( k-\epsilon \) model

Launder and Spalding (1972, 1974), and Jones (1982) developed the standard \( k-\epsilon \) model to close the time-averaged systemic PDEs. The \( k-\epsilon \) model equations are derived from the RANS equations, and the various model constants, relies on phenomenological considerations and empiricism. By using dimensional analysis, the turbulent viscosity \( \mu_t \) can be assumed as

\[ \mu_t = C \rho VL \tag{2-17} \]

where \( C \) is a dimensionless constant. \( V \) is the turbulent velocity scale (m/s), \( L \) is the turbulent length scale (m). According to dimensional analysis, the turbulent velocity scale, \( V \), and the length scale, \( L \), can be defined by using two quantities of turbulent kinetic energy \( k \) and its rate of dissipation \( \epsilon \).

\[ V = k^{1/2} \tag{2-18} \]
\[ L = \frac{k^{3/2}}{\epsilon} \tag{2-19} \]

Thus the turbulent viscosity can be evaluated by \( k \) and \( \epsilon \) as

\[ \mu_t = \rho C_{\mu} \frac{k^2}{\epsilon} \tag{2-20} \]

where \( C_{\mu} \) is a dimensionless constant.

In the standard \( k-\epsilon \) model, the \( k \) and \( \epsilon \) can be obtained from the following transport equations as

\[ \frac{\partial(\rho k)}{\partial t} + \frac{\partial (\rho u_i k)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_i} \right) + G_k + G_b - \rho \epsilon \tag{2-21} \]

\[ \frac{\partial(\rho \epsilon)}{\partial t} + \frac{\partial (\rho u_i \epsilon)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\mu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_i} \right) - \frac{\epsilon}{k} \left( G_k \left( 1 - C_{\epsilon} \right) + \frac{C_{\epsilon_e} \epsilon}{k} \right) - C_{\mu} \rho \epsilon \tag{2-22} \]

where \( G_k \) is the generation of \( k \) due to the turbulent stress as

\[ G_k = - \rho u_i u_j \frac{\partial u_j}{\partial x_i} = \tau_{ij} \frac{\partial u_j}{\partial x_i} \tag{2-23} \]

It can be evaluated by Boussinesq hypothesis as
$G_k = \mu, S^2$ \hspace{1cm} (2-24)

where $S$ is the modulus of the mean strain rate $S_{ij}$ as

$S \equiv \sqrt{2S_{ij}S_{ij}}$ \hspace{1cm} (2-25)

$S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$ \hspace{1cm} (2-26)

$G_b$ is the generation of $k$ due to the buoyancy as

$G_b = \beta g \mu \frac{\partial T}{\partial x_i}$ \hspace{1cm} (2-27)

where $Pr_t$ is the turbulent Prandtl number for temperature or enthalpy (0.85), and $\beta$ is the coefficient of thermal expansion as

$\beta = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p$ \hspace{1cm} (2-28)

The standard $k-\epsilon$ model constants $C_1\epsilon$, $C_2\epsilon$, $C_\mu$, $\sigma_k$, $\sigma_\epsilon$ have the following “standard” values as

$C_1\epsilon = 1.44$, $C_2\epsilon = 1.92$, $C_\mu = 0.09$, $\sigma_k = 1.0$, $\sigma_\epsilon = 1.3$

The boundary conditions for solving the equations of standard $k-\epsilon$ model are summarized in Table 2.1.

<table>
<thead>
<tr>
<th>Boundary Types</th>
<th>Boundary conditions (Launder and Spalding, 1974)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet:</td>
<td>Given $k$ and $\epsilon$ \hspace{1cm} $\partial k/\partial n = 0$ and $\partial \epsilon/\partial n = 0$</td>
</tr>
<tr>
<td>Outlet or symmetry axis:</td>
<td>$k = 0$ and $\epsilon = 0$ \hspace{1cm} Standard wall functions</td>
</tr>
<tr>
<td>Free stream:</td>
<td>$u^* = \frac{1}{\kappa} \ln \left( E y^* \right)$ \hspace{1cm} (2-29)</td>
</tr>
<tr>
<td>Solid walls:</td>
<td>where $u^* = \frac{u_x C_\mu^{1/4} k^{1/2}}{\tau_w/\rho}$ \hspace{1cm} (2-30)</td>
</tr>
<tr>
<td></td>
<td>$y^* = \frac{\rho C_\mu^{1/4} k^{1/2} y_p}{\mu}$ \hspace{1cm} (2-31)</td>
</tr>
<tr>
<td></td>
<td>$u_x$ is the mean velocity at point $P$ near the wall</td>
</tr>
<tr>
<td></td>
<td>$u_\tau = \sqrt{\tau_w/\rho}$ is the friction velocity</td>
</tr>
<tr>
<td></td>
<td>$y_p$ is the distance from point $P$ to the wall</td>
</tr>
<tr>
<td></td>
<td>$\kappa$ is Von Karman constant (0.42)</td>
</tr>
<tr>
<td></td>
<td>$E$ is the wall roughness (9.81 for smooth walls)</td>
</tr>
</tbody>
</table>
where $y^* < 11.225$

Wall-adjacent cells

$u^* = y^*$  \hspace{1cm} (2-33)

Wall-law for temperature

$T^* \equiv (T_w - T_P) \rho c_p C_{\mu}^{1/4} \frac{k_{P}^{1/2}}{k_{P}}$  \hspace{1cm} (2-34)

\[ q_w \begin{cases} 
\text{Pr} y^* + \frac{1}{2} \rho P_{r} \left( C_{\mu}^{1/4} \frac{k_{P}^{1/2}}{k_{P}} - u_{T}^{2} \right); (y^* < y_{T}^*) \\
\left( \frac{1}{k} \ln \left( E_{y}^{*} \right) + P \right) + \\
\frac{1}{2} \rho \left( C_{\mu}^{1/4} \frac{k_{P}^{1/2}}{k_{P}} \right) \left( P_{r} u_{T}^{2} + (P_{r} - P_{T}) u_{T}^{2} \right); (y^* > y_{T}^*)
\end{cases} \]

where $P = \frac{\pi / 4}{\sin(\pi / 4)} \left( \frac{A}{\kappa} \right)^{1/2} \left( \frac{P_{r}}{P_{T}} \right)^{1/4} \left( \frac{P_{T} - 1}{P_{T}} \right)^{1/4}$  \hspace{1cm} (2-35)

$T_w$ is the wall temperature

$T_P$ is the temperature at the cell adjacent to wall

$q_w$ is the wall heat flux

$Pr$ is the molecular Prandtl number

$Pr_t$ is the turbulent Prandtl number (0.85 at the wall)

$A$ is Van Driest constant (26)

$u_t$ is the mean velocity magnitude at $y^* = y_{T}^*$

$y_{T}^*$ is the thermal sublayer thickness

### 2.2.3 The RNG $k-\varepsilon$ model

By using renormalization group (RNG) methods, the RNG $k-\varepsilon$ model can be derived from the instantaneous NS equations (Choudhury 1993). The transport equations for turbulent kinetic energy $k$ and its dissipation rate $\varepsilon$ in RNG $k-\varepsilon$ model have the same forms as in the standard $k-\varepsilon$ model except of the additional quantities of the inverse effective Prandtl numbers $\alpha_k$ and $\alpha_\varepsilon$, and the $R$ term in the $\varepsilon$ equation.

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho u_i k)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \alpha_k \mu_{eff} \frac{\partial k}{\partial x_i} \right) + G_k + G_b - \rho \varepsilon \quad (2-36)
\]

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \alpha_\varepsilon \mu_{eff} \frac{\partial \varepsilon}{\partial x_i} \right) + C_{\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} - R \quad (2-37)
\]

where $\alpha_k = \alpha_\varepsilon = 1.393$ at high Reynolds numbers. $G_k$ and $G_b$ are the same as in Eqs.(2-23, 2-27).
\[ R = \frac{C_\mu \rho \eta^3 (1 - \eta / \eta_0) e^2}{1 + \beta \eta^3} \frac{e}{k} \]  
(2-38)

where \( \eta_0 = 4.38 \), \( \beta = 0.012 \) and

\[ \eta \equiv \frac{Sk}{\varepsilon} \]  
(2-39)

The effective viscosity can be solved by the following equations as

\[ d\left( \frac{\rho^2 k}{\sqrt{\varepsilon \mu}} \right) = 1.72 \frac{\dot{\nu}}{\sqrt{\dot{\varepsilon}^3 - 1 + C_v}} d\dot{\nu} \]  
(2-40)

\[ \dot{\nu} = \frac{\mu_{\text{eff}}}{\mu} \]  
(2-41)

where \( C_v = 100 \). At high Reynolds numbers, Eq.(2-40) becomes Eq.(2-20).

In the RNG \( k-\varepsilon \) model, the effects of swirl can be accounted by modifying the turbulent viscosity as

\[ \mu_t = \mu_{\text{eff}} f(\alpha_s, \Omega, \frac{k}{\varepsilon}) \]  
(2-42)

where \( \alpha_s \) is a swirl constant (0.05 at mildly swirling flows).
\[ \Omega \] is a characteristic swirl number.

The RNG \( k-\varepsilon \) model constants \( C_1 \varepsilon \) and \( C_2 \varepsilon \) have the following values:
\[ C_1 \varepsilon = 1.42, \quad C_2 \varepsilon = 1.68 \]

The boundary condition treatments for solving the equations of RNG \( k-\varepsilon \) model are the same as those for the standard model in Table 2.1.

In both \( k-\varepsilon \) model transport equations (2-22, 2-37), the model constant \( C_{3\varepsilon} \) for buoyancy term can be calculated as

\[ C_{3\varepsilon} = \tanh\left| \frac{\nu}{u} \right| \]  
(2-43)

where \( \nu \) is the velocity component parallel to the gravitational vector.
\( u \) is the velocity component perpendicular to the gravitational vector.

\[ C_{3\varepsilon} = \begin{cases} 
0; & \text{if the mean flow is perpendicular to the gravitational vector} \\
1; & \text{if the mean flow is parallel to the gravitational vector} 
\end{cases} \]
2.2.4 The $k-\varepsilon$ model via heat and mass transfer

The interaction of turbulence and heat transfer can be modeled using the same concept of Reynolds analogy. The turbulent energy transport equations can be written as

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}(u_i (\rho E + p)) = \frac{\partial}{\partial x_i}(k_{\text{eff}} \frac{\partial T}{\partial x_i} + u_j (\tau_{ij} \text{eff})) + S_h$$  \hspace{1cm} (2-44)

where $E$ is the total energy. $k_{\text{eff}}$ is the effective conductivity.

For the standard $k-\varepsilon$ Model,

$$k_{\text{eff}} = k + \frac{c_p \mu_i}{Pr_i}$$  \hspace{1cm} (2-45)

For the RNG $k-\varepsilon$ Model,

$$k_{\text{eff}} = \alpha c_p \mu_{\text{eff}}$$  \hspace{1cm} (2-46)

where $\alpha = 1/Pr$ in the viscosity-dominated region, and $\alpha = 1.393$ in the fully turbulent region (Kays, 1994).

The effective stress tensor, $(\tau_{ij})_{\text{eff}}$, which represents the viscous heating, is defined as

$$(\tau_{ij})_{\text{eff}} = \mu_{\text{eff}} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) - \frac{2}{3} \mu_{\text{eff}} \frac{\partial u_i}{\partial x_i} \delta_{ij}$$  \hspace{1cm} (2-47)

The interaction of turbulence and mass transfer can be modeled similarly. The turbulent mass transport equations can be written as

$$\frac{\partial}{\partial t}(\rho m_i) + \frac{\partial}{\partial x_i}(\rho u_i m_i) = -\frac{\partial}{\partial x_i}(D_{\text{eff}} \frac{\partial m_i}{\partial x_i}) + R_i + S_i$$  \hspace{1cm} (2-48)

where $m_i$ is the local mass fraction of each species in the system. $R_i$ is the mass rate of creation or depletion by chemical reaction. $S_i$ is the rate of creation by addition from the any sources. $D_{\text{eff}}$ is the effective diffusivity. For the standard $k-\varepsilon$ model,

$$D_{\text{eff}} = \rho D_{i,m} + \frac{\mu_i}{Sc_i}$$  \hspace{1cm} (2-49)

where $Sc_i$ is the turbulent Schmidt number (0.7).

For the RNG $k-\varepsilon$ model,

$$D_{\text{eff}} = \alpha c_p \mu_{\text{eff}}$$  \hspace{1cm} (2-50)

where $\alpha = 1/Sc$ in the diffusion-dominated region, and $\alpha = 1.393$ in the fully turbulent region.
2.2.5 The Reynolds stress model

By using Boussinesq relation of Eq.(2-14), the Reynolds stresses ($\rho \overline{u_i' u_j'}$) are linked to the mean flow velocities, such as in $k-\epsilon$ models. However, these kind models of first-moment closure approach are quite limited in predicting the flows with complex strain fields or significant body forces. This drawback advocated Launder et al (1975, 1989) to have developed a more complex second-moment closure approach, so called Reynolds stress model (RSM), in which the Reynolds stresses are modeled using both the mean flow velocities and the first-moment terms.

For the sake of convenience, the Reynolds stresses ($\rho \overline{u_i' u_j'}$) may denote $\rho u_i u_j$ and their transport equations can be derived as

$$
\frac{\partial (\rho u_i u_j)}{\partial t} + C_{ij} = D_{ij}^T + D_{ij}^L + P_{ij} + G_{ij} + \Pi_{ij} - \epsilon_{ij} + \Omega_{ij} \tag{2-51}
$$

where

Convection: $C_{ij} = \frac{\partial (\rho U_k u_i u_j)}{\partial x_k}$ \tag{2-52}

Turbulent diffusion: $D_{ij}^T = -\frac{\partial}{\partial x_k} \left( \rho u_i u_j u_k + p (\delta_{ki} u_i + \delta_{kj} u_j) \right)$ \tag{2-53}

Molecular diffusion: $D_{ij}^L = \frac{\partial}{\partial x_k} \left( \mu \frac{\partial (u_i u_j)}{\partial x_k} \right)$ \tag{2-54}

Stress production: $P_{ij} = -\rho \left( u_j u_k \frac{\partial U_j}{\partial x_k} + u_j u_k \frac{\partial U_i}{\partial x_k} \right)$ \tag{2-55}

Buoyancy production: $G_{ij} = -\rho \beta \left( g_j u_j \theta + g_j u_i \theta \right)$ \tag{2-56}

Pressure-strain interactions: $\Pi_{ij} = \rho \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$ \tag{2-57}

Rate of dissipation: $\epsilon_{ij} = 2\mu \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_j}$ \tag{2-58}

Rotation production: $\Omega_{ij} = -2\rho \Omega_k \left( u_j u_m \epsilon_{ikm} + u_j u_m \epsilon_{jkm} \right)$ \tag{2-59}

Eq.(2-51) contains 6 partial differential equations corresponding to the six Reynolds stresses of $u_1^2$, $u_2^2$, $u_3^2$, $u_1' u_2'$, $u_1' u_3'$, $u_2' u_3'$, and the terms $C_{ij}$, $D_{ij}^T$, $P_{ij}$, $\Pi_{ij}$, $\epsilon_{ij}$ need not any modeling, while terms $D_{ij}^L$, $G_{ij}$, $\Pi_{ij}$, $\epsilon_{ij}$ have to be modeled to close the equations.
Lien and Leschziner (1994) suggested a scalar turbulent diffusivity to model the $D_{ij}^T$ term as

$$D_{ij}^T = \frac{\partial}{\partial x_i} \left( \frac{\mu_i}{\sigma_k} \frac{\partial u_j}{\partial x_k} \right)$$  \hspace{1cm} (2-60)

where $\sigma_k = 0.82$ and the turbulent viscosity $\mu_i$ is calculated by

$$\mu_i = \rho C_\mu \frac{k^2}{\varepsilon}$$  \hspace{1cm} (2-61)

where $C_\mu = 0.09$.

For the most difficult term of pressure-strain interactions, Launder et al (1975, 1989) proposed a comprehensive model, in which different effects are decomposed respectively as

$$\Pi_{ij} = \Pi_{ij,\text{slow}} + \Pi_{ij,\text{rapid}} + \Pi_{ij,\text{wall}}$$  \hspace{1cm} (2-62)

For the slow pressure-strain:

$$\Pi_{ij,\text{slow}} = -C_i \rho \frac{\varepsilon}{k} (u_i u_j - \frac{2}{3} \delta_{ij} k)$$  \hspace{1cm} (2-63)

where $C_1 = 1.8$.

For the rapid pressure-strain:

$$\Pi_{ij,\text{rapid}} = -C_2 \left( \frac{P_{ij} + \Omega_{ij} + G_{ij} - C_{ij}}{2} \right) - \frac{2}{3} \delta_{ij} \left( P + G - C \right)$$  \hspace{1cm} (2-64)

where $C_2 = 0.6$, and $P = \frac{1}{2} P_{kk}$, $G = \frac{1}{2} G_{kk}$, and $C = \frac{1}{2} C_{kk}$.

For the wall-reflection:

$$\Pi_{ij,\text{wall}} = C_1' \frac{\varepsilon}{k} (u_i u_m n_k n_m \delta_{ij} - \frac{3}{2} u_i u_j n_k n_k - \frac{3}{2} u_j u_k n_k n_k - \frac{3}{2} u_k u_i n_k n_k) \frac{k^{1/2}}{C_i \varepsilon d}$$

$$+ C_2' \left( \frac{P_{ik,\text{rapid}} n_k n_m \delta_{ij} - 3 \frac{1}{2} \Pi_{ik,\text{rapid}} n_k n_k - \frac{3}{2} \Pi_{jk,\text{rapid}} n_k n_k} {C_i \varepsilon d} \right)$$  \hspace{1cm} (2-65)

where $C_1' = 0.5$, $C_2' = 0.3$. $n_k$ is the $x_k$ component of the unit normal to the wall. $d$ is the normal distance to the wall. $C_i = C_\mu^{3/4} / \kappa = (0.09)^{3/4} / 0.41 = 0.4$.

Usually, the turbulent pressure-strain term (2-57) can be simplified to use as

$$\Pi_j = -C_1 \frac{\varepsilon}{k} (u_j u_j - \frac{2}{3} k \delta_{ij}) - C_2 \left( P_{ij} - \frac{2}{3} P \delta_{ij} \right)$$  \hspace{1cm} (2-66)

where $C_1 = 1.8$ and $C_2 = 0.6$. 17
In RSM, though the turbulent kinetic energy, $k$, can be directly taken from the Reynolds stress $\frac{1}{2}u'_i u'_j$, the $k$ and its scalar dissipation rate, $\varepsilon$, can be obtained by solving their transport equations similar to that used in the standard $k$-$\varepsilon$ model as

$$\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho u_i k)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} + \frac{1}{2} \left( P_{ii} + G_{ii} \right) - \rho \varepsilon (1 + 2M_i^2) \quad (2-67)$$

$$\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} + \frac{1}{2} C_{\varepsilon 1} \varepsilon (P_{ii} + C_{\varepsilon 3} G_{ii}) - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k} \quad (2-68)$$

where $\sigma_k = 0.82$, $\sigma_\varepsilon = 1.0$, $C_{\varepsilon 1} = 1.44$, $C_{\varepsilon 2} = 1.92$. $C_{\varepsilon 3}$ can be treated as the same as $C_{\varepsilon 3}$ in (2-43) for $k$-$\varepsilon$ models. So, for a three dimensional problem, six Reynolds stress equations (2-51) together with $\varepsilon$ equation (2-68), totally seven equations have to be solved for RSM.

<table>
<thead>
<tr>
<th>Boundary types</th>
<th>Boundary conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet:</td>
<td>Given $u'_i u'_j$, and $\varepsilon$</td>
</tr>
<tr>
<td>Outlet:</td>
<td>$\partial (u'_i u'_j)/\partial n = 0$, and $\partial \varepsilon/\partial n = 0$</td>
</tr>
<tr>
<td>Free stream:</td>
<td>$u'_j u'_i = 0$, and $\varepsilon = 0$</td>
</tr>
<tr>
<td>Solid wall:</td>
<td>standard wall functions</td>
</tr>
</tbody>
</table>

The boundary conditions for the solving the Reynolds stress transport equations for elliptic flows are summarized in Table 2.2. The inlet conditions of Reynolds stresses and dissipation rate $\varepsilon$ can be obtained directly from the turbulent intensity, $I_i$, and the characteristic length, $L$, of the physical domain. In FLUENT, the turbulence is assumed as isotropic that $k = \frac{3}{2} u'_i^2$ and $u'_i u'_j = 0 (i \neq j)$. Two relations have to be used as

$$k = \frac{3}{2} \left( U_{avg} I_i \right)^2 \quad (2-69)$$

$$\varepsilon = C_{\mu}^{3/4} \frac{k^{3/2}}{0.07 L} \quad (2-70)$$

At the solid walls, the standard wall functions as shown in Table 2.1 for standard $k$-$\varepsilon$ model are also used. The wall-adjacent cell values of Reynolds stresses can be calculated by
\[
\begin{align*}
\bar{u}_{\tau\tau} / k &= 1.098 \\
\bar{u}_{\eta\eta} / k &= 0.247 \\
\bar{u}_{\lambda\lambda} / k &= 0.655 \\
-\bar{u}_{\tau\eta} / k &= 0.255
\end{align*}
\] (2-71)

where \( \tau, \eta, \) and \( \lambda \) denote the tangential, normal, and binormal coordinates in a local coordinate system for the wall. The \( k \) near the wall is obtained by solving its transport equation (2-67). However, instead of solving \( k \) transport equation, the wall-shear stress \( \tau_w \) can be employed as

\[
\rho u_{\tau\tau} / \tau_w = 5.1 \\
\rho u_{\eta\eta} / \tau_w = 1.0 \\
\rho u_{\lambda\lambda} / \tau_w = 2.3 \\
-\rho u_{\tau\eta} / \tau_w = 1.0
\] (2-72)

2.3 Radiation models

The energy source due to radiation in Eq.(2-6), \( S_{h,\text{radiation}} \), can be expressed as

\[
S_{h,\text{radiation}} = \frac{4\pi}{ds} I(\Omega) d\Omega
\] (2-73)

where \( I \) is the radiation intensity, a function of position \( s \) and solid angle \( \Omega \).

The radiation transfer equation (RTE) (Siegel and Howell 1992) for an absorbing, emitting, and scattering medium can be expressed as

\[
\frac{dI(s, \Omega)}{ds} + (a + \sigma_s) I(s, \Omega) = \frac{\sigma_s T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(s, \Omega) \Phi d\Omega
\] (2-74)

where, \( a \) is the absorption coefficient. \( \sigma_s \) is the scattering coefficient. \( \sigma \) is the Stefan-Boltzmann constant \((5.672 \times 10^{-8} \text{ W/m}^2 \text{ K}^4)\). \( T \) is the local temperature. \( \Phi \) is the phase function, and \((a + \sigma_s)\) is the optical thickness or opacity of the medium.

2.3.1 Discrete transfer radiation model

The discrete transfer (DT) radiation model (Shah 1979, Carvalho 1991) is a widely used radiation model to a wide range of optical thickness. It assumes that the radiation leaving the surface element in a certain range of solid angles can be approximated by a single ray, and the effect of scattering is neglected. Thus, the RTE is simplified as

\[
\frac{dI}{ds} + aI = \frac{a\sigma T^4}{\pi}
\] (2-75)
This equation is integrated along a series of rays emanating from boundary faces in each discrete control volume, by using the ‘ray tracing’ method that provides a prediction of radiation heat transfer between surfaces without explicit view-factor calculations. Its accuracy is limited mainly by the number of rays traced and the computational grid. The ray paths are calculated and stored firstly, and then are read in for the consequent calculations of fluid flow. To reduce the computational time, the ‘clustering’ method must be applied for a large computational case. In this situation, a number of radiating surfaces and absorbing cells are clustered into surface and volume ‘clusters’. To do so, the volume clusters are formed by starting from a cell and simply adding its neighbors and their neighbors until a specified number of cells per volume cluster is collected. Similarly, surface clusters are made by starting from a face and adding its neighbors and their neighbors until a specified number of face per surface cluster is collected. For the surface and volume clusters, it needs to calculate the incident radiation flux and the volume sources. The temperatures of the surface and volume clusters are then calculated as

\[
T_{sc} = \left| \frac{\sum \frac{A_f T_f^4}{A_f}}{A_f} \right|^\frac{1}{4}
\]

\[
T_{vc} = \left| \frac{\sum \frac{V_c T_c^4}{V_c}}{V_c} \right|^\frac{1}{3}
\]

where \(T_{sc}\) and \(T_{vc}\) are the temperatures of the surface and volume clusters respectively. \(A_f\) and \(T_f\) are the area and temperature of face \(f\). \(V_c\) and \(T_c\) are the volume and temperature of cell \(c\). The summations are carried over all faces of a surface cluster and all cells of a volume cluster.

The boundary conditions for DT radiation model are treated as shown in Table 2.3.
Table 2.3 Radiative boundary conditions for DT radiation model

<table>
<thead>
<tr>
<th>Boundary Type</th>
<th>Boundary Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wall conditions</td>
<td></td>
</tr>
<tr>
<td>The incident radiation heat flux, $q^-_{\text{rad}}$</td>
<td>$q^-_{\text{rad}} = I^- d\Omega$ (2-78)</td>
</tr>
<tr>
<td>The net radiation heat flux from the surface, $q^+_{\text{rad}}$</td>
<td>$q^+<em>{\text{rad}} = (1 - \varepsilon</em>\omega)q^-<em>{\text{rad}} + \varepsilon</em>\omega \sigma T^4$ (2-79)</td>
</tr>
<tr>
<td>The radiation intensity $I_0$ of a ray emanating from the point $P$</td>
<td>$I_0 = q^+_{\text{rad}} / \pi$ (2-80)</td>
</tr>
<tr>
<td>Flow inlets and outlets</td>
<td></td>
</tr>
<tr>
<td>The emissivity of all flow inlets and outlets can be assumed 1.0 as black body absorption but can be redefined.</td>
<td>The net radiation heat flux at flow inlets and outlets is computed in the same manner as at walls as described above.</td>
</tr>
</tbody>
</table>

In the Table 2.3, $\Omega$ is the hemispherical solid angle and $I^-$ is the intensity of the incoming ray. $T_\omega$ is the surface temperature of the point $P$ on the surface and $\varepsilon_\omega$ is the wall emissivity that is inputted as a boundary condition.

2.3.2 Discrete ordinates radiation model

In the discrete ordinates (DO) radiation model (Chui and Raithby 1990, 1993, Murthy and Mathur 1998), the RTE is expressed as

$$\frac{d(I_{s_i})}{dx_i} + (a + \sigma_s)I(r, s) = an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(r, s')\phi(s \cdot s')d\Omega'$$  (2-81)

where $s$ is the direction in terms of the spatial coordinates $x_i$, and $s_i$ are the components of $s$.

Different with DT radiation model, the DO radiation model uses the solution method of solving the fluid flow and energy equations to solve the set of radiation transport equations in terms of different directions, $s$. Furthermore, the DO model can include the radiation effects of a second phase. In this situation, the RTE can be written as

$$\frac{d(I_{s_i})}{dx_i} + (a + a_p + \sigma_s)I(r, s) = an^2 \frac{\sigma T^4}{\pi} + E_r + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(r, s')\phi(s \cdot s')d\Omega'$$  (2-82)

where $a_p$ is the equivalent absorption coefficient for the particulates. $\sigma_p$ is the equivalent particle scattering factor. $E_r$ is the equivalent emission. These parameters are defined as

$$a_p = \lim_{V \to 0, n \to 1} \varepsilon_{mn} \frac{A_{pn}}{V},$$  (2-83)

where $\varepsilon_{mn}$ is the emissivity. $A_{pn}$ is the projected area. $V$ is the volume.
\[ A_{pn} = \frac{\pi D_{pn}^2}{4}, \quad (2-84) \]

where \( D_{pn} \) is the diameter of the \( n \)th particle.

\[ \sigma_p = \lim_{V \to 0 \ n \to 1} N (1 - f_{pn})(1 - \varepsilon_{pn}) \frac{A_{pn}}{V} \quad (2-85) \]

where \( f_{pn} \) is the scattering factor of the \( n \)th particle.

\[ E_p = \lim_{V \to 0 \ n \to 1} N \varepsilon_{pn} A_{pn} \frac{\sigma T_{pn}^4}{\pi V} \quad (2-86) \]

where \( T_{pn} \) is the temperature of the \( n \)th particle.

The boundary condition treatments for the DO radiation model at Gray-Diffuse walls are listed in the Table 2.3.

<table>
<thead>
<tr>
<th>Boundary Type</th>
<th>Boundary Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gray-Diffuse Wall conditions</td>
<td></td>
</tr>
<tr>
<td>The incident radiation heat flux, ( q_{in} )</td>
<td>( q_{in} = I_{in} s \cdot n d\Omega )</td>
</tr>
<tr>
<td>The net radiation heat flux from the surface, ( q_{out} )</td>
<td>( q_{out} = (1 - \varepsilon_{\omega}) q_{in} + n^2 \varepsilon_{\omega} \sigma T_{\omega}^4 )</td>
</tr>
<tr>
<td>The radiation intensity ( I_0 ) of a ray emanating from the point ( P )</td>
<td>( I_0 = \frac{q_{out}}{\pi} )</td>
</tr>
<tr>
<td>Flow inlets and outlets</td>
<td></td>
</tr>
<tr>
<td>The emissivity of all flow inlets and outlets can be assumed 1.0 as black body absorption but can be redefined.</td>
<td>The net radiation heat flux at flow inlets and outlets is computed in the same manner as at walls as described above.</td>
</tr>
</tbody>
</table>

For the variable absorption coefficient, the weight sum of gray model (WSGGM) (Smith 1982) is more realistic than the simple gray gas model. In WSGGM, the total emissivity over the distance \( s \) can be described as

\[ \varepsilon = \sum_{i=0}^{l} a_{\varepsilon,i}(T)(1-\exp(-\kappa_i ps)) \quad (2-90) \]

where \( a_{\varepsilon,i} \) is the emissivity weighting factor for the \( i \)th fictitious gray gas. \( \kappa_i \) is the absorption coefficient of the \( i \)th gray gas. \( p \) is the sum of the partial pressures of all absorbing gases. \( s \) is the path length.
In the work, the values of parameters $a_{ei}$ and $\kappa_i$ are based on the literatures (Copalle 1983, and Smith 1982).

In addition of DT and DO radiation models, in this work, the Rosseland radiation model and P-1 radiation model (Cheng 1964) are also employed. These two radiation models are well addressed in the literatures (Siegel and Howell 1992).

### 2.4 Compressibility effects

In many combustion flows, including in grate fired boilers, the pressure is nearly constant so the heat release principally affects the density which usually decreases by the factor of five to eight as the absolute temperature increases by the same factor. But usually, the speed of travel of a flame is rarely larger than 1 m/s (except in explosions) much lower than the speed of sound and so are the fluid speeds. Thus we have the seemingly incongruous situation of a flow with large density changes that is essentially incompressible. However, on the other hand, the flame thickness is typically much smaller than any relevant fluid dynamic length scale so the density change occurs in a very small region. It is possible to compute these flows by solving the compressible equations of motion (Fletcher 1997). The problem is that methods designed for compressible flows become very inefficient when applied to low speed flows.

Sometimes, such as Ecotube system used in a grate fired boiler, the local velocity in combustion chamber may be very large (Mach number > 0.3), then the compressible flow properties have to be considered.

Compressible flows can be characterized by the value of the Mach number:

$$M = \frac{u}{c} \quad \text{(2-91)}$$

where $c$ is the speed of sound in the gas:

$$c = \sqrt{\gamma RT} \quad \text{(2-92)}$$

and $\gamma$ is the ratio of specific heats ($c_p / c_v$).

For compressible flows, the ideal gas law is written in the following form:

$$\rho = \frac{(p_{op} + p)}{RT_s} \quad \text{(2-93)}$$

where $p_{op}$ is the operating pressure and $p$ is the local static pressure relative to the operating pressure. The static temperature $T_s$ will be computed from the energy equation.
Compressible flows are described by the standard continuity and momentum equations. For high Mach number flows, compressibility affects turbulence through so-called ‘
dilatation’, which is normally neglected in the modeling of incompressible flows. Here, the dilatation dissipation is modeled following Sarkar’s proposal (1990).

In standard $k$-$\varepsilon$ model, the $k$ equation is modified as

$$\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho u_i k)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_b + \rho \varepsilon (1 + 2M_t^2) \quad (2-94)$$

where the turbulent Mach number, $M_t$, is defined as

$$M_t = \sqrt{k / \rho c^2} \quad (2-95)$$

For the heat transfer, the energy equation Eq.(2-44) correctly incorporates the coupling between the flow velocity and the static temperature while the viscous dissipation terms becomes important in high Mach number flows.

2.5 Gaseous turbulent combustion models

The reaction rate of gaseous reaction process is determined by the mixing of the reacting species, and by the reaction kinetics which is usually strongly depended on the reaction temperature in a combustion chamber. Actually, the combustion process, even only a simple fuel combustion, concerns hundreds intermediate reactions which are in practice impossible calculated in detail. Therefore, some simplifications and assumptions have to be done to deal with combustion reaction problems. The Arrhenius rate expressions, the eddy-dissipation concept of Magnussen and Hjertager (1976), and the mixture fraction / PDF approach are well-known and widely used methods of them.

2.5.1 The generalized finite rate reaction modeling

The $k$th reaction taking place in a combustion system that contains $N$ chemical species, can be described in general as

$$v_{r,k}^{i} S_{r}^{i} = k_{f,k}^{i} v_{r,k}^{i} S_{r}^{i} = k_{b,k}^{i} v_{r,k}^{i} S_{r}^{i} \quad (2-96)$$

where $k_{f,k}$ and $k_{b,k}$ are the forward and backward reaction rates for the $k$th reaction, respectively. $v_{r,k}^{i}$ and $v_{r,k}^{j}$ are stoichiometric coefficients for reactant and product in the $k$th reaction. $S_{r}^{i}$ stands for the symbol of chemical species $i$.

The molar reaction rate of species $i'$ in the $k$th reaction, can be expressed as

$$\dot{R}_{r,k} = (v_{r,k}^{i'} - v_{r,k}^{i'}) \left( k_{f,k}^{i} \prod_{j=1}^{N} (C_j)^{\eta_{r,j}} - k_{b,k}^{i} \prod_{j=1}^{N} (C_j)^{\eta_{r,j}} \right) \quad (2-97)$$
where \( C_{j'} \) is the molar concentration of each species \( j' \) (kmol/m\(^3\)). \( \eta_{j',k} \) is the rate exponent for reactant \( j' \) in the \( k \)th reaction. \( \eta_{j',k} \) is the rate exponent for product \( j' \) in the \( k \)th reaction.

The reaction source of species \( i' \), \( R_{i'} \), is the sum of the all reaction sources over the \( N_s \) reactions that the species may participate in, so

\[
R_{i'} = \sum_{k=1}^{N_s} R_{i',k} = M_{i'} \sum_{k=1}^{N_s} \frac{\dot{R}_{i',k}}{M_{i'}}
\]  

(2-98)

where \( R_{i',k} \) is the reaction rate in \( k \)th reaction. \( \dot{R}_{i',k} \) is the molar reaction rate in \( k \)th reaction. \( M_{i'} \) is the molecular weight of species \( i' \).

The reaction rates can be calculated using the standard Arrhenius rate expressions or the eddy-dissipation model, depending on whether the combustion process is controlled by chemical reactions or by the mixing of the turbulent eddies containing fluctuating species concentrations.

### 2.5.1.1 The Arrhenius rate

The Arrhenius rate expression of the forward reaction rate can be written as

\[
k_{f,k} = A_i T^{\beta_i} \exp\left(-\frac{E_i}{RT}\right)
\]

(2-99)

where \( A_i \) is the pre-exponential factor. \( \beta_i \) is the temperature exponent. \( E_i \) is the activation energy for the reaction (J/kmol). \( R \) is the universal gas constant (J/kmolK).

The backward reaction rate can be easily calculated using the equilibrium relation as

\[
k_{b,k} = \frac{k_{f,k}}{K_k}
\]

(2-100)

where \( K_k \) is the chemical equilibrium constant for the \( k \)th reaction. It can be calculated from the change of Gibbs free energy as

\[
K_k = \left(\frac{p}{RT}\right)^{\sum_{i=1}^{N_s} \eta_{i',k}} \exp(\Delta G / RT)
\]

(2-101)

and

\[
\Delta G = \sum_{j=1}^{N} (\nu_{j',k} - \nu_{j',k}) (S_{j'}^0 T - h_{j'}^0)
\]

(2-102)

where \( S_{j'}^0 \) is the standard state entropy, and \( h_{j'}^0 \) is the standard state enthalpy.

### 2.5.1.2 The eddy-dissipation model
Magnussen and Hiertager (1976) first considered the relation of the reaction rate to the dissipation rate of the reactant and product containing eddies, and suggested that the reaction rate can be the smaller of the two expressions below:

\[ R_{i,k} = v'_{i,k} M_j A \rho \frac{\varepsilon}{k} \frac{m_R}{M_R} \]  \hfill (2-103)

\[ R_{i,k} = v'_{i,k} M_j A B \rho \frac{\varepsilon}{k} \frac{m_P}{M_P} \]  \hfill (2-104)

where \( m_p \) is the mass fraction of product species \( P \), \( m_R \) is the mass fraction of a particular reactant \( R \). \( A \) and \( B \) are empirical constants equal to 4.0 and 0.5, respectively. \( k/\varepsilon \) represents the time scale of the turbulent eddies (Spalding 1970).

In the finite-rate/eddy-dissipation modeling, the smallest rate of those from the Arrhenius rate expression or the eddy dissipation model is used as the reaction rate, which is used as the source term in the species conservation and energy equations.

### 2.5.2 The mixture fraction / PDF modeling

Since the turbulence is one kind of random movement, the stochastic method is of course considered as a suitable way to deal with the turbulent reacting flows. It results in the mixture fraction and probability density function (PDF) approach (Sivathanu 1990) that has been developed for simulating the turbulent diffusion flames and similar reaction processes in which turbulent mixing is the limiting rate for reaction progress.

#### 2.5.2.1 Simplification of the combustion chemistry

There are two options for simplifying the combustion chemistry: the flame sheet approach (or mixed-is-burned), and the thermodynamic equilibrium assumption.

The flame sheet approach assumes that the chemical reactions are infinitely fast and irreversible, with fuel and oxidant species never coexisting in space and complete one-step conversion to final products. This simple system description yields linear relationships between the species mass fractions and the mixture fraction.

The equilibrium assumption implies that the chemical reactions are rapid enough for chemical equilibrium to always exist at the molecular level. In this situation, the minimization of Gibbs free energy method (Kuo 1986) can be used to compute species mole fractions from \( f \). The equilibrium model is quite powerful since it can predict the formation of intermediate species and it does not require the knowledge of detailed chemical kinetic rate data.

#### 2.5.2.2 Mixture fraction
A non-dimensional variable $f$ known as the mixture fraction (Sivathanu and Faeth 1990) can be defined as

$$ f = \frac{Z_k - Z_{kO}}{Z_{f} - Z_{kO}} $$  

(2-105)

where $Z_k$ is the mass fraction of the $k$th element, e.g. carbon. Subscript $O$ denotes the value at the oxidizer stream inlets, and subscript $F$ denotes the value at the fuel stream inlets. For a simple fuel/oxidizer system (Pun and Spalding 1967), the mixture fraction can be stated more simple in terms of the local fuel mass fraction as

$$ f = \frac{n_{kF}}{n_{kF} + n_{kO}} $$  

(2-106)

The value of the mixture fraction at each point in the flow domain is computed from the transport equation for the mean (time averaged) value of $f$ in the turbulent flow field as

$$ \frac{\partial (\rho \bar{f})}{\partial t} + \frac{\partial (\rho u_j \bar{f})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu_j}{\sigma_j} \frac{\partial \bar{f}}{\partial x_j} \right) + S_m $$  

(2-107)

where $S_m$ is the $\bar{f}$ source due to transfer of mass into the gas phase from the second phase.

In order to close the turbulence-chemistry model, the mixture fraction variance $\bar{f}^2$ can be computed by solving the transport equation of the variance $\bar{f}^2$ (Jones and Whitelaw 1982) as

$$ \frac{\partial (\rho \bar{f}^2)}{\partial t} + \frac{\partial (\rho u_j \bar{f}^2)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu_j}{\sigma_j} \frac{\partial \bar{f}^2}{\partial x_j} \right) + C_g \mu_j \left( \frac{\partial \bar{f}}{\partial x_j} \right)^2 - C_d \rho \frac{e}{k} \rho f^2 $$  

(2-108)

where the constants $\sigma, C_g$ and $C_d$ take the values 0.7, 2.86, and 2.0, respectively.

In general, an instantaneous thermochemical state of the fluid is related to the mixture fraction, so through calculation of a single conserved scalar field, $f$, other important scalars of interest can be derived without solving individual transport equations to describe them. In other words, given a description of the system chemistry, and certain other restrictions on the system, the mixture fraction value at each point in the flow field can be used to compute the instantaneous values of individual species mole fractions, density, and temperature.

If the reacting system is adiabatic, the instantaneous values of mole fractions, density, and temperature depend solely on the instantaneous mixture fraction as

$$ \phi = \phi (f) $$  

(2-109)

where $\phi$ represents the instantaneous species concentration, density, or temperature. While, in the case of nonadiabatic systems, it becomes as
\[ \phi_i = \phi_i(f, H^*) \]  
where \( H^* \) is the instantaneous enthalpy, computed by

\[
H^* = \sum_j m_j \left( \int_{T_{ref,j}}^T c_{p,j} dT + h_j^0(T_{ref,j}) \right)
\]  

(2-111)

Therefore, to predict the turbulent reacting flow is transformed into predict the time-averaged values of mixture fraction. How these time-averaged values of mixture fraction are related to the instantaneous values depends on the turbulence-chemistry interaction model. Here, the PDF approach (Janicka 1982, Pope 1985) is used as the closure model when the mixture fraction/ PDF modeling approach is used.

### 2.5.2.3 PDF approach

The probability density function, \( p(f) \), is defined as the fraction of time that the fluctuating variable \( f \) takes on a value between \( f \) and \( f + \Delta f \).

\[
p(f) \Delta f = \lim_{\tau_i \to 0} \frac{1}{\tau_i} \tau_i
\]  

(2-112)

where \( \tau_i \) is the time fraction that \( f \) spends in the range of \( \Delta f \).

The shape of \( p(f) \) depends on the nature of the turbulent fluctuations in \( f \), so it can be calculated from the mean mixture fraction, \( \bar{f} \), and its variance, \( \bar{f}^2 \). In practice, one of two mathematical functions, the double delta function and the beta function, can be used (Bilger 1980, Jones and Whitelaw 1982).

The double delta function PDF shape has the form as

\[
p(f) = \begin{cases} 0.5, & f = \bar{f} - \sqrt{\bar{f}^2} \\ 0.5, & f = \bar{f} + \sqrt{\bar{f}^2} \\ 0, & \text{elsewhere} \end{cases}
\]  

(2-113)

with suitable bounding near \( f = 1 \) and \( f = 0 \).

The \( \beta \) function PDF shape has the form as

\[
p(f) = \frac{f^{\alpha-1}(1-f)^{\beta-1}}{\int_0^1 f^{\alpha-1}(1-f)^{\beta-1} df}
\]  

(2-114)

where

\[
\alpha = \bar{f}\left| \frac{\bar{f}(1-\bar{f})}{\bar{f}^2} - 1 \right|
\]  

(2-115)
and

\[
\beta = (1 - \bar{f}) \left| \frac{\bar{f}(1 - \bar{f})}{f^2} - 1 \right|
\]

(2-116)

The double delta function is more easily computed, while the \( \beta \) function is thought to represent more closely experimentally observed PDF.

In an adiabatic single mixture fraction system, time-averaged values of species mole fractions and temperature can be calculated by

\[
\bar{\phi}_i = \frac{1}{\rho} \rho_i \phi_i(f) \, df
\]

(2-117)

The time-averaged fluid density can be calculated as

\[
\frac{1}{\rho} = \frac{1}{\rho} \rho(f) \, df
\]

(2-118)

where \( \rho(f) \) is the instantaneous density obtained using the instantaneous species mole fractions and temperature in the gas law equation. It is more accurate than the approach of using directly the gas law.

In a nonadiabatic system, turbulent fluctuations should be accounted for by means of a joint PDF \( p(f, H^*) \). The computation of \( p(f, H^*) \) is not practical for most engineering applications. However, the problem can be simplified significantly by assuming that the enthalpy fluctuations are independent of the enthalpy level. Then, \( p = p(f) \) is still kept and

\[
\bar{\phi}_i = \frac{1}{\rho} \phi_i (f, H^*) p(f) \, df
\]

(2-119)

Therefore, in order to calculate \( \bar{\phi}_i \), the time averaged enthalpy \( \bar{H}^* \) should be solved first from the modeled transport equation of \( \bar{H}^* \) as

\[
\frac{\partial}{\partial x_i} (\rho u_i \bar{H}^*) = \frac{\partial}{\partial x_i} \left( k_i \frac{\partial \bar{H}^*}{\partial x_i} \right) + \tau_{ik} \frac{\partial u_i}{\partial x_k} + S_h
\]

(2-120)

where \( S_h \) is the source terms due to radiation heat transfer to wall boundaries and heat exchange with the second phase.

2.6 Large eddy simulation
Turbulence can be characterized as a three dimensional, time-dependent, chaotic, random and dissipative flow. According to Kolmogorov theory (1941, 1991), in a turbulent flow, the turbulent energy spectrum has a cascade corresponding to a wide range of length scales from largest eddies (anisotropic integral length scales) to smallest eddies (isotropic Kolmogorov length scales). The largest eddies are typically comparable in size to the characteristic length of the mean flow, while the smallest scales are responsible for the dissipation of the turbulent kinetic energy (Tennekes and Lumley 1972). The direct numerical simulation (DNS) can in principle resolve the whole spectrum of turbulent scales. However, DNS is not feasible for practical engineering problems for the mesh size in three dimensions for DNS is proportional to \(O(Re^{9/4})\), and the number of time steps required for \(n\) cycle iterations for DNS is proportional to \(nO(Re^{9/4})\).

In the large eddy simulation (LES), it only resolves directly the large eddies of turbulent flows, while small eddies are modeled. In non-premixed turbulent combustion, the rate of mixing is determined by the motions of the largest eddies. The size, orientation, and rate of rotation of these eddies depends on the particular flow configuration and the geometry. Reynolds stress model (RSM) cannot directly capture the dynamics of the large, mixing-controlling eddies. Instead, LES is to simulate the motions of the largest eddies in a turbulent flow so that only the small scales of turbulence need to be modeled. Since the small eddies contain only a small portion of the total turbulent kinetic energy, the computed flows are usually less sensitive to the turbulence modeling. This LES strategy results in a significant reduction of both the mesh size with the order of \(O(Re^{3/2})\) and the number of time steps for \(n\) cycles iterations with the order of \(nO(Re^{1/2})\). Thus, LES is more feasible for a higher Reynolds number flow than DNS. The first use of LES can be traced back to the work of Lilly (1966) and Deardorff (1970). Since their pioneering studies, there has been considerable success in utilizing LES for a wide variety of problems (Piomelli and Liu 1995, Jones 1996, Olsson 1997, Moin 1997, Cook 1998, DesJardin 1998, Gullbrand 1999). Different with the time-averaged method used in RANS, in LES, the space filtering procedure is applied to the governing equations with a filter function.

### 2.6.1 Filtered governing equations

For turbulent reacting flows, a Favre-filtered variable \(\tilde{\phi}(x,t)\) can be defined as

\[
\overline{\rho \phi}(x,t) = \overline{\rho \tilde{\phi}}(x,t) = \int_D \rho \phi(x', t) G(x, x') dx'
\]

where the overbar “~” denotes a grid-scale filter. \(D\) is the fluid domain. \(G\) is a top-hat filter function. For the finite volume method, the top-hat filter takes the form as

\[
G(x, x') = \begin{cases} \frac{1}{V}, & x' \in V \\ 0, & x' \notin V \end{cases}
\]
so the filtered variable becomes

\[ \bar{\rho} \tilde{\phi} (x, t) = \frac{1}{V} \int_D \rho \phi (x', t) dx', \quad x' \in V \]  

(2-123)

Then, the filtered governing equations of continuity, momentum, energy and species, can be written as (DesJardin 1998)

\[ \frac{\partial \bar{p}}{\partial t} + \frac{\partial \bar{p} \bar{u}_i}{\partial x_i} = 0 \]  

(2-124)

\[ \frac{\partial \bar{p} \bar{u}_i}{\partial t} + \frac{\partial \bar{p} \bar{u}_i \bar{u}_j}{\partial x_j} = - \frac{\partial \bar{p}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} \]  

(2-125)

\[ \frac{\partial (\bar{p} \bar{u}_i \bar{u}_j + \bar{u}_i \bar{p})}{\partial t} + \frac{\partial (\bar{p} \bar{u}_i \bar{u}_j + \bar{u}_i \bar{p})}{\partial x_j} = \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial \bar{q}_i}{\partial x_j} \]  

(2-126)

\[ \frac{\partial \bar{p} \bar{Y}_m}{\partial t} + \frac{\partial \bar{p} \bar{Y}_m \bar{u}_i}{\partial x_i} = \frac{\partial \bar{r}_m}{\partial x_i} - \frac{\partial \bar{q}_m}{\partial x_i} + \bar{R}_m \]  

(2-127)

where \( E \) is the total energy, \( Q \) is the subgrid kinetic energy. \( Y_m \) is mass fraction of species \( m \) in the mixture. \( \bar{R}_m \) is the filtered chemical reaction rate for species \( m \). \( \tau_{ij} \) is the filtered viscous stress tensor expressed using resolved variables by Newton’s law as

\[ \tau_{ij} = \frac{\mu(\tilde{T})}{Re} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \frac{\mu(\tilde{T})}{Re} \frac{\partial \bar{u}_i}{\partial x_k} \delta_{ij} \]  

(2-128)

\( \bar{q}_i \) is the heat flux vector expressed using resolved variables by Fourier’s law as

\[ \bar{q}_i = - \frac{\mu(\tilde{T})}{(\gamma - 1)M^2 \text{Pr} \text{Re}} \left( \frac{\partial \tilde{T}}{\partial x_i} - \frac{Ce}{Le} \frac{\partial \bar{Y}_p}{\partial x_i} \right) \]  

(2-129)

\( \bar{q}_m \) is the filtered species diffusion vector expressed using resolved variables by Fick’s law as

\[ \bar{q}_m = - \frac{\mu(\tilde{T})}{Sc \text{Re} \frac{\partial \bar{Y}_m}{\partial x_i}} \]  

(2-130)

where \( Sc = 1.0, \text{Pr} = 0.7, Le = 1.43, Ce = 0.5. \bar{Y}_p \) is the product species mass fraction.

In Eqs.(2-124, 125, 126, 127), the unknowns of \( \tau_{ij}, \tau_{ij}, \tau_{ij}, \bar{q}_i, \bar{q}_i, \bar{q}_i, \bar{q}_i, \bar{q}_i, \bar{q}_i \) are subgrid-scale (SGS) correlations and have to be modeled to close the filtered governing equations.
2.6.2 Subgrid-scale turbulent model

In SGS turbulent model (2-125), the SGS stress tensor is defined as

\[ \tau_{u_i u_j} \equiv \rho \ddot{u}_i \ddot{u}_j - \rho \ddot{u}_i \ddot{u}_j \]  \hspace{1cm} (2-131)

Basically, in the simple situation of incompressible flows, the SGS stress tensor can be modeled by the concept of eddy viscosity and the gradient of resolved velocity similar to Boussinesq hypothesis as

\[ \tau_{u_i u_j} - \frac{1}{3} \tau_{u_i u_j} \delta_{ij} = -2 \mu_s \ddot{S}_{ij} \]  \hspace{1cm} (2-132)

where \( \mu_s \) is the sub-grid-scale turbulent viscosity, and \( \ddot{S}_{ij} \) is the rate of strain as

\[ \ddot{S}_{ij} \equiv \frac{1}{2} \left( \frac{\partial \ddot{u}_i}{\partial x_j} + \frac{\partial \ddot{u}_j}{\partial x_i} - \frac{\partial \ddot{u}_k}{\partial x_i} \delta_{jk} \right) \] \hspace{1cm} (2-133)

The SGS turbulent viscosity \( \mu_s \) can be calculated by using Smagorinsky-Lilly model (1963, 1966) as

\[ \mu_s = C_s \rho L_s^2 \sqrt{2 \ddot{S}_{ij} \ddot{S}_{ij}} \] \hspace{1cm} (2-134)

where \( L_s \) is the mixing length for subgrid scales. For the finite volume method, it can be calculated as

\[ L_s = \min(\kappa d, C_s V^{1/3}) \] \hspace{1cm} (2-135)

where \( \kappa = 0.42 \) and \( C_s = 0.1 \). \( d \) is the distance to the closest wall, and \( V \) is the mesh cell volume.

It was found that the SGS stress modeled by the Smagorinsky-Lilly model correlates poorly with the SGS stress obtained from filtering fully resolved DNS and experimental velocity fields (Clark 1979, Liu 1994). Furthermore, the SGS stress model is an absolutely dissipative model, which takes account of the transport of energy only from large-scale eddies to small-scale eddies. Other more sophisticated SGS turbulent models are well addressed in literature (Moin 1991, Germano 1991, Olsson 1997, DesJardin 1998).

2.6.3 LES interaction with combustion

Until recently, LES has not been applied to practical combustion problems yet. There exists a big difficulty for LES to be applied to combustion problems because the flame thickness is typically smaller than the computational mesh size and is therefore not resolved in simulations (Libby 1994). To overcome this difficulty, some approaches have been proposed, such as, simulation of an artificially thickened flame (Butler 1977, O’Rourke 1979), use of a flame-front tracking technique “G-equation” (Kerstein 1988),...
and flame surface density concept (Boger 1998), etc. Usually, there are two different classes of SGS combustion models: the conserved scalar approach and the direct closure approach (Bilger 1980). The first class of SGS combustion model employs an assumed form for the probability density function of a scalar variable within a mesh cell volume, such as the large eddy probability density function (LEPDF) method (Gao 1993). It has been shown that an assumed LEPDF method could be used in LES of non-premixed turbulent reacting flows with both equilibrium and finite rate chemistry (Frankel 1993). Recently, based on an assumed LEPDF method in conjunction with the laminar flamelet concept, a new SGS chemistry model termed the large eddy laminar flamelet model (LELFM), was developed for the filtered chemical species to the incompressible and compressible flows with multi-step, Arrhenius-rate chemistry (Cook 1998). Another class of SGS combustion model attempts to model the effect of SGS fluctuations on the filtered reaction rate $\bar{R}_m$ in Eq.(2-127). Recently, DesJardin (1998) investigated both two classes of SGS combustion models. The tendency seems to develop more complex SGS combustion models that considering the uncertainties of SGS turbulence models. However, for practical combustion problems or some other purposes, it seems advisable to use the simplest SGS turbulent model combined with an eddy dissipation conception (EDC) (Magnussen 1976) combustion model. In this strategy, Bai (1997) proposed a mixing rate modeled using the resolved vorticity scales. This simple SGS combustion model was also used for investigating a high order Cartesian grid method (Gullbrand 1998).

In the present work (paper 6), the hybrid procedures of the standard SGS Smagorinsky model combined with the finite rate/EDC model or mixture fraction/PDF model have been investigated to simulate a single wall jet HPDAC furnace chamber. The incompressible SGS turbulent model as (2-132 to 2-135) is employed to calculate the turbulent flow while the combustion is simulated using the finite rate/EDC model in the RANS framework. To realize this hybrid simulation, a switching-iterative procedure is used as listed in Figure 2.1, in which the results of the RSM/EDC combustion model are set as the initial conditions for the beginning of the LES calculation. After certain long iterations when the LES results become statistically independent of initial conditions, the calculation is then switched to the RSM/EDC model again. This time-dependent switching-iteration cycle should be continued until a convergent and statistical steady state is reached.

```
Start

$t = 0$
```
The boundary conditions for solving incompressible LES models are listed in Table 2.4.

Table 2.4. The boundary conditions for LES

<table>
<thead>
<tr>
<th>Boundary types</th>
<th>Boundary conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet:</td>
<td>( \bar{u} = \bar{u}_i &gt; + I \psi \bar{u} ) \hspace{1cm} (2-136)</td>
</tr>
<tr>
<td></td>
<td>where ( I ) is the intensity of the fluctuation. ( \psi ) is a Gaussian random number.</td>
</tr>
<tr>
<td>Solid wall:</td>
<td>wall function</td>
</tr>
<tr>
<td>Fine mesh:</td>
<td>( \frac{\bar{u}}{u_{\tau}} = \frac{\rho u_{\tau} y}{\mu} = y^+ ) \hspace{1cm} (2-137)</td>
</tr>
<tr>
<td>Coarse mesh:</td>
<td>( \frac{\bar{u}}{u_{\tau}} = \frac{1}{\kappa} \ln E\left( \frac{\rho u_{\tau} y}{\mu} \right) ) \hspace{1cm} (2-138)</td>
</tr>
</tbody>
</table>

For LES, though there are no restrictions on the near-wall mesh spacing, it is better to use a very fine near-wall mesh spacing in the order of \( y^+ = 1 \).

The results of the hybrid LES and RSM/EDC are found in acceptable agreement with the corresponding results of in-furnace measurements and physical modeling. By compared with the pure RSM, it is found that the differences between the two
predictions of the hybrid LES and RSM are insignificant in the near field of the flow. The Smagorinsky constant $C_s$ has been also tuned in the work. It illustrates that $C_s$ value significantly influences the predictions on both near field and far field of the jet flow. Though, further investigations are needed to validate the SGS stress models and parameters, it is found that LES is an attractive tool to simulate the dynamic processes of turbulent reacting flows for the HPDAC furnaces.
Chapter 3
NO\textsubscript{x} Modeling

NO\textsubscript{x} has been considered as one of main air pollutants. The control of NO\textsubscript{x} emissions is therefore one of main tasks for the design and operation of advanced industrial burners and furnaces. The term NO\textsubscript{x} appeared in combustion literature usually represents mainly the nitric oxide NO and insignificant parts of other nitrogen oxides (nitrogen dioxide NO\textsubscript{2} and nitrous oxide N\textsubscript{2}O), hence, the NO\textsubscript{x} denotes the NO only in the this chapter. In the work, a state of the art NO\textsubscript{x} postprocessor in FLUENT for thermal NO, prompt NO and HCN route fuel NO has been used for engineering applications of NO\textsubscript{x} modeling. In addition, the NH\textsubscript{3} route fuel NO based on the global De Soete model, and a selective non-catalytic reduction of nitrogen oxides (SNCR) scheme have been also proposed. The details of NO\textsubscript{x} modeling are described below.

3.1 NO\textsubscript{x} formation in combustion

There are three different chemical mechanisms of NO formation in combustion, corresponding to three different names as thermal NO, prompt NO, and fuel NO. According to Zel'dovich mechanism (1946), the thermal NO is due to the direct oxidation of molecular nitrogen N\textsubscript{2} in hot flames and can be described as

\begin{align*}
N_{2} + O &\rightarrow NO + N \quad (3-1) \\
N + O_{2} &\rightarrow NO + O \quad (3-2) \\
N + OH &\rightarrow NO + H \quad (3-3)
\end{align*}

In a conventional furnace, the thermal NO emission will be much significant when the temperature is over 1500°C. Prompt NO is due to the hydrocarbon fragments, mainly CH and CH\textsubscript{2}, attacking molecular nitrogen N\textsubscript{2}. According to Fenimore (1971), the prompt NO is formed in the fuel rich zone with low temperature and short residence time, and can be described as

\begin{align*}
CH + N_{2} &\rightarrow HCN + N \quad (3-4) \\
CH_{2} + N_{2} &\rightarrow HCN + NH \quad (3-5) \\
N + O_{2} &\rightarrow NO + O \quad (3-6) \\
HCN + OH &\rightarrow CN + H_{2}O \quad (3-7) \\
CN + O_{2} &\rightarrow NO + CO \quad (3-8)
\end{align*}

Fuel NO\textsubscript{x} is due to the oxidation of fuel nitrogen-bound compounds (fuel-N). Generally, the fuel-N is a particularly important source of NO emissions for solid fuels of coal and biomass, which typically contain 0.1~0.4% nitrogen by weight. The extent of conversion of fuel-N to NO is dependent on the local combustion characteristics and its initial concentration. Fuel-N compounds are released into the gas phase when the fuel is heated during the devolatilization stage. From the thermal decomposition of these compounds in the reaction zone, radicals such as HCN, N, CN, and NH can be formed and converted to NO. The above free radicals are subject to a double competitive reaction path. According to Houser (1980, 1988), HCN will be the principal product if fuel-N is present in aromatic or cyclic form, while NH\textsubscript{3} may become the principal product of fuel-N conversion if fuel-N is present in the form of aliphatic amines. The detailed route of fuel NO formation and destruction is still not completely understood, however, it can be drafted using a simplified model (Wendt 1991) as shown in Figure 3.1.
3.2 NO kinetic models

The transport equation of NO species can be written as
\[ \rho \frac{\partial Y_{NO}}{\partial t} + \rho u_i \frac{\partial Y_{NO}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y_{NO}}{\partial x_i} \right) + S_{NO} \] (3-9)
where \( Y_{NO} \) is the mass fraction in the gas phase, and the source term \( S_{NO} \) includes thermal NO, prompt NO and fuel NO. In addition, the transport equations of the important intermediates, HCN and \( NH_3 \) in fuel NO mechanism, can be written as
\[ \rho \frac{\partial Y_{HCN}}{\partial t} + \rho u_i \frac{\partial Y_{HCN}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y_{HCN}}{\partial x_i} \right) + S_{HCN} \] (3-10)
\[ \rho \frac{\partial Y_{NH_3}}{\partial t} + \rho u_i \frac{\partial Y_{NH_3}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y_{NH_3}}{\partial x_i} \right) + S_{NH_3} \] (3-11)
where \( Y_{HCN} \) and \( Y_{NH_3} \) are mass fractions of HCN and \( NH_3 \) in the gas phase, respectively.

3.2.1 Thermal NO kinetics

Considering the reactions (3-1, 3-2, 3-3), the net rate of formation of NO is governed by
\[ \frac{d[N_{\text{NO}}]}{dt} = k_1 [O][N_2] + k_2 [N][O_2] + k_3 [N][OH] \]
\[ - k_{-1} [NO][N] - k_{-2} [NO][O] - k_{-3} [NO][H] \] (3-12)
where \( k_1, k_2, k_3 \) are the rate coefficients for positive reactions, while \( k_{-1}, k_{-2}, k_{-3} \) are for negative reactions. By using the Quasi-Steady assumption for [N] and neglecting the third reaction of [OH], it becomes

\[
\frac{d[NO]}{dt} = \frac{2[O]k_2k_3[O_2][N_2] - k_{-1}k_{-2}[NO]^2}{k_1[O_2] + k_{-1}[NO]} \tag{3-13}
\]

where the rate constants are determined by experiments (Hanson and Salimian 1984) as

\[
k_1 = 1.8 \times 10^8 \exp(-38370/T) \text{ m}^3 \text{ mol}^{-1} \text{ s}^{-1}
\]
\[
k_{-1} = 3.8 \times 10^7 \exp(-425/T) \text{ m}^3 \text{ mol}^{-1} \text{ s}^{-1}
\]
\[
k_2 = 1.8 \times 10^4 T \exp(-4680/T) \text{ m}^3 \text{ mol}^{-1} \text{ s}^{-1}
\]
\[
k_{-2} = 3.8 \times 10^3 T \exp(-20820/T) \text{ m}^3 \text{ mol}^{-1} \text{ s}^{-1}
\]

Furthermore, in the formula (3-13), the [O] can be expressed by using [O_2] according to the assumption of the equilibrium assumption of [O] (Westenberg 1971) as

\[
[O] = 3.97 \times 10^8 T^{-0.5} [O_2]^{0.5} \exp(-31090/T) \text{ mol m}^{-3} \tag{3-15}
\]

So, one has

\[
\frac{d[NO]}{dt} = \frac{7.94 \times 10^5 T^{-0.5} [O_2]^{0.5} \exp(-31090/T)(k_1k_2[O_2][N_2] - k_{-1}k_{-2}[NO]^2)}{k_1[O_2] + k_{-1}[NO]} \tag{3-16}
\]

Thus, the NO source term in Eq.(3-9) due to thermal NO can be written as

\[
S_{thermal, NO} = M_{NO} \frac{7.94 \times 10^5 T^{-0.5} [O_2]^{0.5} \exp(-31090/T)(k_1k_2[O_2][N_2] - k_{-1}k_{-2}[NO]^2)}{k_1[O_2] + k_{-1}[NO]} \tag{3-17}
\]

where \( M_{NO} \) is the molecular weight of NO.

### 3.2.2 Prompt NO kinetics

In prompt NO formation, the process is mainly controlled by reactions (3-4, 3-5) of hydrocarbon radicals, CH and CH_2. Thus, the kinetic equation of prompt NO formation can be simplified as

\[
\frac{d[NO]}{dt} = f_s k_{ps} [O_2]^p [N_2]^{FUEL} \exp \left( - \frac{E_a}{RT} \right) \tag{3-19}
\]

where \( f_s \) is the de Soete model’s correction factor and can be calculated as
\[ f_s = 4.75 + 0.0819n - 23.2\phi + 32\phi^2 - 12.2\phi^3 \]  
(3-20)

where \( n \) is the number of carbon atoms per molecule of the hydrocarbon fuel, and \( \phi \) is the equivalence ratio.

\( k_{pr}' \) and \( E'_a \) are experimental constants (Dupont 1993). \( \alpha \) is the oxygen reaction order that depends on experimental conditions as

\[
\begin{align*}
   a &= 1.0, & \chi_{O_2} < 4.1 \times 10^{-3} \\
   & -3.95 - 0.9 \ln \chi_{O_2}, & 4.1 \times 10^{-3} < \chi_{O_2} < 1.11 \times 10^{-2} \\
   & -0.35 - 0.1 \ln \chi_{O_2}, & 1.11 \times 10^{-2} < \chi_{O_2} < 0.03 \\
   & 0, & \chi_{O_2} > 0.03
\end{align*}
\]

(3-21)

Thus, the NO source term in Eq.(3-9) due to prompt NO can be written as

\[
S_{\text{prompt NO}} = M_{NO} f_s k_{pr}' \left[ O_2 \right] [N_2 FUEL] \exp \left( -\frac{E_a}{RT} \right)
\]

(3-22)

3.2.3.1 Fuel NO\textsubscript{x} kinetics

3.2.3 Fuel NO\textsubscript{x} kinetics

3.2.3.1 HCN route

In Fluent code, the HCN route fuel NO has been employed, in which the HCN is the domain fuel-N species. For liquid fuels, the route can be simplified as shown in Figure 3.2.

![Figure 3.2 The HCN route NO for liquid fuel-N](image)

The source terms in the transport equations (3-9, 3-10) can be described as a set of equations as

\[
\begin{align*}
   S_{NO} &= S_{NO-1} + S_{NO-2} \\
   S_{HCN} &= S_{pHHCN} + S_{HCN-1} + S_{HCN-2}
\end{align*}
\]

(3-23)

(3-24)

\[
\begin{align*}
   S_{pHHCN} &= S_{p,HCN} m_{NF} \frac{M_{HCN}}{M_N} / V \\
   S_{HCN-1} &= -R_1 M_{HCN} P / RT
\end{align*}
\]

(3-25)

(3-26)
\[ S_{HCN-2} = -R_2 M_{HCN} P / RT \]  

(3-27)

where \( S_{pl, HCN} \) is the rate of HCN production which is equal to the rate of fuel release into the gas phase. \( S_r \) is the release rate of fuel into gas phase. \( m_{nf} \) is the mass fraction of nitrogen in fuel. \( V \) is the cell volume. \( P \) is pressure, and \( \bar{T} \) is the mean temperature (K). \( R_1 \) and \( R_2 \) are conversion rates of HCN (1/s) in reactions (1) and (2) respectively. According to De Soete model (1975), the global conversion rates can be expressed as

\[ R_1 = A_1 x_{HCN} x_{O_2}^\alpha \exp(-E_1 / RT) \]  

(3-28)

\[ R_2 = A_2 x_{HCN} x_{NO} \exp(-E_2 / RT) \]  

(3-29)

where \( \alpha \) is the oxygen reaction order as in (3-21). \( T \) is the instantaneous temperature. \( x \) is the mole fraction and

\[ A_1 = 3.5 \times 10^{10} \text{ 1/s} \]
\[ A_2 = 3.0 \times 10^{12} \text{ 1/s} \]
\[ E_1 = 67000 \text{ Cal/mol} \]
\[ E_2 = 60000 \text{ Cal/mol} \]

Considering the relation of mole fraction \( x_{HCN} \) to mass fraction \( Y_{HCN} \) as

\[ x_{HCN} = \frac{Y_{HCN}}{M_{HCN}} \left( \frac{\rho RT}{P} \right) \]  

(3-30)

thus the source term of fuel NO in Eq. (3-23) can be expressed as

\[ S_{fuel, NO} = (R_1 - R_2) \frac{M_{NO} P}{RT} \]  

(3-31)

For solid fuels, the simplified route (Lockwood 1992) can be drafted as shown in Figure 3.3.

![Figure 3.3 The HCN route NO for solid fuel-N](image)

In this route, all char N are assumed to convert to NO directly, thus the source terms for the transport equations (3-9, 3-10) can be written as

\[ S_{NO} = S_{C, NO} + S_{NO-1} + S_{NO-2} + S_{NO-3} \]  

(3-32)

\[ S_{HCN} = S_{pc, HCN} + S_{HCN-1} + S_{HCN-2} \]  

(3-33)
where $S_{NO-1}$, $S_{NO-2}$, $S_{HCN-1}$, and $S_{HCN-2}$ are as the same as in equations (3-23, 3-24). $S_{NO-3}$ due to the third heterogeneous reaction in Figure 3.3 can be calculated from

$$S_{NO-3} = A_{BET} C_s M_{NO} R_3 / 1000 \quad (\text{kg/m}^3/\text{s}) \quad (3-34)$$

where $A_{BET}$ is the BET pore surface area (Brunauer 1943) (m$^2$/kg) and determined by experiments. For coal, the BET area is typically 25,000 m$^2$/kg. For biomass, the BET area may be 100 times larger than that of coal. $C_s$ is the concentration of particles (kg/m$^3$). $R_3$ is the reaction rate of NO reduction on the char surface (mole/s/m$^2_{BET}$) and can be modeled as (Levy 1981)

$$R_3 = A_3 x_{NO} \exp\left(-\frac{E_3}{R T}\right) P \quad (3-35)$$

where $A_3$ is a constant (230 mole/atm/m$^2_{BET}$/s). $E_3$ is 34,100 cal/mole. $T$ is the mean temperature. $P$ is pressure (atm) and $x_{NO}$ is the mole fraction of NO.

$S_{C,NO}$ is the rate of fuel NO production from char-N and can be calculated as

$$S_{C,NO} = S_c m_{NC} M_{NO} / M_N / V \quad (3-36)$$

where $S_c$ is the char burnout rate (kg/s). $m_{NC}$ is the mass fraction of nitrogen in the char. $V$ is the cell volume (m$^3$).

$S_{pvc,HNCN}$ is the rate of HCN production from the volatile and can be calculated as

$$S_{pvc,HCN} = S_v m_{NV} M_{HCN} / M_N / V \quad (3-37)$$

where $S_v$ is the rate of volatile from the solid fuel into gas phase (kg/s). $m_{NV}$ is the mass fraction of nitrogen in the volatile, and $V$ is the cell volume (m$^3$).

### 3.2.3.2 NH$_3$ route

For NH$_3$ precursor of NO generation, there are two widely used reaction rates for the fuel-N. One is the Mitchell and Tarbell model (1982); another is the De Soete model (1975). Both are similar in global forms. The overall reactions are:

$$\text{NH}_3 + \text{O}_2 \rightarrow \text{NO} + \text{H}_2\text{O} + 0.5\text{H}_2 \quad (3-38)$$

$$\text{NH}_3 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O} + 0.5\text{H}_2 \quad (3-39)$$

According to De Soete model, the reaction rates can be expressed as

$$k_1 = 4.0 \times 10^6 x_{NH_3} x_{O_2}^\alpha \exp(-32000/RT) \quad (3-40)$$

$$k_2 = 1.8 \times 10^5 x_{NH_3} x_{NO} \exp(-27000/RT) \quad (3-41)$$

where $\alpha$ is the oxygen reaction order just as in Eq.(3-21). $x_{NH_3}$ and $x_{O_2}$ are the mole fractions of NH$_3$ and O$_2$, respectively.

Reaction (3-39) is also the basic reaction of the SNCR (selective non-catalytic reduction of nitrogen oxides) techniques. For industrial application of SNCR techniques, the reductive agent ammonia or urea (H$_2$NCONH$_2$) solution is injected into the boiler to reduce the NO into
nitrogen N₂. Since reaction (3-38) converts the NH₃ back to NO, there will be existence of optimum operating conditions for NO abatement by SNCR.

For liquid fuels, the simplified route can be drawn as in Figure 3.4.

\[ \text{NH}_3 \text{ injection} \]

1: O₂

\[ \text{Liquid Fuel-N} \rightarrow \text{NH}_3 \rightarrow \text{NO} \]

2: NO

\[ \text{N}_2 \]

Figure 3.4 The NH₃ route NO for liquid fuel-N

The source terms in the transport equations can be described as

\[ S_{\text{NH}_3} = S_{\text{pl,NH}_3} + S_{\text{NH},-1} + S_{\text{NH},-2} \quad (3-42) \]
\[ S_{\text{NO}} = S_{\text{NO}-1} + S_{\text{NO}-2} \quad (3-43) \]

The rate of NH₃ production is composed of two parts. One is the rate of fuel release into the gas phase through devolatization; another is that of injected ammonia liquid release into the gas phase also through devolatization.

\[ S_{\text{pl,NH}_3} = S_{r} m_{NF} M_{\text{NH}_3} / M_{N} / V + S_{a} Y_{\text{NH}_3} \quad (3-44) \]

where \( S_{r} \) is the rate of fuel release to gas phase. \( m_{NF} \) is the mass fraction of nitrogen in fuel. \( V \) is the cell volume. \( S_{a} \) is the rate of ammonia liquid release to gas phase. \( Y_{\text{NH}_3} \) is the NH₃ mass fraction in the ammonia liquid.

\[ S_{\text{NH},-1} = -k_{1} M_{\text{NH}_3} P / RT \quad (3-45) \]
\[ S_{\text{NH},-2} = -k_{2} M_{\text{NH}_3} P / RT \quad (3-46) \]

where \( M_{\text{NH}_3} \) is the molecule weight of NH₃. \( P \) is pressure and \( T \) is the instantaneous temperature.

NO is produced in reaction 1 but destroyed in reaction 2 in Figure 3.4, thus we have

\[ S_{\text{NO}-1} = -S_{\text{NH},-1} \frac{M_{\text{NO}}}{M_{\text{HCN}}} = k_{1} \frac{M_{\text{NO}} P}{RT} \quad (3-47) \]
\[ S_{\text{NO}-2} = S_{\text{NH},-2} \frac{M_{\text{NO}}}{M_{\text{HCN}}} = -k_{2} \frac{M_{\text{NO}} P}{RT} \quad (3-48) \]

where \( \bar{T} \) is the mean temperature.
For solid fuels, the simplified route can be drawn as in Figure 3.5.

![Diagram showing the NH3 route NO for solid fuel-NO]

The source terms for the transport equations (3-9, 3-11) are

\[
S_{NO} = S_{C:NO} + S_{NO-1} + S_{NO-2} + S_{NO-3} \quad (3-49)
\]
\[
S_{NH3} = S_{pvc,NH3} + S_{NH3-1} + S_{NH3-2} \quad (3-50)
\]

where the source contributions \( S_{NO-1} \), \( S_{NO-2} \), \( S_{NO-3} \), \( S_{NO-2} \), and \( S_{NO-3} \) are as the same as in equations (3-45), (3-46), (3-36), (3-47), (3-48), and (3-34).

The overall source of NH3 (\( S_{pvc,NH3} \)) is mainly from the fuel volatile contribution and ammonia injection contribution as

\[
S_{pvc,NH3} = S_{v} m_{NV} \frac{M_{NH3}}{M_{N}} / V + S_{a} Y_{NH3} \quad (3-51)
\]

where \( S_{v} \) is the source of volatile from the solid particles into gas phase (kg/s). \( m_{NV} \) is the mass fraction of nitrogen in the volatile. \( V \) is the cell volume (m³). \( S_{a} \) is the rate of ammonia liquid release into gas phase. \( Y_{NH3} \) is the NH3 mass fraction in the ammonia liquid.

### 3.3 NOx simulation in combustion

Because the NOx concentration is quite small in a practical combustion furnace, its influence on flow field and other scales, such as temperature, pressure, other species concentrations, is negligible. Similar to the decoupled method used in NOx kinetic modeling, for using the NOx models, the most efficient way is to put the NOx simulation as a postprocessor to the main combustion calculation. This NOx simulation strategy is shown in Figure 3.6.
In a practical combustion system, the reacting flow is highly turbulent. The turbulent mixing process results in temporal fluctuations in temperature and species concentrations. Since in the NO\textsubscript{x} models, the NO\textsubscript{x} formation rate with temperature and species concentrations are highly nonlinear, the turbulent influence on the NO\textsubscript{x} formation rate is significant. Therefore, the temperature and composition fluctuations must be taken into account by considering the probability density functions (PDF). To calculate NO\textsubscript{x} concentration, a time-averaged NO\textsubscript{x} formation rate must be computed at each point in the domain using the averaged flow field information. The preceding combustion simulation can use either the generalized finite rate chemistry model and eddy dissipation model by Magnussen and Hjertager, or the mixture fraction / PDF model as described in detail in previous chapter 2.5. The mean turbulent reaction rate of NO\textsubscript{x} formation can be modeled by using the PDF approach.

The time-averaged turbulent reaction rate \( \bar{R} \) can be described in terms of the instantaneous rate \( R \) and a single or joint PDF of various variables. In general,

\[
\bar{R} = R(v_1, v_2, \ldots) P(v_1, v_2, \ldots) dv_1 v_2 \ldots
\]

where \( v_1, v_2, \ldots \) are the quantities of temperature and the various species concentrations. \( P(v_1, v_2, \ldots) \) is the probability density function. For the instantaneous NO source \( S_{NO} \), the time-averaged turbulent production rate of NO, \( \bar{S}_{NO} \), can be expressed as

\[
\bar{S}_{NO} = S_{NO}(v) P(v) dv
\]

where \( P(v) \) is the PDF in the normalized temperature or in a single mixture fraction. Here the integration must be done at every node and at every iteration. The integration limits are determined from the minimum and maximum values of the independent variable such as temperature or single mixture fraction in the previous combustion solution. The HCN or NH\textsubscript{3} source terms can be treated in the same way. The PDF \( P(v) \) is assumed to be a two-moment beta function as appropriate for combustion calculations (Missaghi 1987, Hand 1989), in which the independent variable \( v \) must be normalized to assume values between 0 and 1. Just as in Eqs.(2-108, 109, 110), the beta function is defined as
\[ P(v) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} v^{\alpha-1}(1 - v)^{\beta-1} = \frac{v^{\alpha-1}(1 - v)^{\beta-1}}{v^{\alpha-1}(1 - v)^{\beta-1}} \] (3-54)

where \( \Gamma \) is the Gamma function.

\[ \alpha = m\left(\frac{m(1 - m)}{\sigma^2} - 1\right) \] (3-55)

\[ \beta = (1 - m)(\frac{m(1 - m)}{\sigma^2} - 1) \]

where \( m \) is the mean value of the variable \( v \). It is directly from the main combustion calculation. \( \sigma^2 \) is the variance of the variable \( v \). It can be calculated by solving the variance transport equation as

\[
\frac{\partial}{\partial t}(\rho \sigma^2) + \frac{\partial}{\partial x_i}(\rho \mu_i \sigma^2) = \frac{\partial}{\partial x_i} \left( \frac{\mu_i}{\sigma_i} \frac{\partial \sigma^2}{\partial x_i} \right) + C_g \mu_i \left( \frac{\partial m}{\partial x_i} \right)^2 - C_d \rho \varepsilon \sigma^2 \] (3-56)

where the constant \( \sigma_i, C_i \) and \( C_d \) take the values 0.7, 2.86, and 2.0, respectively. Assuming equal production and dissipation of variance, then Eq.(3-54) becomes

\[ \sigma^2 = \frac{\mu_i k}{\rho \varepsilon C_d} \left( \frac{\partial m}{\partial x_i} \right)^2 \] (3-57)

where the term in the brackets is the dissipation rate of the independent variable.
Chapter 4
Numerical Methods

In this thesis work, the commercial Fluent/UNS solver (Fluent 1996, 1998) has been used. The finite volume method (FVM) and the iterative method together with convergence acceleration approach are applied to solve the governing PDE system in integral forms of a series of physical models for turbulent combustion.

4.1 The unstructured mesh and discretization schemes

For a practical furnace with a complex geometry, its physical/computational domain can be divided into discrete control volumes (3D cell or mesh) using unstructured tetrahedral-type grids (Baker 1994). The benefit of unstructured grid generation is its ability to adaptively refine the mesh in areas that contain complex flow structures, such as multi-jet flows inside the domain. In this thesis, the CAD software codes of Geomesh and Tgrid are employed to generate the unstructured grid and mesh cases. Then, the governing partial differential equation system can be integrated on the individual control volumes to construct the algebraic equation system for discrete unknowns.

For space discretization, by neglecting the time derivative and applying Gauss divergence theorem, the integration for (2-10 or 2-15) on an arbitrary control volume $V$ yields the integral form of stead-state transport equation as

$$\nabla \cdot \Gamma \phi = S \phi \quad \text{d}V$$  \hspace{1cm} (4-1)

where $\mathbf{v}$ is the velocity vector, $A$ is the surface area vector, $\Gamma$ is the diffusion coefficient for $\phi$, $S$ is the source of $\phi$ per unit volume. It is integrated on a given control volume and yields the following algebraic equation as

$$\sum_{f}^{N_{faces}} v_f \phi_f A_f \cdot \nabla \phi = \sum_{f}^{N_{faces}} \Gamma_{\phi} (\nabla \phi)_n A_f + S \phi \quad \text{d}V$$  \hspace{1cm} (4-2)

where $N_{faces}$ is the number of faces enclosing the cell. $\phi_f$ is the value of $\phi$ convecting through the face $f$. $v_f$ is the mass flux through the face $f$. $A_f$ is the area of the face $f$. $(\nabla \phi)_n$ is the magnitude of $\nabla \phi$ normal to the face $f$. This equation can be linearized as

$$a_p \phi = a_{nb} \phi_{nb} + b$$  \hspace{1cm} (4-3)

where $nb$ represents the neighbor cells. $b$ is the constant part of the source term $S_c$ in linearized $S_\phi = S_c + S_p \phi$ and of the boundary conditions. $a_p$ and $a_{nb}$ are the linearized coefficients and meet

$$a_p = a_{nb} - S_p$$  \hspace{1cm} (4-4)

Since the grid is unstructured, all discrete values for variable $\phi$ are stored at the cell centers. The diffusion terms are second-order central-differenced, while the
convection terms can be discretized using upwind scheme (first-order or second-order), power-law scheme (first order) (Patankar 1980) and QUICK scheme (third-order) (Leonard 1979, 1990). If the first-order upwind scheme is employed, the face value $\phi_f$ can be selected as the cell-centered value $\phi$ of the upstream cell. If the second-order upwind scheme (Barth 1989) is used, the face value of $\phi_f$ can be calculated using a Taylor series expansion for $\phi$ about the cell centroid as

$$
\phi_f = \phi + \nabla \phi \cdot \Delta s
$$

(4-5)

where $\phi$ and $\nabla \phi$ are the cell-centered value and its gradient in the upstream cell. $\Delta s$ is the displacement vector from the upstream cell centroid to the face centroid. The gradient can be calculated by using the Gauss divergence theorem as

$$
\nabla \phi = \frac{1}{V} \sum_{f}^{N_{faces}} \tilde{\phi}_f A
$$

(4-6)

where $\tilde{\phi}_f$ is the averaged $\phi$ of the two cells adjacent to the face.

The traversal of linearized equation Eq.(4-3) on each cell in the whole computational domain, results in a set of algebraic equations which can be solved using a point implicit Gauss-Seidel linear equation solver in conjunction with an algebraic multigrid (AMG) method. In addition, in order to overcome the difficulty of convergence due to the nonlinearity of the equation set, the underrelaxation approach (Patankar 1980) can be used as

$$
\phi = \phi^* + \alpha \Delta \phi
$$

(4-7)

where $\phi$ is the new value of the variable in a cell. $\phi^*$ is the old value from the previous iteration. $\alpha$ is the underrelaxation factor. $\Delta \phi$ is the correction standing for the computed change.

For large eddy simulation, the flow is time-dependent, so the implicit second-order difference of time stepping scheme and the second-order upwind scheme or third-order QUICK scheme for convection term can be used. Since the scheme is fully implicit, there are no strict limitations on the size of the time step. However, the following three conditions may be considered.

Full resolution in time as

$$
\Delta t < \tau
$$

(4-8)

where $\tau$ is the Kolmogorov time scale.

CFL (Courant-Friedrichs-Lewy) condition

$$
C = \frac{c \Delta t}{\Delta x}
$$

(4-9)
where $C$ is the Courant number and $c$ is a characteristic constant.

Viscous stability condition

$$C_{vis} = \frac{D \Delta t}{Re \Delta x^2}$$

(4-10)

where $C_{vis}$ is the viscous stability number.

Usually, the limitation (4-10) is not significant, however, the limitations of (4-8, 4-9) are equally restrictive to LES (Olsson 1997) for explicit treatment.

4.2 Pressure-velocity coupling

The coupling between the velocity field and pressure field is strong to solve the incompressible flows. An effective way is using SIMPLE (Patankar 1980) or SIMPLEC (SIMPLE-Consistent) (Vandoormaal 1984) algorithms to handle the discretization of the momentum and continuity equations with pressure-velocity coupling problems. The SIMPLE uses a relationship between velocity and pressure corrections to enforce mass conservation and to obtain the pressure field. Firstly, guess a pressure field to solve the momentum equations to obtain a preliminary velocity field. The pressure correction and the velocity corrections are then calculated by using the continuity equation. The SIMPLEC procedure is similar to the SIMPLE procedure. The only difference lies in the expression used for the face flow rate correction, and the SIMPLEC is used where pressure-velocity coupling is the main deterrent to obtain a solution.

4.3 Segregated solution method

The algebraic equations discretized from the governing PDEs can be solved sequentially and iteratively by using segregated solution method. Since the governing equations are non-linear and coupled, the iterative method, such as Gauss-Seidel underrelaxation scheme, should be used to obtain a set of converged solutions for unknowns at each grid. Figure 4.2 illustrates the solution procedure.
4.4 The unstructured multigrid method

The linearized equations on unstructured meshes can be solved using the point-iterative solver of the Gauss-Seidel underrelaxation method. It can rapidly remove local errors in the solution but its global errors are reduced at a rate inversely related to the grid size. In other words, when the mesh being refined to a certain level with a large number of control volumes, the iterative process maybe stall for the convergence rate becomes prohibitively low. An effective way to solve this problem is using multigrid (MG) method, which allows the global error or long-wavelength errors to be addressed by using a sequence of successively coarser meshes. The long-wavelength error on a fine mesh becomes a short-wavelength or local error on a coarse mesh. Each grid in the mesh hierarchy reduces those error components that the Gauss-Seidel solver handles well on that grid. Since computations can be performed at exponentially decaying expense in both CPU time and storage as the mesh is coarsened, a very efficient mechanism can be devised for reducing long wavelength...
errors. There are two significant characteristics for the MG method that the convergence is grid level independent and the solution to the level of truncation errors can be obtained with much less computational work. Basically, consider a set of linearized algebraic equations having the exact solution $\phi_{\text{exact}}$, as

$$A\phi_{\text{exact}} + b = 0$$

(4-11)

where $A$ is the original fine mesh level operator. Assume an approximate solution $\phi$ and a defect $d$ on the original fine mesh level, as

$$A\phi + b = d$$

(4-12)

The correction $\psi$ is

$$\psi = \phi_{\text{exact}} - \phi$$

(4-13)

So, one can obtain an equation for the correction and the defect on the original fine mesh level, as

$$A\psi + d = 0$$

(4-14)

Next step, on the coarse mesh level, one has

$$A^H\psi^H + Rd = 0$$

(4-15)

where $A^H$ is the coarse mesh level operator. $\psi^H$ is the coarse mesh level correction. $R$ is the restriction operator for transferring the fine mesh level defect $d$ down to the coarse mesh level.

Then the approximate solution on the fine mesh level can be updated by

$$\phi^{\text{new}} = \phi + P\psi^H$$

(4-16)

where $P$ is the prolongation operator for transferring the coarse mesh level correction up to the fine mesh level.

To get the final convergent solution, the $V$-cycle or $W$-cycle, or their mixture of $F$-cycle MG schemes can be applied. Basically, the traversal of the mesh hierarchy can be conducted in the following process:

- Pre-relaxation sweeps/smoothings on the current mesh level to reduce the high-frequency components of the local error. (For AMG, the pre-relaxation is not necessary.)
- Restriction to the next coarser mesh level using an appropriate restriction operator $R$.
- The error on the coarse mesh level is reduced by performing the $V$ or $W$ MG cycles.
- The cumulative correction calculated on the coarse mesh level is interpolated back to the fine mesh level using an appropriate prolongation operator.
Post-relaxation sweeps/smoothings to remove the high-frequency error introduced on the coarse mesh level.

Fluent/UNS has an AMG linear equation solver to accelerate the convergence of the Gauss-Seidel underrelaxation iterations. The algorithm of the restriction and prolongation is an unstructured version of the additive correction (AC) strategy (Hutchinson and Raithby 1986, Maruszewski 1989). The prolongation operator is obtained from the transpose of the restriction operator as

$$P = R^T$$  \hspace{1cm} (4-17)

The coarse mesh level operator $A^H$ is constructed using a Galerkin approach and has the following expression as

$$A^H = RAP$$  \hspace{1cm} (4-18)

For AMG, the residual reduction rate criteria is defined as

$$R_i > \beta R_{i-1}$$  \hspace{1cm} (4-19)

where $R_i$ is the residual or defect on the current mesh level after the $i$th relaxation. $\beta$ is the residual reduction tolerance ($0 \sim 1$, default 0.7) controlling the frequency of visiting the coarser mesh level. While, the convergence or termination criteria can be defined as if the error in the correction solution is reduced to a some fraction $\alpha$ ($0 \sim 1$, default 0.1) of the original error on this mesh level as

$$R_i < \alpha R_0$$  \hspace{1cm} (4-20)

where $R_i$ is the residual or defect on the current mesh level after the $i$th relaxation. $R_0$ is the residual initially obtained on this mesh level at the current global iteration.

**4.5 Convergence and accuracy**

Actually, there are no universal measures to judge convergence. However, for most practical problems, the convergence criterion can be set that the scaled residuals drop three orders to $10^{-3}$ for solved equations (for energy equation, the convergence criterion is $10^{-6}$). The scaled residual $R^\phi$ for Eq. (4-3) can be defined as

$$R^\phi = \left| \sum_{\text{cells}, p} \sum_{\text{nb}} a_{ab} \phi_{ab} + b - a_p \phi_p \right|$$

There are two error sources coming from the discretization error, $D$ ($D = \text{analytical solution of governing PDE} - \text{exact solution of discretized algebraic equation}$) and numerical error, $\varepsilon$ ($\varepsilon = \text{numerical solution} - \text{exact solution of discretized algebraic equation}$). If the discretization error shrinks in progression of refining the mesh, the discretization scheme is consistent. While, if the numerical error $\varepsilon$ in the cell $P$ shrinks in the iterative procedure from step $n$ to $n + 1$, as
\[
\varepsilon_{n+1}^p \leq 1
\]

(4-22)

then, the numerical solution is stable. Dahlquist (1956) proved that a linear multistep scheme is convergent if and only if it is consistent and stable. However, for the practical combustion problem, the governing PDEs are highly non-linear, so there are no exact measures for judging convergence. Instead, in order to obtain the physically realistic results and stable iterative solutions, the discretization scheme should possess three properties of conservativeness, boundedness and transportiveness (Patankar 1980, Versteeg and Malalasekera 1995). For conservativeness, the flux of the transported \( \phi \) through a common face must be in a consistent manner of the same expression in adjacent control volume. For boundedness, all coefficients of the discretized equations should all be positive, and in the absence of sources the internal nodal values of the variable \( \phi \) should be bounded by its boundary values. For transportiveness (Roache 1976), the discretized scheme should be able to recognise the direction of the flow or the strength of convection relative to diffusion by the measure of cell Peclet number, \( Pe \), as

\[
Pe = \frac{\text{convection}}{\text{diffusion}} = \frac{\rho u}{\Gamma / \Delta x}
\]

(4-23)

where \( \Delta x \) is the cell width. It can be shown that upwind schemes possess these three properties, thus they are highly stable. While, the QUICK scheme may be unbounded under certain flow conditions, thus it is conditional stable.

It is apparent that there are two ways to enhance the solution accuracy by using higher-resolution discretization (refining the mesh) or/and using the higher-order schemes. For higher-resolution discretization, since the computer source is always limited, therefore a wise strategy is to use the unstructured grid together with the adaptive mesh technique (Mavriplis 1996) for local mesh refinement for the complex geometry and flow structures. In principle, one may refine the mesh until the numerical solution being grid non-sensitive (grid-independent). For higher-order schemes, the second-order upwind scheme and the third-order QUICK scheme can be applied. However, for a large mesh case, the higher-order schemes will cost more computational time and may be less stable. Therefore, in practice, a balance among the convergence, accuracy and computational source should be considered and evaluated always.

4.6 Custom field functions and user-defined-functions

In Fluent/UNS, the custom field functions (CFFs) can be used to define user’s field functions, such as the degree of mixing (Dong 2000, paper 3). In addition of CFFs, the user-defined functions (UDFs) can be used to code the sub-models for the boundary conditions, source terms, property definitions, reaction rates, solution of user-defined scalars, etc. UDFs should be written in the C language and compiled and grouped in a shared library using Makefile.udf and makefile.udf. The complied UDFs can completely access to the main solver to perform the computational tasks for sub-models.
Chapter 5
Grate Bed Modeling

5.1 Introduction

In modeling of grate fired furnaces, it is essential to develop a sub-model of grate bed (in chemical engineering, grate bed also called fuel bed, fixed-bed or packed-bed), where the interaction of the solid phase and the gas phase is very complicated.

Generally, a combustible element in the fuel bed is heated primarily by radiation from the over-bed region and from the burning fuel bed. As its temperature rises, it loses its free moisture at 100 °C, pyrolyses at 260 °C, ignites at 316 °C and then burns vigorously until either the oxygen surrounding the element is depleted or all the element is devolatized, leaving a carbonaceous char. The residual charred or partly charred element may undergo further pyrolysis, be gasified by CO₂ or H₂O to yield CO or CO and H₂, or be oxidized by free oxygen directly to CO₂. Figure 5.1 shows a typical grate fired furnace.

![Fig.5.1 Schematic of a grate fired furnace (Smoot L. D., 1993)](image)

In the heterogeneous grate bed, all the above processes may be occurring simultaneously within a section of the bed, since neighboring fuel elements vary widely in size and composition. In addition, complexity is also introduced by the substantial temperature and concentration gradients that may be present in the larger fuel elements. It seems convenient for the purposes of bed modeling to divide the bed combustion mechanisms as physical process and chemical process.

The physical process includes heating-up and drying of fuel particles, motion of particles on the moving grate, and interaction between gas and solid phases, while the chemical process includes pyrolysis and devolatilization of fuel particles and char gasification and combustion.
For the purpose of modeling, the most demanding approach is a Lagrangian granular flow method which calculates the movement of individual fuel elements (or representative Cluster of elements), continuously considering the contact with neighboring elements and the associated forces. This kind of microscopic bed sub-model would have the advantage that no empirical information would be needed to describe the transport and stoking process. Although this approach seems to be feasible, it needs very detailed information about the fuel composition and mechanical properties of the fuel, which are generally not available.

For the most common grate combustion of countercurrent process, one of the first comprehensive and well-documented grate bed models, called UD/MIT Model, was developed at the University of Delaware and the Massachusetts Institute of Technology. Since then, some zero-dimensional, one-dimensional and less two-dimensional fixed-bed models have been developed. These bed sub-models have common features for simplification as below:

- Single particle size
- No momentum transport for gas and solid phase
- Uniform bed
- Instantaneous drying
- Simplified devolatilization with yields from proximate analysis
- Char combustion and gasification with kinetic parameters for small particles
- Fixed combustion product distribution (CO/CO\(_2\))
- Simplified gas phase chemistry usually reduced to water-gas shift equilibrium
- Limited sensitivity analysis and validation

Yet, model development has not reached the point where significant use is made in process development for solid fuels utilization. Recently, some authors attempted (Hobbs 1992, A.M. dos Santos 1993, Peters 1997, Dong, 1997) to develop a robust grate bed sub-model based on single particle models. However, due to the heterogeneous properties of fuel and insufficient knowledge about the strong interaction between the gas and solid phases, there is still a need for broader investigations in both experimental ways and numerical ways.

5.2 Hobbs 1-Dimensional fixed-bed submodel

This one-dimensional sub-model of countercurrent fixed-bed, considers separate gas and solid temperature, axially variable solid and gas flow rates, variable bed void fraction, fuel drying and devolatilization based on chemical functional group composition, oxidation and gasification of char, and partial equilibrium in the gas phase.

A schematic of the countercurrent fixed-bed combustion model is shown in Figure 5.2. The fuel is fed to the top and move down under gravity, countercurrent to the rising primary air stream. The bed is divided into five zones corresponding to drying, devolatilization, gasification, combustion and ash, in which, the differentiation between
The gasification zone and the combustion zone is based on the presence or absence of free oxygen. The exothermic combustion reactions provide the necessary energy for the endothermic gasification, devolatilization and drying.

![Schematic of Hobbs bed model](image)

The governing equations are based on the conservation of mass and energy, as listed in Table 5.1. Shrinking-core char sub-model describes char oxidation and gasification, while the chemical equilibrium is used to calculate gas concentration and temperature. Turbulence is not treated in slowly moving bed with low gas velocities.

Primary assumptions for the one-dimensional bed sub-model include negligible aerodynamic drag, ideal gases, and particles locally isothermal throughout, one particle size and type exists in the feed fuel. The constitutive relations for solids flow have been proposed by D.D.Gray (1988) and no solution for these equations has been attempted.

Hobbs bed sub-model has been used to simulate some commercial coal gasifiers and reasonable agreement with experimental temperature and pressure profile data for gasification of different coal has been obtained. However, this bed sub-model seems hardly to be used in grate fired furnaces directly.
Table 5.1 Governing equations and boundary conditions for Hobbs bed model
(M.L. Hobbs et al, 1992)

| Overall gas species continuity | \( \frac{dW_g}{dz} = \sum_{i=1}^{n} r_i \) (5-1) |
| Overall solid species continuity | \( \frac{dW_s}{dz} = -\sum_{i=1}^{n} r_i \) (5-2) |
| Gas phase energy | \( \frac{dW_g h_g}{dz} = A \left( Q_{ig} - Q_{gw} + \sum_{i=1}^{n} r_i h_{ig} \right) \) (5-3) |
| Solid phase energy | \( \frac{dW_s h_s}{dz} = A \left( -Q_{sg} - Q_{sw} - \sum_{i=1}^{n} r_i h_{ig} \right) \) (5-4) |
| Solid species continuity |
| Moisture | \( \frac{dW_{moisture}}{dz} = A r_{moisture} \) (5-5) |
| Non-volatile carbon | \( \frac{dW_{Non-volC}}{dz} = A r_{Non-volC} \) (5-6) |
| Organic functional groups | \( \frac{dy_i}{dz} = \frac{1}{U_s} k_i y_i \) (5-7) |
| Tar fraction | \( \frac{dx}{dz} = \frac{1}{U_s} k_i x \) (5-8) |
| Gas phase elemental continuity | \( \frac{dW_j}{dz} = \sum_{i=1}^{n} r_{i,j} \) (5-9) |
| Gas phase tar species continuity | \( dW_{tar} = \sum_{i=1}^{n} r_{i, tar} \) (5-10) |
| Gas phase tar elemental continuity | \( \frac{dW_{tar, i}}{dz} = \sum_{i=1}^{n} r_{i, tar} \) (5-11) |
| Boundary conditions |
| Feed coal/gas mass flow rate | Feed coal/gas enthalpy or temperature |
| Proximate and functional group analysis | Feed gas and tar composition |
| Heat and mass transport corrections used can be found in the reference of M.L. Hobbs et al, 1992 |

5.3 Goh 1-dimensional continuum bed submodel

For modeling the solid waste incineration in a travelling grate fired furnace, Goh (1998), has developed a one dimensional bed sub-model, in which, the bed is divided into four layers whose thickness vary along the travelling grate. Different layers are separated by the drying front, the pyrolysis front and the gasification front. The model mechanism is schematically shown in Figure 5.3. The solid fuel is assumed as having four main components: free moisture, volatiles, bound ash and char. While in the model, it is supposed that the fuel bed consists of seven key components: gas space (1), moisture (2), volatiles (3), bound ash (4), fixed carbon (5), internal pore space (6), free ash (7).
In this model, several simplifications are considered as below:

1. The properties of the fuel remain constant and temperature-independent;
2. The void fraction remains constant;
3. Drying and pyrolysis temperatures are constant;
4. The rates of drying and pyrolysis depend on the latent heats of the process;
5. The gasification takes place at 600K, and the rate of gasification is proportional to the square root of the temperature at the gasification front;
6. The combustion of gaseous volatiles occurs in the freeboard region;
7. Interaction between the preheated air and the gases within the voids and the bed solids are neglected;
8. A high value of “effective” thermal conductivity is used to compensate the effect of radiation.

The detailed governing equations are summarized in Table 5.2. This macroscopic bed submodel considers the bed as a continuum so far as to avoiding to deal with the complicated granular flow problems. However, this model is apparently lack of a firm basis, and has not yet been used and validated in practical applications.
Table 5.2 Governing equations in Goh bed submodel (Goh, 1998)

<table>
<thead>
<tr>
<th>Equation Description</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume conservation in L layer</td>
<td>$\varepsilon_L + (1 - \varepsilon_L) \omega_{NL} = 1$</td>
</tr>
<tr>
<td>Volume of solid removed in L layer</td>
<td>$\Delta V_{L(\rightarrow)} = (1 - \varepsilon_L) \Delta V_{L(\rightarrow)}$</td>
</tr>
<tr>
<td>Volume of component N removed in L layer</td>
<td>$\Delta V_{L(\rightarrow)N} = \omega_{NL} \Delta V_{L(\rightarrow)S}$</td>
</tr>
<tr>
<td>Volume of internal pore space formed</td>
<td>$\Delta V_{L(\rightarrow)S} = (1 - \omega_{NL}) \Delta V_{L(\rightarrow)S} + F_N \Delta V_{L(\rightarrow)N}$</td>
</tr>
<tr>
<td>Total volume added in L layer</td>
<td>$\Delta V_{L(\rightarrow)} = \frac{\Delta V_{L(\rightarrow)S}}{(1 - \varepsilon_{L+1})}$</td>
</tr>
<tr>
<td>Volume changes of layer B</td>
<td>$\frac{\partial V_B}{\partial t} = \frac{(R_p)<em>2}{\rho_2 \omega</em>{2B} (1 - \varepsilon_B)}$</td>
</tr>
<tr>
<td>Volume changes of layer C</td>
<td>$\frac{\partial V_C}{\partial t} = \frac{(R_p)<em>3}{\rho_2 \omega</em>{2B} (1 - \varepsilon_C)} - \frac{(R_p)<em>3}{\rho_3 \omega</em>{3C} (1 - \varepsilon_C)}$</td>
</tr>
<tr>
<td>Volume changes of layer D</td>
<td>$\frac{\partial V_D}{\partial t} = \frac{(R_p)<em>3}{\rho_3 \omega</em>{3D} (1 - \varepsilon_D)} - \frac{(R_p)<em>5}{\rho_5 \omega</em>{5D} (1 - \varepsilon_D)}$</td>
</tr>
<tr>
<td>Volume changes of layer A</td>
<td>$\frac{\partial V_A}{\partial t} = \frac{(R_p)<em>5}{\rho_3 \omega</em>{3D} (1 - \varepsilon_A)} - \frac{(R_p)<em>5}{\rho_5 \omega</em>{5D} (1 - \varepsilon_A)}$</td>
</tr>
<tr>
<td>Enthalpy balance of boundary at two immediately adjacent layers</td>
<td>$q_{in} - q_{out} = (R_p \Delta H_p)_{N,N=2,3,or.5}$</td>
</tr>
<tr>
<td>Mass rate of removal of N from the solid</td>
<td>$(R_p)<em>N = \frac{\rho_N \Delta V</em>{L(\rightarrow)N}}{\Delta t}$</td>
</tr>
<tr>
<td>Mass flow rate of materials C</td>
<td>$m_C = \frac{(\rho_C)}{\rho_2} \frac{(R_p)<em>2}{\omega</em>{2B} (1 - \varepsilon_B)} \left[1 - \frac{(1 - F_2) \omega_{2B}}{(1 - \varepsilon_C)} \right]$</td>
</tr>
<tr>
<td>Mass flow rate of materials D</td>
<td>$m_D = \rho_D \left{ \frac{(R_p)<em>2}{\rho_2 \omega</em>{2B} (1 - \varepsilon_B)} \left[1 - \frac{(1 - F_2) \omega_{2B}}{(1 - \varepsilon_C)} \right] \right.$</td>
</tr>
<tr>
<td>Mass flow rate of materials A</td>
<td>$m_A = \rho_A \left{ \frac{(R_p)<em>3}{\rho_2 \omega</em>{2B} (1 - \varepsilon_B)} \left[1 - \frac{(1 - F_2) \omega_{2B}}{(1 - \varepsilon_C)} \right] \right.$</td>
</tr>
</tbody>
</table>

\[\text{(5-12) to (5-25)}\]
5.4 Saastamoinen 1-dimensional bed submodel

Saastamoinen (1998) has developed another kind of simplified one-dimensional grate sub-model, in which, the whole bed is divided into three zones corresponding to drying, pyrolysis and char gasification, as shown in Figure 5.4. The governing equations are summarized in Table 5.3.

![Fig.5.4 Schematic of the fuel bed zones](image)

**Table 5.3 Governing equations for Saastamoinen submodel**

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho l_v \frac{d \delta}{dt} = \frac{\lambda}{\delta} (T_v - T_v) = q )</td>
<td>Heat and drying</td>
</tr>
<tr>
<td>( L_d = H \frac{w_{gr}}{w_{ig}} )</td>
<td>Pyrolysis and combustion</td>
</tr>
<tr>
<td>( \Delta n \delta C_H = \min(\eta f_d, \eta O_2, \eta H_2) )</td>
<td>The length of the zone</td>
</tr>
<tr>
<td>( \frac{dn \delta H_C}{dz} = -f \Delta n \delta O_2 )</td>
<td>The mass flux density of volatiles</td>
</tr>
<tr>
<td>( C + \frac{1}{2}(1 + \gamma)O_2 \rightarrow (1 - \gamma)CO + \gamma CO_2 )</td>
<td>The consumption of char</td>
</tr>
<tr>
<td>( \Delta H_C = (1 - \gamma)\Delta H_{CO} + \gamma \Delta H_{CO_2} )</td>
<td>Char oxidation</td>
</tr>
</tbody>
</table>

The properties of the bed are solved as a function of the distance \( z \) from the fuel fed opening, the beginning of the grate. In three-dimensional flow simulations, the bed is modeled as a wall boundary condition. The grate bed submodel is then solved separately for each one-dimensional cross section of the wall.
Pättikangas (1999) declared that this one-dimensional submodel has been used to simulate a 60MW grate coal fired furnace at Vanaja power plant in Finland. However, in this model, the bed velocity distribution has not been considered, and the parameters of \( \eta \) and \( \gamma \) are not available.

5.5 Black-box bed sub-model

Due to the over complexity, there is no any practically detailed bed sub-model. In other word, a general theoretical or deductive bed model does not exist at all. However, for a certain furnace boiler case, the biomass fuel composition and moisture content could be derived from the operating data and exhausted flue gas composition, and this information enables us to insure a global mass balance on the C, H, O components of the biomass fuel. In fact, it is possible to adopt a simplified assumption based on global mass and local element transfer balances and experimental bed data of composition and temperature distributions that are from measurements taken in situ over the bed. In this way, fuel flow rate and primary air flow rates are included implicitly in these contributions, and all these bed data are used as inlet boundary conditions in the experimental combustion model.

This strategy is based on the global and local mass balances according to the fuel composition analysis, proximate analysis and the experimental solid fuel pyrolysis data.

5.5.1. Chemical species and their distributions in the grate bed

For the sake of the practical application at the current work, an important simplification is made to only consider the homogeneous off-bed gas phase reactions, in which the chemical reactions can be assumed in different complicated levels depending on the experimental pyrolysis data and computer capacity. Because all the chemical species in the off-bed gas phase come from the different bed zones, it is reasonable and for convenience to divide the bed as three ideal zones, named drying zone, pyrolysis zone and char gasification zone. The mass balance of all species in the global system is based on the basic processes and their reaction formulas taken place in these zones as follows:

(i) Drying zone

\[
\text{Fuel} \cdot n\text{H}_2\text{O} \rightarrow \text{Fuel} + n\text{H}_2\text{O}(g) \quad (5-32)
\]

(ii) Pyrolysis (or volatilization) zone

\[
\text{C}_x\text{H}_y\text{O}_z(s) + q\text{H}_2\text{O} \rightarrow p_1\text{C}_m\text{H}_n + p_2\text{CO} + p_3\text{H}_2 \quad (5-33)
\]

where \( \text{C}_x\text{H}_y\text{O}_z \) is the equivalent fuel, in which the number \( x, y, \) and \( z \) are depended on the composition analysis data of the solid fuel. \( \text{C}_m\text{H}_n \) is the equivalent component of \( \text{CH}_4 \) and \( \text{C}_1-\text{C}_3 \) hydrocarbons, in which the number \( m \) and \( n \) are depended on the experimental data of solid fuel pyrolysis. \( q, p_1 \ p_2 \) and \( p_3 \) are stoichiometric coefficients of the pyrolysis reaction and have to satisfy the following relationships:
\[ x = mp_1 + p_2 \]
\[ y + 2q = np_1 + 2p_3 \]
\[ z + q = p_2 \] (5-34)

(iii) Char Gasification zone

\[ \text{C (char)} + \text{O}_2 \rightarrow \text{CO} \] (5-35)

For the gas phase combustion, the typical two-step or three-step gas phase reaction sets can be selected as follows:

- CO and H\(_2\)
  \[ \text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2 \]
  \[ \text{H}_2 + \frac{1}{2}\text{O}_2 \rightarrow \text{H}_2\text{O} \] (5-36)

- \(\text{C}_{m}\text{H}_n\) CO and H\(_2\)
  \[ \text{C}_{m}\text{H}_n + (m/2 + n/4)\text{O}_2 \rightarrow m\text{CO} + (n/2)\text{H}_2\text{O} \]
  \[ \text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2 \]
  \[ \text{H}_2 + \frac{1}{2}\text{O}_2 \rightarrow \text{H}_2\text{O} \] (5-37)

5.5.2 Temperature distribution in the grate bed

Theoretically, it is possible to evaluate the temperature distribution in the grate bed by using the energy balance approach. But the problem is that there is lack of detail information about the energy processes taking place in the grate bed. However, it is reasonable to assume that the temperatures at drying zone should be from 373 K to 530 K, at the pyrolysis zone from 530 K to 590 K, and at the char gasification zone from 900 K to 1300 K or a little higher (Nasserzaden 1991, Dos Santos 1993).

Therefore, to use the black-box bed model we only need the original fuel composition and its mass flow rate, primary air mass flow rate, and pyrolysis data. In our experiences and considering the computer capacity, the chemical reaction species can be selected six or seven components, such as \(\text{C}_{m}\text{H}_n\) or \(\text{C}_x\text{H}_y\text{O}_z\), \(\text{CO}\), \(\text{H}_2\), \(\text{H}_2\text{O}\), \(\text{O}_2\), \(\text{CO}_2\), and \(\text{N}_2\), etc.

5.6 Discussion

Since the first fixed-bed model was established in 1976 for the packed bed reactor of coal gasification and combustion, it has been still a big challenge to build a general moving grate bed submodel that will be flexible, robust in a wide range of solid fuels under different operating conditions.

Nasserzaden (1991) used a porous-media model in investigating the solid refuse bed on top of a roller grate. Dos Santos(1993), Kim (1996) used the in-furnace measurement data as the inlet boundary conditions for the modeling of the over-bed gas phase simulation. Goh (1998) developed a continuum bed model but lack of a firm basis and validation. Saastamoinen (1998) developed a simplified bed model and coupled with a three-dimensional flow simulation for evaluation of different fireplace designs.
Päättikangas (1999) used Saastamoinen's submodel couple with three-dimensional flow simulation to calculate a utility power plant grate fired furnace, however, it is lack of validation and sensitive analysis.

The black-box bed model has been used together with the three-dimensional flow simulation, to calculate two different utility grate fired furnaces, one is the 17MV biomass boiler, another is the 45MW coal boiler (Dong 1997, 1998). The output data from the black-box bed model, are directly used as the inlet conditions for the next step simulation of the over-bed gas phase.
Chapter 6
Summary of Papers

This doctoral thesis describes the fundamentals of mathematical modeling for the industrial furnaces and boilers and presents the results from the numerical simulations of some typical applications in advanced industrial furnaces and boilers. The main objective of this thesis work is to employ computational fluid dynamics (CFD) technology as an effective computer simulation tool to study and develop the new combustion concepts, phenomena and processes in advanced industrial furnaces and boilers. The applications concern on from retrofitted conventional grate boilers to the most advanced highly preheated and diluted air combustion (HPDAC) furnaces. In this work, several topics are specially concerned when applying CFD technology to combustion cases. These topics are including grate bed model, NOx modeling, mixing problem, Ecotube system, and highly preheated and diluted air combustion technology.

In this work, the current development of grate bed models is reviewed and it is noted that until now there is no really realistic grate bed model which can be used satisfactorily to solve practical problems. Thus, a black-box grate bed model is developed and used in modeling of grate fired furnaces and boilers. It is based on the thermodynamic calculations and a set of conservation equations of mass, energy of fuel and air on the grate bed. One of this bed model’s benefits is simple and feasible to be put into use in industry. For NOx modeling, besides the thermal NO and prompt NO, the HCN route fuel NO has been employed to predict the fuel NO emissions in coal/biomass fired furnaces. In addition, based on NH3 route of fuel NO formation, a SNCR scheme for NOx abatement has been proposed also. For mixing problem, the concepts of global degree of mixing and individual degree of mixing have been proposed and used successfully in prediction of the mixing field in HPDAC and other practical applications. The proposed parameter “degree of mixing” completely overcomes some shortages of existed mixing parameters, such as the mixing factor and the degree of non-mixing, which are non-normalized and may lose physical meaning in some regions of the system. The Ecotube system is a new air supply technique. It is used to improve the secondary or over-fire air configuration, thus to reduce the pollutant emissions and to enhance the combustion facilities’ efficiencies. In this work, the Ecotube system has been installed in a biomass fired grate furnace and a coal fired grate boiler. The performance of Ecotube has been investigated and evaluated numerically. In addition, the optimization of Ecotube air system also has been carried out by using numerical modeling method together with physical modeling method. It is found that the location of Ecotube influences the flow field, temperature field and pollutant emissions in a boiler. The Ecotube air system should be installed close to grate bed as a secondary air system or be installed far from the grate bed as a over-fire-air system to reduce the unburned species, thus Ecotube air system may reduce about 35% NOx emissions. Results show that the Ecotube system gives a considerably more uniform velocity, temperature and concentration distribution from the secondary air tubes to the upper part of the bark boiler. The upper part of the boiler works almost as a ‘plug flow reactor’ which gives sufficient residence time for CO conversion and low NOx emission. The calculations of flow and mixing patterns in the bark and coal boilers conclude that the Ecotube system is
quite effective for secondary air distribution and improves combustion after retrofitting the furnace in an old boiler.

The flow and mixing process inside an entrained power boiler for co-firing of pulverized coal and biomass has been investigated numerically. It is found that the mixing is very good inside the new boiler. The volume averaged mixing degree is very close to unity, so the design of the burner's configuration in the boiler is excellent. It is also shown that the numerical method is a very good tool to help design, analysis, and evaluate the industrial-scale combustion systems.

Recently, the highly preheated and diluted air combustion has been regarded as the new generation energy technology for advanced industrial furnaces and boilers. In this work, the HPDAC phenomena have been studied by using different numerical models. The finite rate/eddy dissipation model and the mixture fraction/PDF model are used to investigate the single fuel jet reacting flows under the conditions of highly preheated and diluted air combustion. Some important features and characteristics of HPDAC are investigated by means of numerical simulations. It is found that mixture fraction/PDF model is better to predict the thermal field of HPDAC than the finite/eddy dissipation model. In the work, a 580KW semi-industrial HPDAC test furnace at IFRF, Netherlands, has been investigated by using mixture fraction/PDF model. The results show that the conditions of highly preheated air combustion make the furnace being a well-stirred reactor. The mixing process is very effective. The temperature and chemistry fields are quite uniform in the furnace. Globally, the combustion in the furnace is mixing controlled. It is found that the invisible flame may be captured by monitoring the OH radical, and the thermal NO dominates the NOx emissions in the furnace. It is NO that should take charge of 94.6% total NOx generation.

In this work, a hybrid procedure of the large-eddy simulation based on the SGS stress model and standard Smagorinsky model, together with the Reynolds stress model and finite rate/eddy dissipation model, has been carried to simulate the single fuel jet under the conditions of highly preheated and diluted air combustion. Results show that this hybrid procedure of standard Smagorinsky model and finite rate/eddy dissipation model seems to be acceptable to the practical engineering problems, and LES is a good tool to simulate the dynamical process of turbulent combustion in an HPDAC furnace.

Paper 1: CFD modeling of Ecotube system in coal and biomass grate combustion

Perfect combustion in a conventional grate furnace is difficult to achieve, because the mixing process is poor in the fuel bed on the grate and in the gas phase region above the grate. This problem can be alleviated by using different combustion air systems. Also, a turbulent jet performs the mixing, so a number of free turbulent jets or some combination of turbulent jets may be applied to improve the mixing process in a grate furnace. This paper presents an evaluation of one such innovative multi-jet air system called Ecotube. Two modeling methods, mathematical modeling and physical modeling, are applied in the work. For the mathematical modeling, the Reynolds transport equations and the perfect gas state equation together with the standard $k-\varepsilon$ turbulence model and the discrete transfer (DT) radiation model are used to model the
turbulent flows. The simulation of gas phase combustion is based on the multi-step chemical reactions where the Arrhenius finite-rate reaction mechanism and the Magnussen and Hiertager eddy-dissipation model are used simultaneously to calculate the interaction between turbulence and chemical reactions. Also, three different types of NO mechanism, such as Zeldovich’s thermal NO, De Soete’s prompt NO and the cyanogen route fuel NO are used as a postprocessor to the main combustion calculation to predict the NO emissions. The finite volume method with a second order upwind scheme is used to discrete the elliptical partial differential equations while the physical/computational domain is divided using the unstructured grid technique. The point-implicit Gauss-Seidel relaxation iterative method together with the SIMPLE or SIMPLEC algorithm for pressure-velocity coupling are used to solve the discretized equations. In order to accelerate the convergence rate, the unstructured algebraic multigrid (AMG) method is also used in the solver. In addition, the heterogeneous processes in the grate bed and off-bed gas phase, such as char combustion and the soot or ash processes, are neglected in this work. The boundary conditions at the grate bed inlets are simply derived based on the mass and energy balance according to the fuel pyrolysis reactions.

For physical modeling, a three-dimensional water model is established to represent the gaseous combustion and to demonstrate the mixing process. The flow patterns are visualized by using dyes or color indicators. The process is recorded by a camera and a computer controlled video system and then analyzed. The water model is used primarily to provide qualitative information of flow patterns to justify the performance of the Ecotube system for mixing purpose and to validate the mathematical modeling.

Two types of boilers were used in this project. One is a biomass waste fired boiler with 15 MW thermal power, installed at Bäckhamars AB in Sweden, another is a coal fired boiler with 29 MW thermal power, installed at the Zamosc power plant in Poland. The CFD study is based on three-dimensional cases, while for physical modeling study, only two-dimensional cases of the coal-fired boiler have been carried out. The mesh case of the biomass boiler employs 284,399 unstructured (tetrahedral) cells and a total computational volume of 255 m$^3$. While the mesh case of the coal fired boiler employs 194,332 unstructured cells and a total computational volume of 100 m$^3$.

Results from the mathematical modeling are verified partly by physical modeling and also by in-furnace measurements of flue gas velocities, temperatures and concentrations. Results show that the new Ecotube air system generates a considerable improvement in efficiency for coal and biomass waste combustion in industrial boilers and furnaces. The upper furnace works almost as a ‘plug flow reactor’, which gives sufficient residence time for CO conversion and low NOx emission, while the main combustion chamber can acts as a well-stirred reactor. The modeling of flow and mixing patterns in the biomass waste boiler and the coal boiler concludes that the Ecotube air system is quite effective for secondary/over-fire air distribution. It improves grate combustion environment in a grate furnace by facilitating much better mixing, resulting in a more uniform flame. It also reduces the level of NOx and CO emissions in a grate furnace or boiler. These comprehensive simulations provide useful information concerning the combustion performance of industrial grate fired furnaces equipped with the new Ecotube air system. Such means
can be used to aid design, retrofit and improve existing industrial boilers and furnaces. Thus, it is apparent that the numerical simulation is successful in the work and the Ecotube technique has good potential for future application in industry.

**Paper 2: Design and optimizing Ecotube air system for clean combustion of coal in a grate fired boiler**

Based on the results of paper 1, an improved design of Ecotube air system for optimizing the secondary and over-fired air (SOFA) configuration is proposed for a 25MW industrial travelling grate fired boiler for coal combustion. The CFD technique is applied to simulate and optimize the performance of the furnace with its SOFA system. The mathematical models described in paper 1 are also used. The heterogeneous grate bed is modeled by using a black-box bed model that is based on the balance of mass and energy according to the fuel pyrolysis and volatilization, char gasification and combustion in the grate bed layer. Only homogenous gas phase processes above the grate bed are simulated using CFD. In addition, the residence time distribution (RTD) of fluid flow in the boiler is modeled by using Lagrangian particle trajectory and turbulent dispersion of particles model. The time of small tracer particles that move with the fluid is solved by step-wise integrated through each particle paths.

The simulated coal boiler has a horizontal moving grate with seven wind boxes for primary air supply. Very complicated phenomena take place in the grate bed. According to the black-box bed model (chapter 5), boundary conditions at the grate bed inlets are derived based on the mass and energy balance for the fuel pyrolysis and combustion reactions.

The gas phase combustion simulation is based on the multi-step chemical reactions. According to the mass balance based on the coal composition analysis and the ratio of volatile, the equivalent composition of coal and the equivalent volatile can be obtained, thus the pyrolysis and combustion reactions for coal are proposed.

A new advanced secondary/over-fire air (SOFA) system using Ecotube technique is thus studied and five different air configurations are comprehensively calculated for optimizing the SOFA configuration in the boiler. The results of numerical modeling show that the Ecotube system can generate a local strong mixing zone, which renders a good mixing and enhances the residence time. The strong mixing zone generated by SOFA from the Ecotube system plays an important role in controlling the combustion process. The low position Ecotube air configuration is favorable to perfect combustion, while the upper position Ecotube air configuration is favorable to minimizing the NO emission. It can be concluded that the Ecotube technique is quite effective to distribute the secondary/over-fire air, to improve the grate combustion and to reduce CO and NOx emissions. The good combustion can be achieved if using low position Ecotube air configuration, while the NOx can be reduced about 35% if using the upper position Ecotube air configuration in the boiler. Therefore, for the grate combustion, the Ecotube system is effective and has strong potential to be put into application in industry for future.
In this paper, the flow and mixing patterns in an entrained boiler for co-firing of pulverized coal and renewable biomass fuels have been studied by using numerical modeling and water modeling methods. In order to reach the complete combustion of fuels, the strong turbulent flows in a boiler always are expected for fuel/air mixing. The co-firing process can be realized in one burner (coal and biomass are fed to the same burner) or between different burners or burner levels (coal and biomass are fed to different burners or burner levels). The simulated boiler is a 365 MW industrial entrained boiler fired with pulverized coal and biomass. The boiler is equipped with 13 highly swirling burners and 24 over-fire air (OFA) jets on its wall sides. Each burner has a separate system for feeding the pulverized fuel and has four levels of coaxial air jets in which primary and secondary air are highly swirling by internal turbulators. In the boiler, the burners are operated in different rotating directions of flows. This aerodynamic configuration is expected to generate much better turbulent mixing pattern while it also creates additional difficulties for modeling. Different with the paper 1 and paper 2, in this work, the renormalization group (RNG) \( k-\varepsilon \) turbulence model is employed to deal with the strong turbulent swirling flows. In order to simulate the interaction between different flames with different coaxial-jet swirling flows in the co-firing process, a 3-D mesh case of whole boiler together with all 13 burners is established. Totally 70 inlets are taken into account to describe the boiler and burners with whole detail geometry. For grid generation, the unstructured finite volume grid with multi-block concept is employed to divide the very complicated geometry of the flow domain into discrete segments with high grid quality. This approach is very important to get a convergent and accuracy solution. In the work, the total volume of computational domain is about 2536m\(^3\), and total 281,847 tetrahedral cells are employed to discrete the computational domain. The finite volume method and first-order upwind scheme are used to discrete the elliptical partial differential equations into algebraic equations, which are solved by using the point-implicit Guass-Seidel iteration method. The standard SIMPLE scheme is used for pressure–velocity coupling, while the under-relaxation method is used to control the update of computed variables during the iteration process. In order to increase the convergent rate, the algebraic multigrid method is also used. In addition, a parameter, the degree of mixing, is defined and used to quantitatively describe the mixing pattern of the fluid flow in the boiler.

On the other hand, a 3-D water model has been established to simulate the aerodynamic pattern of the boiler and burners. The water modeling is used to evaluate the performance of the boiler with its burners, as well as the CFD simulation results. In the work, the acid/alkali neutralization flame modeling technique is employed to visualize the 3-D fluid flow field and mixing pattern in the boiler and burners. The results of numerical and water modeling illustrate that the design of the pulverized fuel boiler is successful. The mixing inside the boiler is perfect and the boiler can be regarded as a well-stirred reactor. It has been shown that using unstructured grid and multi-block concept is a good solution to cater for the complex flow and geometry in an industrial entrained boiler. Thus detailed information about the complicated fluid flow and mixing patterns in the boiler can be obtained. Just as expected, the agreement is quite good between the results of 3D full-scale CFD simulation and those of the 3D small-scale water modeling. Having these tools
checked and learned, the in-burner co-firing or between burners co-firing processes can be studied in a whole range of operating conditions in future work.

**Paper 4: Study on mathematical modeling of highly preheated air combustion**

Highly preheated and diluted air combustion (HPDAC) has been considered as a promising energy technology for next generation of advanced industrial furnaces and boilers. In this paper, the important features and characteristics of highly preheated and diluted air combustion are investigated by means of numerical modeling method. Two turbulent models of RNG $k-\varepsilon$ model and Reynolds stress model (RSM) and two turbulent-chemistry interaction models of finite rate/eddy-dissipation model (FRED) and the mixture fraction/probability density function (MPDF) model, have been applied to study the turbulent jet flames under the HPDAC conditions in a single chamber and a test furnace with two switching burners. In addition, the Rosseland model and discrete transfer (DT) radiation model are used to model the radiation, while the Zeldovich’s thermal NO and De Soete’s prompt NO mechanisms are employed to model the NO emissions. A single jet HPDAC test apparatus with fuel direct injection (FDI) technique, and a two-burner switching HPDAC test furnace are simulated. The unstructured grid technique is used and the local mesh refinements near the jet are especially treated in sake of numerical convergence requirements.

Both the finite rate/eddy dissipation model and the mixture fraction/probability density function model are investigated and compared each other. The numerical results are also partially validated by some experimental measurements. Results show that the mixture fraction/probability density function model is better than the finite rate/eddy dissipation model for predicting of the thermal fields of the turbulent jet flames, and thus can give out reasonable prediction of NOx formation. The numerical simulation results in the flow patterns, thermal fields, chemical species profiles and NOx emissions in the HPDAC chamber and furnace that could be used to draw the following conclusions: The RSM/MPDF model is better than $k-\varepsilon$/FRED model to predict the turbulent diffusion flame. A detailed reaction system is needed to add into the CFD modeling framework that will result in next stage research work for development of more realistic models. The main features and characteristics of highly preheated air combustion have been successfully investigated by using mathematical modeling method. A more detailed and comprehensive mathematical modeling for both HPDAC fundamental research and large-scale industrial HPDAC utilities is still a challenge.

**Paper 5: Numerical modeling of highly preheated air combustion in a 580KW testing furnace at IFRF**

Based on the progress on paper 4, a comprehensive numerical simulation has been conducted for a highly preheated air combustion (HPAC) furnace fired with natural gas. The geometry of the simulated burner and furnace, as well as the operating conditions, are based on the actual experimental NFK burner and IFRF furnace. The numerical results are compared with the experimental results from a 580kW semi-industrial furnace at IFRF, Netherlands, and are expected as the supplement to the experimental demonstration, to provide detail information about the new combustion system. Meanwhile, the numerical results are also validated by the experimental measurements. For the numerical modeling, the Reynolds transport equations and the
perfect gas state equation together with the standard $k$-$\varepsilon$ turbulence model and the discrete ordinates (DO) radiation model are used to model the turbulent flows. The mixture fraction/probability density function model (MPDF) is used to calculate the interaction between turbulence and chemical reactions. The MPDF model is based on the solution of the mixture fractions instead of each species transport equations. The turbulence effects are accounted for with the help of a probability density function (PDF), while the kinetics of chemical reactions are not explicitly defined but treated in thermodynamics using assumption of chemical equilibrium. In the present simulation, total 11 species, such as CH$_4$, C$_2$H$_6$, C$_3$H$_8$, C$_4$H$_{10}$, O$_2$, OH, CO, CO$_2$, H$_2$, H$_2$O and N$_2$ are calculated in this model. In addition, the Zeldovich’s thermal NO and De Soete’s prompt NO mechanisms are used to predict the NO emissions. The finite volume method with a second order upwind scheme is used to discrete the elliptical partial differential equations while the physical/computational domain is divided using the unstructured grid technique. The point-implicit Guass-Seidel relaxation iterative method together with the SIMPLE algorithm for pressure-velocity coupling are used to solve the discretized equations. In order to accelerate the convergence rate, the unstructured algebraic multigrid (AMG) method is also applied. A new parameter of the global degree of mixing has been proposed based on the individual degree of mixing defined in paper 3 and can be easily used to quantify the mixing process for non-reacting or reacting flows. Both the global and the individual parameters of the degree of mixing have been compared with the other mixing parameters to study the mixing process in the HPAC furnace. Both the modeling and the experiment illustrate that the conditions of highly preheated air combustion make furnace being a well-stirred reactor, thus the temperature and chemistry fields are quite uniform in the furnace. A new parameter, the degree of mixing, is proposed to quantify the mixing process of the turbulent reacting flows in the furnace. Modeling shows that the combustion in the furnace is mixing controlled, and the invisible flame of HPAC can be captured by monitoring the profile of hydroxyl radical. Furthermore, the calculation illustrates that the thermal NO takes about 94.6% of total NO generation in the furnace, thus it is thermal NO that dominates the global NO$_x$ emissions from the furnace. The numerical results and the IFRF measurements have been compared with each other. It has been found that the conditions of highly preheated air combustion make the 580kW semi-industrial furnace being a well-stirred reactor under. The mixing process is very effective. The temperature and chemistry fields are quite uniform in the furnace. The global degree of mixing ($\xi$) and the individual degree of mixing ($\xi_i$) are well-defined parameters to quantify the mixing process in non-reacting or reacting flows. Globally, the combustion in the furnace is mixing controlled. The invisible flame of HPAC can be captured by monitoring the profile of hydroxyl radical. The thermal NO dominates the NO$_x$ emissions from the furnace. It takes 94.6% of total NO generation. The numerical results are in good agreement with the measurements in velocity field, temperature, and species except the radiation heat flux and the intermediates of CO and H$_2$. It needs a further investigation on both experiments and numerical models.

**Paper 6: Large eddy simulation of a single jet flow in highly preheated and diluted air combustion**

In a HPDAC furnace, the highly turbulent flow field is time dependent controlled by the switching regenerative burners. This is the motivation in this paper to use the large
eddy simulation to simulate a single fuel jet flame under the conditions of highly preheated and diluted air combustion (HPDAC). In addition of paper 4 and paper 5, in the work, a hybrid procedure of LES subgrid scale (SGS) Smagorinsky-Lille model and with Reynolds stress model and the finite rate / eddy dissipation conception (EDC) combustion model has been employed to simulate a single wall jet HPDAC furnace chamber. The propane-air two-step combustion system is selected for modeling under two different HPDAC inlet air conditions corresponding to 3% w/w oxygen at 1300K and 21% w/w oxygen at 1300K. The global two-step reactions of propane combustion are considered in the modeling. The finite volume method with the unstructured mesh is used to obtain a solution of the spatially averaged governing equations. The inlet boundary conditions are mainly based on the experimental operating conditions and the diluted air is assumed containing 14 % CO₂. The wall solid is treated using standard wall function, while the thermal condition on the wall is set as the constant temperature at 600K. The first convergent RSM/EDC results are set as initial conditions for beginning of LES modeling. In this work, the convective terms are approximated via second-order upwind scheme, while time derivatives are discretized via a second-order implicit scheme. For the velocity-pressure coupling, the SIMPLE scheme is employed. The resulting algebraic equations are solved iteratively and the algebraic multigrid (AMG) method is used to accelerate the convergent speed. The numerical results show that the hybrid procedure of the SGS Smagorinsky modeling and the RSM/EDC modeling is capable of predicting the global flame effects on the flow, such as flow velocities, mixing patterns, temperatures and turbulent parameters. The predictions are found in acceptable agreement with the corresponding results of in-furnace measurements and physical modeling. By compared with the pure Reynolds stress model, it is found that the differences between the two predictions of LES and RSM are insignificant in the near field of the flow. The Smagorinsky constant $C_s$ has been also tuned in the work. It illustrates that $C_s$ value significantly influences the predictions on both near field and far field of the jet flow. For further work, a more dense discretization mesh together with carefully checked boundary conditions should be established and performed on a more powerful computer. In addition, there always exists a need to further investigate some uncertainties of SGS model’s parameters and to develop more adequate SGS stress models for the turbulent combustion flames.
Paper 1

CFD Modeling of Ecotube System in Coal and Biomass Grate Combustion

Wei Dong and Wlodzimierz Blasiak
Division of Heat and Furnace Technology
Royal Institute of Technology
10044 Stockholm, Sweden


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CFD Modeling of Ecotube System in Coal and Biomass Grate Combustion

Wei Dong* and Wlodzimierz Blasiak
Division of Heat and Furnace Technology
Royal Institute of Technology
10044 Stockholm, Sweden

Abstract: This paper presents a comprehensive numerical simulation for the advanced secondary/over fired air Ecotube system. The computational fluid dynamics (CFD) technique is applied to simulate and analyze the performance of this new air system in two typical coal and solid waste fired furnaces. Results show that the numerical simulation is successful and the Ecotube technique has good potential for future application in industry.

Keywords: Numerical Simulation, Grate Combustion, Aerodynamics, Solid Fuel Combustion

1. Introduction

Grate combustion is the oldest method of utilizing coarse solid fuels, but is still very widely used. The air supply is divided into the primary combustion air, which is introduced at the bottom of the grate, and the secondary, or sometimes over-fire air, which is introduced above the grate. The amount of primary air controls the rate of combustion in the fuel bed, while the amount of secondary air controls the overall combustion efficiency. Sufficient secondary air must be added to completely oxidize any unburned or partially oxidized species originating from the solid fuel bed.

Perfect combustion in a conventional grate furnace is difficult to achieve, because the mixing process is poor in the fuel bed on the grate and in the gas phase region above the grate. This problem can be alleviated by using different combustion air systems. Also, a turbulent jet performs the mixing, so a number of free turbulent jets or some combination of turbulent jets may be applied to improve the mixing process in a grate furnace. This paper presents an evaluation of one such innovative multi-jet air system called Ecotube[1]. This evaluation of Ecotube air system is based on mathematical modeling using computational fluid dynamics (CFD) technique to simulate two different grate fired boilers. One boiler is fired by solid biomass waste while the other is coal fired. Results from the mathematical modeling are verified partly by physical modeling and also by in-furnace measurements of flue gas velocities, temperatures and concentrations.

2. Description of the Ecotube Air System

Ecotube, a new air supply system, was developed in Sweden, and has been used in demonstrations to retrofit already existing grate boilers since 1996. It aims to distribute the secondary air inside the boiler more evenly and to make the aerodynamic configuration more effective for the combustion of solid fuels. It also aims to reduce pollutant emissions from the furnace chamber. As shown in Figure 1, the Ecotube air system in a boiler consists of two air tubes that are mounted parallel to each other above the grate bed.

* Corresponding author. Fax: +46-8-149338. Email: dong@metallurgi.kth.se
Each tube has a set of small air jets on opposite sides and points in suitable directions. There are total 36 air jets in the Ecotube system. Each jet is 10 mm in diameter and the injection velocity of the jet air can exceed 150 m/s. This arrangement with the high speed air injection is expected to mix the secondary/over-fire air more efficiently with the off-bed gases. The first combustion zone may then be considered as a well-stirred reactor while the gas flow from the secondary combustion zone up through the boiler can be treated as a plug flow.

3. Modeling Methods

Two modeling methods, mathematical modeling and physical modeling\cite{2,3}, are available in the Heat and Furnace Laboratory at the Royal Institute of Technology. Mathematical modeling using CFD technique is a very strong and effective tool to simulate the flow and combustion in an industrial boiler. It is based on Navier-Stokes equations or Reynolds transport equations, together with the gas state equation and the k-ε turbulence model. The finite volume method with a second order upwind scheme is used to discrete the elliptical partial differential equations. Radiation heat transfer is modeled by the discrete transfer method. The SIMPLE-Consistent algorithm is employed for pressure-velocity coupling. The Arrhenius finite-rate reaction mechanism and the Magnussen and Hiertager eddy-dissipation model are used simultaneously to calculate the interaction between turbulence and chemical reaction flows. Also, three different types of NO mechanism, such as Zeldovich’s thermal NO\cite{4}, De Soete’s prompt NO and the cyanogen route fuel NO\cite{5} are used to predict the NO emission. The NO model serves as a postprocessor to the main combustion calculation. To accelerate the convergent rate, the unstructured multigrid method is also used in the solver. All the simulations in this work are performed using FLUENT code\cite{6} on an IBM Risc 6000/591 workstation computer with 512 MB main memory running under the AIX4.1 operating system.

Physical modeling can be used to obtain flow patterns and mixing information pertaining to a grate furnace. It uses water to represent the combustion gases and to demonstrate the mixing process. The flow patterns are visualized by using dyes or
color indicators. The process is recorded by a camera and a computer controlled video system and then analyzed. A three-dimensional water model is used primarily to provide qualitative information of flow patterns, on which, it is possible to justify the performance of the Ecotube system for mixing purpose, and to validate the mathematical modeling.

4. Simulated Boilers

Two types of boilers were used in this project. One is a biomass waste fired boiler with 15 MW thermal power, installed at Bäckhamars AB in Sweden, another is a coal fired boiler with 29 MW thermal power, installed at the Zamosc power plant in Poland. The CFD study is based on three-dimensional cases, while for physical modeling study, only two-dimensional cases of the coal-fired boiler have been carried out.

4.1 Geometry and Mesh

As shown in Figure 2, the mesh case of the biomass waste boiler has 284,399 tetrahedral cells and a total computational volume of 255 m³. The mesh case of the coal fired boiler employs 194,332 tetrahedral cells and a total computational volume of 100 m³.

![Figure 2. The mesh cases of two boilers with Ecotube air system](image)

4.2. Combustion bed and boundary conditions

The simulated biomass waste boiler case has an inclined moving grate with four wind boxes for primary air supply, while the simulated coal boiler case has a horizontal moving grate with seven wind boxes for primary air supply. The solid fuel particles move slowly along the grate and are normally burnt out before reaching the final vibrating plate near the ash outlet. Very complicated phenomena take place in the combustion bed. These phenomena include heating and drying of fuel particles, motion of particles on moving grate, the interaction between gas and solid phases, fuel...
pyrolysis and volatilization, and finally char gasification and combustion. Although fixed-bed combustion modeling has received significant attention over the last decade, little application of the bed model technology has been implemented for practical grate furnaces and boilers. This is due to the intangible complexity of the actual bed combustion processes. This complexity can be simplified, however, by subdividing the grate bed into well-defined zones according to the under grate primary air inlets. For further simplification, only homogenous gas phase processes above the grate bed are simulated. The heterogeneous processes in the grate bed and off-bed gas phase, such as char combustion and the soot or ash processes, are neglected in this CFD simulation. In this simplified model, boundary conditions at the grate bed inlets are derived based on the mass and energy balance according to the fuel pyrolysis reactions\cite{7}.

The solid fuel compositions and thermal data used in the mathematical modeling are listed in Table 1.

<table>
<thead>
<tr>
<th>Elements</th>
<th>Biomass waste</th>
<th>Coal</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>51 %</td>
<td>65 %</td>
</tr>
<tr>
<td>H</td>
<td>6 %</td>
<td>4 %</td>
</tr>
<tr>
<td>N</td>
<td>0.3 %</td>
<td>&lt; 1 %</td>
</tr>
<tr>
<td>O</td>
<td>41 %</td>
<td>10 %</td>
</tr>
<tr>
<td>Inertial</td>
<td>1.7 %</td>
<td>11 %</td>
</tr>
<tr>
<td>Volatile</td>
<td>35 %</td>
<td></td>
</tr>
<tr>
<td>Water content</td>
<td>50 %</td>
<td>10 %</td>
</tr>
<tr>
<td>Low Heat value</td>
<td>9 MJ/kg</td>
<td>26 MJ/kg</td>
</tr>
</tbody>
</table>

The gas phase combustion simulation is based on the following multi-step chemical reactions. According to the mass balance based on the biomass composition analysis, and the previous work of in furnace measurements\cite{7,8}, we can get the equivalent composition of biomass as $C_{4.25}H_{6}O_{2.56}$ and the equivalent volatile of biomass as $C_{1.54}H_{4.28}$.

Thus, in this simulation, the pyrolysis and combustion reactions for biomass waste are assumed to be as

$$C_{4.25}H_{6}O_{2.56} + 0.15H_2O \rightarrow C_{1.54}H_{4.28} + 2.71CO + 0.935H_2$$

$$C_{1.54}H_{4.28} + 1.84O_2 \rightarrow 1.54CO + 2.14H_2O$$

$$CO + 0.5O_2 \rightarrow CO_2$$

$$CO_2 \rightarrow CO + 0.5O_2$$

$$H_2 + 0.5O_2 \rightarrow H_2O$$

and for coal, an high-volatile coal combustion system in FLUENT is modified to be as

79% Raw coal ($C_{5.417}H_{4}O_{0.625}$) $\rightarrow$ 34% Volatile ($CH_{2.834}O_{0.221}$) + 45% Char(C)

Char (C) + 0.5 O$_2$ $\rightarrow$ CO

Volatile + O$_2$ $\rightarrow$ CO + H$_2$O
\[ \text{CO} + 0.5 \text{ O}_2 \rightarrow \text{CO}_2 \]
\[ \text{CO}_2 \rightarrow \text{CO} + 0.5\text{O}_2 \]

where, the kinetic data of volatile reactions for both biomass and coal are directly adopted from the data generated by methane combustion reactions.

5. Results and Discussions

The global flow fields in the biomass waste boiler and coal boiler are shown in Figures 3 and 4.

![Figure 3 Velocity profiles in the biomass and coal boilers](image)
![Figure 4 Comparison of flow patterns (velocity contours) for the old biomass boiler and the new retrofitted one](image)
It is obvious that large eddies are created by the high-speed secondary air, so the main combustion chamber can be regarded as a well-stirred reactor. The mixed gases, however, travel up to the outlet in a plug flow pattern. The figures also provide important information concerning how the Ecotube air system controls the flow field and improves the gas mixing by comparing the conventional biomass boiler to the retrofitted one. It is obvious that once modified with the Ecotube air system in a grate furnace, the secondary air plays a more important role in flow field.

The Ecotube flow fields obtained by the numerical and physical modeling of the coal boiler are compared in Figure 5. The patterns are quite similar, thus results from these two different modeling are in good agreement.

Figure 5 Comparison of physical and numerical results of Ecotube air flow patterns in the coal boiler

The temperature in the layer of 1m above the Ecotube in the biomass waste boiler was in-situ measured by using platinum/platinum-rhodium thermocouples.

Figure 6 Comparison of temperatures in the middle line 1 m above the Ecotube in the biomass boiler
Figure 6 plots the comparison of measured and predicted temperatures in the middle line parallel to the Ecotube. The horizontal axis indicates the horizontal distances of six testing points to the wall of the boiler. In this testing line, the maximum temperature difference between measurement and prediction is less than 8%. However, the maximum temperature difference between measurements and predictions may reach to 15% in other directions in the same measuring layer 1m above the Ecotube system in the biomass boiler. The main reason maybe due to the strongly unstable flows around the Ecotube, which results in a large uncertainty of the local thermal field.

The temperature profiles of the biomass case and the coal case are plotted in Figure 7. For the coal boiler, the time averaged temperature at a point 0.65 m below the top ceiling of the boiler was measured as 695 °C, while the corresponding prediction is 728 °C. The difference is less than 5%, so the agreement is good. However, because there are no access ports in main combustion chamber of the coal boiler, it is lack of measurement data to compare with the numerical predictions inside the combustion chamber where the Ecotube system is installed.
Numerical calculation shows that the carbon monoxide in the flue gas is to be about 1050 mg/m$^3$ and 260 mg/m$^3$ for the retrofitted biomass boiler and the retrofitted coal boiler, respectively.

The profiles of CO mass fraction in the old and retrofitted coal boiler are plotted in Figure 8. It shows that CO emissions in the retrofitted coal boiler equipped with the Ecotube air system will be reduced about one order of magnitude when compared to those in the old coal boiler without the Ecotube air system.

Correspondingly, the O$_2$ profiles are shown in Figure 9. The oxygen mass fractions in the flue gas are predicted to be 3.2 % and 8.9 % for these two retrofitted boilers. These values are corresponding to the different excess air ratios of 1.1 and 1.5, respectively.

![Figure 9 Oxygen profiles in the retrofitted biomass waste and coal boilers](image)

NO$_x$ emission of biomass waste combustion in a conventional grate furnace is a quite significant problem. During 1997 to 1998, by using the chemiluminescent method, a series of in-situ measurements in the utility biomass combustion boiler, was carried out to compare with the numerical predictions of NO emissions.

The calculated NO ppm in the new retrofitted biomass waste boiler is plotted in Figure 10. According to the results, the average NO concentration in the outlet is about 45 ppm, which is very close to that measured in flue gas, 48–60 ppm. In this numerical case, it is found that the contributions of thermal and prompt NO are insignificant. So, fuel-NO completely dominates the NO$_x$ emission level in the flue gas.
These results show that the Ecotube air system facilitates much better mixing, resulting in a more uniform flame in a grate combustion chamber with fewer pollutant emissions.

6. Conclusions

Using unstructured grids, CFD technique is a good tool to perform comprehensive simulations for the complex flow and geometry in an industrial boiler with realistic computing source power. Detailed information about the flow patterns and mixing processes in industrial boilers can be obtained though mathematical modeling accompanied with physical modeling.

Results show that the new Ecotube air system generates a considerable improvement in efficiency for coal and biomass waste combustion in industrial boilers and furnaces. The upper furnace works almost as a ‘plug flow reactor’, which gives sufficient residence time for CO conversion and low NO\textsubscript{x} emission, while the main combustion chamber can acts as a well-stirred reactor. The modeling of flow and mixing patterns in the biomass waste boiler and the coal boiler concludes that the Ecotube air system is quite effective for secondary/over-fire air distribution. It improves grate combustion environment in a grate furnace by facilitating much better mixing, resulting in a more uniform flame. It also reduces the level of NO\textsubscript{x} and CO emissions in a grate furnace or boiler.

These comprehensive simulations provide useful information concerning the combustion performance of industrial grate fired furnaces equipped with the new Ecotube air system. Such means can be used to aid design, retrofit and improve existing industrial boilers and furnaces.
Acknowledgements

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Design and Optimizing Ecotube Air System for Clean Combustion of Coal in a Grate Fired Boiler

Wei Dong* and Wlodzimierz Blasiak
Division of Heat and Furnace Technology
Department of Metallurgy, Royal Institute of Technology
10044 Stockholm, Sweden
*Fax: +46-8-149338, Email: dong@metallurgi.kth.se

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The computational fluid dynamics (CFD) technique together with a black-box bed model are used to simulate and optimize the performance of a 25MW industrial travelling grate fired boiler for coal combustion. A new advanced secondary/over-fire air (SOFA) system using Ecotube technique is studied and five different air configurations are comprehensively calculated for optimizing the SOFA configuration in the boiler. The results of numerical modeling show that the Ecotube system can generate a local strong mixing zone, which renders a good mixing and enhances the residence time. Results show that the Ecotube technique is quite effective to distribute the secondary/over-fire air, to improve the grate combustion and to reduce CO and NOₓ emissions. The perfect combustion can be achieved if using low position Ecotube air configuration, while the NOₓ can be reduced about 35% if using the upper position Ecotube air configuration in the boiler. Therefore, for the grate combustion, the Ecotube system is effective and has strong potential to be put into application in industry for future.

1. Introduction

Grate fired furnace is still a widely used technology for solid fuel combustion. However, perfect combustion in a conventional grate fired furnace is difficult to achieve, particularly in a large industrial furnace chamber. It is due to the mixing process is usually poor in the fuel bed on the grate and in the gas phase region above the grate. Since clean combustion of coal in power generation industry has become an essential task due to the more strict requirements for environmental protection, it is therefore always expected to use different combustion air systems to improve the coal combustion in grate fired furnaces.

* Corresponding author. Fax: +46-8-149338, Email: dong@metallurgi.kth.se
A new multiple jet system, called Ecotube system, has been proposed and used in some grate fired furnaces and boilers. It is a patent technique designed to retrofit an already existing furnace, to distribute the secondary/over-fire air (SOFA) inside the boiler more evenly and to make the aerodynamic configuration more effective for the combustion of solid fuels. The Ecotube air system also aims to reduce the emissions of pollutants, such as CO and NOx, from the furnace chamber. The performance of Ecotube system in different grate fired furnaces and boilers has been also evaluated by the numerical method and the in-furnace measurements. Since the location of Ecotube system strongly influences the flow pattern, it is therefore interesting to search for the optimum position of Ecotube system in the furnace chamber.

In the last decade, the computational fluid dynamics (CFD) technique has been proven to be a valuable tool to simulate the flow and combustion processes in industrial furnaces and boilers. Although there are still some deficiencies with a detailed modeling of the interaction between turbulence and chemical reactions, numerical simulation has been successfully used to support design improvements and optimization effects for large-scale industrial combustion utilities. However, for grate fired furnaces and boilers, CFD has been applied very seldom since a large portion of the necessary boundary conditions has to be estimated or properly modeled. In this work, a black-box grate bed model is employed as the preprocessing step to define the boundary conditions for the next step of CFD calculation. This black-box bed model is only based on the balance of mass and energy according to the fuel pyrolysis and volatilization, char gasification and combustion in the grate bed, thus it avoids to take into account the details of the very complicated dynamic processes of the grate bed. In the work, both CFD tool and black-box bed model are employed to investigate the
optimum aerodynamic configuration of Ecotube system in a utility travelling grate fired boiler for coal combustion. The experimental validation has been done for a base case (A).

2. Simulated boiler, Ecotube and air configurations

The simulated boiler, 9m height, is a typical grate fired coal boiler with 25 MW output thermal power. It has an 8m long horizontal traveling grate with seven wind-boxes under the grate for primary air supply. Inside the furnace chamber, a new SOFA system is installed. It consists of two air tubes, so called Ecotube, which are mounted parallel to each other above the grate bed in a certain height. Each tube has a set of small air jets (16×φ10, 8×φ15, air speed 160m/s) distributed on two opposite sides, pointed in suitable directions, as shown in Figure 1. Using this arrangement, the secondary/over-fire air is expected to mix more efficiently with the off-bed gases, thus to improve the combustion in the furnace.

![Fig.1 Ecotube system](image)

In order to optimize the aerodynamic design of SOFA in the boiler, several geometrical cases are studied corresponding to four different SOFA configurations for the boiler as shown in Figure 2.
Fig. 2 Four configurations of SOFA system designed for the coal boiler

For grid generation, the unstructured finite volume grid and multi-block concept are employed to divide the very complicated geometry of the complex flow domains in a grate fired furnace into discrete segments with high grid quality, which is very important to get a convergent solution. Geometry case (A) stands for the original boiler, in which the secondary air inlets (10×Ø32) are located on one side of the wall, 2m high above the grate. Since the case (A) is symmetry in geometry (there exists a symmetrical plane in the boiler), only half part of the boiler is therefore considered. The 3-D unstructured mesh case (A) has total 47,463 tetrahedral cells. Geometry case (B) stands for the low position Ecotube configuration, in which the Ecotube system is installed 2m high above the grate. The 3-D unstructured mesh case (B) has total 192,320 tetrahedral cells. Geometry case (C) stands for the middle position Ecotube configuration, in which the Ecotube system is installed 3m high above the grate. The 3-D unstructured mesh case (C) has total 193,337 tetrahedral cells. Geometry case (D) stands for the middle position Ecotube configuration, in which the Ecotube system is installed 5m high above the grate. The 3-D unstructured mesh case (D) has total 192,332 tetrahedral cells.
3. Mathematical models

Basically, for homogenous Newtonian fluid flows, the mathematical modeling is based on a set of coupled conservation equations of mass, momentum, energy, and chemical species transport and reactions, in their time-averaged steady-state forms also known as the averaged Navier-Stokes equations or Reynolds transport equations. In the work, the fluid is treated as ideal gas and the turbulence is modeled by using the standard ‘two-equation’ k-ε model. The simulation of gas phase combustion is based on the multi-step chemical reactions where Arrhenius’ finite rate reaction model and Magnussen and Hiertager’s eddy-dissipation model are used simultaneously to calculate the interaction between turbulence and chemical reactive flows.

In the work, three different types of NO mechanism, such as thermal NO model (Zeldovich, 1946), prompt NO model and the cyanogen route fuel NO model (De Soete, 1975), are used to predict the NO emissions. The NO model serves as a postprocessor to the main combustion calculations.

The 3-D elliptical partial differential equations are transformed into a set of discrete algebraic equations by using the finite volume method. The well-known SIMPLE algorithm and a second-order upwind scheme are applied to solve the algebraic equation set of the discrete system. To accelerate the convergent rate, the unstructured multigrid method is also used in the solver.

The heterogeneous grate bed is modeled by using a black-box bed model that is based on the balance of mass and energy according to the fuel pyrolysis and volatilization, char gasification and combustion in the grate bed layer. In addition, the residence time distribution (RTD) of fluid flow in the boiler is modeled by using Lagrangian particle
trajectory and turbulent dispersion of particles model\textsuperscript{10}. The time of small tracer particles that move with the fluid is solved by step-wise integrated through each particle paths.

4. Coal grate bed and boundary conditions

The simulated coal boiler has a horizontal moving grate with seven wind boxes for primary air supply. The coal particles move slowly along the grate and are normally burnt out before reaching the final vibrating plate near the ash outlet. Very complicated phenomena take place in the grate bed. These phenomena include heating and drying of fuel particles, motion of particles on moving grate, the interaction between gas and solid phases, fuel pyrolysis and volatilization, and finally char gasification and combustion.

Although grate bed modeling has received significant attention over the last decade, little application of the bed model technology has been implemented for practical grate furnaces and boilers. This is due to the intangible complexity of the actual bed combustion processes. This complexity can be simplified, however, by subdividing the grate bed into well-defined zones according to the under grate primary air inlets. For further simplification, only homogenous gas phase processes above the grate bed are simulated. The heterogeneous processes in the grate bed and off-bed gas phase, such as char combustion and the soot or ash processes, are neglected in this CFD simulation. According to the black-box bed model\textsuperscript{2}, boundary conditions at the grate bed inlets are derived based on the mass and energy balance for the fuel pyrolysis and combustion reactions. Figure 3 demonstrates the black-box bed model and the bed boundary conditions used in the modeling.
The coal composition and thermal data used in the modeling are listed in Table 1. The gas phase combustion simulation is based on the following multi-step chemical reactions. According to the mass balance based on the coal composition analysis and the ratio of volatile, we can get the equivalent composition of coal as C_{5.417}H_{6}O_{0.6} and the equivalent volatile as CH_{2.4}O_{0.36}. Thus, in this simulation, the pyrolysis and combustion reactions for coal are assumed to be as

79% Raw coal (C_{5.417}H_{6}O_{0.6}) \longrightarrow 34\% \text{ Volatile (CH}_{2.4}\text{O}_{0.36}) + 45\% \text{ Char(C)}

or C_{5.417}H_{6}O_{0.6} (s) \longrightarrow 1.667 \text{ CH}_{2.4}\text{O}_{0.36} (g) + 3.75\text{C(s)}

\text{CH}_{2.4}\text{O}_{0.36} (\text{Volatile}) + 1.42\text{O}_{2} \longrightarrow \text{CO}_{2} + 1.2\text{H}_{2}\text{O}

\text{C + 0.5 O}_{2} \longrightarrow \text{CO}

\text{CO + 0.5 O}_{2} \longrightarrow \text{CO}_{2}

where, the kinetic data of volatile reactions for coal are directly adopted from the data for methane combustion reactions.\textsuperscript{11}
Table 1 Coal element and approximate analysis

<table>
<thead>
<tr>
<th>Elements</th>
<th>Coal</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>65 %</td>
</tr>
<tr>
<td>H</td>
<td>4 %</td>
</tr>
<tr>
<td>N</td>
<td>&lt; 1 %</td>
</tr>
<tr>
<td>O</td>
<td>9.6 %</td>
</tr>
<tr>
<td>Inertial</td>
<td>11 %</td>
</tr>
<tr>
<td>Volatile</td>
<td>34 %</td>
</tr>
<tr>
<td>Water content</td>
<td>10 %</td>
</tr>
<tr>
<td>Low Heat value</td>
<td>26 MJ/kg</td>
</tr>
</tbody>
</table>

5. Results and discussions

In the work, total five computational cases A1, A2, B, C and D have been investigated. All five cases have the same bed boundary conditions as shown in Figure 3 and wall conditions (constant temperature at 530 K for the water-cooling wall). The case A1 has no secondary air while case A2 has the same amount of secondary air (10% of primary air) as cases B, C and D.

All the simulations in the work are performed using FLUENT code on a SUN workstation with 512MB main memory running under the Solaris operating system.

5.1 Flow fields, residence times and mixing patterns

The flow fields of the cases A1, A2, B, C and D are demonstrated in Figure 4. It is apparent that the SOFA strongly affects the flow patterns. For case A1, there is no secondary air or over-fire air, the whole flow of over-bed gases is approximately as the plug flow pattern, so the mixing is poor. While the case A2 has the secondary air (SA) from the wall side air jets, so the mixing is improved but still not good since the mixing zone generated due to SA injection is very close to the wall near the SA jets.
It can be seen from the Figure 4 (B, C and D) that due to the Ecotube system, the combustion domain of the boiler is composed of three different zones: the main combustion (MC) zone, the strong mixing (SM) zone, and the upper flow (UF) zone. For the case B, since the Ecotube system is located at low position (2 m high above the grate bed), the MC zone is short and significantly affected by the secondary air from the Ecotube. Therefore, the MC zone together with the SM zone can be regarded as a well-stirred reactor, while the UF zone can be considered as a plug flow reactor. For the case C, the Ecotube system is installed in the middle of the boiler combustion chamber, so the MC zone and UF zone are approximately the plug flow reactors while the SM zone can be regarded as a typical well-stirred reactor.

Figure 5 shows a set of particle tracks from the grate bed for the different air configurations. Correspondingly, the average residence times are plotted in the Figure 6.
It is obvious that the case A2 has a short residence time, only 2.73 seconds, meaning the mixing is poor, while the cases B, C and D have long residence times, increasing about 30%, so the mixing is significantly improved by using the Ecotube system.

### 5.2 Thermal fields

The temperature profiles of the five air configurations for the coal boiler are demonstrated in the Figure 7. It illustrates that the SOFA controls the combustion process in the grate fired boiler.

The case A1 has no SOFA, so the peak flame is very high, almost outside of the combustion chamber, meaning the combustion is poor in the main chamber. In case
A2, the combustion is improved by using the secondary air from the wall side air jets, and the combustion flame is kept in the main combustion chamber.

It is interesting for the cases B, C and D with installing the Ecotube system in different high levels, since there are no significant peak flames. The higher the Ecotube system, the lower the peak temperature will be, from 1620K in case B, 1500K in case C to 1300K in case D, for the fuel concentration will be small at upper part of the boiler.

![Fig.8 Temperature distributions in x-direction at 4m level in the boiler](image)

It is also obvious that the SOFA from the Ecotube or the SM zone mainly controls the combustion, and makes the flame volume bigger thus more uniform thermal fields in the combustion chamber as shown in Figure 8.

### 5.3 CO emissions

The predicted CO profiles in the coal boiler for the five air configurations are demonstrated in Figure 9. Since the total excess air ratio $\lambda = 1.53$, so the coal volatiles
and CO should be consumed up in the combustion chamber and their concentrations in flue gas are very low.

![Fig.9 The CO mass fractions in the boiler for different air configurations](image)

For the case A1, the flame is very high and the CO from the coal gasification can not be burned out perfectly inside the main combustion chamber of the boiler. The situation in case A2 is improved by injecting the secondary air from the wall side air jets but still not good. Cases B, C and D show that CO can be completely consumed in the main combustion chamber by using Ecotube system. In addition, it is very clear that it is the strong turbulent SOFA of Ecotube system, or SM zone, which controls the combustion process. Figure 10 plots a set of averaged CO mass fractions distributed in different high levels for the cases of the five air configurations. Obviously, for the purpose of perfect combustion, the case B seems to be the best air configuration for the boiler, in which the CO mass fraction in flue gas reaches the minimum of $1.3 \times 10^{-10}$.

![Fig.10 Plot of CO mass fractions at different high levels for different air configurations](image)
5.4 NO emissions

In the work, three different NO mechanisms, thermal NO, prompt NO and fuel NO, have been considered. Through the calculations separately, it is found that thermal NO takes less than 5% amount of total NO at 1500K, and the prompt NO is at least three orders of magnitude less than fuel NO. Therefore, the prompt NO can be neglected and only thermal NO and fuel NO are included in the final calculations. In addition, if the temperature is less than 1500K, the thermal NO will be also non-significant, so the fuel NO dominates the total NO contribution in the furnace chamber and in flue gas.

Since the fuel-N is assumed mainly existing in the coal volatile, releasing from the bed zone 2, so the fuel NO is mainly generated in the front part of the boiler chamber as shown in Figure 11. Due to the fuel NO generation is very sensitive with local volatile-N concentrations, so the high NO concentration region locates in the volatile region between the bed zone 2 and the SOFA as seen in Figure 11 and Figure 12 mutually.
The NO generation is also sensitive to the local oxygen concentrations and the globule O$_2$ is controlled by the operating conditions, such as fuel rate and air rate. In the work, the total excess air ratio is controlled at the $\lambda=1.53$ (the bed excess air ratio $\lambda_b = 1.39$), so the O$_2$ mass fraction in the flue gas is about 10.3%, while the NO ppm in the flue gas correspondingly is from 40ppm (case D) to 60ppm(case A). The oxygen mass fraction profiles in the boiler for different air configurations are shown in Figure 13.
The average NO ppm concentrations in different high levels in the boiler for different air configurations, are plotted in Figure 14. It is interesting that compared to other cases, the NO ppm distribution in the case B is quite uniform trending to about 50ppm.

![Fig.14 The NO ppm distributions at different high levels](image)

It also illustrates that the case D has the minimum NO generation and emission because in this case, the temperature and the local concentration of volatile (containing fuel-N) are lower that those in the other cases. The flue gas line in Figure 14 shows that from the case A1 to case D, the NO emission is reduced about 35%.

6. Conclusion

In the work, the computational fluid dynamics together with a black-box bed model are used to simulate a 25MW industrial travelling grate fired boiler for coal combustion. A new advanced secondary/over-fire air (SOFA) system using Ecotube technique is studied and five different air configurations are comprehensively calculated for optimizing the SOFA configuration in the boiler. The results of numerical modeling show that the Ecotube system can generate a local strong mixing zone, which renders a good mixing and enhances the residence time. The strong
mixing zone generated by SOFA from the Ecotube system plays an important role in controlling the combustion process.

The numerical simulation results show that the Ecotube technique is an effective SOFA supply tool to improve the grate combustion and to reduce the pollutant emissions. The low position Ecotube air configuration (case B) is favorable to perfect combustion, while the upper position Ecotube air configuration (case D) is favorable to minimizing the NO emission.

It can be concluded that the Ecotube technique is quite effective to distribute the secondary/over-fire air, to improve the grate combustion and to reduce CO and NOx emissions. The perfect combustion can be achieved if using low position Ecotube air configuration, while the NOx can be reduced about 35% if using the upper position Ecotube air configuration in the boiler. Therefore, for the grate combustion, the Ecotube system is effective and has strong potential to be put into application in industry for future.
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Paper 3

CFD simulation and physical modeling of fluid-flow patterns in an entrained boiler for co-firing of pulverized coal and biomass waste

Wei Dong*, Jiri Vaclavinek and Wlodzimierz Blasiak
Division of Heat and Furnace Technology
Royal Institute of Technology
10044 Stockholm, Sweden

* Fax: +46-8-149338  E-mail: dong@metallurgi.kth.se

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Modeling of fluid flow and mixing patterns in an entrained boiler

Wei Dong*, Jiri Vaclavinek and Wlodzimierz Blasiak
Division of Heat and Furnace Technology
Royal Institute of Technology
10044 Stockholm, Sweden

Abstract

In the present work, the flow and mixing patterns in an entrained boiler have been studied by using numerical modeling and water modeling. In the work, the renormalization group (RNG) $k$-$\varepsilon$ turbulence model is employed to deal with the strong swirling flows. In addition, a parameter, the degree of mixing, is defined and used to quantitatively describe the mixing pattern of the fluid flow in the boiler. The results of numerical and water modeling illustrate that the design of the pulverized fuel boiler is successful. The mixing inside the boiler is perfect and the boiler can be regarded as a well-stirred reactor.

Keywords: CFD, numerical modeling, co-firing, entrained boiler, pulverized coal, biomass

1. INTRODUCTION

Co-firing of pulverized coal and biomass fuels in an entrained boiler is a technical test for sustainable development in Nordic energy industry. This paper presents results of numerical simulation and physical modeling of fluid-flow structures and mixing patterns in an entrained boiler for co-firing of pulverized coal and renewable bio-fuel, such as solid wastes from agriculture and forestry. This research work aims to use computational fluid dynamics (CFD) and water modeling tools to study the fluid flow and mixing patterns in the boiler. In order to reach the complete combustion of fuels, the strong turbulent flows in a boiler always are expected for fuel/air mixing. The co-firing process can be realized in one burner (coal and biomass are fed to the same burner) or between different burners or burner levels (coal and biomass are fed to different burners or burner levels). The simulated boiler is a 365 MW industrial entrained boiler fired with pulverized coal and biomass [1]. The boiler is equipped with 13 highly swirling burners and 24 over-fire air (OFA) jets on its wall sides. Each burner has a separate system for feeding the pulverized fuel and has four levels of coaxial air jets in which primary and secondary air are highly swirling by internal turbulators. In the boiler, the burners are operated in different rotating directions of flows. This aerodynamic configuration is expected to generate much better turbulent mixing pattern while it also creates additional difficulties for modeling. Finally, a combustion case of modeling the swirling burner also has been carried out.

2. MATHEMATICAL MODELING

In the last decade, the CFD technique has been proven to be a valuable tool to simulate the flow and combustion processes in industrial furnaces and boilers. It is based on a set of coupled conservation equations of mass, momentum, energy, and chemical species transport and reactions in general Reynolds transport equations. In the present work, the gas is treated as the ideal gas and the turbulent swirling flows are modeled using the renormalization group (RNG) $k$-$\varepsilon$ turbulence model [2]. In order to simulate the interaction between different flames with different coaxial-jet swirling flows in the co-firing process, a 3-D mesh case of whole boiler together with

* Corresponding author. Fax: +46-8-149338. Email: dong@metallurgi.kth.se
all 13 burners is established. Totally 70 inlets are taken into account to describe the boiler and burners with whole detail geometry. For grid generation, the unstructured finite volume grid with multi-block concept is employed to divide the very complicated geometry of the flow domain into discrete segments with high grid quality. This approach is very important to get a convergent solution. The well-known SIMPLE algorithm [3] and the multigrid method [4] are applied with a first-order upwind scheme to solve the set of algebraic equations of the discrete system.

3. PHYSICAL MODELING

In addition of CFD simulation, the water modeling, a common physical modeling tool, is used to evaluate the performance of the boiler with its burners, as well as the CFD simulation results. In water model, water is used as fluid as combustion gas based on the similarity theory. In the work, a 3-D water model [5] is established to simulate the aerodynamic pattern of the boiler and burners. The acid/alkali neutralization flame modeling technique is employed to visualize the 3-D fluid flow field and mixing pattern in the boiler and burners.

4. SIMULATED BOILER AND CALCULATION METHODS

The simulated boiler manufactured by Burmeister and Wain company is installed in Uppsala, Sweden. It is a 365 MWth boiler fired with pulverized coal and/or biomass fuels. As shown in Figure 1, the boiler is equipped with 13 highly swirling burners and 24 over-fire air (OFA) nozzles. Every burner has four levels of air placed as a set of coaxial jets where primary air and secondary air are highly swirled by internal turbulators.
coupling, while the under-relaxation method is used to control the update of computed variables during the iteration process. In order to increase the convergent rate, the multigrid method is also used. All calculations are performed on an IBM Risc 6000/59 workstation with 512 MB main memory.

5. RESULTS AND DISCUSSION

5.1 Air inlet conditions for the boiler

The boiler has 13 co-firing burners with 10 transport air inlets, 10 primary air inlets, 13 secondary air inlets and 13 tertiary air inlets, and 24 over-fire air inlets. There are therefore total 70 different air inlets among which all of the primary air and secondary air are highly swirling and needs to be specially treated. The values of all of inlets input data are listed in Table 1.

<table>
<thead>
<tr>
<th>Name</th>
<th>Mean velocity m/s</th>
<th>Axial velocity m/s</th>
<th>Tangential velocity m/s</th>
<th>Turbulence %</th>
<th>Hydraulic Diameter m</th>
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<td>81.29</td>
<td>81.29</td>
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<td>10</td>
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<tr>
<td>OFA2</td>
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<td>69.15</td>
<td>0</td>
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<td>For 1–10 burners</td>
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<td>17.86</td>
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<tr>
<td>Primary air</td>
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<td>25.91</td>
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<tr>
<td>Tertiary air</td>
<td>2.24</td>
<td>2.24</td>
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<td>1</td>
<td>0.15</td>
</tr>
<tr>
<td>For 11–13 burners</td>
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<td></td>
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<td>Secondary air</td>
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<tr>
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<td>2.24</td>
<td>0</td>
<td>1</td>
<td>0.15</td>
</tr>
</tbody>
</table>

5.2 Flow field and mixing pattern

The isothermal case is calculated to study the aerodynamic configuration of flow and mixing patterns in the pulverized fuel boiler. Figure 2 displays the velocity vectors in different positions and the swirling flows from the burners, the over-fire air flow and the main flow in the central plane inside the boiler.

Fig.2. The velocity vectors in different positions
In the view of engineering, turbulence means mixing. So, it is a common knowledge to use a turbulator to generate a strong swirling flow that greatly benefits the mixing of fuel and air. This is especially important for design of a pulverized fuel boiler. In this case, all the 13 burners generate swirling flows to help the mixing process inside the combustion domain. In order to study the mixing process inside the boiler more accurately, an appropriate concept of degree of mixing is essential and should be well defined. Here, the individual degree of mixing ($\xi_i$) at a given point in the computational domain, is defined as

$$ \xi_i = \exp \left( \frac{(x_i - \bar{x}_i)^2}{x_i(x_i - x_{i,\text{max}})} \right) $$

where $x_i$ is the local mass fraction of $i$th component in the system, $\bar{x}_i$ is the mass-averaged mass fraction of $i$th component, and $x_{i,\text{max}}$ is the maximum mass fraction of $i$th component in the system. For non-reacting flow system, $x_{i,\text{max}}$ stands for the initial/boundary inlet mass fraction $x_{i,0}$. The value of $\xi_i$ varies between 0, non-mixing, to 1, perfect mixing.

Furthermore, the global degree of mixing ($\bar{\xi}$) at a given point in the computational domain can be defined as

$$ \bar{\xi} = \exp \left( \frac{1}{N} \sum_{i=1}^{N} \frac{(x_i - \bar{x}_i)^2}{x_i(x_i - x_{i,\text{max}})} \right) $$

where $N$ is the total number of species in the system.

In this work, the carbon monoxide is added into primary air as tracer, so, both the CO mass fraction and the degree of mixing for CO in the whole computational domain are calculated. Figure 3 displays (a) the CO profile in a cross-section plane (11.5m height), and (b) the profile of the degree of mixing ($\xi_{\text{co}}$) ($i = \text{CO}$).

Fig.3. The profiles of the tracer CO mass fraction and the degree of mixing
It illustrates that mixing inside the boiler is very well. The mean degree of mixing is 0.992 in the whole computational domain, so that the boiler can be regarded as a well-stirred reactor.

It is very clear that mixing inside the boiler is very well. The volume averaged degree of mixing is 0.992 in the whole computational domain, so that the boiler can be regarded as a well-stirred reactor.

Figure 4 displays the visualization of water modeling of mixing pattern, and correspondingly, the calculated path lines showing the mixing path from the swirling burners.

![Comparison of mixing patterns](image)

Both the mixing patterns are very similar for water modeling and numerical modeling. It is obvious that the flows from the opposite directions strongly bump each other and a perfect mixing takes place in a wide range around the center zone of boiler chamber.

The results of numerical and physical modeling are in reasonable agreement each other. It can be believed that the aerodynamic design of the boiler is very successful. The boiler can be considered as a well-stirred reactor.

6. CONCLUSIONS

In the present work, the flow and mixing pattern of an entrained boiler has been studied by using numerical modeling and water modeling. The results of numerical and water modeling illustrate that the design of the pulverized fuel boiler is successful. The mixing inside the boiler is perfect and the boiler can be regarded as a well-stirred reactor.

It has been shown that using unstructured grid and multi-block concept is a good solution to cater for the complex flow and geometry in an industrial entrained boiler. Thus detailed information about the complicated fluid flow and mixing patterns in the boiler can be obtained. Just as expected, the agreement is quite good between the results of 3-d full-scale CFD simulation and those of the 3-D small-scale water
Having these tools checked and learned the in-burner co-firing or between burners co-firing processes can be studied in a whole range of operating conditions in the future work.

References

Paper 4

Study on Mathematical Modeling of Highly Preheated Air Combustion

Wei Dong and Wlodzimierz Blasiak
Division of Heat and Furnace Technology
Royal Institute of Technology
10044 Stockholm, Sweden

Fax: +46-8-149338, E-mail: dong@metallurgi.kth.se

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Study on Mathematical Modeling of Highly Preheated Air Combustion

Wei Dong and Wlodzimierz Blasiak
Division of Heat and Furnace Technology
Royal Institute of Technology
10044 Stockholm, Sweden
Fax: +46-8-149338, E-mail: dong@metallurgi.kth.se

Keywords: mathematical modeling, furnace, highly preheated air combustion

Brief abstract
In this paper, the mathematical modeling of turbulent jet flame under the highly preheated air combustion conditions are conducted. The finite rate/eddy dissipation model and the mixture fraction/probability density function model are investigated and compared each other. The numerical results are also partially validated by some experimental measurements. In addition, some important features and characteristics of highly preheated air combustion are also investigated by means of numerical simulation. Results show that the mixture fraction/probability density function model is better than the finite rate/eddy dissipation model for predicting of the thermal fields of the turbulent jet flames, and thus can give out reasonable prediction of NOx formation, etc.

1. Introduction

Since 1993 Hasegawa and Tanaka, et al\textsuperscript{[1,2,3]} first proposed a new green combustion technology, researches have been very actively ongoing on this new combustion method now known as highly preheated air combustion (HPAC) technology. It aims to reach simultaneously over 30\% fuel saving (or say, cut-down 30\% CO\textsubscript{2} emission), low NO\textsubscript{x} emissions and down sizing of furnaces by exhaust gas recirculation and uniform thermal field in HPAC furnaces\textsuperscript{[4]}. The principle of this combustion method can be simply described as varying the periodic time of the alternate combustion to provide a suitable heat flux profile for each particular application. An improvement is combining heat recirculation with hot combustion product recirculation in a furnace, which decreases the maximum flame temperature and creates a more uniform profile of combustion gas temperature in the furnace. In order to obtain enough knowledge of the main features of HPAC, Hasegawa and Mochida\textsuperscript{[5,6]}, and Lille\textsuperscript{[7]} conducted some small-scale experimental studies for characteristics and visualization of HPAC. In addition, Ishii\textsuperscript{[8]} and Shimada\textsuperscript{[9]} conducted mathematical modeling applied industrial codes FLUENT and STAR-CD respectively to simulate the large-scale industrial testing furnaces, in which the standard k-\varepsilon model and probability density function (PDF) model were used to deal with the turbulence-reaction flows. Though the numerical results seem satisfied in predicting the temperature distributions in HPAC testing furnaces, it still needs a more comprehensive investigation in mathematical modeling for fundamental understanding and the best implementation of the HPAC technology into the industrial furnaces.

The general objective of this work is to simulate the phenomena of turbulent combustion, emphasizing on jet flames under the highly preheated air combustion conditions, thus different models are used and compared each other based on modeling of the preliminary HPAC test apparatus at Royal Institute of Technology, Sweden. In the present work, the computational fluid dynamics (CFD) technology involved the eddy-dissipation model with global kinetic reactions and the probability density function approach with equilibrium assumption for modeling of turbulent-
reaction flows are investigated. A single jet HPAC test apparatus with fuel direct injection (FDI) technique, and a two-burner switching HPAC test furnace are simulated by using a commercial CFD-software FLUENT code.

2. Mathematical Modeling

Computational fluid dynamics technique is a very strong and effective tool to simulate the flow and combustion. It is based on Navier-Stokes equations or Reynolds transport equations, together with fluid state equation, different turbulence models and turbulent reaction models, etc. In the present work, the following models are used:

- Turbulence: RNG k-ε model and Reynolds stress model (RSM)
- Radiation: Rosseland model and Discrete Transfer Radiation model
- Heat transfer: Standard wall function
- NOx formation: Zeldovich’s thermal NO and De Soete’s prompt NO mechanisms
- Turbulent-chemistry interaction: finite-rate/eddy-dissipation model and mixture fraction/PDF model

The finite-rate/eddy-dissipation model (FRED) is based on the Arrhenius finite rate chemistry and the eddy-dissipation concept of Magnussen and Hjertager. The solution of transport equations of chemical species, with n-step chemical reactions under the influence of turbulence on the reaction rate is expected to describe the turbulent combustion taken place in a HPAC furnace. According to our preliminary HPAC furnace burning propane, total six species, such as C3H8, O2, CO, CO2, H2O, and N2, and the two-step reactions of propane are selected in this model.

The mixture fraction/PDF model (MPDF) is based on the solution of the mixture fractions instead of each species transport equations. The turbulence effects are accounted for with the help of a probability density function, while the kinetics of chemical reactions are not explicitly defined but treated in thermodynamics using one of two assumptions, ‘flame sheet or mixed-is-burned’ or ‘chemical equilibrium’. In the present simulation, total ten species, such as C3H8, O2, CO, CO2, H2O, N2, C2, OH, CH and O are calculated in this model.

3. Simulated HPAC Test Furnaces

In this work the propane-air system is selected for modeling and experimental study. The test HPAC set-up at The Royal Institute of Technology (KTH) in Stockholm, Sweden, has a combustion chamber in dimension of 160×200×280mm³ with a fuel jet (diameter from 0.3mm to 1mm) on one side of the wall. The operating conditions in experiments are kept in the 0.4 m/s, 1300K of main flow of diluted air and 25 m/s, 300K of the propane flow. The HPAC furnace has the dimension of 0.5×0.5×1m³ with two switching burners. Each burner has 25KW thermal power firing propane and the switch time is assumed 20 seconds. Figure 1 shows the three-dimensional mesh cases of the HPAC test set-up chamber and the test furnace respectively. The former has 67,730 unstructured tetrahedral cells while the latter employs 93,460 the same type cells to discrete the physical spaces of the chamber and the furnace. The local mesh refinements near the jet or nozzles are especially treated in sake of numerical convergence requirements.
4. Results and Discussions

4.1 Turbulent diffusion flames

- Flow patterns

Figure 2 shows a serial of the k-ε/FRDE turbulent jet flow patterns and another serial of RSM/MPDF turbulent jet flow patterns in conditions of 3%, 8%, 15% and 21% O₂ diluted air at 1300K.

It demonstrates that the flow pattern is not so sensitive to oxygen concentration, though the lower oxygen concentration renders the longer flame. Compared with the on-line experimental photos, the RSM/MPDF model gives out a more realistic prediction for flow pattern than the k-ε/FRDE model does.
- Temperature profiles
Figure 3 shows a serial profiles of k-ε/FRDE turbulent jet thermal fields and another serial profiles of RSM/MPDF turbulent jet thermal fields in conditions of 3%, 8%, 15% and 21% diluted air at 1300K, compared with those of experimental photos.

![FRDE model]

![MPDF model]

![Experimental photos]

Figure 3. Comparison of temperature predictions with experimental photos

It is obvious that the RSM/MPDF model is quite good in prediction of thermal fields while the k-ε/FRED model overestimates the peak temperatures of jet flames. Both of models show that under the condition of high temperature, the lower oxygen concentration of the main combustion flow leads to a more uniform thermal field.

- Chemical species profiles
In this work total ten species including C₃H₈, CO, CO₂, O₂, OH, CH, O₂, NOₓ, N₂ and C₂ are calculated. Figure 4 shows a serial profiles of C₃H₈, CO, OH, CH, O₂ and NOₓ mass fractions in conditions of 3%, 15%, and 21% O₂ diluted air at 1300K. The profiles of C₃H₈ and CO listed are predicted by using FRED model while other chemical species listed are calculated by using MPDF model. In present calculations, because FRED model gives out overestimated peak temperatures, it therefore overestimates the thermal NOₓ emissions.
Figure 4. Comparison of chemical species profiles in conditions of 3%, 15% and 21% O₂ diluted air
In contrary, the MPDF model gives out quite reasonable results for NO\textsubscript{x} predictions, though the NO\textsubscript{x} level in 3\% O\textsubscript{2} diluted air condition is extremely low. It needs to be evaluated more detail in future work. The results also show that CH and OH radicals are insignificant in the condition of lower oxygen diluted air combustion system.

In addition, an interesting phenomenon is that according to MPDF calculation, C\textsubscript{2} seems insignificant for propane/air system while Hasegawa’s experimental work\textsuperscript{[4]} shows that C\textsubscript{2} radical contributes the green luminous intensity in the higher temperature and lower oxygen concentration zone. That means in order to improve the CFD calculation a detailed reaction system has to be added into the modeling framework.

4.2 HPAC test furnace

In this first phase work, the finite rate/eddy dissipation model is used to simulate the HPAC test furnace which has two switching burners. Each burner has two φ1.2 nozzles with fuel (propane) flow of 50m/s at 330K. There are two operating conditions of diluted air. The first one is 21\%O\textsubscript{2} normal air, 20m/s at 1300K, and the second one is 5\%O\textsubscript{2}, 10\%CO\textsubscript{2}, 2\%H\textsubscript{2}O, 60m/s at 1500K. The furnace wall is assumed as the water-cooling wall at the constant temperature of 530K. The switch time for two burners is 20 seconds that is long enough for twin-burner system to be simulated in steady-state situation, though the time-dependent simulations also have been carried out for comparison.

- Flow patterns
  Figure 5 displays the velocity vectors on the central horizontal plane of the furnace during the periodic switching time.

  ![Figure 5: Flow structures in the HPAC test furnace](image)

  Both flow patterns are similar. From the calculation by the incompressible fluid assumption, the outlet velocity is larger than the air inlet velocity because the combustion reaction of propane-air generates more volume of flue gas as well as there exits the thermal expansion of gas phase for the temperature increase.

- Temperature distributions
  Figure 6 displays the thermal fields on the central horizontal plane of the furnace under the two operating conditions.
Figure 6. The temperature profiles in the PHAC furnace

It demonstrates that the lower oxygen concentration leads to a longer diffusion flame, a lower but more uniform temperature distribution in the furnace.

- NO\textsubscript{x} emissions
  Figure 7 displays the profiles of NO\textsubscript{x} mass fractions corresponding with the profiles of oxygen mass fractions.

As discussed above that the FRED model overestimates the peak temperature of the diffusion flame, the thermal NO\textsubscript{x} formation in the HPAC furnace therefore also be overestimated. But by comparing these two numerical results, it can conclude that to decrease the oxygen concentration by means of exhaust gas recirculation is an effective way to abate the NO\textsubscript{x} emission in a furnace.
5. Conclusions

In this first stage research work of mathematical modeling for highly preheated air combustion, two turbulent models and two turbulent-chemistry interaction models have been applied to study the turbulent jet flames under the HPAC conditions in a single chamber and a test furnace. The numerical simulation results in the flow patterns, thermal fields, chemical species profiles and NO\textsubscript{x} emissions in the HPAC chamber and furnace that could be used to draw the following conclusions:

- The RSM/MPDF model is better than k-\(\varepsilon\)/FRED model to predict the turbulent diffusion flame.
- A detailed reaction system is needed to add into the CFD modeling framework that will result in next stage research work for development of more realistic models.
- The main features and characteristics of highly preheated air combustion have been successfully investigated by using mathematical modeling method.
- A more detailed and comprehensive mathematical modeling for both HPAC fundamental research and large-scale industrial HPAC utilities is still a challenge.

References


Paper 5

Numerical modeling of highly preheated air combustion in a 580KW testing furnace at IFRF

Wei Dong* and Wlodzimierz Blasiak
Division of Heat and Furnace Technology
Royal Institute of Technology
10044 Stockholm, Sweden

* Fax: +46-8-149338, E-mail: dong@metallurgi.kth.se

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Numerical modeling of highly preheated air combustion in a 580KW testing furnace at IFRF

Wei Dong* and Wlodzimierz Blasiak
Division of Heat and Furnace Technology
Royal Institute of Technology
10044 Stockholm, Sweden

Abstract
In this paper, a comprehensive numerical simulation has been conducted for a 580kW highly preheated air combustion furnace fired with natural gas. The numerical results are compared to the experimental results from a 580kW semi-industrial furnace at IFRF, Netherlands. Both the modeling and the experiment illustrate that the conditions of highly preheated and diluted air combustion (HPDAC) make furnace being a well-stirred reactor, thus the temperature and chemistry fields are quite uniform in the furnace. A new parameter, the degree of mixing, is proposed to quantify the mixing process of the turbulent reacting flows in the furnace. Modeling shows that the combustion in the furnace is mixing controlled, and the invisible flame of HPDAC can be captured by monitoring the profile of hydroxyl radical. Furthermore, the calculation illustrates that the thermal NO takes about 94.6% of total NO generation in the furnace, thus it is thermal NO that dominates the global NOx emissions from the furnace.

1. Introduction

Industrial furnaces utilizing highly preheated and diluted air combustion (HPDAC), as shown in Figure 1, provide very high performance for energy savings and low NOx emissions. It has long been recognized that substantial fuel savings can be gained when a combustion system is equipped with a reheat cycle by using recuperative or regenerative burners [1].

Fig.1. Schematic of a HPAC furnace

However, because of material problems, the previous recuperative and regenerative burners could offer only modest fuel savings since the combustion air could not be preheated to high temperatures. Recent developments on new honeycomb type regenerators at Nippon Furnace Kogyo (NFK) make it possible to preheat the combustion air up to temperatures higher than 1000 °C by recirculating the hot exhaust gas and, thus, fuel savings up to 50%, as well as significant decreasing of CO2 and NOx emissions. This highly preheated and diluted air combustion technology has

* Corresponding author, Fax: +46-8-149338, E-mail: dong@metallurgi.kth.se
now been considered as the emerging furnace design methodology for next generation of high performance combustion systems \cite{2}.

Since September 1997, the International Flame Research Foundation (IFRF), Netherlands, has carried out a semi-industrial scale experimental project \cite{3} to estimate the combustion of natural gas with air preheated up to 1300 °C. The experimental furnace was equipped with a NFK burner and operated as a well-stirred reactor. In this project, the behavior of this HPDAC burner was demonstrated by measuring the thermal field, CO and NO\textsubscript{x} emissions \cite{4}. The objective of this paper is to demonstrate the behavior of this new HPDAC burner by using a comprehensive numerical simulation of the fluid flow and combustion of natural gas in the experimental furnace. The geometry of the simulated burner and furnace, as well as the operating conditions, are based on the actual experimental NFK burner and IFRF furnace. The numerical results are expected as the supplement to the experimental demonstration, to provide detail information about the new combustion system. Meanwhile, the numerical results are also validated by the experimental measurements.

2. Experimental HPDAC furnace

The experimental furnace, the IFRF furnace No.1, is refractory lined and has the inner dimensions of 2 by 2 meters and the inner length is 6.25m, as shown in Figure 2. It has 11 water cooled segments. For each segments the wall temperatures on the top and on the side of the furnace are monitored using type B thermocouples (Pt6\%Rh/Pt30\%Rh). The heat extraction is monitored by measuring the temperature rise and mass flow of the cooling water. All these segments are equipped with ports for detailed in-flame measurements on both sides. The furnace pressure is kept at about +0.5mm water pressure throughout the trail to avoid air in-leakage.

The burner (NFK) used in the experiments is shown in Figure 3. It has four gas injectors and a hot air injector. In experiments, two of the four injectors are used at a time. The hot air injector has an inner diameter of 124mm, resulting in an injection velocity of 75m/s at 1300°C.

(a) The IFRF test furnace No.1
3. Mathematical models

Computational fluid dynamics technique is a very strong and effective tool to simulate the flow and combustion. It is based on Navier-Stokes equations or Reynolds transport equations, together with fluid state equation, different turbulence models and turbulent reaction models, etc. In the present work, the following models are used:

- Turbulence: Standard $k$-$\varepsilon$ model
- Radiation: Discrete ordinate model [5]
- Heat transfer: Standard wall function
- NO$_x$ formation: Zeldovich’s thermal NO [6] and De Soete’s prompt NO [7] mechanisms
- Turbulent-chemistry interaction: Mixture fraction/PDF model [8]

The mixture fraction/PDF model (MPDF) is based on the solution of the mixture fractions instead of each species transport equations. The turbulence effects are accounted for with the help of a probability density function, while the kinetics of chemical reactions are not explicitly defined but treated in thermodynamics using assumption of chemical equilibrium. In the present simulation, total 11 species, such as CH$_4$, C$_2$H$_6$, C$_3$H$_8$, C$_4$H$_{10}$, O$_2$, OH, CO, CO$_2$, H$_2$, H$_2$O and N$_2$ are calculated in this model.
4. Results and discussions

4.1. Computational case and boundary conditions

Figure 4 shows the three dimensional mesh of the simulated furnace. Total 86571 tetrahedral cells are employed to discrete the whole computational domain.

In the work, the natural gas (NG) is used as fuel. Its composition and properties are listed in Table 1. The boundary conditions in numerical modeling are based on the experimental operating conditions, as shown in the Table 2. However, the thermal condition on the wall is set as the constant temperature at 1500K.

The CFD code FLUENT is employed and all the numerical simulations are performed on a SUN Ultra 60 workstation with 512Mb main memory.

![Fig.4. The 3-D mesh of the simulated furnace](image)

<table>
<thead>
<tr>
<th>Table 1. Natural gas composition and properties</th>
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<tr>
<td>Property</td>
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<td>CH₄</td>
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<tr>
<td>C₂H₆</td>
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<td>C₃H₈</td>
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<th>Table 2. Experimental conditions</th>
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<td>Flow rate</td>
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<tr>
<td>Natural</td>
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<tr>
<td>Vitiated</td>
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<td>Furnace</td>
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4.2. Flow field and mixing patterns

The flow field shown in Figure 5 is corresponding to the horizontal central plane through the air jet and the two fuel jets (y=0 plane). Fig.5.(a) shows the flow vector profile. In Fig.5.(b), the stream lines from the air jet and the fuel jets demonstrate two big eddies inside the furnace. Fig.5.(c) is the velocity contour, which is in good agreement with the measured velocity contour shown in (d).
Fig. 5. The flow pattern and velocity profiles in the $y=0$ plane.

The local comparisons of predicted and measured velocity magnitudes in two cross sections are plotted in Figures 6 and 7. It can be seen that the predicted velocity contour near the jets is a little bit wider than the measured one.

Mixing between oxidant and fuel is one of the most important features of diffusion combustion. However, how to describe the mixing process in a combustion system seems to be also a tough problem. In the IFRF experiments, the concept of mixing factor ($m$) \(^{(9)}\) was used to study the mixing process. It is defined as follows:

$$m = \frac{(kgO_2/kgfuel)_{flamepoint}}{(kgO_2/kgfuel)_{stochiometric}}$$  \hspace{1cm} (1)
where all products that are not completely burned are referred to as fuel, and \( m = 1 \) means the perfect mixing.

Kim S. \(^{10}\) proposed a mixing parameter to quantify the degree of mixing. It is defined as

\[
\alpha = \sqrt{\frac{\sum_{j=1}^{N} (x_j - x_{j,0})^2}{N}}
\]  

(2)

where \( x_j \) is the local mass fraction of the \( j \)th tracer and \( x_{j,0} \) is the mass fraction under the completely mixed condition. The parameter value of \( \alpha \) at a given location represents the degree of non-mixing, and \( \alpha = 0 \) means the perfect mixing.

However, both the mixing factor \( m \) and the mixing parameter \( \alpha \) are non-normalized. Furthermore, the Eq.(1) cannot be used out of the flame where there may be no fuel at all and the mixing factor \( m \) will be indefinite.

In this modeling work, the new concepts of the global degree of mixing and individual degree of mixing are proposed. The global degree of mixing (\( \xi \)) at a given point in the computational domain is defined as

\[
\xi = \exp \left( \frac{1}{N} \sum_{i=1}^{N} \frac{(x_i - \bar{x}_i)^2}{x_i(x_i - x_{i,max})} \right)
\]  

(3)

and the individual degree of mixing (\( \xi_i \)) at a given point is defined as

\[
\xi_i = \exp \left( \frac{(x_i - \bar{x}_i)^2}{x_i(x_i - x_{i,max})} \right)
\]  

(4)

where \( x_i \) is the local mass fraction of \( i \)th component in the \( N \)-components system. \( \bar{x}_i \) is the mass-averaged mass fraction of \( i \)th component. \( x_{i,max} \) is the maximum mass fraction of \( i \)th component in the computational domain, while, for the non-reacting flow system, \( x_{i,max} \) stands for the initial/boundary inlet mass fraction \( x_{i,0} \). The value of \( \xi (\xi_i) \) varies between 0, non-mixing, to 1, perfect mixing.

The calculated global and individual degrees of mixing for the highly preheated air combustion case are visualized in Figure 8. For the dominated components of \( \text{O}_2 \) (oxidant) and \( \text{N}_2 \) (inert), their individual degrees of mixing are close to unit in the most part of the domain as shown in Fig.8.(b) and (c). While, for the fuel components, such as \( \text{CH}_4 \), a flame-shaped mixing zone is very clearly demonstrated in Fig.8.(d). It can be clear also that no fuel existed outside of the mixing zone means no mixing physically for the fuel. Comparison Fig.8.(a) to (d), it is found that the global degree of mixing \( \xi \) is dominated by that of the fuel, the lean component.
It is interesting to compare the degree of mixing ($\xi$) to the mixing factor ($m$) and the degree of non-mixing parameter ($\alpha$). The results are shown in Figure 9, in which the experimental profile of mixing is calculated according to the mixing factor ($m$) from Eq.(1).

All the mixing pictures of Fig.9.(a), (b), (c) and (d), in which the (b) presents the non-reaction situation, exhibit that the mixing process in the furnace is very well and the furnace can be regarded as a well-stirred reactor. Fig.9.(b) and (d) is in inverse in describing the mixing process, while the Fig.9.(a) can display the maximum mixing region with really physical meaning. It is noticed that the mixing factor, $m$, is difficult to use and may loss its physical meaning in the computational domain. Both $m$ and the degree of non-mixing, $\alpha$, are non-normalized and can not tell the individual mixing processes of each components in the system. It is obvious that the degree of mixing, $\xi$, proposed in this paper, overcomes these shortages and can be easily used in quantitative analysis of the mixing process in non-reacting or/and reacting flows.
4.3. Thermal field and heat flux

The thermal fields from the numerical modeling and the experimental measurements are demonstrated in Figure 10. The agreement between temperature predictions and measurements are quite good.

Fig. 10. Comparison of temperature (°C) profiles for the $y=0$ plane

The local comparisons of temperatures in cross sections and axial-direction are plotted in Figures 11, 12 and 13. The predicted peak temperature is about 20% higher than the measured one in the central line of the furnace. The maximum difference of the predicted and the measured temperatures, as shown in Figure 11, is about 40% in the fuel jet zone, where the in-flame agitation error of measurement is usually large. While, the agreement of predicted and measured temperatures out of the jet zone to far field is good with the range of error in 5%.

Fig. 11. Comparison of predicted and measured temperatures in the cross section at $x=0.15$ m in the $y=0$ plane
Since the mixing is very good, the temperature under the conditions of highly preheated air combustion is quite uniform, thus a lower peak flame temperature inside the furnace. In the modeling work, the wall temperature is set as constant at 1500K. The influence of radiation can be estimated by computing the Boltzmann number

\[
Bo = \frac{(\rho U c_p)_{domain}}{\sigma T_{AF}^4} \frac{convection}{radiation}
\]

where \(\sigma = 5.729 \times 10^{-8} \text{ W/m}^2\text{K}^4\), the Boltzmann constant and \(T_{AF}\) is the adiabatic flame temperature. As an estimate, assume \(T_{AF} = 2000\text{K}\), \(\rho = 1 \text{ kg/m}^3\), averaged velocity in the domain \(U = 5 \text{ m/s}\), and \(c_p = 1000 \text{ J/kgK}\). The resulting Boltzmann number is \(Bo = 10\), which means that radiation is only tenth of convection in the combustion domain. The modeling predicted radiation heat fluxes on the top wall and one of the side walls are plotted in Figure 14. The maximum predicted value is about 12 kW/m\(^2\) on the top wall. It was reported in IFRF experiments that the measured radiation heat flux on the wall is high up to 340 kW/m\(^2\), which means the whole furnace is close to be a black body. This value can be compared to the total surface incident radiation flux, as plotted in Figure 15.
The values of wall surface incident radiation are around 280~310 kW/m², which very close to the measured values of radiative heat flux. So, the question is in that whether the measured radiative heat flux could be the total surface incident radiation flux. Otherwise, the measured radiative heat flux would be thirty times larger than the maximum value 11 kW/m² of modeling predicted radiation heat flux. It needs further investigations both on experiments and on radiation transfer models.

4.4. H₂ and CO formation

Figure 16 exhibits the profiles of modeling predicted and experimental measured H₂ %vol. concentrations in the furnace domain. In the IFRF experiments, it was reported that about 0.5% H₂ was found in the middle part of the furnace, which indicates the slow combustion as well as cracking of the fuel of natural gas.

![Figure 16. The profiles of H₂ %vol.](image)

![Figure 17. The profiles of CO %vol.](image)

Figure 17 displays the profiles of modeling predicted and experimental measured CO %vol. concentrations in the furnace domain. Comparison to the measurements in Fig. 17.(b), it seems that the modeling underestimates the CO formation from the fuel of natural gas in the front part of the furnace as shown in Fig. 17.(a).

![Figure 18. The profiles of CO %vol.](image)

Figure 18 displays the local comparison of predicted and measured CO concentrations in the cross section through the jet zone. It shows that according to the prediction, the CO should be formed in the fuel jet zone immediately, however, the measurement
shows that CO is generated far from the fuel jet zone. In the modeling, both CO (0 ~ 10% vol.) and H₂ (0 ~ 30% vol.) are only exist near the fuel and air jet zones, which means that in the modeling both mixing and chemical reaction are fast. This is not agreement with the measurement, since the crack of hydrocarbon is a slow reaction process. Therefore, the PDF model in the work needs a further improvement.

Both modeling results and experimental measurements show that the highest concentrations of CO and H₂ appear in the high temperature region that is located at the boundary of the vitiated air jet and natural gas jets.

4.5. O₂, OH and flame zone

Figure 19 shows the profiles of O₂ %vol. concentrations of (a) modeling predicted, and (b) experimental measured, in the furnace domain. In the modeling, the averaged O₂ concentration is about 2.1 %vol. in the computational domain, and the flue gas has 2.06 %vol. oxygen. In macroscopic view, the numerical predictions and the measurements are in good agreement. However, it is practically impossible for experiment to map the chemical species fields due to the limited access for in-flame measurements.

![Fig.19. The Profiles of O₂ %vol.](image)

![Fig.20. The predicted OH mass fraction](image)

The low oxygen zone near the jets in Fig.19.(a) indicates the most intense combustion is taking place in the near burner zone where the oxygen is mostly consumed. Correspondingly, Figure 14 of OH radical profile of mass fraction exhibits the maximum flame region that is in good agreement with the temperature profile shown in Fig.10.(b). According to the IFRF experiments, no flame has been observed. The whole furnace is “glowing” without any visible presence of a flame under the conditions of highly preheated air combustion. This “disappearance” of flames has already been identified as one of characteristic features of combustion taking place in the presence of a substantial amount of combustion products [11], such as in flameless combustion (FLOX) and HPDAC [12, 13]. Therefore, in order to capture the invisible flame in HPDAC furnaces, to monitor the OH concentration may be a good way. It also needs further experimental investigations.
4.6. NO\textsubscript{x} emissions

In the IFRF measurements, the NO emissions at the furnace exit were found to be in range of 190~210 ppm. About 90 ppm of NO enters the furnace with the vitiated air stream and a fraction of this NO is likely to be reduced by the reactions with CH\textsubscript{i} radicals.

Correspondingly, in the modeling work, the prediction of NO ppm in the furnace domain is demonstrated in Figure 15. Both thermal and prompt NO are considered in calculations. The average NO ppm in the furnace is about 191.8 ppm, and the NO ppm in the flue gas at exit is 191.6 ppm, very close to the measured value. So, the prediction value of NO emissions is in good agreement to the measurement results.

In order to judge whether the thermal or prompt mechanism is responsible for the furnace NO emissions, the thermal and prompt NO are calculated separately and the results are visualized in Fig.21.(b) and (c). It is obvious that both thermal and prompt NO are formed very close to the natural gas jets with the maximum thermal NO of 282 ppm and the maximum prompt NO of 17.6 ppm.

It is found that average thermal NO is about 171 ppm corresponding to only 9.6 ppm of prompt NO in the furnace. The thermal NO takes possession of 94.6% contribution of total NO emissions in the furnace, while the prompt NO is insignificant, only taking 5.4% of total NO emissions. So, the NO\textsubscript{x} emissions from the furnace are dominated by thermal NO.

Actually, the NO emissions of 191 ppm are not high for the furnace exit temperature of 1250 °C. If the vitiated air (22%vol. oxygen) is changed as the highly diluted air (2~10%vol. Oxygen) from a real regenerative burner, it can be believed that the NO emissions will be dramatically lower under the similar operating conditions.
5. Conclusions

In the work, a comprehensive numerical modeling of a 580kW highly preheated air combustion furnace has been conducted. The numerical results are compared to the IFRF experimental measurements with good agreements. Meanwhile, the numerical modeling provides plenty of detail information about flow and mixing patterns, thermal field and heat transfer, combustion process and NO emissions, etc.

A new concept of degree of mixing is proposed and can be easily used to quantify the mixing process for non-reacting or reacting flows.

All the numerical simulations can result in the following conclusions

- The conditions of highly preheated air combustion make the 580kW semi-industrial furnace being a well-stirred reactor under. The mixing process is very effective. The temperature and chemistry fields are quite uniform in the furnace.
- The degree of mixing ($\xi$) is a well-defined parameter to quantify the mixing process in non-reacting or reacting flows.
- Globally, the combustion in the furnace is mixing controlled.
- The invisible flame can be captured by monitoring the OH radical.
- The thermal NO dominates the NOx emissions from the furnace. It takes 94.6% of total NO generation.
- The numerical results are in good agreement with the measurements except the radiation heat flux. It needs a further investigation on both experiments and numerical models.

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References


Paper 6

Large Eddy Simulation of a Single Jet Flow in Highly Preheated and Diluted Air Combustion

Wei Dong and Wlodzimerz Blasiak

Division of Heat and Furnace Technology
Royal Institute of Technology
10044 Stockholm
Sweden

Fax: +46-8-149338, E-mail: dong@metallurgi.kth.se

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Wei Dong* and Wlodzimerz Blasiak
Division of Heat and Furnace Technology
Royal Institute of Technology
10044 Stockholm
Sweden

Abstract

In the present work, the large eddy simulation (LES) has been used to simulate a single fuel jet reacting flow under the conditions of highly preheated and diluted air combustion (HPDAC). A hybrid procedure of the standard subgrid scale (SGS) Smagorinsky-Lille model and Reynolds stress model (RSM) together with the finite rate/eddy dissipation reaction model has been employed to simulate a single wall jet HPDAC furnace chamber. The propane-air two-step combustion system is selected for modeling under two different HPDAC inlet air conditions corresponding to 3% w/w oxygen at 1300K and 21% w/w oxygen at 1300K. The numerical results show that the standard Smagorinsky model and Reynolds stress model together with the finite rate/eddy dissipation model are capable of predicting the global flame effects on the flow, such as flow velocities, mixing patterns, temperatures and turbulent parameters. The predictions are found in acceptable agreement with the corresponding results of in-furnace measurements and physical modeling. By compared with the pure Reynolds stress model, it is found that the differences between the two predictions of LES and RSM are insignificant in the near field of the flow. Though, further development of SGS stress and combustion models is needed, it is found that LES is an attractive tool to simulate the dynamic processes of turbulent reacting flows for the HPDAC furnaces.

Keywords: large eddy simulation, highly preheated and diluted air combustion, jet flow, Reynolds stress model, numerical simulation

1. Introduction

Highly preheated and diluted air combustion (HPDAC) has been considered as a promising energy technology for next generation of advanced industrial furnaces and boilers [1]. In a HPDAC furnace, the high turbulent flow field is time dependent controlled by the switching regenerative burners. Although the thermal field in a HPDAC furnace is quite uniform compared to the conventional furnace, the whole combustion process is time developed. In order to capture this kind dynamic process in modeling, some new dynamic model methods are needed to be developed.

In non-premixed turbulent combustion, the rate of mixing is determined by the motions of the largest eddies. The size, orientation, and rate of rotation of these large eddies depends on the particular flow configuration and geometry. Reynolds stress model (RSM) [2] can not directly capture the dynamics of the large, mixing-controlling eddies. Large eddy simulation (LES) resolves directly the large eddies of turbulent flows, while small eddies are modeled. The small eddies contain only a small portion of the total turbulent kinetic energy, thus, the computed flows are usually less sensitive to the turbulence modeling. Moreover, the small eddies tend to be more universal in character, so that the models should be more reliable. The use of LES was due to the work of Lilly [3] and Deardorff [4]. Since their pioneering studies, there has been considerable success in utilizing LES for a wide variety of

* Corresponding author. Fax: +46-8-149338. E-mail: dong@metallurgi.kth.se
problems [5-8]. However, there exists a difficulty for LES to be applied to combustion problems because the flame thickness is typically smaller than the computational mesh size and is therefore not resolved in simulations [9]. To overcome this difficulty, some approaches have been proposed, such as, simulation of an artificially thickened flame [10, 11], use of a flame-front tracking technique “G-equation” [12], and flame surface density concept [13], etc. Usually, there are two different classes of SGS combustion models: the conserved scalar approach and the direct closure approach [14]. The first class of SGS combustion model employs an assumed form for the probability density function of a scalar variable within a mesh cell volume, such as the large eddy probability density function (LEPDF) method [15]. It has been shown that an assumed LEPDF method could be used in LES of non-premixed turbulent reacting flows with both equilibrium and finite rate chemistry [16]. Recently, based on an assumed LEPDF method in conjunction with the laminar flamelet concept, a new SGS chemistry model termed the large eddy laminar flamelet model (LELFM), was developed for the filtered chemical species to the incompressible and compressible flows with multi-step, Arrhenius-rate chemistry [8]. Another class of SGS combustion model attempts to model the effect of SGS fluctuations on the filtered reaction rate. Recently, DesJardin [17] investigated both two classes of SGS combustion models. The tendency seems to develop more complex SGS combustion models that considering the uncertainties of SGS turbulence models. However, for practical combustion problems or some other purposes, it seems advisable to use the simplest SGS turbulent model combined with an eddy dissipation conception (EDC) [18] combustion model. In this strategy, Bai [19] proposed a mixing rate modeled using the resolved vorticity scales, which was also used for investigating a high order Cartesian grid method [20]. In this work, the Smagorinsky model combined with EDC combustion model is employed to simulate a single jet reacting flow under the conditions of highly preheated and diluted air combustion.

2. Mathematical models

2.1. Governing equations

The governing equations for an incompressible Newtonian fluid flow are continuity equation and Navier-Stokes equations as follows:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0
\]

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \tau_{ij}
\]

where \( p \) is the static pressure. \( \tau_{ij} \) is the stress tensor which is defined by

\[
\tau_{ij} \equiv \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}
\]

A filtered variable is defined by

\[
\tilde{\phi} = D \phi(x')G(x,x')dx'
\]

where the filter is denoted by “\( \cdot \)”, \( D \) is the fluid domain, and \( G \) is a filter function that determines the scale of the resolved eddies.
For the finite volume method, the volume of a mesh cell, $V$, implicitly provides the filtering operation as

$$\bar{\phi}(x) = \frac{1}{V} \int \phi(x') dx', x' \in V$$  \hspace{1cm} (5)

Filtering the Eqs(1) and (2), one obtains

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \overline{u}_i}{\partial x_i} = 0$$  \hspace{1cm} (6)

$$\frac{\partial}{\partial t} \left( \rho \overline{u}_i \right) + \frac{\partial}{\partial x_j} \left( \rho \overline{u}_i \overline{u}_j \right) = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \overline{u}_i}{\partial x_j} \right) - \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j}$$  \hspace{1cm} (7)

where $\tau_{ij}$ is the subgrid-scale (SGS) stress defined by

$$\tau_{ij} = \rho \mu_{ij} - \rho \overline{u}_i \overline{u}_j$$  \hspace{1cm} (8)

The small unresolved scales influence the large resolved scales through the SGS stress term.

### 2.2. Subgrid-scale model

In Eq.(7), the subgrid-scale stress can be modeled by the concept of eddy viscosity similar to the Boussinesq hypothesis as

$$\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2 \mu_s \overline{S}_y$$  \hspace{1cm} (9)

where $\mu_s$ is the subgrid-scale turbulent viscosity, and $\overline{S}_y$ is the rate of strain tensor as

$$\overline{S}_y = \frac{1}{2} \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right)$$  \hspace{1cm} (10)

The subgrid-scale turbulent viscosity is approximated by using the standard Smagorinsky-Lilly model [21, 22] as

$$\mu_s = \rho L_s^2 \left| \overline{S} \right|$$  \hspace{1cm} (11)

where $L_s$ is the mixing length for subgrid scales and $\left| \overline{S} \right|$ is the Smagorinsky constant.

$$L_s = \min(\kappa d, C_s V^{1/3})$$  \hspace{1cm} (12)

where $\kappa = 0.42$ and $C_s = 0.1$. $d$ is the distance to the closest wall, and $V$ is the volume of the cell.

$$\left| \overline{S} \right| = C_s \sqrt{2 \overline{S}_{yy} \overline{S}_{yy}}$$  \hspace{1cm} (13)

### 2.3. LES with combustion

The spatially filtered transport equations of energy and chemical species can be rewritten as
\[
\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho u_i E + \rho u_i p)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( k + c_p \mu \frac{\partial T}{\partial x_i} \right) + \frac{\partial u_i \tau_{ij}}{\partial x_i} + \frac{\partial (\rho c_p T \overline{d_i})}{\partial x_i} \tag{14}
\]
\[
\frac{\partial (\rho m_i)}{\partial t} + \frac{\partial (\rho u_i m_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D_{i,m} \frac{\partial m_i}{\partial x_i} \right) + \overline{R_i} \tag{15}
\]

where \( E \) is the total energy, \( m_i \) is the local mass fraction of each species. \( c_p \) is the specific heat. \( Pr \) is the Prandtl number. \( Sc_i \) is the turbulent Schmidt number (0.7). \( \overline{R_i} \) is the filtered chemical reaction rate and requires a closure model.

Since the SGS combustion modeling is a very difficult task and is still under the development, until currently, LES has not been applied to practical combustion problems yet. However, as an option for the practical problem, the flow field can be solved using LES, while the combustion can be solved in Reynolds-averaged framework, in which the influence of turbulence on the reaction rate is taken into account by employing the EDC model. In EDC model, the mean chemical reaction rate \( \overline{R_i} \) is modeled as

\[
\overline{R_{i,k}} = \nu_{i,k} M_i A \rho \min \left( \frac{m_R}{\nu'_{R,k} M_R}, \frac{\sum_{p} m_p}{\sum_{p} \nu'_{p,k} M_p} \right) \frac{\varepsilon}{k} \tag{16}
\]

where \( \nu_{i,k} \) is the stoichiometric coefficient of the species \( i' \) for the \( k \)th reaction. \( M_i \) is the molecular weight of species \( i' \). \( m_p \) is the mass fraction of any product species. \( m_R \) is the mass fraction of a particular reactant. \( A \) and \( B \) are empirical constants equal to 4.0 and 0.5 respectively. \( k/\varepsilon \) represents the time scale of the turbulent eddies [23].

3. Simulated HPAC furnace and calculation methods

In the work, the propane-air system is selected for modeling and experimental study. The global two-step reactions of propane combustion are considered as:

\[
\begin{align*}
\text{C}_3\text{H}_8 + 3.5\text{O}_2 & \rightarrow 3\text{CO} + 4\text{H}_2\text{O} \\
\text{CO} + 0.5\text{O}_2 & \rightarrow \text{CO}_2
\end{align*}
\]

The test HPAC set-up at the Royal Institute of Technology (KTH) in Stockholm, Sweden, has a combustion chamber in dimension of 160\( \times \)200\( \times \)280mm\(^3\) with a fuel jet (diameter 0.5mm, height 0.05m from bottom) on the cross side of the wall. The experimental main flow rate of diluted air (air + N\(_2\)) is 2m/s at 1300K, while the propane flow rate is 125 m/s at 300K. The Reynolds number at the main inlet is about \( Re = 27,000 \), and the Reynolds number for the jet inlet based on the nozzle width fuel injection velocity is about \( Re = 4200 \).

In the work, the finite volume method and the unstructured grid are used for spatial discretization of the computational domain. Two mesh cases corresponding to the coarse grid (193,228 Tgrid cells) and the moderate grid (506,232 Tgrid cells) are established, in which the moderate grid case is only used to compare the LES with RSM. Figure 1 displays the computational domain and the three dimensional mesh of the moderate grid case of the simulated HPAC furnace.
The incompressible SGS turbulent model is employed to calculate the turbulent flow while the combustion is simulated using the finite rate/EDC model in the RANS framework. To realize this hybrid simulation, a switching-iterative procedure is used, in which the results of the RSM/EDC combustion model are set as the initial conditions for the beginning of the LES calculation. After certain long iterations when the LES results become statistically independent of initial conditions, the calculation is then switched to the RSM/EDC model again. This time-dependent switching-iteration cycle should be continued until a convergent and statistical steady state is reached. In numerical modeling, the boundary conditions of inlet are mainly based on the experimental operating conditions. The diluted air is assumed containing 14% CO₂. On the solid wall, the wall function is used and the thermal condition on the wall is set as the constant temperature at 600K.

In the work, the second-order central-difference scheme is used for the approximation of diffusive terms and the second-order upwind scheme is employed for the discretization of convective terms, while a second-order implicit scheme is utilized with time derivatives. For the velocity-pressure coupling, the SIMPLE scheme [24] is employed. The resulting algebraic equations are solved iteratively and an algebraic multigrid (AMG) method [25] is used to accelerate the convergent speed. The CFD code FLUENT is employed and all calculations are performed on an IBM/590 workstation with 512MB main memory.

4. Results and discussions

In the work, the total integration time corresponded to at least four residence times \( t_r = (H/u_b) \), where \( u_b \) is the bulk velocity of the cross-flow and \( H \) is the height of the computational domain. The LES solution will reach statistically stationary after \( t_r > 0.4s \). The current two mesh cases are still relatively coarse since the current used computer’s capacity is quite limited in main memory and speed. A much more dense and accurate discretization mesh will be employed in further work.
4.1. Flow fields, thermal fields and mixing patterns

For the coarse mesh case under the condition of low oxygen (3%) diluted air, the LES calculation results of dynamic development of velocity field, temperature and the mass fraction of CO in the central plane of the furnace, are displayed in Figure 2. The eddy structures are not clear due to the grid size is not enough fine. However, the moderate mesh case under the same condition shows that large eddy simulation can capture eddy structures while Reynolds stress model can not. The comparison of statistically steady velocity profiles for LES and RSM is shown in Figure 3.
In principle, the SGS model can be evaluated via the DNS (direct numerical simulation) numerical tests or high-precision experiments to the “true” SGS stress. Unfortunately, both DNS and in-furnace high-precision measurements are unavailable at the moment to this practical engineering problem. Although there are no enough precision measurements of velocity, temperature and chemical species in the present testing experiments, the current experiments (Lille 1999, [26]) and physical modeling (Olsson 1999, [27]) can be used to exhibit whether the LES calculation results are reasonably agreement with the experiments and the water-modeling results.

Figure 4 displays comparisons of the temperature profiles from LES and experiments under different oxygen concentrations. The agreements are acceptable. It is obvious that the flame width corresponding to 3% O₂ highly diluted air is much wider than that in the 21% O₂ air condition, thus the thermal field is more uniform under the lower oxygen condition.
Actually in a turbulent flow, the mixing is controlled by the large eddies. In Fig.2.(c), the corresponding CO profiles demonstrate the flow and mixing patterns from the transition to fully developed turbulence. Figure 5 exhibits the comparison mixing patterns of LES calculation and physical modeling. The quantified mixing pattern of fully developed turbulent flow under the condition of 3% O₂ diluted air, is shown in Fig.5.(a), in which the global degree of mixing is calculated by using the following formula [28] as:

$$\xi = \exp \left( \frac{1}{N} \sum_{i=1}^{N} \frac{(x_i - \bar{x}_i)^2}{x_i (x_i - x_{i,max})} \right)$$  \hfill (21)

where $x_i$ is the local mass fraction of $i$th component in the $N$-components system. $\bar{x}_i$ is the mass-averaged mass fraction of $i$th component in the system, and $x_{i,max}$ is the maximum mass fraction of $i$th component in the system.

Compared with the water modeling of Fig.5.(b), it is found that the calculated mixing pattern is in good agreement with the water-modeling results.

4.2. LES to conventional Reynolds stress model

Figure 6 shows the comparison of LES/S model to pure Reynolds stress model for predicting the mean x-axial (cross-section) velocity of the fully developed turbulent flow, from the level of 0.01m to 0.10m downstream of the jet exit.

It is found that the differences between the two predictions are not large. In the near field of the flow, the differences are insignificant, while in the far field the flow, the differences are a little bit increased.

4.3 S-model parameter of $C_s$

The Smagorinsky constant $C_s$ has been also tuned in the work. For the Eq.(12), the Smagorinsky constant $C_s = 0.1$ with length scale $V^{1/3}$, other $C_s = 0.165$ (Schmidt, 1989, [29]) to $C_s = 0.3$ (Jones, 1996, [6]), three different values are investigated for
the present case. Corresponding to these three different $C_s$ values, the comparison of mean x-axial velocities are plotted in Figure 7.

Fig. 6. Mean x-axial (cross-section) velocities at the heights of 0.01m, 0.03m, 0.05m, 0.10m downstream above the jet exit.
Fig. 7. Comparison of mean x-axial velocities corresponding to different Smagorinsky constant $C_s$

![Comparison of mean x-axial velocities](image)

Fig. 8. Comparison of profiles of the subgrid eddy viscosity ratio

Figure 8 displays the big difference of the SGS eddy viscosity ratios corresponding to $C_s=0.1$ and $C_s=0.3$. It is obvious that $C_s$ value influences significantly the predictions on both the near field and the far field of the flow. Therefore, the further investigations are needed on tuning the SGS-stress/S model parameters and more adequate SGS models.
5. Conclusions

In the present work, the large eddy simulation (LES) has been used to simulate a single fuel jet reacting flow under the conditions of highly preheated and diluted air combustion (HPDAC). The standard sub-grid scale (SGS) Smagorinsky-Lille model along with the Reynolds stress model and eddy dissipation reaction model have been employed to simulate a single wall jet HPDAC furnace chamber. The propane-air two-step combustion system is selected for modeling under two different HPDAC inlet air conditions corresponding to 3% w/w oxygen at 1300K and 21% w/w oxygen at 1300K. The numerical results show that the standard Smagorinsky model and the Reynolds stress model together with finite rate/eddy dissipation model are capable of predicting the global flame effects on the flow, such as flow velocities, mixing patterns, temperatures and turbulent parameters. The predictions are found in acceptable agreement with the corresponding results of in-furnace measurements and physical modeling. By compared with the pure Reynolds stress model, it is found that the differences between the two predictions of LES and RSM are insignificant in the near field of the flow. The Smagorinsky constant $C_s$ has been also tuned in the work. It illustrates that the value of $C_s$ significantly influences the predictions on both near field and far field of the jet flow. Though, further investigations are needed to validate the SGS-stress models and parameters, it can be concluded that the LES is an attractive tool to simulate the dynamic processes of turbulent reacting flows for the HPDAC furnaces.

However, for further work, a more dense discretization mesh together with carefully checked boundary conditions should be established and performed on a more powerful computer. In addition, there always exists a need to further investigate some uncertainties of SGS model’s parameters and to develop more adequate SGS stress and combustion models for the turbulent reacting flows.

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