AUTOMATED PROCESS AND GEOMETRY DESIGN
OPTIMIZATION OF A COAL COMBUSTION REACTOR

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ABSTRACT OF THE DISSERTATION

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The importance of design of an optimized and efficient combustion or gasification system, the complexity of such an optimization problem with conflicting objectives and the inadequacy of traditional optimization methods in searching the entire design space and their intuitive and random nature, presents the significant importance of proposing an automated multi-objective optimization method in the field of combustion and gasification design. In the current research, automated multi-objective optimization has been implemented in geometry and process design of a coal combustion reactor. A coal combustion reactor with four tangential inlets is considered in order to create a swirl flow. Coal particles are mixed with air and are injected into the reactor via four tangential inlets. A combination of single-phase and multi-phase reactions has been considered to simulate the combustion process. All the steps of geometry creation, grid generation and CFD simulation have been integrated automatically using macro files to run in batch mode in an optimization platform, i.e., modeFrontier. Three sets of multi-objective optimization problems have been solved with two, four and six input variables respectively. The $\epsilon$ constraint method has been implemented for multi-objective optimization. Each multi-objective optimization problem consists of individual single objective problems which are solved by the SIMPLEX method.
Two conflicting objectives, i.e., NO mass fraction and $CH_4$ mass fraction, have been selected for all optimization problems. Results from all single objective optimizations have been summarized to obtain the Pareto Set. It is presented that automated multi-objective optimization proposes a reliable and promising method to integrate CAD and CFD tools with optimization methods in an automated fashion to perform faster, more accurate, more efficient and more cost-effective designs in the field of combustion and gasification.
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Dedication

To my family who is my everything in life
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Chapter 1
Introduction

1.1 Motivation

There have been many studies in the literature about CFD modeling of coal combustion and gasification processes and some of these studies suggest design improvement and optimization applications based on individual computational simulations. However, modifications of process parameters and/or geometry step-by-step and CFD simulation of each of these modifications individually to achieve the optimal answer by trial and error is a very intuitive, inefficient, random and time-consuming process and it does not necessarily cover the entire design space. Also, optimization by trial and error is not a suitable and accurate candidate for problems with several input variables. In addition, there are many engineering problems in the field of coal combustion and gasification in which the objectives of the optimization problem are conflicting with each other and therefore, a set of best optimal results (i.e., the Pareto Set) must be introduced. In such cases, the analysis of the optimal set of design variables via individual computational simulations and judgement on the results would be even more challenging. Automated design optimization provides a reliable method to search the entire design space that otherwise would not be entirely searchable in a rational fashion by conventional methods. In addition, this method eliminates the effect of human error in handling significant amounts of data in engineering design problems and optimizes the time to solve the design problem by running continuously and automatically.

The optimizations studies developed in the field of coal combustion and gasification mostly implement experimental data in neural network and multi-objective genetic algorithms or other optimization methods. Some other studies utilize process integration methods to analyze power generation systems via combustion/gasification processes in order to perform a thermo-economical optimization. Although all the results of these studies
represent good agreement with experimental data and introduce a promising method to optimize combustion/gasification processes, nevertheless, the cost of combustion characteristics measurements and the limitations by the geometry, time, number of instruments and required skills [31] impose many limitations to accurate data collection and therefore the optimization process.

These limitations motivate the current study to integrate CFD modeling of coal combustion with automated multi-objective process and design optimization. The proposed approach suggests a set of optimal process and design parameters in an automatic paradigm with regard to CFD simulations and comparison of CFD modeling results according to the defined objectives and constraints.

1.2 Literature Review

With recent developments in computer power, Computational Fluid Dynamics (CFD) simulation has become a powerful tool for different geometry and process design and optimization. Coal combustion is one of the fields that gains the advantage of CFD simulation. Related studies in the literature are categorized in four different groups.

1. CFD simulation in coal combustion

2. CFD simulation in gasification

3. Coal combustion optimization using experimental data

4. Gasification systems optimization using process integration

1.2.1 CFD Modeling in Coal Combustion

Magel et al. [21] numerically studied a pulverized coal flame and a coal-fired utility boiler. They used a 3D-prediction code for quasi-stationary turbulent reacting flow which is based on a conservative finite-volume solution procedure. Their combustion model is based on an extended Eddy Dissipation concept combined with finite rate chemistry and they validated their data with measurements from a 350kW swirled flame and air staging semi-industrial
pulverized coal combustion facility. They studied temperature distribution, oxygen and CO concentrations and axial and tangential velocities at various axial and wall distances.

Sahajwalla et al. [24] performed numerical simulation of pulverized coal combustion using FLUENT. They modeled combustion in a 2D, 12m × 1m duct employing two different methods, a finite rate formulation, known as the Magnussen model, which is based on the solution of species transport equations for reactants and product concentrations, and a mixture fraction/ Probability Density Function (PDF) formulation which solves a single conserved scalar (the mixture fraction) transport equation. They analyzed \( O_2 \) mass fraction and char burnout rate in the reactor for both models and noticed that the mixture fraction/PDF modeling approach models the turbulent combustion more realistically.

Monir Hossain and Jamal Naser [18] modeled a 600 MW full scale industrial furnace using the CFX4 package. They utilized the \( k-\epsilon \) turbulence model, Shahs discrete transfer model for radiation, single reaction devolatilization, an eddy-break-up model for gaseous combustion and Fields model for char oxidation. They validated their numerical data with the predicted and measured results of Magel et al. [21].

Ryoichi Kurose et al. [19] performed a 3D numerical simulation of a pulverized coal combustion field in a test furnace with an advanced low-\( NO_x \) burner. They used STAR-CD to numerically analyze their problem. They specifically examined the validities of existing \( NO_x \) formation and reduction models for the combustion fields produced with the low-\( NO_x \) burner. They improved the accuracy of the \( NO \) model by lessening the effect of \( NO \) reduction in the model of Levy et al. [20] and taking into account the \( NO \) formation from char \( N \).

Chejne et al. [6] also developed a time-dependent mathematical model and a numerical algorithm to simulate the combustion of piled coal particles in two directions: along the coal stack and inside each particle. The model predicts unburned solid fraction along the bed height, gas composition, heat of reaction, gas and coal temperature. They also specifically mention that their model can be used to optimize the combustion process by varying the excess air, particle size distribution, coal type, geometry of the reactor and different types of ignition mechanism.

Chui et al. [7] also numerically studied oxy-fuel combustion in order to investigate
burner design concepts to improve $O_2$ management in the combustor and reduce $NOx$ emissions. They used a commercial software, CFX-TASC flow, jointly developed by CETC and ANSYS Canada Limited, to model the flame and $NOx$ characteristics of an existing 0.3MW cylindrical, down-fired vertical combustor and two other improved designs with different combustor sizes. Their numerical results present reduced $NOx$ emission for one of the new burner designs and supports the idea of enlarging the diameter of the current combustor to minimize wall effects in order to expand flame volume and therefore, improve $O_2$ management. They performed a set of experiments based on their numerical simulations and the results validated their numerical improvements.

The Chui et al. study is a very good example of design optimization using CFD by trial and error and emphasizes the importance and necessity of developing automated design optimization in the field of coal combustion process and design.

A comprehensive study was performed by Williams et al. [28] about the current state of coal combustion modelling. Their main purpose was to outline recent progress in the application of CFD models in the assessment of coal firing in boilers or furnaces employing $NOx$ abatement technologies and in this process their main concern was coal combustion sub-models. The application of these sub-models to two combustion situations, a drop tube furnace and a low $NOx$ burner, has been studied. The accuracy of the sub-models has been investigated via the experimental data from four well-studied coals. It is shown that using these submodels in coal combustion modeling allows for a more accurate description of the coal devolatilization stage by using network coal pyrolysis models as a pre-processor to generate realistic input data. Other advanced features in these sub-models are the use of a mixture fraction/PDF approach to represent volatile combustion and the use of an intrinsic char reactivity model.

P. J. Stopford [26] in his study in 2002 has reviewed some of the recent applications of the CFX-4 code in the power generation and combustion industry. Examples include coal-fired low-$NOx$ burner design, furnace optimization, over-fire air, gas reburn and laminar flames. In his review study of a low-$NOx$ burner design, effects of coal quality on $NOx$ emission and carbon burnout in pulverized coal boilers, over-fire air installment design of a cyclone boiler and $NOx$ reburn in corner-fired furnaces, he concludes that CFD models are
capable of predicting furnace NO\textsubscript{x} emissions with 10\% accuracy provided that operating conditions of the boiler are well characterized. Also he mentions that it is more difficult to accurately predict the amount of char burnout.

### 1.2.2 CFD Simulation in Gasification

In the literature, there are also studies related to CFD modeling the gasification process and gasifier reactors which were found very informative for the purpose of the current study.

Y. Wang and L. Yan [27] in their comprehensive study in 2008, reviewed CFD studies on Biomass Thermochemical Conversion. They illustrate the mathematical equations governing the fluid flow, heat and mass transfer, chemical reactions involved in thermochemical systems and submodels for individual processes. They provide summaries of their comparisons of different CFD applications in biomass combustion, gasification and pyrolysis in addition to CFD applications in NO\textsubscript{x} formation studies from biomass thermochemical conversions.

Wurzenburger et al. [30] studied thermal conversion of biomass as a combined transient single particle and fuel-bed model in a packed-bed furnace. They used a finite volume method to discretize their space and solved their equations by using a linear-implicit extrapolation routine (LIMEX), [9] and validated their results with experimental studies. They claim that their model can be used to investigate different furnace conditions in order to optimize the existing furnace model and the reason is their important simulation results about the time needed for the complete burnout of the bed. This time depends on the fuel condition such as moisture content and type of biomass, as well as operation conditions such as the primary air flow rate and temperature, bed height and the temperature of combustion chamber. The total burnout time is an important design factor in grate length and overall furnace size.

Another study which has been very interesting in the scope of the current research (both from combustion modelling and also design optimization point of view) is that of Fletcher et al. in 1998 [13]. They computationally modelled biomass gasification process, first the flow within the reactor and then the combustion process.

In the first case, they utilized their computational analysis to optimize the geometry
of the reactor in order to minimize the slagging problem and promote char recirculation. In their first study in 1998, Fletcher et al. [13] utilized the CFD package CFX4 to study the flow within an entrained flow biomass gasifier. Their gasifier was designed to convert sawdust and chopped cotton gin trash into a low calorific value gas which could be burned in a modified engine to run a generator. They performed their analysis using two turbulence methods of $k-\epsilon$ and DSM (Differential Stress Model) and compared the results in predicting the complex swirling flow in the reactor. They also performed a particle tracking study to determine means of avoiding slagging in the gasifier base. Their computational results proved to be very useful to the designers to improve and optimize the geometry design to avoid slagging and promote char recirculation.

In another study in 2000, Fletcher et al. [14] performed a CFD analysis of the combustion model of the entrained flow biomass gasifier. Their aim was to use CFD to prove the design of a pilot plant and then use the validated model to design a 1MW plant. In their study, they analyzed the swirl velocity, temperature, methane, hydrogen, CO, CO$_2$, steam and oxygen distributions in the reactor. They conclude that the larger volume flow rates associated with combustion flows and the fact that gasification reactions are not that sensitive to the detailed velocity field around particles but rather on the residence time, causes the results in the combustion case not to be sensitive to the choice of the turbulence model.

1.2.3 Coal Combustion Optimization Using Experimental Data

There are some optimization studies related to coal combustion and biomass gasification in the literature. Some of these studies have adopted experimental data to perform a multi-objective optimization such as the research performed by Hao et al. [32] and Da-Zhang and Jing-Yan [5].

Hao et al. [32] optimized low-NOx combustion for a pulverized coal burned utility burner using neural network and genetic algorithms. Experimental results include the NOx emission characteristics of a 600MW capacity boiler. An artificial neural network is used to describe its NOx emission property and develop a neural network based model. A genetic algorithm is employed to search for the optimum solution. In their experiment, they carried out a total of 12 different cases on the boiler, changing the boiler load, over fire air (OFA)
distribution pattern, secondary air distribution pattern, coal quality, nozzles tilting angle and observing their effect on the \(NOx\) emissions. \(NOx\) and \(O_2\) concentrations are constantly monitored in the boiler outlet. Their result suggest that there is a close correlation between the \(NOx\) emission characteristics of the boiler and the operating parameters and the coal quality. By using 11 cases as the training samples in the neural network and the 12th case as the input to verify the accuracy of the model, they found that their relative error is 3.3%. After establishing the neural network correctly, the genetic algorithm is used to determine the optimum operating parameters. In their study, they chose a total of eight damper opening values of the secondary air and over fire air damper opening value as the parameters to be optimized. Their optimized results agree well with the experimental experience of air staging leading to low-\(NOx\) emissions.

Da-Zhang and Jing-Yan [5] performed their study on experimental data from a biomass (sawdust) gasifier and based on least square support vector machine (LSSVM). They chose gasification temperature and the adding catalyst as restrictive conditions and gas production rate, gas heating value and gasification efficiency as gasification performance indicators. They used the method of particle swarm optimization to optimize their multi-objective function. Their results represent the variation of gasification yield, lower heating value and gasification efficiency with catalyst addition in different gasification temperatures and indicate close agreement with experimental values.

1.2.4 Gasification Systems Optimization Using Process Integration

There are also some research studies in the literature which have implemented process integration technology to perform a thermo-economic analysis and multi-objective optimization for biomass gasification energy systems.

Gassner and Marechal [15] focused on production of SNG (Synthetic Natural Gas) from wood (thermochemical conversion of wood into methane). The whole concept of their study is based on decomposition of the problem into several parts. First the block flow diagram of the conversion process is set up then energy-flow, energy-integration and economic models of the equipment and their interactions are integrated in a multi-objective optimization
framework in order to calculate a set of optimal process configurations. They utilized thermodynamic, economic, and environmental performance indicators for their optimization objectives such as energy and exergy efficiencies, total production cost and avoided emissions. Their optimization procedure aims at identifying a set of Pareto optimal process configurations. For their research they have used a set of computational platforms such as BELSIM-VALI, LENI-OSMOSE, LENI-EASY and LENI-MOO (an advanced multi-objective genetic algorithm) for energy-flow modeling, economic modeling, energy-integration modeling and multi-objective optimization respectively.

In another study, Brown et al. [4] addressed the thermo-economic assessment of a 20MW wood gasification, gas cleaning and energy conversion process with particular attention to electricity generation and tar control. For this purpose they derived a modified equilibrium model from experimental data to formulate gasification products under changing operating conditions and formulated a flowsheet optimization superstructure based on the methods previously described by Godat and Marechal [16] and Marechal et al. [22]. The flowsheets are simulated as energy-flow models of wood drying, gasification, gas cleaning and energy conversion processes, using the VALI4 software. They utilized exergy efficiency and total grass roots costs as optimization objectives and implemented a queing multi-objective optimization evolutionary algorithm (MOO-LENI). They considered the use of air, oxygen or steam fluidized bed gasifiers coupled with an internal combustion engine combined cycle with cold gas cleaning or a gas turbine combined cycle with hot gas cleaning.

1.3 Objectives

As mentioned previously, optimization of process and geometry parameters of coal combustion based on trial and error and comparison of individual CFD simulations is very intuitive, random and inefficient and it does not necessarily cover the entire design space. In addition, using experimental data to build a population and using optimization methods such as Genetic Algorithm (GA) in order to propose a set of optimal results, is also not desirable. The reason is, although literature verifies acceptable agreement between the results of such optimization approaches with experiments, however, high costs of measurement methods and instruments is an important impediment.
The objective of this research is to automatically optimize the geometry design and operational parameters of a coal combustion reactor with swirl flow. The proposed methodology in the current research integrates CFD simulation of coal combustion with multi-objective optimization methods and therefore, achieves automated multi-objective optimization. This approach takes advantage of CFD simulation in the design of a coal combustion reactor and at the same time utilizes optimization methods to suggest a set of optimal designs in an automatic continuous paradigm.

The proposed method, or automated multi-objective design optimization, has several advantages over other conventional optimization approaches. The current method searches across the entire design space; therefore, it suggests an optimal set of solutions which is closest to the Pareto Set. Also, it maximizes the use of available computer power as it can be run automatically and continuously, eliminating human error in handling numerous files.

In the current study, a set of process and geometry parameters is proposed in order to obtain the least amount of emissions, i.e., methane and oxides of nitrogen, at the outlet. The main focus of this research is not on proposing the most suitable grid generation, turbulence or combustion model in order to simulate the process of coal combustion but is rather on implementation of automated multi-objective design optimization method in coal combustion process.

To achieve this goal, four steps of geometry creation (in SolidWorks, Windows operating system), grid generation (in ICEMCFD, Linux operating system), CFD simulation and post processing (in ANSYS-CFX, Linux operating system) have been integrated via modeFrontier, a multi-objective optimization tool. A set of input variables are generated via DOE (Design of Experiments) methods in the range defined for each input variable. Process parameters input variables of the optimization problem include the mass flow rate of coal particles and air into the reactor, inlet temperature and coal particle diameters. Geometry input variables include the heights of the upper and the lower cylinders.

In the first step, a coal combustion reactor is created in a CAD software, Solidworks. The reactor consists of two cylinders, connected via a reverse cone with two pairs of tangential inlets, two located at the lower cylinder and two at the upper cylinder in a shape that creates swirl flow inside the reactor. An unstructured tetrahedral grid is generated inside
the reactor via ICEMCFD, another ANSYS package and then coal combustion process consisting of devolatilization, fuel gas oxidation and char oxidation is modeled utilizing ANSYS-CFX, a commercial CFD package. All the above mentioned steps are integrated in modeFrontier, in the Windows operating system.

The multi-objective optimization method performed is the classic $\epsilon$-constraint method. ModeFrontier will provide a Pareto Set of designs as a result of multi-objective optimization introducing the optimal parameter and geometry design scenarios in order to achieve the desired objectives, i.e., to obtain the least amount of emissions in the reactor outlet. Mass fractions of methane and oxides of nitrogen are calculated emissions in the outlet as well.
Chapter 2

Problem Definition

As mentioned in the previous chapter, the purpose of the current research is to propose a set of parameter and design configurations for a coal combustion reactor in order to achieve the minimum amount of emissions at the outlet, i.e., the minimum amount of methane and oxides of nitrogen. Therefore, the main theme of this study is to apply automated geometry and process design optimization in design of a coal combustion reactor. The focus in this research is not the computational simulation of coal combustion phenomena per se but rather is on implementing the automated design optimization method, which has been widely used in other areas such as the aerospace industry, in the field of coal combustion and investigate its capabilities in design and optimization problems in this field. To achieve this goal, a sample entrained flow coal combustion reactor with tangential inlets to create swirl flow inside the reactor has been selected. Homogeneous and heterogeneous chemical reactions for simulation of the multi-phase phenomena of coal combustion are simplified. Individual preliminary CFD simulations have been performed prior to the optimization in order to evaluate the conflicting objectives on the optimization problem. A combination of process and geometry input variables are selected in order to evaluate the automated design optimization method while simulating a simplified coal combustion phenomena.

ModeFrontier, a multi-objective optimization software, has been used to solve the optimization problems in the current study. Since all the steps of the design problem such as geometry creation, grid generation, CFD simulation and post-processing, are performed interactively using commercial software, in order to design optimization in an automated fashion, all these steps are performed by running in batch mode via created macro files. Execution of batch runs has been possible by shell scripting in modeFrontier integration nodes. File handling from process to process in a serial pattern and also from local machine
to remote servers and vice versa is performed by using capabilities of modeFrontier in SFTP transfers. The following steps summarizes the implemented optimization processes:

1. Geometry creation in SolidWorks (local machine, Windows operating system)
2. Grid generation in ICEMCFD (remote server, Linux operating system)
3. CFD simulation in ANSYS-CFX (remote server in 4 processors, Linux operating system)
4. Post processing in ANSYS-CFX (remote machine, Linux operating system)
5. Integration of all the steps above and design optimization in modeFrontier (local machine, Windows operating system)

### 2.1 Geometry and Grid Details

The reactor geometry is created in SolidWorks. The reactor studied in the current research consists of two cylinders connected to each other via a reverse cone. Four tangential inlets are located in pairs on the upper and lower cylinders in order to create a swirl flow inside the reactor and achieve better mixing by turbulent flow. In order to produce a compact device, which also gives long residence times for the particulate it is usual to generate swirl [13].

The outlet is located on top of the upper cylinder. The geometry details are summarized in Table 2.1 and Fig. 2.1 represents the shape of the reactor created in Solidworks.

An unstructured grid with 338,896 tetrahedral elements has been utilized to generate the grid domain. The computations were run on tupolev, a 12 node Linux cluster with two dual
core processors per node at 2.2 GHz, 1 GByte RAM per processor, operating under Ubuntu Linux. Each computation ran for 56 hours wall clock time, 224 hours processor time (56 hours on each core).

2.2 Solution Details, Boundary and Initial Conditions in ANSYS-CFX

In the current research coal particles with specified mass flow rate, diameter distribution and temperature are mixed with air at the same temperature and are uniformly injected into the reactor from four tangential inlets creating a swirl flow inside the reactor. The most robust boundary conditions at the inlets and outlet have been set, i.e., mass flow rates of air and coal particles at the inlets and static pressure at the outlet. The inlet total pressure will be the result of the prediction and the flow and will be normal to the boundary which assumes that a uniform mass influx exists over the entire inlets boundary. Coal particles have zero slip velocity at the inlets and are equally spaced and are uniformly injected from all four inlets. In different simulations performed in the current research either a set of discrete diameter distribution or a specific particle diameter has been set at the inlets. At the outlet, a static pressure boundary condition sets a zero relative pressure and the flow direction is an implicit result of the computation. A smooth, insulated and no-slip
wall boundary condition has been set for the body of the reactor. A medium turbulence intensity of 5 and viscosity ratio, $\mu_t/\mu$, equal to 10 have been used at the inlets. The static temperature has also been set at the inlets. The solution domain inside the reactor consists of a continuous phase of gas mixture and a particle transport solid phase of coal particles. The initial conditions applied to the problem consist of air at an inlet temperature of 1500K and Cartesian $X$-velocity of 26$m/s$. Oxygen with a mass fraction of 0.232 is the only initial gas component in the simulation and $N_2$ would be set as a constraint.

A series of homogeneous and heterogeneous reactions take place and create gaseous products and ash. The whole simplified coal combustion process includes three steps of devolatilization, char oxidation and fuelgas-oxygen oxidation among which the first two are heterogenous (multi-phase) and the last one is a homogeneous (single-phase) reaction.

The $k-\epsilon$ turbulence model and eddy dissipation combustion model for homogeneous reactions are utilized. A finite rate chemistry model is used for heterogeneous reactions. The transient flow model is solved until steady state solution is reached.

Typical Reynolds numbers are of the oder of $10^4$. Under relaxation factors of 0.75 have been utilized for velocity, mass and energy of particles and the average mass residual per cell is reduced to $10^{-5}$ which is acceptable compared to the total mass flow rate of 0.01 – 0.001 kg/s. Average global balances and average convergence rate are typically 0.1% and 0.6%, respectively.

### 2.3 Design Optimization

All the steps of geometry creation in Solid Works, grid generation in ICEMCFD, CFD simulation in ANSYS-CFX and post processing in CFX-post are integrated and operated in batch mode in modeFrontier which is a multi-objective optimization software. Three different optimization problems have been studied with two, four and six input variables. The first two problems consist of process input variables only but the last one covers both process and geometry input variables. Objectives of the optimization problems are similar for all three scenarios, i.e, minimization of methane and oxides of nitrogen at the outlet. A DOE table is created by modeFrontier using the method of random variables in the ranges
defined for the input variables. The classic method of $\epsilon - constraint$ has been implemented for the multi-objective optimization problem and the SIMPLEX method is used to calculate each single objective optimization.
Chapter 3
Conservation Equations and Thermochemistry Model of Coal Combustion

In this chapter, the governing equations and thermochemistry model applied to the coal combustion problem are discussed. Combustion of a coal particle consists of three stages: devolatilization of the raw coal particles, oxidation of the residual char that produces gaseous products and incombustible ash, and finally oxidation of the gaseous products.

In this chapter the governing equations applied to the gas phase will be discussed first. Then, the particle transport model for the coal particles will be described and finally, the chemical reactions used to model different stages of coal combustion will be introduced. At the end of the chapter, we will focus on the numerical method applied to simulate the process.

3.1 Conservation Equations

A multi-component, heterogeneous, reacting mixture of particles and gas is considered. The gas consists of $K$ species in $K$ distinct coexisting continua, and thus there exists at each point in space at each moment in time a Cartesian velocity vector $v_i^k$, density $\rho^k$, static enthalpy $h^k$, and all other thermodynamic properties for each specie.

3.2 Favre-Averaging in Gas Phase

Mass-weighted averaging (Favre-averaging) has been used to model the turbulent quantities. For any intensive variable $f(x_i, t)$, a Favre-averaged value and a corresponding fluctuating value are defined as
\[ f(x_i, t) = \tilde{f}(x_i, t) + f''(x_i, t) \]  

(3.1)

where

\[ \tilde{f}(x_i, t) = \frac{\bar{\rho f}}{\bar{\rho}} \]  

(3.2)

where \( \bar{\cdot} \) is the ensemble average. The Reynolds conditions are assumed to hold for the ensemble average. These include the property that the ensemble average and partial derivatives commute.

### 3.3 Conservation of Mass in Gas Phase

A volume \( \tau^k \) containing an identifiable amount of species \( k \) is considered. The conservation of mass is

\[ \frac{d}{dt} \int_{\tau^k} \rho^k \, dV = \int_{\tau^k} w^k \, dV \]  

(3.3)

where \( w^k \) is the net rate of production of mass of species \( k \) per unit volume per unit time. Since \( \tau^k \) moves with the species \( k \) at velocity \( v_i^k \), the Reynolds Transport Theorem yields

\[ \frac{d}{dt} \int_{\tau^k} \rho^k \, dV = \int_{\tau^k} \left[ \frac{\partial \rho^k}{\partial t} + \frac{\partial \rho^k v_i^k}{\partial x_i} \right] \, dV \]  

(3.4)

where the repeated subscript\(^1\) \( i \) implies summation over all values of \( i \). Therefore

\[ \int_{\tau^k} \left[ \frac{\partial \rho^k}{\partial t} + \frac{\partial \rho^k v_i^k}{\partial x_i} - w^k \right] \, dV = 0 \]  

(3.5)

Since the volume \( \tau^k \) is arbitrary, the integrand must be exactly zero, and therefore

\[ \frac{\partial \rho^k}{\partial t} + \frac{\partial \rho^k v_i^k}{\partial x_i} = w^k \]  

(3.6)

A mass-averaged bulk velocity \( v_i \) is defined as

\(^1\)Note that a repeated \textit{superscript} does \textit{not} imply summation over all values of the superscript unless specifically noted by the summation symbol \( \sum \).
\[ v_i = \sum_k Y^k v_i^k \]  

(3.7)

where

\[ Y^k = \frac{\rho^k}{\rho} \quad \text{and} \quad \rho = \sum_k \rho^k \]  

(3.8)

*Diffusion velocity* \( V_i^k \) is defined as

\[ V_i^k = v_i^k - v_i \]  

(3.9)

It is therefore evident that

\[ \sum_k \rho^k V_i^k = 0 \quad \text{or equivalently} \quad \sum_k Y^k V_i^k = 0 \]  

(3.10)

The conservation of mass becomes

\[
\frac{\partial \rho^k}{\partial t} + \frac{\partial \rho^k v_i}{\partial x_i} = w_k + \frac{\partial}{\partial x_i} \left( -\rho^k V_i^k \right) 
\]  

(3.11)

and equivalently

\[
\frac{\partial \rho Y^k}{\partial t} + \frac{\partial \rho Y^k v_i}{\partial x_i} = w_k + \frac{\partial}{\partial x_i} \left( -\rho Y^k V_i^k \right) 
\]  

(3.12)

We express the mass-averaged bulk velocity as

\[ v_i = \tilde{v}_i + v''_i \]  

(3.13)

where from (3.2)

\[ \tilde{v}_i = \frac{\bar{v}_i}{\bar{\rho}} \quad \text{and} \quad v''_i = v_i - \tilde{v}_i \]  

(3.14)

Furthermore from (3.2)

\[ \overline{\rho Y^k} = \tilde{\bar{\rho}} Y^k \]  

(3.15)

Note also that
\[
\sum_k \rho Y^k = \sum_k \rho \bar{Y}^k = \rho \bar{Y}^k = \bar{\rho} \tag{3.16}
\]
and therefore from (3.15)
\[
\sum_k \bar{Y}^k = 1 \tag{3.17}
\]
Taking the ensemble average of (3.12)
\[
\frac{\partial \rho \bar{Y}^k}{\partial t} + \frac{\partial \rho \bar{Y}^k \bar{v}_i}{\partial x_i} = \bar{w}^k + \frac{\partial}{\partial x_i} \left( -\rho Y^k v''^i - \rho Y^k V^k_i \right) \tag{3.18}
\]
which holds for \(k = 1, \ldots, K\). Summing over \(k\) yields
\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{v}_i}{\partial x_i} = \sum_k w_k \tag{3.19}
\]
since
\[
\sum_k \rho Y^k v''^i = \left( \sum_k \rho Y^k \right) v''^i = \rho \bar{v}'^i = 0 \tag{3.20}
\]
and
\[
\sum_k \rho Y^k V^k_i = \sum_k \rho \bar{Y}^k \bar{V}^k_i = \rho \sum_k \bar{Y}^k \bar{V}^k_i = 0 \tag{3.21}
\]
Note that \(\sum_k w_k\) represents the net generation of gas by phase change.
The terms on the right side of (3.18) are modeled as
\[
-\rho Y^k v''^i = \frac{\mu_t}{S_{Cl}} \frac{\partial \bar{Y}^k}{\partial x_i} \text{ turbulent diffusion of species } k \tag{3.22}
\]
\[
-\rho Y^k V^k_i = \bar{\rho} D^k \frac{\partial \bar{Y}^k}{\partial x_i} \text{ molecular diffusion of species } k \tag{3.23}
\]
where \(\mu_t\) is the *dynamic turbulent viscosity*, \(S_{Cl}\) is the *turbulent Schmidt number*, and \(D^k\) is the *molecular species diffusivity*.
The final form of the conservation of mass is therefore
\[
\frac{\partial \bar{\rho} \bar{Y}^k}{\partial t} + \frac{\partial \bar{\rho} \bar{Y}^k \bar{v}_i}{\partial x_i} = \bar{w}^k + \frac{\partial}{\partial x_i} \left( \Gamma_{\text{eff}}^k \frac{\partial \bar{Y}^k}{\partial x_i} \right) \quad (3.24)
\]

where

\[
\Gamma_{\text{eff}}^k = \bar{\rho}D^k + \frac{\mu_t}{Sc_t} \quad (3.25)
\]

Summing (3.24) on \( k \) and using (3.17) yields

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{v}_i}{\partial x_i} = \sum_k \bar{w}^k + \frac{\partial}{\partial x_i} \left( \sum_k \Gamma_{\text{eff}}^k \frac{\partial \bar{Y}^k}{\partial x_i} \right) \quad (3.26)
\]

Equation (3.26) must be identical to (3.19); otherwise, there is a fictitious source/sink of mass. Therefore

\[
\frac{\partial}{\partial x_i} \left( \sum_k \Gamma_{\text{eff}}^k \frac{\partial \bar{Y}^k}{\partial x_i} \right) = 0 \quad (3.27)
\]

This can be achieved by assuming

\[
D^k = D \quad (3.28)
\]

and using (3.17). In other words, \( D^k \) is independent of \( k \).

Equation (3.24) is identical to Equation(125) in the ANSYS CFX manual[2]. Note, however, that there are several typographical errors in the manual. The conservation of mass in CFX is shown in Fig. 3.1.

\[
\frac{\partial \bar{\rho} \bar{Y}_i}{\partial t} + \frac{\partial \bar{\rho} \bar{U}_i \bar{Y}_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \Gamma_{\text{eff}} \frac{\partial \bar{Y}_j}{\partial x_j} \right) + S_i
\]

Figure 3.1: Conservation of mass in CFX

The term \( w^k \) mentioned in conservation of mass equation as the net rate of production of mass of species \( k \) per unit volume per unit time can be calculated considering the chemical reactions and mass transfer. In general, an arbitrary chemical reaction can be written in terms of \( N \) elementary reactions involving \( K \) species,
\[
\sum_{k=1,2,...}^{K} \gamma'_{nk} \mathbb{R}_k \longrightarrow \sum_{k=1,2,...}^{K} \gamma''_{nk} \mathbb{R}_k \tag{3.29}
\]

where \(\gamma'_{nk}\) and \(\gamma''_{nk}\) are the stoichiometric coefficients of species \(k\) in reaction \(n\) appearing as a reactant and as a product respectively and \(\mathbb{R}_k\) is the chemical symbol for species \(k\) and \(K\) is the number of species.

The net rate of production/consumption, \(w^k\), for species \(k\) can be written as the sum of the rate of progress for all the elementary reactions in which species \(k\) participates,

\[
w^k = M_k \sum_{n=1}^{N} \dot{c}_{kn} \tag{3.30}
\]

where \(M_k\) is the molecular weight and \(\dot{c}_{kn}\) is the rate of changes of the concentration of species \(k\) in reaction \(n\) and is calculated as,

\[
\dot{c}_{kn} = (\gamma''_{nk} - \gamma'_{nk}) R_n \tag{3.31}
\]

where \(R_n\) is the specific reaction rate. In the current study, The Eddy Dissipation model has been used to model the homogeneous reaction (single phase reaction) and calculate \(R_n\). Analysis of heterogeneous reactions (multi-phase reactions) in current study is performed via a finite rate chemistry model.

### 3.4 The Eddy Dissipation Model for Single Phase Reaction

The Eddy Dissipation model is very robust in modeling turbulent reacting flows. This model is based on the concept that chemical reaction is fast relative to the transport processes in the flow and assumes that reaction rate is related to the time required to mix reactants at the molecular level, since as soon as reactants are mixed in this level, products are created instantaneously. In turbulent flows, the mixing time is dominated by the eddy properties, therefore, the rate is proportional to a mixing time defined by the turbulent kinetic energy, \(k\), and dissipation, \(\epsilon\),

\[
\text{rate} \propto \frac{\epsilon}{k} \tag{3.32}
\]
In the Eddy Dissipation model, the specific reaction rate, \( R_n \), is determined by the smallest of the reactant limiter and the product limiter. The reactant limiter is defined as,

\[
R_n = A^\epsilon_k \text{min}(\frac{[c_{mol}]}{\gamma_{nk}})
\]

(3.33)

where, \([c_{mol}]\) is the molar concentration of species \( k \) which includes reactants only. The product limiter is defined as,

\[
R_n = A^\epsilon_k \text{min}(\frac{\sum_k [c_{mol}] M_k}{\sum_k \gamma_{nk}'' M_k})
\]

(3.34)

where the summation includes products only. \( A \) and \( B \) are constants that are by default set to 4 and \(-1\) respectively. Negative values for \( B \) makes the product limiter to be turned off by default. Therefore, the reaction rate is determined by reactant concentrations and turbulence.

### 3.5 Finite Rate Chemistry Model for Multi-Phase reactions

The only option available in ANSYS-CFX for multi-phase reactions is finite-rate chemistry. This model is very suitable in situations where the chemical time scale is rate-limiting. In the model the rate of reaction \( R_n \) is defined as,

\[
R_n = F_n \prod_{k=1}^{K} [c_{mol}]^{r'_{nk}} - B_n \prod_{k=1}^{K} [c_{mol}]^{r''_{nk}}
\]

(3.35)

where \( F_k \) and \( B_k \) are forward and backward rate constants respectively and \( r \) represents the reaction order of species \( k \) in reaction \( n \). Forward and backward rate reactants are calculated by the Arrhenius equation,

\[
F_n = A_n T^{\beta_n} e^{\frac{-E_n}{RT}},
\]

(3.36)

\[
B_n = A_n T^{\beta_n} e^{\frac{-E_n}{RT}}
\]

(3.37)

where \( A_n, \beta_n, E_k \) and \( T \) are pre-exponential factor, temperature exponent, activation energy and temperature respectively. These values are listed in Table 3.4. In the current study, forward reactions have been considered only.
3.6 Conservation of Momentum in Gas Phase

A volume $\tau^k$ containing an identifiable amount of species $k$ is considered. The Cartesian stress tensor acting on species $k$ is denoted by $\sigma_{ij}^k$, and the body force per unit mass of species $k$ acting on species $k$ is $f_i^k$. The rate of generation of momentum per unit volume of species $k$ is $w^k m_i^k$ where $m_i^k$ is the momentum per unit mass of species $k$ created. The conservation of momentum is

$$\frac{d}{dt} \int_{\tau^k} \rho^k v_i^k dV = \int_{\partial \tau^k} \sigma_{ij}^k n_j dA + \int_{\tau^k} f_i^k dV + \int_{\tau^k} w^k m_i^k dV$$  \hspace{1cm} (3.38)

where $\partial \tau^k$ is the surface of the volume $\tau^k$ and $n_j$ is the outward unit normal. Using the Reynolds Transport Theorem,

$$\frac{\partial \rho^k v_i^k}{\partial t} + \frac{\partial \rho^k v_i^k v_j^k}{\partial x_j} = \frac{\partial \sigma_{ij}^k}{\partial x_j} + \rho^k f_i^k + w^k m_i^k$$  \hspace{1cm} (3.39)

Consider the summation on $k$ of (3.39). The first term on the left side becomes

$$\sum_k \frac{\partial \rho^k v_i^k}{\partial t} = \frac{\partial}{\partial t} \left( \sum_k \rho^k v_i^k \right) = \frac{\partial \rho v_i}{\partial t}$$  \hspace{1cm} (3.40)

The second term on the left side becomes

$$\sum_k \frac{\partial \rho^k v_i^k v_j^k}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \sum_k \rho^k v_i^k v_j^k \right]$$

$$= \frac{\partial}{\partial x_j} \left[ \sum_k \left( \rho^k v_i v_j + \rho^k v_i V_j^k + \rho^k V_i^k v_j + \rho^k V_i^k V_j^k \right) \right]$$

$$= \frac{\partial}{\partial x_j} \left[ \rho v_i v_j + \sum_k \rho^k V_i^k V_j^k \right]$$  \hspace{1cm} (3.41)

Assuming the body force $f_i^k$ is the same for all species$^2$,\n
$$\sum_k \rho^k f_i^k = \rho f_i$$  \hspace{1cm} (3.42)

$^2$For example, gravity.
Define

\[
\sigma_{ij} = \sum_k \sigma_{ij}^k \quad (3.43)
\]

\[
\tau_{ij}^d = -\sum_k \rho^k V_i^k V_j^k \quad (3.44)
\]

then the summation on \( k \) of (3.39) is

\[
\frac{\partial \rho v_i}{\partial t} + \frac{\partial \rho v_i v_j}{\partial x_j} = \frac{\partial \sigma_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}^d}{\partial x_j} + \rho f_i + m_i \quad (3.45)
\]

where \( m_i = \sum_k w^k m_i^k \) is the net production of momentum. It is typically postulated \[29\] that momentum is neither created nor destroyed by chemical reaction. Therefore, \( m_i \) represents the net production of momentum per unit volume per time by phase change\(^3\).

The stress tensors \( \sigma_{ij}^k \) are

\[
\sigma_{ij}^k = -p^k \delta_{ij} + \tau_{ij}^k \quad (3.46)
\]

where \( \delta_{ij} \) is the Kronecker delta and

\[
p_k = -\frac{1}{3} \sigma_{ii}^k \quad (3.47)
\]

Define

\[
p = \sum_k p^k \quad (3.48)
\]

\[
\tau_{ij}^v = \sum_k \tau_{ij}^k \quad (3.49)
\]

and the conservation of momentum is

\[
\frac{\partial \rho v_i}{\partial t} + \frac{\partial \rho v_i v_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}^v}{\partial x_j} + \frac{\partial \tau_{ij}^d}{\partial x_j} + \rho f_i + m_i \quad (3.50)
\]

The ensemble average of (3.50) yields

\[
\frac{\partial \tilde{\rho} \tilde{v}_i}{\partial t} + \frac{\partial \tilde{\rho} \tilde{v}_i \tilde{v}_j}{\partial x_j} = -\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial \tilde{\tau}_{ij}}{\partial x_j} + \tilde{\rho} f_i + \tilde{m}_i \quad (3.51)
\]

\(^3\)Note that the units of \( m_i^k \) and \( m_i \) are different.
where

$$
\tau_{ij} = -\rho v_i'^\prime v_j'^\prime + \bar{\tau}_v^{ij} + \bar{\tau}_d^{ij}
$$  \hfill (3.52)

The Reynolds stress is assumed defined by means of a dynamic turbulent eddy viscosity $\mu_t$ as

$$
-\rho v_i'^\prime v_j'^\prime = \mu_t \left( \frac{\partial \bar{v}_i}{\partial x_j} + \frac{\partial \bar{v}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left( \bar{p}k + \mu_t \frac{\partial \bar{v}_l}{\partial x_l} \right)
$$  \hfill (3.53)

The trace of (3.53) yields

$$
\rho v_i'^\prime v_i'^\prime = 2\bar{p}k \quad \text{and thus} \quad k = \frac{1}{2} \frac{\rho v_i'^\prime v_i'^\prime}{\rho} \quad \text{(3.54)}
$$

where the summation on $i$ is indicated. Therefore, (3.54) defines the turbulence kinetic energy per unit mass $k$.

The sum of the laminar and diffusion stresses is modeled as

$$
\bar{\tau}_v^{ij} + \bar{\tau}_d^{ij} = \mu \left( \frac{\partial \bar{v}_i}{\partial x_j} + \frac{\partial \bar{v}_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \bar{v}_l}{\partial x_l} \right)
$$  \hfill (3.55)

This model effectively combines $\bar{\tau}_d^{ij}$ and $\bar{\tau}_v^{ij}$ and models their sum.

From (3.51) the total stress tensor can be written as

$$
\sigma_{ij\text{tot}} = -\bar{p} \delta_{ij} + \tau_{ij}
$$  \hfill (3.56)

and thus

$$
\sigma_{i\text{tot}} = -3\bar{p} + \tau_{ii}
$$  \hfill (3.57)

$$
\sigma_{i\text{tot}} = -3\bar{p} - \rho v_i'^\prime v_i'^\prime
$$

and therefore

$$
\frac{1}{3} \sigma_{i\text{tot}} = -\frac{1}{3} \left( \bar{p} + \frac{1}{3} \rho v_i'^\prime v_i'^\prime \right)
$$  \hfill (3.58)

---

$^4$Note summation on index $l$. The Reynolds stress is assumed defined by means of a dynamic turbulent eddy viscosity $\mu_t$ as
In other words, $\bar{p} + \frac{1}{3} \overline{\rho v_i^p v_i^p}$ is the (negative of the) average normal stress on a fluid element.

The shear stress tensor therefore becomes

$$
\tau_{ij} = (\mu_t + \mu) \left( \frac{\partial \tilde{v}_i}{\partial x_j} + \frac{\partial \tilde{v}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left[ \bar{p} k + (\mu_t + \mu) \frac{\partial \tilde{v}_i}{\partial x_j} \right]
$$

(3.59)

where $\mu$ is the dynamic molecular viscosity of the mixture.

A modified pressure $p'$ is defined by

$$
p' = \bar{p} + \frac{2}{3} \bar{\rho} k + (\mu_t + \mu) \frac{\partial \tilde{v}_i}{\partial x_j}
$$

(3.60)

ANSYS CFX omits the term in $\partial \tilde{v}_i / \partial x_j$.

The effective dynamic viscosity is defined as

$$
\mu_{\text{eff}} = \mu_t + \mu
$$

(3.61)

The conservation of momentum is

$$
\frac{\partial \bar{\rho} \tilde{v}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{v}_i \tilde{v}_j}{\partial x_j} = - \frac{\partial p'}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu_{\text{eff}} \left( \frac{\partial \tilde{v}_i}{\partial x_j} + \frac{\partial \tilde{v}_j}{\partial x_i} \right) \right] + \tilde{\rho} \tilde{f}_i + \bar{m}_i
$$

(3.62)

Eq (3.62) is identical to the conservation of momentum in the ANSYS CFX Manual [2].

The conservation of momentum in CFX is shown in Fig. 3.2.

Equation 3.62: Conservation of momentum in CFX

### 3.7 Conservation of Energy in Gas Phase

It is postulated [29] that energy is neither created nor destroyed by chemical reactions. The First Law of Thermodynamics is therefore

$$
\sum_k \frac{d}{dt} \int_{\tau_k} \rho^k \left( u^k + \frac{1}{2} v_i^k v_i^k \right) dV \bigg|_{\tau_k=\tau} = \sum_k \left[ \int_\sigma \sigma_{ij}^k n_j v_i^k dA + \int \rho^k f_j^k v_j^k dV \right]
$$

(3.63)
\[- \sum_k \int_{\partial \tau} q_j^k n_j \, dA + \int_{\tau} q_c \, dV\]

Since the First Law applies to a system \(i.e.,\) an identifiable collection of mass), and assuming that the gas consists of \(N\) distinct coexisting continua, at time \(t\) we consider the \(N\) systems defined by \(\tau_k\) which coincide with each other (and the volume \(\tau\)). However, each system \(\tau_k\) moves with a different instantaneous velocity \(v^k_i\) and thus the Reynolds Transport Theorem must be applied to the left side (3.63) individually to each system. Here \(\tau\) is the elemental volume, \(\partial \tau\) is the surface of \(\tau\), \(u^k\) is the absolute internal energy of species \(k\) per unit mass of species \(k\), \(q_j^k\) is the molecular heat flux associated with species \(k\), and \(q_c\) is the energy added per unit volume per unit time by phase change.

To evaluate the left side of (3.63), define

\[\beta^k = Y^k \left( u^k + \frac{1}{2} v^k_i v^k_i \right) \]  
(3.64)

The Reynolds Transport Theorem yields\(^5\)

\[\sum_k \frac{d}{dt} \int_{\tau_k} \rho^k \left( u^k + \frac{1}{2} v^k_i v^k_i \right) \, dV \bigg|_{\tau_k = \tau} = \sum_k \int_{\tau_k} \left[ \frac{\partial \rho \beta^k}{\partial t} + \frac{\partial \rho \beta^k v^k_j}{\partial x_j} \right] \bigg|_{\tau_k = \tau} \, dV \]  
(3.65)

Now

\[\rho \beta^k = \rho Y^k \left( u^k + \frac{1}{2} v^k_i v^k_i + v_i V^k_i + \frac{1}{2} V^k_i V^k_i \right) \]  
(3.66)

and thus interchanging the summation and differentiation,

\[\sum_k \rho \beta^k = \rho \left[ u + \frac{1}{2} v_i v_i + \frac{1}{2} \sum_k Y^k V^k_i V^k_i \right] \]  
(3.67)

where

\[u = \sum_k Y^k u^k \]  
(3.68)

The total energy per unit mass is defined as

\(^5\)Note that \(v^k_j\) appears in the second term in the integrand, \(not\ \nu_j\).
\[ e = u + \frac{1}{2} v_i v_i \]  

(3.69)

and the \textit{diffusion kinetic energy per unit mass} is defined as

\[ \varphi = \frac{1}{2} \sum_k Y^k V_i^k V_j^k \]  

(3.70)

and thus

\[ \sum_k \rho \beta^k = \rho (e + \varphi) \]  

(3.71)

Similarly

\[ \sum_k \rho \beta^k v_j^k = \rho (e + \varphi) v_j - \varpi_j \]  

(3.72)

where

\[ \varpi_j = - \sum_k \rho Y^k \left( u_i^k V_j^k + v_i^k V_j^k + \frac{1}{2} V_i^k V_j^k \right) \]  

(3.73)

Hence the left side of (3.63) is

\[ \int_{\tau} \left[ \frac{\partial \rho (e + \varphi)}{\partial t} + \frac{\partial \rho (e + \varphi) v_j}{\partial x_j} - \frac{\partial \varpi_j}{\partial x_j} \right] dV \]  

(3.74)

From Gauss’ Theorem, the first term on the right of (3.63) becomes

\[ \sum_k \int_{\partial \tau} \sigma_i^k n_j v_i^k dA = \int_{\tau} \frac{\partial \sigma_i^j}{\partial x_j} dV + \int_{\tau} \frac{\partial}{\partial x_j} \left( \sum_k \sigma_i^k V_i^k \right) dV \]  

(3.75)

Similarly,

\[ \sum_k \int_{\partial \tau} q_i^k n_j dA = \int_{\tau} \frac{\partial q_i}{\partial x_j} dV \]  

(3.76)

where

\[ q_j = \sum_k q_i^k \]  

(3.77)

Therefore, (3.63) becomes
\[
\frac{\partial \rho (e + \varphi)}{\partial t} + \frac{\partial \rho (e + \varphi) v_j}{\partial x_j} = \frac{\partial \sigma_{ij} v_i}{\partial x_j} + \rho f_j v_j + \frac{\partial \Pi_j}{\partial x_j} + q_c + \frac{\partial}{\partial x_j} \left( \sum_k \sigma_{ij}^k v_i^k \right) \quad (3.78)
\]

where
\[
\Pi_j = -q_j + \omega_j \quad (3.79)
\]

Assuming \( \varphi \ll e \) and \( V_j^k \ll v_j \),
\[
\frac{\partial \rho e}{\partial t} + \frac{\partial \rho e v_j}{\partial x_j} = \frac{\partial \sigma_{ij} v_i}{\partial x_j} + \rho f_j v_j + \frac{\partial \Pi_j}{\partial x_j} + q_c \quad (3.80)
\]

Define
\[
\rho^k h^k = \rho^k u^k + p^k \quad (3.81)
\]

where \( h^k \) is the static enthalpy per unit mass of species \( k \). Then
\[
\rho \sum_k Y^k h^k = \rho \sum_k Y^k u^k + \sum_k p^k \quad (3.82)
\]
\[
= \rho u + p
\]

and therefore the mixture static enthalpy per unit mass \( h \) is defined as
\[
h = \sum_k Y^k h^k \quad \text{and therefore} \quad h = u + \frac{p}{\rho} \quad (3.83)
\]

The mixture total enthalpy per unit mass \( H \) is defined as
\[
H = h + \frac{1}{2} v_i v_i \quad \text{and therefore} \quad H = e + \frac{p}{\rho} \quad (3.84)
\]

Substituting
\[
\sigma_{ij} = -p \delta_{ij} + \tau_{ij}^v \quad (3.85)
\]

into (3.80) and using (3.84)
\[
\frac{\partial \rho H}{\partial t} + \frac{\partial \rho H v_j}{\partial x_j} = \frac{\partial p}{\partial t} + \frac{\partial \tau_{ij}^v v_i}{\partial x_j} + \rho f_j v_j + \frac{\partial \Pi_j}{\partial x_j} + q_c
\] (3.86)

The ensemble average of (3.86) introduces

\[
\bar{\rho H} = \rho \left( h + \frac{1}{2} v_i v_i \right)
= \bar{\rho} h + \frac{1}{2} \bar{\rho} \tilde{v}_i \tilde{v}_i + \bar{\rho} k
\] (3.87)

and thus

\[
\bar{H} = \bar{h} + \frac{1}{2} \bar{v}_i \bar{v}_i + k
\] (3.88)

Furthermore

\[
\bar{\rho H} v_j = \rho \left[ h + \frac{1}{2} (\tilde{v}_i + v''_i)^2 \right] \left[ \tilde{v}_j + v''_j \right]
= \bar{\rho} \bar{H} + \bar{\rho} h v''_j + \bar{\rho} v''_i v''_j \tilde{v}_i + \frac{1}{2} \bar{\rho} v''_i v''_i v''_j
\] (3.89)

The molecular stress work term is approximated as

\[
\bar{\tau}_{ij}^v v_i = \bar{\tau}_{ij}^v \tilde{v}_i
\] (3.90)

The ensemble average of (3.86) becomes

\[
\frac{\partial \bar{\rho} \bar{H}}{\partial t} + \frac{\partial \bar{\rho} \bar{H} \tilde{v}_j}{\partial x_j} = \frac{\partial \bar{p}}{\partial t} + \frac{\partial \left[ (-\rho v''_i v_j + \bar{\tau}_{ij}^v) \tilde{v}_i \right]}{\partial x_j} + \frac{\partial \left( -\rho h v''_j + \Pi_j \right)}{\partial x_j} + \bar{\rho} f_j \tilde{v}_j + \bar{q}_c
\]

The total stress term is modeled as

\[
-\rho v''_i v_j + \bar{\tau}_{ij}^v = (\mu + \mu) \left( \frac{\partial \tilde{v}_i}{\partial x_j} + \frac{\partial \tilde{v}_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{v}_l}{\partial x_l} \right)
\] (3.91)

The term \( \partial \tilde{v}_l / \partial x_l \) is dropped in CFX. The total heat flux is modeled as
\[-\rho \hat{h} v_j + \Pi_j = \frac{\mu_t}{Pr_t} \frac{\partial \hat{h}}{\partial x_j} + \lambda \frac{\partial \hat{T}}{\partial x_j} \] (3.92)

where \( Pr_t \) is the turbulent Prandtl number and \( \lambda \) is the thermal conductivity of the mixture.

The energy equation is therefore

\[
\frac{\partial \rho \tilde{H}}{\partial t} + \frac{\partial \rho \tilde{H} \tilde{v}_j}{\partial x_j} = \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} \left[ (\mu_t + \mu) \left( \frac{\partial \tilde{v}_i}{\partial x_j} + \frac{\partial \tilde{v}_j}{\partial x_i} \right) \tilde{v}_i \right] + \frac{\partial}{\partial x_j} \left[ \frac{\mu_t}{Pr_t} \frac{\partial \hat{h}}{\partial x_j} + \lambda \frac{\partial \hat{T}}{\partial x_j} \right] + \rho f_j \tilde{v}_j + \bar{q}_c \] (3.93)

Eq (3.93) is identical to the conservation of energy in the ANSYS CFX Manual[2]. The conservation of energy in CFX is shown in Fig. 3.3.

It should be mentioned that body forces have been neglected in current research.

### 3.8 Equation of State in Gas Phase

It is assumed that the static partial pressure of each species \( k \) is given by Dalton’s Law with a common temperature

\[ p^k = n^k RT \] (3.94)

where \( n^k \) is the molar concentration of species \( k \) and \( R \) is the Universal Gas Constant. Since

\[ n^k = \frac{\rho^k}{M^k} \] (3.95)

where \( M^k \) is the molecular weight of species \( k \), then

\[ p = \sum_k \frac{\rho^k Y^k}{M^k} RT \] (3.96)

Thus
\[
\bar{p} = \sum_k \rho Y^k RT \frac{M_k}{M}
\] (3.97)

The numerator is approximated by assuming \(Y^k \approx \tilde{Y}^k\) and thus

\[
\rho Y^k RT = \rho \tilde{Y}^k R \tilde{T}
\] (3.98)

The ensemble averaged pressure is therefore

\[
\bar{p} = \sum_k \rho \tilde{Y}^k \frac{R \tilde{T}}{M_k}
\] (3.99)

### 3.9 Turbulence Model in Gas Phase

The Jones-Launder turbulence model is defined by equations for the turbulence kinetic energy \(k\) and the rate of dissipation of turbulence kinetic energy \(\epsilon\) by

\[
\frac{\partial \bar{\rho} k}{\partial t} + \frac{\partial \bar{\rho} k \bar{v}_j}{\partial x_j} = P_k + P_{kb} - \bar{\rho} \epsilon + \frac{\partial}{\partial x_j} \left[ \left( \frac{\mu_t}{\sigma_k} + \mu \right) \frac{\partial k}{\partial x_j} \right]
\] (3.100)

\[
\frac{\partial \bar{\rho} \epsilon}{\partial t} + \frac{\partial \bar{\rho} \epsilon \bar{v}_j}{\partial x_j} = C_{\epsilon_1} \frac{\epsilon}{k} (P_k + P_{eb}) - C_{\epsilon_2} \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left[ \left( \frac{\mu_t}{\sigma_\epsilon} + \mu \right) \frac{\partial \epsilon}{\partial x_j} \right]
\] (3.101)

where \(C_{\epsilon_1}, C_{\epsilon_2}, \sigma_k\) and \(\sigma_\epsilon\) are constants. The turbulence production term is

\[
P_k = \mu_t \left( \frac{\partial \bar{v}_i}{\partial x_j} + \frac{\partial \bar{v}_j}{\partial x_i} \right) \frac{\partial \bar{v}_i}{\partial x_j} - \frac{2}{3} \frac{\partial \bar{v}_i}{\partial x_i} \left( 3 \mu_t \frac{\partial \bar{\rho} \epsilon_{mn}}{\partial x_m} + \bar{\rho} k \right)
\] (3.102)

and the turbulence production due to buoyancy is

\[
P_{kb} = -\frac{\mu_t}{\bar{\rho} \sigma_\rho} f_i \frac{\partial \bar{p}}{\partial x_i}
\] (3.103)

### 3.10 Particle Transport Model

Pulverized coal particles are treated in CFX as non-interacting spheres with internal reactions, heat transfer and fully coupled to the continuous fluid. Fully coupled particles exchange momentum with the continuous phase, allowing the continuous flow to affect the
particles, and the particles to affect the continuous flow. Two-way coupling requires that the particle source terms are included in the momentum equations. The momentum sources could be due to turbulent dispersion forces or drag. The particle source terms are generated for each particle as they are tracked through the flow. Particulates are tracked through the flow in a Lagrangian way. The tracking is carried out by forming a set of ODEs in time for each particle, consisting of an equation for position, velocity, temperature and masses of species. These equations are integrated using a simple integration method to calculate the behavior of the particles as they traverse the flow domain.

Particle sources are applied in the control volume that the particle is in during the timestep. The particle sources in the momentum equations are obtained by solving transport equations for the sources. The generic equation for particle sources is:

$$\frac{dS_P}{dt} = C_S \Phi_P + R_S$$  \hspace{1cm} (3.104)

Where $C_S \Phi_P$ are the contributions from the particles that are linear in the solution variable and $R_S$ contains all other contributions. The source to be added to the continuous phase is then multiplied by the number flow rate for that particle, which is the mass flow rate divided by the mass of the particle.

### 3.11 Momentum Transfer

When a discrete particle is traveling in a continuous fluid medium, the forces acting on the particle that affect the particle acceleration are due to the difference in velocity between the particle and fluid, as well as to the displacement of the fluid by particle. For a Lagrangian description of particle motion, the conservation of momentum for a particle is

$$m_p \frac{dv^P_i}{dt} = F_{di} + F_{bi} + F_{ri} + F_{(vm)i} + F_{(ba)i}$$  \hspace{1cm} (3.105)

where $m_p$ is the mass of the particle, $v^P_i$ are the Cartesian components of the particle velocity, and $F_{di}$, $F_{bi}$, $F_{ri}$, $F_{(vm)i}$ and $F_{(ba)i}$ are the aerodynamic drag, buoyancy forces, rotation forces, virtual or added mass forces and pressure gradient forces, respectively. The effects of particle rotation, virtual mass, pressure gradient and history (Basset term) are neglected. The drag force is
\[ F_{d_i} = \frac{1}{2} C_D \rho A |v - v^p| (v_i - v_i^p) \]  

(3.106)

where \( v = (v_1, v_2, v_3) \) is the mass-averaged flow velocity vector, \( v^p \) is the particle velocity vector and \( A \) is the particle cross-sectional area assuming spherical particles.

The drag coefficient is a complicated function of Reynolds number, which must be determined from experiment. Assuming spherical particles, the Schiller Naumann drag model proposes:

\[ C_D = 24(1 + 0.15 Re^{0.687})/Re \]  

(3.107)

where \( Re \) is the slip Reynolds number given by \( Re = \frac{\rho |v - v^p| d}{\mu F} \). In turbulent flow, the instantaneous fluid velocity is decomposed into Favre-Averaged value, \( \tilde{v}_i \), and fluctuating value, \( v''_i \). In turbulent tracking, particle trajectories are not deterministic, i.e., two identical particles, injected from a single point, at different times, may follow separate trajectories due to the random nature of the instantaneous fluid velocity and the fluctuating part of fluid velocity causes the dispersion of particles in a turbulent flow.

The effect of turbulence on the particles is modelled according to Gosman and Loannides and assumes that a particle is always within a single turbulent eddy. Each eddy has a characteristic fluctuating velocity, \( v''_f \), life time, \( \tau_e \), and length, \( l_e \). When a particle enters the eddy, the fluctuating velocity for the eddy is added to the local mean fluid velocity to obtain the instantaneous fluid velocity. The fluctuating part of fluid velocity is assumed to prevail as long as the particle-eddy interaction time is less than eddy life time and the displacement of the particle relative to the eddy is less than eddy length. If either of these conditions exceeds, the particle will enter a new eddy with new characteristics [2]. The turbulent velocity, length and life time are calculated as follows:

\[ v''_f = \Gamma \left( \frac{2k}{3} \right)^{0.5} \]  

(3.108)

\[ l_e C_\mu^{3/4} k^{2/3} \]  

(3.109)
\[
\tau_c = \frac{l_v}{(2k^3)^{1/2}} \tag{3.110}
\]
where \( k \) and \( \epsilon \) are the local turbulent kinetic energy and dissipation, respectively and \( C_\mu \) is turbulence constant. \( C_\mu^{3/4} \) is a factor chosen to relate the characteristic length scale to the Eddy Dissipation length. The variable \( \Gamma \) is a normally distributed random number which accounts for the randomness of turbulence about a mean value.

### 3.12 Heat Transfer

Heat transfer to the particle is modelled as the sum of contributions from convective heat transfer, latent heat transfer associated with mass transfer and radiation heat transfer which is neglected in our model. The convective heat transfer \( Q_c \) is given by,

\[
Q_C = \pi d \lambda N u (T_g - T) \tag{3.111}
\]
where \( \lambda \) is the thermal conductivity, \( T_g \) and \( T \) are temperatures of gas and particle respectively. The Nusselt number is given as,

\[
N u = 2 + 0.6 Re^{0.5} (\mu \frac{C_p}{\lambda})^{1/3} \tag{3.112}
\]
where \( \mu \frac{C_p}{\lambda} \) is the Prandtl number. Convective heat transfer has a correction based on the rate of mass transfer from the particle [2]:

\[
Q_C = Q_C \xi e^{-\xi} \tag{3.113}
\]
where \( \xi \) is given by \( \xi = C_p \frac{|dm|}{\pi d \lambda N u} \) in which \( \frac{dm}{dt} \) is total mass transfer rate of particle. The latent heat transfer is given by,

\[
Q_M = \Sigma \frac{dm_i}{dt} V \tag{3.114}
\]
where the sum is taken over all components of the particles. The latent heat of vaporization \( V \) is temperature dependent and is obtained directly from the material modeling section of CFX, defined by the NASA formulation in our case.
\[ V = \int_{T_{ref}}^{T} (C_{pgi} - C_{ppi})dT \] (3.115)

where \(C_{pgi}\) and \(C_{ppi}\) are tabulated in the SANDIA report based on NASA Chemical Equilibrium program [1].

The rate of change of temperature for the particle is then obtained from

\[ \sum (m_i C_p) \frac{dT}{dt} = Q_C + Q_M \] (3.116)

where the sum is taken over all components of the particle. Also, radiation heat transfer has been neglected in current study.

### 3.13 Mass Transfer

Each component of mass being transferred between the continuous and particle phases satisfies the following equation.

\[ \frac{dm_k}{dt} = -\pi d_p \rho D_F Sh (EY_{P,k} - Y_{F,k}) \] (3.117)

where \(m_k\) is the mass of constituent in the particle, \(Y_{P,k}\) is the mass fraction of component \(C\) in the particle. \(Y_{F,k}\) is the mass fraction of component \(k\) in the surrounding fluid, \(E\) is the equilibrium mass fraction ratio (default value is 1), \(\rho D_F\) is the dynamic diffusivity of the mass fraction in the continuum and \(Sh\) is the Sherwood number given by,

\[ Sh = 2 + 0.6 Re^{0.5} \left( \frac{\mu}{\rho D} \right)^{1/3} \] (3.118)

where \(\frac{\mu}{\rho D}\) is Schmidt number which is the ratio of convective mass transfer to diffusion mass transfer. This mass transfer correlation is analogous to heat transfer correlation mentioned in Eq.(3.112). This model assumes that the mass transfer is driven only by concentration differences.
### Table 3.1: Proximate analysis

<table>
<thead>
<tr>
<th>Composition</th>
<th>Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ash Fraction</td>
<td>0.024</td>
</tr>
<tr>
<td>Fixed Carbon Fraction</td>
<td>0.581</td>
</tr>
<tr>
<td>Moisture Fraction</td>
<td>0.043</td>
</tr>
<tr>
<td>Volatiles Fraction</td>
<td>0.352</td>
</tr>
</tbody>
</table>

### Table 3.2: Ultimate analysis

<table>
<thead>
<tr>
<th>Composition</th>
<th>Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ash Fraction</td>
<td>0.024</td>
</tr>
<tr>
<td>Carbon Fraction</td>
<td>0.7405</td>
</tr>
<tr>
<td>Chlorine Fraction</td>
<td>0.000</td>
</tr>
<tr>
<td>Hydrogen Fraction</td>
<td>0.0531</td>
</tr>
<tr>
<td>Nitrogen Fraction</td>
<td>0.0160</td>
</tr>
<tr>
<td>Oxygen Fraction</td>
<td>0.1199</td>
</tr>
<tr>
<td>Sulphure Fraction</td>
<td>0.0035</td>
</tr>
</tbody>
</table>

### 3.14 Materials Defined in CFX

The ccl file imported into CFX sets up the following materials such as ash, char, fuel gas, gas mixture, HC fuel, HC fuel gas binary mixture and raw combustible. HC fuel and gas mixture are defined in order to represent the phase in which species react. They are defined as hydrocarbon fuel in the material group of particle solids and reacting mixture in the material group of gas phase combustion respectively. Tables 3.1 and 3.2 represent proximate and ultimate analysis of coal (HC fuel).

Fuel gas and raw combustible are defined in order to represent the reacting species and they are set as pure substance in the material group of gas phase combustion and pure substance in the material group of particle solids respectively. The HC fuel gas binary mixture is defined as homogeneous binary mixture in two material groups of gas phase combustion and particle solids and it represents the phase boundary between two chemically equivalent materials in different thermodynamic states. Table 3.3 represents the properties of ash and char.
Table 3.3: Ash and char properties

<table>
<thead>
<tr>
<th>Material</th>
<th>Density ([kgm^{-3}])</th>
<th>Molar Mass ([kgmol^{-1}])</th>
<th>Specific Heat Capacity ([Jkg^{-1}K^{-1}])</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ash</td>
<td>1000</td>
<td>12</td>
<td>800</td>
</tr>
<tr>
<td>Char</td>
<td>2000</td>
<td>12</td>
<td>1600</td>
</tr>
</tbody>
</table>

3.15 Reactions Defined in CFX

Reactions imported into CFX by the ccl file are HC fuel devolatilization, HC fuel char field and fuel gas-air oxidation. The first reaction is multi-phase and represents volatilization/pyrolysis of coal into fuel gas and char. The second reaction is again multi-phase and represents oxidation of char with air which creates \(CO_2\) as a product. Finally, the last reaction is single step and represents the oxidation of fuel gas with air which creates \(CO_2\) and \(H_2O\) as products. Reaction rates for the mentioned reactions are summarized in Table 3.4 and have been discussed in the following sections.

\[
\text{Devolatilization: } Coal \rightarrow fualgas + Char \quad (3.119)
\]

\[
\text{Field char oxidation: } Char + O_2 \rightarrow CO_2 \quad (3.120)
\]

\[
\text{Fuel gas oxidation: } fualgas + 2O_2 \rightarrow CO_2 + 2H_2O \quad (3.121)
\]

3.16 Devolatilization Reaction Rate

Devolatilization can be modeled by one or more reaction steps using Arrhenius multiphase reactions rates. The single reaction model which is also the simpler model is called Badzioch and Hawksley [3]. In this model, the rate of conversion of coal is,

\[
\frac{dC_0}{dt} = -k_vC_0 \quad (3.122)
\]

where, \(C_0\) is the mass fraction of unreacted raw coal in the coal particle at the time \(t\). The rate of production of volatiles in the gas phase are given by,
Table 3.4: Reaction rates

\[
\frac{dV}{dt} = Y k_v C_0
\]

in which, \( Y \) is the actual yield of products (proximate yield multiplied by a factor to correct for the enhancement of yield due to rapid heating). The rate constant \( k_v \) is expressed in Arrhenius form as,

\[
K_v = A_v \exp\left(\frac{-T}{T_p}\right)
\]

where, \( T_p \) is temperature of coal particles and \( A_v \) and \( E_v \) are determined experimentally.

Therefore, the rate of char formations is,

\[
\frac{dC_{ch}}{dt} = (1 - Y) k_v C_0
\]

### 3.17 Char Oxidation Reaction Rate

Char reaction rate is determined by defining a particle user routine written in FORTRAN and imported into CFX. In this routine char reaction rate has been defined as the rate of chemical reaction at the surface and the rate of diffusion has been neglected. Char oxidation rate per unit area of particle surface is given as \( k_c \),

\[
k_c = A_c T_p^n \exp\left(\frac{T_c}{T_p}\right)
\]

In the above equation, \( A_c \) and \( T_c \) depend on type of coal and the recommended values for them are 497\( kg/m^2s \) and 8540\( K \) respectively as presented in Table 3.4. The default value of \( n \) is zero and the unit of \( k_c \) is \( kg/m^2s \).
3.18 Fuel Gas Oxidation Reaction Rate

The rate of reaction for fuel gas oxidation is given by the Arrhenius equation as follows,

\[ k = A T^n \exp\left(\frac{-E}{RT}\right) \]  \hspace{1cm} (3.127)

where \( A \) and \( E \) are pre-exponential factor and the activation energy respectively and the values are given in Table 3.4. Activation energy is the minimum barrier height which reactants must acquire before they can react. At the microscopic level, the collision of the reactant molecules can produce products only if the energy of the reactants exceeds this minimum amount.

3.19 NO Formation

\( NO_x \) formation is a complicated process which involves different mechanisms such as Thermal NO and Prompt NO.

3.20 Thermal NO

The thermal \( NO \) mechanism is a predominant source of \( NO_x \) in gas flames at temperatures above 1800\( K \). In this mechanism \( NO \) is formed from the combination of free radical \( O \) and \( N \) species. The two step mechanism which dominates the process is called the Zeldovich mechanism.

\[ O + N_2 \rightarrow NO + N \]  \hspace{1cm} (3.128)

\[ N_2 + O_2 \rightarrow NO + ON \]  \hspace{1cm} (3.129)

In near stoichiometric conditions a third reaction may be important,

\[ OH + N \rightarrow NO + H \]  \hspace{1cm} (3.130)

Combination of these three steps is called the extended Zeldovich mechanism. Rates of these three reactions are given as follows.
\[ k_1 = 1.8 \times 10^{11} \exp\left(-\frac{38370}{T}\right) \]  \hfill (3.131)

\[ k_2 = 6.4 \times 10^9 \exp\left(-\frac{3162}{T}\right) \]  \hfill (3.132)

\[ k_3 = 3 \times 10^{13} \]  \hfill (3.133)

These reaction rates are multiplied by reactants concentrations and they yield rates in terms of \textit{kmol/m}^3/\textit{s}, which can be converted to a volumetric mass source term. The first reaction is rate limiting. The \textit{N} radicals created in this step are oxidized either in reaction (3.129) or (3.130). These oxidation reactions are assumed to be fast. Therefore the thermal \textit{NO} formation, \( S_{\text{NO,thermal}} \), in [\( \text{kg/m}^3/\text{s} \)] is related to the rate of reaction (3.128).

\[ S_{\text{NO,thermal}} = W_{\text{NO}}k_{\text{thermal}}[O][N_2] \]  \hfill (3.134)

\[ k_{\text{thermal}} = 2k_1 \]  \hfill (3.135)

where \( W_{\text{NO}} \) is the molecular mass of \textit{NO}.

### 3.21 Prompt \textit{NO}

At temperatures lower than 1800\( K \), \textit{NO} concentrations in hydrocarbon flames are too high to be explained by the Zeldovich mechanism. Hydrocarbon radicals react with molecular Nitrogen to form \textit{HCN} which will be oxidized to make \textit{NO} under lean flame conditions.

\[ \text{CH} + \text{N}_2 \rightarrow \text{HCN} + \text{N} \]  \hfill (3.136)

\[ \text{HCN} + \text{O}_2 \rightarrow \text{NO} + \ldots \]  \hfill (3.137)

According to De Soete [25], a single reaction rate can describe the \textit{NO} source by the Fenimore mechanism.
\[ S_{NO,prompt} = W_{NO} k_{prompt} \rho [O]^{1/2} [N_2][fuel] \left( \frac{W}{\rho} \right)^{3/2} \] (3.138)

\[ k_{prompt} = A_{prompt} \exp\left( -\frac{T_{A,prompt}}{T} \right) \] (3.139)

where \( W_{NO} \) and \( W \) are molar mass of \( NO \) and the mean molar mass of the mixture, respectively. The Arrhenius coefficients depend on the fuel. De Soete [25] proposed \( A_{prompt} = 6.4 \times 10^6[1/s] \) and \( T_{A,prompt} = 36510[K] \) for methane.
3.22 Numerical Method

ANSYS CFX implements the Finite Volume method to discretize the spatial domain and numerically solve it. The Finite Volume method utilizes the integral form of the conservation equations. The generic conservation equation for a quantity $\phi$, assuming that the velocity field and all other fluid properties are known, is as follows:

$$\frac{\partial}{\partial t} \int_{\Omega} \rho \phi d\Omega + \int_{S} \rho \phi v \cdot n dS = \int_{S} \Gamma \nabla \phi \cdot n dS + \int_{\Omega} q \phi d\Omega$$  \hspace{3cm} (3.140)

The solution domain is divided into a finite number of control volumes generated by a grid. In contrast to the finite difference method, the grid defines the boundaries of the control volume rather than each computational node. The integral conservation equation (3.140) can be applied to both each individual control volume and the whole domain. To obtain an algebraic equation for each control volume, the surface and volume integrals need to be approximated using quadratic formulae [12].

3.23 Approximation of Surface Integrals

Fig.3.4 represents a typical 2D Cartesian control volume. The extension to the 3D problem is straightforward.

The control volume surfaces in 2D are divided into four plane faces. The net flux through the control volume boundary is the sum of integrals over the four control volume faces.

$$\int_{S} f dS = \sum_{k} \int_{S_{k}} f dS$$  \hspace{3cm} (3.141)

where $f$ is the component of the convective, $\rho \phi v \cdot n$, or diffusive, $\Gamma \nabla \phi \cdot n$, vector in the normal direction to the control volume face. As mentioned previously, the velocity field and the fluid properties are assumed to be known, therefore, the only unknown is $\phi$. If the velocity field is unknown, we will have a more complex problem involving non-linear coupled equations. For example, if we want to calculate the surface integral in eq. (3.141) in face $e$, the simplest approximation is the midpoint rule: the integral is approximated as a product of the integrand at the cell face center, which itself is an approximation to the
mean value over the surface, and the cell face area.

\[ F_e = \int_{S_e} f dS = \bar{f}_e S_e \approx f_e S_e \]  

(3.142)

Provided the value of \( f \) at location \( e \) is known, the approximation of the integrals is of second order. There are other approximations for the surface integral in which the variable values in more than one locations on the cell face are utilized such as the trapezoidal and Simpson rule.

### 3.24 Approximation of Volume Integrals

The simplest second-order approximation for the volume integrals is to replace the volume integral by the product of the mean value at the control volume center.

\[ Q_P = \int_{\Omega} q d\Omega = \bar{q}\Delta\Omega \approx q_P \Delta\Omega \]  

(3.143)

where \( q_P \) is for the value of \( q \) at the control volume center. Higher order approximations require more values of \( q \) at more locations than just the center.
3.25 Approximations in Conservation Equations

To illustrate the Finite Volume scheme for our problem we should consider integration of conservation equations, (3.24), (3.62) and (3.93) over the control volume. Gauss’s divergence theorem is applied to convert volume integrals to surface integrals. If control volumes do not deform in time, the time derivatives can be moved out of the volume integrals. The integral equations will be,

\[
\frac{d}{dt} \int_{V} \bar{\rho} \bar{Y}^k dV + \int_{S} \bar{p} \bar{v}_i dn_i = \int_{V} \bar{w}^k dV + \int_{S} \Gamma_{\text{eff}}^k \bar{Y}^k dn_i
\]

\[
\frac{d}{dt} \int_{V} \bar{p} \bar{v}_i dV + \int_{S} \bar{p} \bar{v}_i \bar{v}_j dn_j = - \int_{S} \bar{p}' dn_i + \int_{S} \left[ \mu_{\text{eff}} \left( \frac{\partial \bar{v}_i}{\partial x_j} + \frac{\partial \bar{v}_j}{\partial x_i} \right) \right] d_n \]

\[
+ \int_{S} \left[ \frac{\mu_{t}}{P_{t}} \frac{\partial \bar{h}}{\partial x_j} + \lambda \frac{\partial \bar{T}}{\partial x_j} \right] d_n + \int_{V} \bar{f}_i dV + \int_{V} \bar{m}_i dV
\]

(3.144)

where, \( V, S \) and \( dn_j \) are volume and surface regions of integration and differential Cartesian components of the outward normal surface vector. The next step is to approximate or discretize the integrals. Volume integrals are discretized within each element while surface integrals are discretized at the integration points (ip) located at the center of each surface segment within an element. Discretized integral equations will become,

\[
V \left( \frac{\bar{\rho} \bar{Y}^k - \bar{\rho}^0 \bar{Y}^k,0}{\Delta t} \right) + \sum_{ip} (\bar{p} \bar{Y}^k \bar{v}_i \Delta n)_{ip} = V \bar{w}^k + \sum_{ip} (\Gamma_{\text{eff}}^k \bar{Y}^k \Delta n)_{ip}
\]

(3.147)

\[
V \left( \frac{\bar{p} \bar{v}_i - \bar{p}^0 \bar{v}_i,0}{\Delta t} \right) + \sum_{ip} (\bar{p} \bar{v}_i \bar{v}_j \Delta n)_{ip} = - \sum_{ip} (\bar{p}' \Delta n)_{ip} + \sum_{ip} \left[ \mu_{\text{eff}} \left( \frac{\partial \bar{v}_i}{\partial x_j} + \frac{\partial \bar{v}_j}{\partial x_i} \right) \bar{v}_i \right] \Delta n_{ip}
\]

\[
+ V(\bar{f}_i) + V(\bar{m}_i)
\]

(3.148)

\[
V \left( \frac{\bar{p} \bar{H} - \bar{p}^0 \bar{H}^o}{\Delta t} \right) + \sum_{ip} (\bar{p} \bar{H} \bar{v}_j \Delta n)_{ip} = - \sum_{ip} (\bar{p} \Delta n)_{ip} + \sum_{ip} \left[ (\mu_{t} + \mu) \left( \frac{\partial \bar{v}_i}{\partial x_j} + \frac{\partial \bar{v}_j}{\partial x_i} \right) \bar{v}_i \right] \Delta n_{ip}
\]
\[ + \sum_{ip} \left[ \mu \frac{\partial h}{Pr \partial x_j} + \lambda \frac{\partial T}{\partial x_j} \right] \Delta n_{jp} + V(\tilde{\rho} f_j \tilde{v}_j) + V(\tilde{f}_j) \]  

where \( \Delta t \) is the time step and \( \Delta n_j \) is discrete outward surface vector and the summation is over all the integration points. The first order backward Euler scheme has been assumed in discretization. The discrete outward surface vector, \( \Delta n_j \), is the product of surface area of the control volume and the unit normal to the surface, \( n_j \). In order to approximate the solution field or solution gradients in each integration point, CFX utilizes finite-element shape functions. Finite-element shape functions describe the variation of a variable within an element such as,

\[ \phi = \sum_{i=1}^{N_{node}} N_i \phi_i \tag{3.150} \]

where \( N_i \) is the shape function at node \( i \) and \( \phi_i \) is the value of \( \phi \) at node \( i \). The shape functions used in CFX are linear in terms of parametric coordinates. Shape functions for tetrahedral elements which are used in our mesh are as follows,

\begin{align*}
N_1(s, t, u) &= 1 - s - t - u \\
N_2(s, t, u) &= s \\
N_3(s, t, u) &= t \\
N_4(s, t, u) &= u
\end{align*}

We also specify how some certain terms such as control volume gradients, advection terms, diffusion terms, pressure gradient term and mass flows are being approximated. In case of control volume gradients approximation, CFX utilizes a form of the Gauss’ divergence theorem to evaluate the control volume gradient.

\[ \nabla \phi = \frac{1}{V} \sum_{ip} (\phi \Delta \vec{n})_{ip} \tag{3.151} \]

where \( \Delta \vec{n} \) is the outward surface vector at \( ip \). It should be mentioned that \( \phi \) will be evaluated at integral points via finite-element shape functions.

In order to approximate advection terms, the integral point values of \( \phi \) must be known in terms of the nodal values.
\( \phi_{ip} = \phi_{up} + \beta \nabla \phi \cdot \Delta \vec{r} \)  

(3.152)

where \( \phi_{up} \) is the value at the upwind node and \( \vec{r} \) is the vector from the upwind node to the \( ip \). The value of \( \beta = 0 \) yields a first order Upwind Differencing Scheme (UDS) which is very robust but introduces diffusive discretization errors.

In order to evaluate spatial derivatives for diffusion terms, shape function are used such as,

\[
\frac{\partial \phi}{\partial x}|_{ip} = \sum_n \frac{\partial N_n}{\partial x}|_{ip} \phi_n
\]

(3.153)

The Cartesian derivatives of the shape functions can be expressed in terms of their local derivatives via the Jacobian transformation matrix.

\[
A = \begin{bmatrix}
\frac{\partial N}{\partial x} \\
\frac{\partial N}{\partial y} \\
\frac{\partial N}{\partial z}
\end{bmatrix} = \begin{bmatrix}
\frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} & \frac{\partial z}{\partial s} \\
\frac{\partial x}{\partial t} & \frac{\partial y}{\partial t} & \frac{\partial z}{\partial t} \\
\frac{\partial x}{\partial u} & \frac{\partial y}{\partial u} & \frac{\partial z}{\partial u}
\end{bmatrix}^{-1} \begin{bmatrix}
\frac{\partial N}{\partial s} \\
\frac{\partial N}{\partial t} \\
\frac{\partial N}{\partial u}
\end{bmatrix}
\]

(3.154)

In order to approximate pressure gradient surface integral, we need to evaluate \( (P \Delta n_{ip})_{ip} \) in which \( P_{ip} \) is evaluated using the shape function.

\[
P_{ip} = \sum_n N_n(s_{ip}, t_{ip}, u_{ip}) P_n
\]

(3.155)

Approximation of the transient terms, assuming the control volumes do not deform in time, and using first order Euler backward scheme, would be,

\[
\frac{\partial}{\partial t} \int_V \rho \phi dV = V \left( \frac{\rho_0 \phi - \rho^0 \phi^0}{\Delta t} \right)
\]

(3.156)

This method is first order accurate in time, robust and fully implicit.

### 3.26 Linear Equation Solution

After application of Finite Volume method to all elements of domain, an algebraic system of equations is arised in the form,
\[ \sum_{nb_i} a_{nb_i}^i \phi_i = b_i \] (3.157)

where \( \phi \) is the solution, \( b \) is the right hand side, \( a \)'s are the coefficients of the equation, \( i \) is the identifying number of the element and \( nb \) means "neighbour" but also includes the central coefficient multiplying the solution at the \( i^{th} \) location.

The discrete system of linear equations are solved using a multigrid (MG) accelerated Incomplete Lower Upper (ILU) factorization technique in CFX which is an iterative solver. The linear systems of equations can be written in matrix form as,

\[
[A] [\phi] = [b] \tag{3.158}
\]

where \([A]\) is the coefficient matrix, \([\phi]\) is the solution vector and \([b]\) is the right hand side. This equation can be solved iteratively starting from an approximated solution, \([\phi^n]\), that is to be improved by a correction, \([\phi']\), to yield a better solution, \([\phi^{n+1}]\),

\[
\phi^{n+1} = \phi^n + \phi' \tag{3.159}
\]

where \(\phi'\) is calculated as,

\[
A\phi' = r^n \tag{3.160}
\]

where \(r^n\) is the residual obtained from

\[
r^n = b - A\phi^n \tag{3.161}
\]

In the multigrid approach which enhances the convergence behavior of the matrix inversion technique, the early iterations are carried on a fine grid and later iterations are carried on progressively coarser virtual grids. The results are then transferred back from the coarsest grid to the original fine grid. Algebraic multigrid creates a virtual coarsening of the grid spacing by forming a system of discrete equations for a coarse grid by summing the fine grid equations.
The raw residual, \( r \), mentioned in equation (3.160) is calculated as the imbalance in the linearized system of discrete equations. The raw residual is normalized as,

\[
\tilde{r}_\phi = \frac{r_\phi}{a_p \Delta \phi}
\]  

(3.162)

where \( r_\phi \) is the raw residual control volume imbalance, \( a_p \) is representative of the control volume coefficient and \( \Delta \phi \) is a representative range of the variable in the domain.

CFX uses a coupled solver, which solves the hydrodynamic equations (for \( u, v, w, p \)) as a single system. This approach uses a fully implicit discretization of the equations at each timestep [2]. Fig. (3.5) represents the solution procedure in CFX. The solution of each set of equations in the flow chart consists of two numerical operations:

1. The non-linear equations are linearized (coefficient iteration) and assembled into the solution matrix.

2. The linear equations are solved (equation solution iteration) using an algebraic multi-grid method.

The time step iteration is controlled by the global physical time step.

CFX implements a single cell, unstaggered, collocated grid to overcome the decoupling of pressure and/or velocity. Also, CFX uses Rhie-Chow interpolation scheme, 4\(^{th}\) order smoothing of pressure, to locale the solution of the pressure and velocity fields at the same nodal locations in the grid [2] and therefore to avoid velocity pressure decoupling and oscillation. This method allows physically sensible solutions on collocated grids and ties together the pressure fields to yield smooth solutions and it minimally affects the mass carrying velocities. The adjustment to the mass carrying velocities appears as a 3\(^{rd}\) order zero term multiplying a higher derivative of pressure.
Figure 3.5: Solution Process in CFX
Chapter 4
Design of Experiments and Optimization Method

4.1 Design of Experiments

Design of Experiments (DOE) is a methodology first originated in 1920 by a British Scientist, Sir R. A. Fisher, as a tool to design and analyze experiments. DOE eliminates redundant observations and reduces the time and resources to perform the experiments. In the current study Design of Experiments based on random sequence has been used to provide an initial population of designs for the optimization algorithm. This method is based on the mathematical theory of random number generation and it fills the design space randomly with a uniform distribution.

4.2 Optimization Method

The design optimization problem faced in the current study is a multi-objective optimization problem, i.e, it involves more than one objective function. In real multi-objective optimization problems, different solutions may produce trade-offs (conflicting scenarios) among different objectives. In such cases a solution that is extreme (in a better sense) with respect to one objective requires a compromise in other objectives. Therefore, it is not possible to choose a solution which is optimal with respect to only one objective [8].

A general multi-objective optimization problem is in the following form:

\[
\begin{align*}
\text{Minimize/maximize} & \quad f_m(x), \quad m = 1, 2, \ldots, M; \\
\text{subject to} & \quad g_j(x) \geq 0, \quad j = 1, 2, \ldots, J; \\
& \quad h_k(x) = 0, \quad k = 1, 2, \ldots, K; \\
& \quad x_i^{(L)} \leq x_i \leq x_i^{(U)}, \quad i = 1, 2, \ldots, n.
\end{align*}
\]

As mentioned previously, there are cases when solutions of the optimization problem are
non-dominated or equally important with respect to all objectives. These solutions are called *Pareto-optimal solutions* and can form a curve (surface) called the *Pareto Set*. In multi-objective optimization the task is to find the Pareto-optimal solutions. In fact, there are two goals in a multi-objective optimization:

1. To find a set of solutions as close as possible to the Pareto optimal front.

2. To find a set of solutions as diverse as possible [8].

It is worthwhile to mention about the concept of domination which is used in most multi-objective optimization algorithms. It is assumed that there are $M$ objective functions. Operator $\triangleleft$ denotes a better solution in order to avoid complexity of several relation symbols. This operator covers both minimization and maximization of objective functions. $i \triangleleft j$ denotes that solution $i$ is better than solution $j$ on a particular objective. For example, if an objective function is to be minimized, the operator $\triangleleft$ would mean the $<$ operator. A solution $x^{(1)}$ is said to dominate the other solution $x^{(2)}$, if both conditions 1 and 2 are true:

1. The solution $x^{(1)}$ is no worse than $x^{(2)}$ in all objectives, or $f_j(x^{(1)}) \leq f_j(x^{(2)})$ for all $j = 1, 2, ..., M$.

2. The solution $x^{(1)}$ is strictly better than $x^{(2)}$ in at least one objective, or $f_{\bar{j}}(x^{(1)}) \triangleleft f_{\bar{j}}(x^{(2)})$ for at least one $\bar{j} \in 1, 2, ..., M$.

As an example, a two objective optimization problem is considered with five different solutions shown in the objective space. Objective function 1, $f_1$, needs to be maximized while objective function 2, $f_2$, needs to be minimized, Fig. 4.1.

The domination definition can be used to decide which solution is better among any two given solutions in terms of both objectives. For example, between solutions 1 and 2, solution 1 is better than 2 in both objectives but between solutions 3 and 5, it is observed that solution 3 is better than 5 in objective 2 while solution 5 is better than 3 in objective 1. When this happens, it is said that solutions 3 and 5 are *non-dominated* with respect to each other. According to [8], if for every member $X$ in a set $P$ there exists no solution $Y$ (in the neighborhood of $X$ such that $\|Y - X\|_\infty \leq \epsilon$, where $\epsilon$ is a small positive number)
dominating any member of the set $P$, then solutions belonging to the set $P$ constitute a \textit{locally} Pareto-optimal set. Accordingly, the non-dominated set of the entire feasible search space $S$ is the \textit{globally} Pareto-optimal set.

The classical method of $\epsilon$ – \textit{constraint} has been utilized for the current research multi-objective problem. This method was suggested by Haimes et al. in 1971 [17]. In this method, the multi-objective optimization problem is reformulated by just keeping one of the objectives and restricting the rest of the objectives within user-specified values [8]. Therefore, the modified optimization problem will become:

\[
\begin{align*}
\text{Minimize} & \quad f_{\mu}(x), \\
\text{subject to} & \quad f_m(x) \leq \epsilon_m, \quad m = 1, 2, ..., M \text{and } m \neq \mu; \\
\text{subject to} & \quad g_i(x) \geq 0, \quad j = 1, 2, ..., J; \\
& \quad h_k(x) = 0, \quad k = 1, 2, ..., K; \\
& \quad x_i^{(L)} \leq x_i \leq x_i^{(U)}, \quad i = 1, 2, ..., n.
\end{align*}
\]

In this method we retain one objective and treat others as constraints. Then the original
feasible objective space will be divided to different portions according to the constraints. In each portion, the objective will be solved and this way, Pareto-optimal solutions can be obtained. For instance, in the case of two objective optimization, \( f_2 \) is retained as an objective and \( f_1 \) is treated as a constraint (\( f_1(X) \leq \epsilon_1 \)). Fig. 4.2 represents four scenarios with four different \( \epsilon_1 \) values. If the third scenario, \( \epsilon = \epsilon_c^1 \), is considered, the resulting problem with the constraint divides the original feasible objective space into two portions, \( f_1 \leq \epsilon_c^1 \) and \( f_1 \geq \epsilon_c^1 \). The left portion is the feasible solution of the problem and now the task is to find the solution which minimizes this feasible region. From Fig. 4.2, it is clear that the minimum solution is \( C \). Pareto-optimal solutions can be found this way.

4.3 The SIMPLEX Method

The SIMPLEX algorithm has been used for single objective optimizations in the current study. SIMPLEX is the well-known Nelder and Mead downhill method (1965) which is commonly used for multidimensional minimization problems. SIMPLEX is an algorithm
for non-linear optimization problems and is different from simplex method for linear programming. As this algorithm does not need derivatives evaluation, it is more robust than algorithms based on local gradients. In modeFrontier, the SIMPEX algorithm has been modified to take into account discrete variables and constraints [23].

In geometry, a simplex is a polyhedron which contains \(N + 1\) points in an \(N\) dimensional space. Therefore, in two dimensions a simplex is a triangle, in the three dimensions it is a tetrahedron. The SIMPLEX is initialized by \(N + 1\), number of variables + 1, corners that are given by the first DOE values. The scheduler compares the values of the objective functions at the \(N + 1\) vertices and moves these points towards the optimal point during the iterative process until the scheduler either exceeds its maximum number of iteration or converges. The movement of the simplex is given by three operations: Reflection, Expansion and Contraction.

**Reflection**

In the reflection movement, the worst vertex, i.e, the worst value of the objective function among all the vertices, is reflected in the opposite face to obtain a new value. The reflection usually moves towards a favourable direction as the direction of movement is away from the worst result. Fig. 4.3 shows a simplex in two dimensions. Suppose that in this simplex, the vertex \(A\) is the highest and \(C\) is the lowest. Therefore, we can expect that the point \(D\) which is obtained by reflecting \(A\) in the opposite face, has a smaller value than at point \(C\).

After the reflection to obtain point \(D\), the value of the objective function at all four points (in 2D) is examined and the worst point (i.e., in the case of minimization the point with the highest value of the objective function) is removed to form the new simplex. This new simplex is represented in Fig. 4.4.

Mathematically, the reflected point can be written as:

\[
D = (1 + \alpha)H - \alpha A
\]  

(4.1)

where \(\alpha > 0\) is a reflection coefficient, \(A\) is the vertex corresponding to the maximum function value and \(H\) is the centroid of all the points except \(A\), in our case \(H = (B + C)/2\).
Expansion

After obtaining a new minimum by reflection process, it is generally expected that by further moving along the same direction, the function value will be decreased. In Fig. 4.5 it is observed that after obtaining $D$, expanding the simplex in the same direction gives a better value. Then the new vertex $E$ is used to create a new simplex.

Mathematically, this expanded point can be written as:

$$E = \beta D + (1 - \beta)H$$

where $\beta > 1$ is a expansion coefficient, $D$ is the vertex created by the reflection and $H$ is the centroid of all the points except $D$, in our case $H = (B + C)/2$.

Contraction

Contraction is used when the reflection process gives a new point that is worse than all the other vertices. The new point is obtained by contraction from the worst point, [23]. Then a new simplex can be formed by replacing the worst vertex, $D$, by the newly obtained point, $E$.

Mathematically, the new point can be written as:
Figure 4.4: Reflected simplex \((A, B, C)\) with the reflected point \((D)\), [8]

\[
E = \beta D + (1 - \beta)H
\]

where \(\beta \in [0, 1]\) is a contraction coefficient, \(D\) is the vertex created by the reflection and \(H\) is the centroid of all the points except \(D\), in our case \(H = (B + C)/2\).

**Constraint Violation Penalty**

The original Nelder and Mead downhill method has been modified in modeFrontier to consider both the minimization of the function and the enforcement of feasibility. A common method for handling constraints is based on penalty functions, i.e., the objective function is increased according to the intensity of the constraint violation. Therefore, it is ensured that the vertices do not deviate too much from the constraint. The penalty function can be defined as:

\[
P(x, \rho) = f(x) + \rho \times c(x)
\]

where \(f(x)\) is the objective function, \(\rho\) is the penalty parameter and \(c(x)\) is the sum of all constraint violations.

A disadvantage of this method is that the penalty parameter is problem dependant and may
cause premature convergance. A solution to this problem is to define the penalty parameter as the difference of maximum and minimum function values.

\[ \rho = f_{\text{max}}(x) - f_{\text{min}}(x) \]  

(4.5)

Each \( c_i(x) \) can be transformed into a fuzzy which introduces a *tolerance parameter* \( k \) in the \( i^{th} \) constraint definition. If \( c_i(x) \leq 0 \) then \( x \) would be a feasible value for the \( i^{th} \) constraint, if \( c_i(x) \geq k \) then \( x \) would be infeasible. For \( 0 < c_i(x) < k \) the distinction between feasible and infeasible is fuzzy.

The SIMPLEX algorithm stops when it cannot find solution with improvements higher than some tolerance.

### 4.4 Optimization Loop, Data and Process Flow

The purpose of this design and process optimization is to define a set of optimal parameter and design configurations for the coal combustion reactor to achieve the minimum amount of emissions, i.e., methane and oxides of nitrogen at the outlet. In order to achieve this goal, three sets of optimizations have been performed in the current study. In the first one, two process parameters, inlet air mass flowrate and inlet coal particles mass flowrate are
defined as input variables of the optimization. In the second optimization problem, two more process input variables, i.e., inlet flow temperature and inlet coal particle diameters are also added. In the third optimization problem, the height of the upper cylinder and the height of the lower cylinder are added as geometry input variables as well.

The output variables in all optimization loops are methane mass fraction at the outlet and \( NO \) mass fraction at the outlet. According to the classical multi-objective optimization method of \( \epsilon - constraint \), one objective, \( NO \) mass fraction at the outlet has been remained as objective to be minimized. Methane mass fraction at the outlet has been defined as a constraint.

Based on the individual CFD simulations of DOE to investigate the design space behavior, it is noticed that the AF ratio has a critical impact on the amount of mass fraction of \( NO \) at the outlet. Therefore, one more constraint, AF ratio, has been added to the optimization loop as well. Ranges of these constraints have been selected based on the individual CFD analysis of DOE prior to the optimization.

ModeFrontier, a multi-objective optimization software, provided by ESTECO, has been utilized for the current study optimization problems. ModeFrontier provides a workflow canvas consisting process nodes and links to define the design optimization problem. Process nodes utilized for definition of the problem include logic nodes, input/output variable nodes,
goal nodes and integration nodes. Logic nodes consist of DOE and scheduler nodes. DOE nodes are used to define the Design Of Experiments algorithm to create the initial set of designs to be evaluated. Scheduler nodes determine which designs need to be evaluated. In other words, this node defines the strategy used to select the DOE design and generate new designs. Input/Output variable file nodes are utilized to connect input/output variables to application nodes. The input file is dynamically generated at run-time by inserting into its fix structure, values of variables for each design. The output file node also identifies a text file from which output variables can be extracted. Transfer variable nodes transfer numeric variables computed within the workflow from one application to another. Goal nodes, such as objective node and constraint node, define the strategy(method) of optimization. Objective node identifies a numeric value computed within the data flow as a function of input/output variables. Constraint nodes determine constraints of the optimization problem that should not be violated by any design. Integration nodes define external applications used in optimization process. These external applications can include script nodes, CAD nodes, CAE nodes, networking nodes, etc. Integration nodes used in current optimization problem canvases include SH shell script node, SolidWorks node, SFTP node and SSH script node. SH shell script node includes a script in a UNIX system’s supported language such as Bourne Shell, C Shell, Korn Shell, etc. Bourne Shell scripting has been used in current workflow definition. During the run, this node will spawn an external UNIX shell interpreter to execute user defined scripts. All of the processes involved in CFD simulation of coal combustion require using interactive software. Therefore, automated design optimization is possible by shell scripting to run all the necessary applications in batch mode via macro files. These macro files include *.jrf files to create the grid, *.pre files to create the CFD problem set-up, *.def file to solve the CFD simulation set-up and *.cse file to post-process the results. All of these macro files are run in batch mode using Bourne shell scripting in SH script nodes or SSH script nodes. In SolidWorks node, a SolidWorks document such as *.sldprt or *.sldasm file is wrapped and data is transferred from and to the document by executing a macro file. The correct definition of PATH variable, i.e., SLDWORKS.exe, is of critical importance. Also, it is
important to assign the path to the correct library file, i.e., cosworks.sll. Desired geometry
input variables in SolidWorks will be defined in modeFrontier by introspection application
in the node. In process-geometry optimization problem of the current study, the data needs
to be transferred from and to the local Windows based workstation (sevilla) to a remote
Linux based workstation (rondine) and a remote Linux based server (tupolev). An SFTP
node is used to transfer files using the SFTP protocol. This node stores all the required
information for the connection and authentication to the remote server and resources to
transfer. In order to use an SFTP node, the user needs to have the privilege to connect
to the server remotely, authenticate itself and have read/write permission to access remote
files. The SSH node is the secured shell script node that is used to store, edit and execute
UNIX shell scripts on remote machines using SSH protocol.

In any optimization problem performed in modeFrontier, two main flows can be defined:

1. **Process Flow** defines the chronological sequence of the application utilized in the
   optimization process.

2. **Data Flow** defines all the necessary actions for merging input variables into input
template files and the mining operation to extract the output variables from the
output files [10].

Figures 4.8 and 4.7 summarize the process flow and data flow respectively in the more
general case of process-geometry design optimization.

In the current setting, modeFrontier and Solidworks are running in the Windows operating
system in a local machine (sevilla) while the CFX package is running on the Linux operating
system. Grid generation and CFD simulation is performed on a remote Linux based server
(tupolev) with four processors and post-processing in ANSYS CFX-post is performed in
another remote Linux based machine (rondine). The optimization loop starts with geometry
creation in the Solidworks node. The geometry created in the form of *.step file is transferred
to ICEMCFD, ANSYS based software, for grid generation. The generated grid, *.cfx5
file, is transferred to the ANSYS-CFX package for CFD simulation. Post-processing which
includes calculation of methane and NO mass fractions at the outlet and AF ratio at the
inlet are performed in CFD-post, part of the CFX package and the output file is sent back to
modeFrontier to be evaluated according to the objective and constraints. The SolidWorks operation in current problem utilizes the defined equations in the *.sldprt file created by SolidWorks as mentioned before. However, all other processes, i.e., grid generation, CFD simulation and post processing are performed by batch run of these applications via macro files and shell scripting. Batch run of these processes is the key element of automated design optimization and the strong capability and advantage of this method over conventional optimization methods. Figures 4.10 and 4.9 represent the process design optimization loop and process-geometry design optimization loop respectively.
Figure 4.8: Process Flow

Figure 4.9: Process Design Optimization Loop
Figure 4.10: Process-Geometry Design Optimization Loop
Chapter 5

Results

In this chapter the results of the current study are discussed. For each optimization problem, results of the optimization are first explained and then some selected CFD simulation results are described for that problem. We start with a simple optimization with two process input variables, air and coal particles mass flow rates. Then we discuss more complicated optimization problems with four process input variables and a combination of four process and two geometry input variables. By increasing the number of input variables, the capability of automated design optimization in providing a set of optimum design variables in order to achieve the objectives, has been presented. According to the preliminary CFD studies on coal combustion, it is observed that amounts of mass fractions of $NO$ and $CH_4$ produced from coal combustion have conflicting behaviors. This conflicting behavior creates a multi-objective optimization problem for which we can find several non-dominated results (Pareto Set). In other words, it is impossible to propose a set of design variables that creates the least amount of $NO$ and $CH_4$ mass fractions at the same time. Therefore, a set of optimal input variables must be proposed. Therefore, in all optimizations similar objectives are considered, i.e., minimization of mass fractions of methane and oxides of nitrogen at the outlet. Also, since the amount of Air-Fuel ratio has a critical role in the amount of production of oxides of nitrogen and methane, it is implemented in the problem as a constraint. According to the $\epsilon$ – constraint optimization method described in Chapter 4, each multi-objective optimization problem in the current study consists of three different single objective optimizations in which $NO$ mass fraction is the objective. The three single objective optimizations are defined by the selected ranges of the second objective, i.e., $CH_4$ mass fraction. This second objective is defined as a constraint according to the $\epsilon$ – constraint optimization method. The created design tables from each of these three
Table 5.1: List of the input variables and the assigned indices

<table>
<thead>
<tr>
<th>Input Variable</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Air Mass Flow Rate, [kg/s]</td>
<td>IV1</td>
</tr>
<tr>
<td>Inlet Coal Particles Mass Flow Rate, [kg/s]</td>
<td>IV2</td>
</tr>
<tr>
<td>Inlet Temperature, [K]</td>
<td>IV3</td>
</tr>
<tr>
<td>Coal Particle Diameter, [micron]</td>
<td>IV4</td>
</tr>
<tr>
<td>Height of Upper Cylinder, [m]</td>
<td>IV5</td>
</tr>
<tr>
<td>Height of Lower Cylinder, [m]</td>
<td>IV6</td>
</tr>
</tbody>
</table>

Table 5.2: Summary of the optimization problems

<table>
<thead>
<tr>
<th>Optimization Problem</th>
<th>IV1</th>
<th>IV2</th>
<th>IV3</th>
<th>IV4</th>
<th>IV5</th>
<th>IV6</th>
</tr>
</thead>
<tbody>
<tr>
<td>problem 1</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
<td>no</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>problem 2</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>problem 3</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
</tbody>
</table>

single objective optimizations have been combined based on the acceptable ranges for NO mass fraction, the values of NO vs. CH\textsubscript{4} mass fractions have been charted and the Pareto Set has been presented in the figures.

Table 5.1 and Table 5.2 summarize the list of input variables and the optimization problems we are focusing in this research, respectively.

5.1 Problem 1: Two Process Input Variables

5.1.1 Optimization Analysis

In the first optimization problem, we focus on a simple optimization with two input variables only, air and coal particles mass flow rates. The first objective as mentioned above is minimization of NO mass fraction at the outlet. The second objective, mass fraction of methane at the outlet, is set as a constraint according to the ε - constraint optimization method described in Chapter 4. The second constraint is Air-Fuel ratio at the inlets since AF ratio is a critical parameter affecting the amount of NO and CH\textsubscript{4} mass fraction at the outlet. The ranges for these constraints are set based on a series of individual CFD analysis and in the first optimization problem the second constraint is set to AF < 2 in order to achieve NO mass fractions in the desired range. This set up has been repeated three times
Table 5.3: DOE’s for the first optimization problem

<table>
<thead>
<tr>
<th></th>
<th>IV1</th>
<th>IV2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.008</td>
<td>0.005</td>
</tr>
<tr>
<td>2</td>
<td>0.003</td>
<td>0.004</td>
</tr>
<tr>
<td>3</td>
<td>0.001</td>
<td>0.008</td>
</tr>
</tbody>
</table>

with three segmentations for the first constraint, mass fraction of methane at the outlet in order to cover as many as possible designs in the domain. In these segmentations, NO mass fraction has set to be less than 0.1, 0.2 and 0.3. Inlet temperature is set to 600K for all single objective optimizations and coal particles have a diameter distribution of 12, 38, 62 and 88 micron. The optimization is started with three DOE’s randomly chosen from the ranges defined for the input variables. The maximum number of iterations is set to 7 and a final termination accuracy of $10^{-5}$ has been selected. The algorithm will stop when it cannot find solutions with better improvements than the convergence accuracy of $10^{-5}$. Fig. 5.1 represents the optimization network in modeFrontier.

Figure 5.1: Optimization Loop for problem 1
Table 5.4: Selected designs for the first optimization problem

<table>
<thead>
<tr>
<th>Designs</th>
<th>Type</th>
<th>IV1</th>
<th>IV2</th>
<th>AF</th>
<th>(CH_4) mass fraction</th>
<th>(NO) mass fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>DOE</td>
<td>0.001</td>
<td>0.008</td>
<td>0.125</td>
<td>0.274</td>
<td>0.027</td>
</tr>
<tr>
<td>2</td>
<td>SIMPLEX</td>
<td>0.001</td>
<td>0.007</td>
<td>0.143</td>
<td>0.264</td>
<td>0.039</td>
</tr>
<tr>
<td>3</td>
<td>SIMPLEX</td>
<td>0.003</td>
<td>0.005</td>
<td>0.600</td>
<td>0.170</td>
<td>0.099</td>
</tr>
<tr>
<td>4</td>
<td>SIMPLEX</td>
<td>0.002</td>
<td>0.006</td>
<td>0.333</td>
<td>0.216</td>
<td>0.055</td>
</tr>
<tr>
<td>5</td>
<td>SIMPLEX</td>
<td>0.003</td>
<td>0.006</td>
<td>0.500</td>
<td>0.191</td>
<td>0.073</td>
</tr>
<tr>
<td>6</td>
<td>SIMPLEX</td>
<td>0.001</td>
<td>0.005</td>
<td>0.200</td>
<td>0.227</td>
<td>0.087</td>
</tr>
<tr>
<td>7</td>
<td>DOE</td>
<td>0.003</td>
<td>0.004</td>
<td>0.750</td>
<td>0.151</td>
<td>0.140</td>
</tr>
<tr>
<td>8</td>
<td>SIMPLEX</td>
<td>0.001</td>
<td>0.009</td>
<td>0.111</td>
<td>0.282</td>
<td>0.019</td>
</tr>
</tbody>
</table>

Table 5.3 represents a list of DOE’s selected by the software for the optimization problem 1 and table 5.4 summarizes the selected designs for all three optimizations for the first problem in addition to the objective and two constraints. These designs are selected from the results of the three single objective optimizations according to the acceptable ranges for \(NO\) mass fraction.

Fig. 5.2 represents the behavior of AF ratio, outlet \(CH_4\) and \(NO\) mass fractions in all the designs. It is noticed that \(NO\) and \(CH_4\) mass fractions have opposite behaviors. Therefore, they are suitable candidates for two-objective optimization since minimization of one objective does not necessarily result in minimization of the other one. In this figure, it is also noticeable that AF ratio and \(NO\) mass fraction at the outlet follow almost similar trends. In other words, a higher AF ratio results in more \(NO\) creation at the outlet. Fig. 5.3 represents the amount of air and coal particle mass flow rates at the inlets for all DOE’s.

Fig. 5.4 represents DOE’s in terms of \(NO\) mass fraction vs. \(CH_4\) mass fraction. The Pareto Set which is the representative of the best optimal solutions can be observed in this figure.

### 5.1.2 CFD Analysis

In this section CFD results of coal combustion simulation for two extreme cases among designs of the first optimization problem have been analyzed. These cases represent high and low amounts of \(NO\) and \(CH_4\) mass fractions. Table 5.5 lists the two cases selected for CFD analysis. These two cases are represented by red dots in Fig. 5.4.
Figure 5.2: AF ratio, NO and Methane behavior

<table>
<thead>
<tr>
<th>Problem</th>
<th>IV1</th>
<th>IV2</th>
<th>AF</th>
<th>$CH_4$ mass fraction</th>
<th>NO mass fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>case 1</td>
<td>0.003</td>
<td>0.005</td>
<td>0.600</td>
<td>0.170</td>
<td>0.099</td>
</tr>
<tr>
<td>case 2</td>
<td>0.001</td>
<td>0.009</td>
<td>0.111</td>
<td>0.282</td>
<td>0.019</td>
</tr>
</tbody>
</table>

Table 5.5: Designs selected for CFD analysis of optimization 1

Figures 5.5(a) and 5.5(b) represent temperature profiles inside the reactor for case 1 and case 2 respectively. The temperature is higher around the tangential inlets. The outlet temperature is 3188$K$ and 3992$K$ for case 1 and case 2 respectively. As noticed, the temperature ranges in the outlet are high compared to the typical flame temperatures expected from hydrocarbon combustion. In the current study, the selected inlet temperatures of air and coal particles are much higher than a typical coal combustion reactor. Typically, coal particles are injected with temperatures close to the ambient temperature. Combustion with highly preheated air shows significantly different combustion characteristics from that obtained with normal temperature or moderately preheated air [11]. Also, in the current
study, reverse reactions have been neglected. Reverse reactions play an important role in reaching the chemical equilibrium. Moreover, the maximum flame temperature option in the defined multi-phase reactions is not selected in our combustion model. This flame temperature, specifies a limit for the flame temperature in Eddy Dissipation model. Hiroshi et al. [11] describes the problem of temperature calculation in common commercial softwares in high temperature air combustion. He indicates the critical role of preheated air temperature and declares that it is difficult to introduce the effects of fluctuating properties of turbulent combustion into a chemically controlled reaction model such as Arrhenius model and although it is reasonable to use this model for high temperature air combustion, the validity of the recommended empirical constants are not examined for high temperature air combustion. He also mentions that it is extremely difficult to predict flame temperature in high temperature air combustion using the existing combustion models for numerical simulation and it might be possible only by using full scale reaction mechanism in complex flows with a considerably short time step. According to [11], the only practical way to obtain a

Figure 5.3: Air and coal particles mass flow rate
reasonable value of combustion temperature for high temperature air combustion without full reaction mechanism (such as neglecting reverse reactions) is to correct the calculated combustion temperature or to introduce a limit so that reactions do not overshoot chemical equilibrium.

The aforementioned reasons result in unreasonably high temperatures in the outlet of the reactor of the current study. It is, however, worth to mention that the purpose of the current study is not to propose the most accurate combustion and thermochemistry model but is rather on implementation of automated multi-objective design optimization method in coal combustion process.

In figures 5.6(a) and 5.6(b) streamlines inside the reactor for case 1 and case 2 can be seen. The streamlines show a strong swirl flow behavior inside the reactor. It is observed that case
2 creates stronger swirl flow and also higher combustion temperature and outlet velocity. Figures 5.7(a) and 5.7(b) represent the average vertical velocity contours inside the reactor for case 1 and case 2, respectively. The average vertical velocity at the outlet for case 1 and case 2 are 5.4 m/s and 14.9 m/s respectively. Figures 5.8(a) and 5.8(b) represent the vertical velocity profiles with respect to Z-coordinates in the outlet. In figures 5.9(a) and 5.9(b) NO mass fraction distribution inside the reactor for case 1 and case 2 can be seen respectively. As observed, more AF ratio leads to more mass fractions of NO inside the reactor which is expected due to the nature of Zeldovich and prompt NO reactions. Figures 5.10(a) and 5.10(b) compare CH$_4$ mass fraction distribution inside the reactor for case 1 and case 2 respectively. Higher AF ratios leads to lower mass fractions of methane. Again, according to the combustion reactions, methane which is a production of devolatilization is oxidized by oxygen to create CO$_2$ and H$_2$O. Therefore, more AF ratios result in more consumption of methane due to its oxidization. Figures 5.11(a) and 5.11(b) represent H$_2$O mass fraction distribution for case 1 and case 2 respectively. Figures 5.12(a) and 5.12(b) compare CO$_2$ mass fraction distribution inside the reactor between case 1 and case 2. Based on the Eddy Dissipation model for fuel gas oxidation reaction the amounts of mass fractions of products depend on the turbulence kinetic energy and dissipation in addition to molar concentrations of species.

Table 5.6 summarizes the amounts of mass fractions of different species, temperature and velocity at the outlet for case 1 and case 2. In Table 5.6, the summation of mass fractions at the outlet in case 1 and case 2 are 1.099063 and 1.01898, respectively. The amounts of mass fractions in excess of 1.0 are exactly the NO mass fractions in each case. This is due to the method implemented in CFX, i.e., Chemistry post processing which is one-way coupled to the main simulation. In other words, it is calculated separately from the solution of the Reynolds-averaged Navier-Stokes equations. Therefore, the computation of NO mass fraction is accurate only if the mass fraction of NO is small relative to the bulk mixture, i.e., less than 10%.
|
|---|---|---|
|Parameter| case 1 | case 2 |
|NO mass fraction| 0.099 | 0.019 |
|CO₂ mass fraction| 0.621 | 0.654 |
|CH₄ mass fraction| 0.170 | 0.282 |
|H₂O mass fraction| 0.004 | 0.001 |
|N₂ mass fraction| 0.205 | 0.064 |
|O₂ mass fraction| 0.000 | 0.000 |
|Temperature| 3188K | 3991K |
|Vertical velocity| 5.4m/s | 14.9m/s |

Table 5.6: Outlet summary for case 1 and case 2 for optimization 1
Figure 5.5: Temperature profiles for optimization 1

(a) Temperature profile for case 1

(b) Temperature profile for case 2
Figure 5.6: Streamlines for optimization 1

(a) Streamlines for case 1

(b) Streamlines for case 2
Figure 5.7: Vertical velocity contours for optimization 1

(a) Vertical Velocity Contours for case 1

(b) Vertical Velocity Contours for case 2
Figure 5.8: Vertical velocity profiles for optimization 1

(a) Vertical Velocity Profile for case 1

(b) Vertical Velocity Profile for case 2
Figure 5.9: NO mass fraction distributions for optimization 1

(a) NO mass fraction distribution for case 1

(b) NO mass fraction distribution for case 2
Figure 5.10: $CH_4$ mass fraction distributions for optimization 1

(a) $CH_4$ mass fraction distribution for case 1

(b) $CH_4$ mass fraction distribution for case 2
Figure 5.11: $H_2O$ mass fraction distributions for optimization 1
Figure 5.12: $CO_2$ mass fraction distributions for optimization 1

(a) $CO_2$ mass fraction distribution for case 1

(b) $CO_2$ mass fraction distribution for case 2
Table 5.7: DOE's for the second optimization problem

<table>
<thead>
<tr>
<th>DOE</th>
<th>IV1</th>
<th>IV2</th>
<th>IV3</th>
<th>IV4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.008</td>
<td>0.003</td>
<td>40</td>
<td>700</td>
</tr>
<tr>
<td>2</td>
<td>0.01</td>
<td>0.01</td>
<td>10</td>
<td>1000</td>
</tr>
<tr>
<td>3</td>
<td>0.01</td>
<td>0.004</td>
<td>90</td>
<td>700</td>
</tr>
<tr>
<td>4</td>
<td>0.003</td>
<td>0.002</td>
<td>50</td>
<td>900</td>
</tr>
<tr>
<td>5</td>
<td>0.007</td>
<td>0.004</td>
<td>20</td>
<td>600</td>
</tr>
</tbody>
</table>

5.2 Problem 2: Four Process Input Variables

5.2.1 Optimization Analysis

In the second optimization problem, two more input variables have been added to problem 1. The process input variables of this problem are inlet air and coal particles mass flow rate, inlet temperature and coal particle diameter. The objective and constraints of the optimization problem are the same as the first problem. For this optimization problem, the second constraint, AF ratio, is set to $AF < 2.5$. Again, this problem has been repeatedly solved for three segmentations of the first constraint, mass fraction of methane at the outlet, in order to cover as many as possible designs in the domain. Similar to the first optimization problem, in these segmentations $NO$ mass fraction is set to be less than 0.1, 0.2 and 0.3. The optimization is started with five DOE's randomly selected from the ranges defined for the input variables. Table 5.7 lists these selected DOE's by modeFrontier. The maximum number of iterations is set to 7 and a final termination accuracy of $10^{-5}$ has been selected. Fig. 5.13 represents the optimization network in modeFrontier and Table 5.8 lists the selected designs, objective and constraints for all three optimizations for the second problem. These designs have been selected from the results of the three single objective optimization problems according to the accepted ranges for $NO$ mass fraction.

Fig. 5.14 represents the behavior of AF ratio, outlet $CH_4$ and $NO$ mass fractions in all the designs. Again, it is noticed that $NO$ and $CH_4$ mass fractions are suitable candidates for two objective optimization because of their opposite behaviors. On the other hand, AF ratio and $NO$ mass fractions at the outlet follow almost similar trends. Figures 5.15 and 5.16 represent the amount of air and coal particles mass flow rate at the inlets and $NO$
mass fraction vs. $CH_4$ mass fraction at the outlet for different designs respectively. In Fig. 5.16 a Pareto Set is recognizable which introduces a set of best optimum results.

5.2.2 CFD Analysis

Two cases of interest have been selected among all the designs for the purpose of CFD analysis. These cases represent high and low amounts of $NO$ and $CH_4$ mass fractions. These two cases have been listed in Table 5.9 and have been represented by red color in Pareto front, Fig. 5.16.

As it is observed in figures 5.17(a) and 5.17(b), the temperature is higher around the tangential inlets. In case 1, larger diameter coal particles and more AF ratio results in higher outlet temperature and velocity. It is also noticed that higher inlet temperature does not necessarily result in higher outlet temperature. The outlet temperature is $3048K$ and $3021K$ for cases 1 and 2 respectively. Again as noticed, the temperature ranges in
Table 5.8: Selected designs for the second optimization problem

<table>
<thead>
<tr>
<th>Design</th>
<th>Type</th>
<th>IV1</th>
<th>IV2</th>
<th>IV3</th>
<th>IV4</th>
<th>AF</th>
<th>CH₄ mass fraction</th>
<th>NO mass fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>SIMPLEX</td>
<td>0.01</td>
<td>0.01</td>
<td>10</td>
<td>1000</td>
<td>1</td>
<td>0.153</td>
<td>0.080</td>
</tr>
<tr>
<td>2</td>
<td>DOE</td>
<td>0.003</td>
<td>0.002</td>
<td>50</td>
<td>900</td>
<td>1.5</td>
<td>0.115</td>
<td>0.256</td>
</tr>
<tr>
<td>3</td>
<td>SIMPLEX</td>
<td>0.007</td>
<td>0.007</td>
<td>50</td>
<td>900</td>
<td>1</td>
<td>0.148</td>
<td>0.228</td>
</tr>
<tr>
<td>4</td>
<td>SIMPLEX</td>
<td>0.004</td>
<td>0.008</td>
<td>10</td>
<td>1000</td>
<td>0.5</td>
<td>0.198</td>
<td>0.027</td>
</tr>
<tr>
<td>5</td>
<td>SIMPLEX</td>
<td>0.008</td>
<td>0.008</td>
<td>80</td>
<td>1000</td>
<td>1</td>
<td>0.147</td>
<td>0.250</td>
</tr>
<tr>
<td>6</td>
<td>SIMPLEX</td>
<td>0.005</td>
<td>0.005</td>
<td>50</td>
<td>900</td>
<td>1</td>
<td>0.147</td>
<td>0.176</td>
</tr>
</tbody>
</table>

Table 5.9: Selected designs for CFD analysis for optimization 2

<table>
<thead>
<tr>
<th>Problem</th>
<th>IV1</th>
<th>IV2</th>
<th>IV3</th>
<th>IV4</th>
<th>AF</th>
<th>CH₄ mass fraction</th>
<th>NO mass fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>case 1</td>
<td>0.01</td>
<td>0.01</td>
<td>10</td>
<td>1000</td>
<td>1</td>
<td>0.153</td>
<td>0.080</td>
</tr>
<tr>
<td>case 2</td>
<td>0.004</td>
<td>0.008</td>
<td>10</td>
<td>1000</td>
<td>0.5</td>
<td>0.198</td>
<td>0.027</td>
</tr>
</tbody>
</table>

the outlet are high compared to the typical flame temperatures expected from hydrocarbon combustion. In the current study, the selected inlet temperatures of air and coal particles are much higher than a typical coal combustion reactor. Typically, coal particles are injected with temperatures close to the ambient temperature. Combustion with highly preheated air shows significantly different combustion characteristics from that obtained with normal temperature or moderately preheated air [11]. Also, in the current study, reverse reactions have been neglected. Reverse reactions play an important role in reaching the chemical equilibrium. Moreover, the maximum flame temperature option in the defined multi-phase reactions is not selected in our combustion model. This flame temperature specifies a limit for the flame temperature in Eddy Dissipation model. Hiroshi et al. [11] describes the problem of temperature calculation in common commercial softwares in high temperature air combustion. He indicates the critical role of preheated air temperature and declares that it is difficult to introduce the effects of fluctuating properties of turbulent combustion into a chemically controlled reaction model such as Arrhenius model and although it is reasonable to use this model for high temperature air combustion, the validity of the recommended empirical constants are not examined for high temperature air combustion. He also mentions that it is extremely difficult to predict flame temperature in high temperature air combustion using the existing combustion models for numerical simulation and it might be possible
Figure 5.14: AF ratio, NO and Methane behavior for optimization 2

only by using full scale reaction mechanism in complex flows with a considerably short time step. According to [11], the only practical way to obtain a reasonable value of combustion temperature for high temperature air combustion without full reaction mechanism (such as neglecting reverse reactions) is to correct the calculated combustion temperature or to introduce a limit so that reactions do not overshoot chemical equilibrium.

The aforementioned reasons result in unreasonably high temperatures in the outlet of the reactor of the current study. It is, however, worth to mention that the purpose of the current study is not to propose the most accurate combustion and thermochemistry model but is rather on implementation of automated multi-objective design optimization method in coal combustion process.

Figures 5.18(a) and 5.18(b) represent swirl flow behavior of streamlines inside the reactor. The average vertical velocity contours are shown in figures 5.19(a) and 5.19(b). The average vertical velocity at the outlet for case 1 and case 2 are $33.4m/s$ and $21.3m/s$ respectively. Figures 5.20(a) and 5.20(b) represent the vertical velocity profiles with respect
Figure 5.15: Air and coal particles mass flow rate for optimization 2

to Z-coordinates in the outlet.

In figures 5.21(a) and 5.21(b), NO mass fraction distribution inside the reactor for case 1 and case 2 can be seen respectively. Similar to the previous problem, it is observed that more AF ratio results in more mass fractions of NO inside the reactor. Figures 5.22(a) and 5.22(b) compare CH4 mass fraction distribution inside the reactor for case 1 and case 2 respectively. Again as it was mentioned before, higher AF ratios results in lower mass fractions of methane and this phenomena is expectable according to the nature of combustion reactions. Figures 5.23(a), 5.23(b), 5.24(a) and 5.24(b) compare mass fraction distributions of products, i.e., H2O and CO2 inside the reactor. According to the Eddy Dissipation model, the amounts of mass fractions of products inside the reactor depend on the turbulence kinetic energy and dissipation in addition to molar concentrations of species.

Table 5.10 summarizes CFD results at the outlet for both cases of optimization problem 2. Here again, the excess amounts of NO mass fractions with regard to the summation of all components’ mass fractions are visible in both case 1 and case 2. The reason is again, as
Figure 5.16: Design Set for optimization 2

described before, the method of calculation of NO mass fraction in which this amount is calculated separately from the rest of the simulation.
Figure 5.17: Temperature profiles for optimization 2
Figure 5.18: Streamlines for optimization 2

(a) Streamlines for case 1

(b) Streamlines for case 2
Figure 5.19: Vertical velocity contours for optimization 2
Figure 5.20: Vertical velocity profiles for optimization 2
Figure 5.21: NO mass fraction distributions for optimization 2
Figure 5.22: $CH_4$ mass fraction distributions for optimization 2
Figure 5.23: $H_2O$ mass fraction distributions for optimization 2

(a) $H_2O$ mass fraction distribution for case 1

(b) $H_2O$ mass fraction distribution for case 2
Figure 5.24: $CO_2$ mass fraction distributions for optimization 2
<table>
<thead>
<tr>
<th>Parameter</th>
<th>case 1</th>
<th>case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO mass fraction</td>
<td>0.080</td>
<td>0.027</td>
</tr>
<tr>
<td>CO$_2$ mass fraction</td>
<td>0.594</td>
<td>0.628</td>
</tr>
<tr>
<td>CH$_4$ mass fraction</td>
<td>0.153</td>
<td>0.198</td>
</tr>
<tr>
<td>H$_2$O mass fraction</td>
<td>0.004</td>
<td>0.001</td>
</tr>
<tr>
<td>N$_2$ mass fraction</td>
<td>0.249</td>
<td>0.173</td>
</tr>
<tr>
<td>O$_2$ mass fraction</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Temperature</td>
<td>3048K</td>
<td>3021K</td>
</tr>
<tr>
<td>Vertical velocity</td>
<td>33.4m/s</td>
<td>21.3m/s</td>
</tr>
</tbody>
</table>

Table 5.10: Outlet summary for case 1 and case 2 for optimization 2
### 5.3 Problem 3: Process and Geometry Input Variables

#### 5.3.1 Optimization Analysis

In the third problem, both process and geometry input variables are integrated to create a more complex optimization problem. Here, in addition to the four process input variables discussed in the previous problems, the heights of the upper and lower cylinders have been considered as geometric input variables as well. The objective is to introduce a list of input variables that create a set of most optimum results. Similar optimization method, approach and settings have been used as the previous optimization problems. AF ratio constraint has been set to be less than 2. The second constraint, \( NO \) mass fraction, for the three single objective optimization problems is set to be less than 0.1, 0.2 and 0.3.

Fig. 5.25 represents a schematic of the combined optimization problem and Table 5.11 lists the DOE’s selected by modeFrontier for the optimization problem 3. Table 5.12 summarizes the selected designs, objective and constraints for optimization problem 3. Similar to the previous optimization problems, these designs have been selected from the results of all the three single objective optimization problems with regard to the acceptable range for \( NO \) mass fraction.

Fig. 5.26 represents the behavior of AF ratio, \( CH_4 \) mass fraction and \( NO \) mass fractions for all the designs of optimization problem 3. The same opposite behavior of \( NO \) and \( CH_4 \) mass fractions is noticeable in this problem as well. Also, as stated before, it is noticed that AF ratio and \( NO \) mass fraction have almost similar trends. Fig. 5.27 shows the amount of air and coal particles mass flow rate at the inlets for all the designs. Fig. 5.28 compares

<table>
<thead>
<tr>
<th>DOE</th>
<th>IV1</th>
<th>IV2</th>
<th>IV3</th>
<th>IV4</th>
<th>IV5</th>
<th>IV6</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.003</td>
<td>0.004</td>
<td>70</td>
<td>800</td>
<td>1.48</td>
<td>0.7000</td>
</tr>
<tr>
<td>2</td>
<td>0.01</td>
<td>0.01</td>
<td>90</td>
<td>1000</td>
<td>1.16</td>
<td>0.7767</td>
</tr>
<tr>
<td>3</td>
<td>0.002</td>
<td>0.008</td>
<td>30</td>
<td>800</td>
<td>1.32</td>
<td>0.7000</td>
</tr>
<tr>
<td>4</td>
<td>0.007</td>
<td>0.009</td>
<td>40</td>
<td>600</td>
<td>1.00</td>
<td>0.8530</td>
</tr>
<tr>
<td>5</td>
<td>0.005</td>
<td>0.006</td>
<td>70</td>
<td>600</td>
<td>1.32</td>
<td>0.7000</td>
</tr>
<tr>
<td>6</td>
<td>0.001</td>
<td>0.002</td>
<td>40</td>
<td>600</td>
<td>1.00</td>
<td>0.8530</td>
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<tr>
<td>7</td>
<td>0.005</td>
<td>0.01</td>
<td>30</td>
<td>800</td>
<td>1.32</td>
<td>0.8500</td>
</tr>
</tbody>
</table>

Table 5.11: DOE’s for the third optimization problem
inlet and outlet temperature behaviors. It is noticed that inlet temperature, coal particle
diameter and height variation do not have significant trackable effect on the amount of NO
and CH\textsubscript{4} mass fractions at the outlet. Fig. 5.29 represents the designs in terms of NO
mass fraction vs. CH\textsubscript{4} mass fraction. This figure shows the Pareto set for the optimization
problem 3.

5.3.2 CFD Analysis

Similar to the previous problems, two cases with high and low amounts of NO and CH\textsubscript{4}
have been analyzed. Table 5.13 lists these two cases which are also shown by red color in
Fig. 5.29.

Figures 5.30(a) and 5.30(b) represent temperature profiles inside the reactors of case 1 and
case 2. It is evident that temperature is higher around the tangential inlets. The outlet
temperature for case 1 and case 2 are 4477\textsuperscript{K} and 3560\textsuperscript{K} respectively. In optimization 3,
Table 5.12: Selected designs for the third optimization problem

<table>
<thead>
<tr>
<th>Designs</th>
<th>Type</th>
<th>IV1</th>
<th>IV2</th>
<th>IV3</th>
<th>IV4</th>
<th>IV5</th>
<th>IV6</th>
<th>AF</th>
<th>CH₄ mf</th>
<th>NO mf</th>
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<tr>
<td>1</td>
<td>DOE</td>
<td>0.003</td>
<td>0.004</td>
<td>70</td>
<td>800</td>
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<td>0.7000</td>
<td>0.75</td>
<td>0.1551</td>
<td>0.0230</td>
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<tr>
<td>2</td>
<td>DOE</td>
<td>0.01</td>
<td>0.01</td>
<td>90</td>
<td>1000</td>
<td>1.16</td>
<td>0.7767</td>
<td>1</td>
<td>0.1447</td>
<td>0.0085</td>
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<td>3</td>
<td>DOE</td>
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<td>0.008</td>
<td>30</td>
<td>800</td>
<td>1.32</td>
<td>0.7000</td>
<td>0.25</td>
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<td>0.009</td>
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<td>0.83</td>
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<tr>
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<td>0.002</td>
<td>40</td>
<td>600</td>
<td>1.00</td>
<td>0.8530</td>
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<td>0.1653</td>
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<td>7</td>
<td>SIMPLEX</td>
<td>0.004</td>
<td>0.003</td>
<td>90</td>
<td>700</td>
<td>1.16</td>
<td>0.7000</td>
<td>1.33</td>
<td>0.1286</td>
<td>0.0562</td>
</tr>
<tr>
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<td>SIMPLEX</td>
<td>0.009</td>
<td>0.01</td>
<td>70</td>
<td>900</td>
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<td>0.7000</td>
<td>0.9</td>
<td>0.1508</td>
<td>0.0050</td>
</tr>
<tr>
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<td>0.009</td>
<td>0.01</td>
<td>60</td>
<td>700</td>
<td>1.00</td>
<td>0.7800</td>
<td>0.9</td>
<td>0.1462</td>
<td>0.0133</td>
</tr>
<tr>
<td>10</td>
<td>SIMPLEX</td>
<td>0.003</td>
<td>0.005</td>
<td>60</td>
<td>600</td>
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<td>0.7800</td>
<td>0.6</td>
<td>0.1741</td>
<td>0.0123</td>
</tr>
</tbody>
</table>

Table 5.13: Selected designs selected for CFD analysis for optimization 3

<table>
<thead>
<tr>
<th>Problem</th>
<th>IV1</th>
<th>IV2</th>
<th>IV3</th>
<th>IV4</th>
<th>IV5</th>
<th>IV6</th>
<th>AF</th>
<th>NO mf</th>
<th>CH₄ mf</th>
</tr>
</thead>
<tbody>
<tr>
<td>case 1</td>
<td>0.004</td>
<td>0.003</td>
<td>90</td>
<td>700</td>
<td>1.16</td>
<td>0.7</td>
<td>1.33</td>
<td>0.0562</td>
<td>0.1286</td>
</tr>
<tr>
<td>case 2</td>
<td>0.002</td>
<td>0.008</td>
<td>30</td>
<td>800</td>
<td>1.32</td>
<td>0.7</td>
<td>0.25</td>
<td>0.0016</td>
<td>0.2414</td>
</tr>
</tbody>
</table>

Table 5.14: Outlet summary for case 1 and case 2 for optimization 3

<table>
<thead>
<tr>
<th>Parameter</th>
<th>case 1</th>
<th>case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO mass fraction</td>
<td>0.0562</td>
<td>0.0016</td>
</tr>
<tr>
<td>CO₂ mass fraction</td>
<td>0.5325</td>
<td>0.6420</td>
</tr>
<tr>
<td>CH₄ mass fraction</td>
<td>0.1286</td>
<td>0.2414</td>
</tr>
<tr>
<td>H₂O mass fraction</td>
<td>0.0093</td>
<td>0.1488</td>
</tr>
<tr>
<td>N₂ mass fraction</td>
<td>0.3296</td>
<td>0.1150</td>
</tr>
<tr>
<td>O₂ mass fraction</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Temperature</td>
<td>4477K</td>
<td>3560K</td>
</tr>
<tr>
<td>Vertical velocity</td>
<td>14.1 m/s</td>
<td>15.9 m/s</td>
</tr>
</tbody>
</table>
Figure 5.26: AF ratio, NO and Methane behavior for optimization 3

similar to the previous optimization problems, it is noticed that the temperature ranges in the outlet are high compared to the typical flame temperatures expected from hydrocarbon combustion. In the current study, the selected inlet temperatures of air and coal particles are much higher than a typical coal combustion reactor. Typically, coal particles are injected with temperatures close to the ambient temperature. Combustion with highly preheated air shows significantly different combustion characteristics from that obtained with normal temperature or moderately preheated air [11]. Also, in the current study, reverse reactions have been neglected. Reverse reactions play an important role in reaching the chemical equilibrium. Moreover, the maximum flame temperature option in the defined multi-phase reactions is not selected in our combustion model. This flame temperature, specifies a limit for the flame temperature in Eddy Dissipation model. Hiroshi et al. [11] describes the
Figure 5.27: Air and coal particles mass flow rate for optimization 3

problem of temperature calculation in common commercial softwares in high temperature air combustion. He indicates the critical role of preheated air temperature and declares that it is difficult to introduce the effects of fluctuating properties of turbulent combustion into a chemically controlled reaction model such as Arrhenius model and although it is reasonable to use this model for high temperature air combustion, the validity of the recommended empirical constants are not examined for high temperature air combustion. He also mentions that it is extremely difficult to predict flame temperature in high temperature air combustion using the existing combustion models for numerical simulation and it might be possible only by using full scale reaction mechanism in complex flows with a considerably short time step. According to [11], the only practical way to obtain a reasonable value of combustion temperature for high temperature air combustion without full reaction mechanism (such as neglecting reverse reactions) is to correct the calculated combustion temperature or to introduce a limit so that reactions do not overshoot chemical equilibrium.

The aforementioned reasons result in unreasonably high temperatures in the outlet of the
In figures 5.31(a) and 5.31(b) streamlines inside the reactor and strong swirl behavior for case 1 and case 2 can be observed. The average vertical velocity at the outlet for case 1 and case 2 is 14.1 m/s and 15.9 m/s respectively. Figures 5.33(a) and 5.33(b) represent the vertical velocity profiles with respect to Z-coordinates in the outlet. Figures 5.34(a) and 5.34(b) compare NO mass fraction distribution inside the reactor for case 1 and case 2 and figures 5.35(a) and 5.35(b) compare CH4 mass fraction distributions inside both reactors. As it was stated before, AF ratio has a similar trend with NO mass fraction but an opposite trend with CH4 mass fraction. Therefore, more concentrations of NO mass fraction and less concentrations of CH4 mass fraction can be observed in case 1. Figures 5.36(a), 5.36(b), 5.37(a) and 5.37(b) represent mass fraction distributions of products inside the reactor. The amounts of products depend on turbulence kinetic energy, dissipation and molar concentrations of species. Table 5.14 summarizes outlet CFD results for optimization
Figure 5.29: Design Set for optimization 3
(a) Temperature profile for case 1

(b) Temperature profile for case 2

Figure 5.30: Temperature profiles for optimization 3
Figure 5.31: Streamlines for optimization 3
Figure 5.32: Vertical velocity contours for optimization 3

(a) Vertical Velocity Contours for case 1

(b) Vertical Velocity Contours for case 2
(a) Vertical Velocity Profile for case 1

(b) Vertical Velocity Profile for case 2

Figure 5.33: Vertical velocity profiles for optimization 3
Figure 5.34: NO mass fraction distributions for optimization 3
(a) $CH_4$ mass fraction distribution for case 1

(b) $CH_4$ mass fraction distribution for case 2

Figure 5.35: $CH_4$ mass fraction distributions for optimization 3
Figure 5.36: $H_2O$ mass fraction distributions for optimization 3
Figure 5.37: $CO_2$ mass fraction distributions for optimization 3
Chapter 6

CFX Combustion Model Validation

In this chapter, a coal combustion problem has been solved and the results have been compared with CFX manual analysis. The purpose is to validate the correct usage of the CFX code in the research (including the combustion model for coal) by replicating the results of the CFX coal combustion tutorial example. It should be noted, however, that the CFX manual provides only a qualitative description of the results of this tutorial example and therefore, the comparison of the results of the replication of the coal combustion tutorial example with the CFX manual is qualitative.

The analyzed problem is CFD simulation of coal combustion in a cylindrical reactor which has two annular inlets at the top and the outlet is located at the bottom of the reactor. The reactor has 5m height and 0.8m diameter. Figure 6.1 shows the geometry of the reactor. Coal particles with mass fraction of $1.015 \times 10^{-3}$ are mixed with air with mass fraction of $1.624 \times 10^{-3}$ and are injected into the reactor from the inner inlet with 0.1m diameter. Outer inlet with 0.2m diameter is where air is injected into the reactor with mass fraction of $1.035 \times 10^{-2}$. Coal particles are injected with 343K from the coal inlet and Air is injected with 573K from the air inlet. Outlet of the reactor is in 1 atm pressure. Furnace wall is maintained at 1400K.

Eddy Dissipation Model for coal combustion and $k - \epsilon$ method for turbulence model have been used. Chemical reactions applied to simulate combustion are identical to the single phase and multi-phase reactions used in the current research. These reactions include devolatilization, char oxidation and fuel gas oxidation. Two cases with and without swirl flow have been studied and the results are compared with CFX analysis. In the case for swirl flow, air is injected into the reactor from the air inlet with an axial velocity and a specific angle.
Figure 6.1: Geometry of the coal combustion reactor

Figure 6.2 represents the convergence of mass and momentum residuals for the case without swirl flow and the case with swirl flow. As CFX manual suggests [2], swirl flow stabilizes the flame and makes the convergence faster compared to the non-swirl flow.

Figures 6.3, 6.4, 6.5 and 6.6 represent temperature profile and $H_2O$ mass fraction in both cases without swirl flow and with swirl flow. According to the CFX manual [2] for a non-swirl case, the flame appears in a significant distance from the burner as it is noticed in the Fig. 6.3. The flame is unstable in non-swirl case and the rate of convergence is low. Fig. 6.4 verifies that as the CFX manual suggests, swirl flow stabilizes the flame and locates it closer to the burner. The swirl component applied to air from the inlet entrains coal particles and keeps them near the burner for a longer time, hence helping them to burn. Flame stabilization by swirl flow results in better convergence rate.

The CFX manual indicates that the $H_2O$ mass fraction is high where the temperature is
Figure 6.2: Mass and momentum residuals convergency

(a) Non-swirl flow

(b) Swirl flow
As we notice in Fig. 6.5, water mass fraction is high at a significant distance from the burner and where high temperature is noticed. Fig. 6.6 indicates that as the CFX manual suggests, the swirl flow moves the location of high concentration of \( H_2O \) mass fraction to the top of the reactor, closer to the burner.
Chapter 7
Conclusions

At the current situation of the world with the rising demand of energy consumption, increasing energy prices and environmental concerns, design of efficient combustion and gasification processes becomes an important engineering problem. Moreover, design of an efficient and environmental friendly system, with all the complexities and conflicting objectives is a challenging process which is not solvable by conventional design and optimization methods. Computational Fluid Dynamics (CFD) has been a powerful design tool in the past decade in the combustion and gasification fields. However, this method alone cannot be a suitable solution for engineering multi-objective design optimization problems because of its random and inefficient procedure which does not necessarily cover the entire design space. The purpose of the current study is to integrate CFD simulation of coal combustion with multi-objective optimizations in an automated fashion. This method is capable of searching the entire design space and therefore, suggesting an optimal set of solutions which is the closest to the Pareto Set. Also, it utilizes the most of computer power as it can be run automatically and continuously, eliminating human error in handling numerous files.

In order to achieve this goal, a coal combustion reactor with swirl flow has been considered. Coal particles are mixed with air and are injected into the reactor via four tangential inlets to create swirl flow in order to achieve better turbulence and better combustion. Simplified single phase and multi-phase reactions have been considered to simulate combustion process. All the steps of geometry creation, grid generation and CFD simulation have been integrated automatically using macro files to run in batch mode in an optimization platform, i.e., modeFrontier.

Three sets of multi-objective optimization problems have been solved with two, four and six input variables respectively. Each multi-objective optimization problem consists of
individual single objective problems solved by the SIMPLEX method. The $\epsilon - constraint$ method has been implemented for multi-objective optimization. Two conflicting objectives have been selected for all optimization problems: minimizing $NO$ mass fraction and $CH_4$ mass fraction. It is noticed that the $AF$ ratio has considerable influence on $NO$ and $CH_4$ mass fractions. Therefore, this parameter has been added as a constraint to the optimization problem. Results from all single objective optimizations have been summarized and graphed in a chart to obtain the Pareto Set. The Pareto Set proposes a set of optimal solutions for the multi-objective problems, i.e., a set of optimal process and geometry design input variables that can result in the least possible combination of emissions in the outlet.

Automated multi-objective optimization proposes a reliable and promising method to integrate CAD and CAE tools with optimization methods in an automated fashion to perform faster, more accurate, more efficient and more cost-effective designs in the field of coal combustion and gasification.
Chapter 8
Future Work

The importance of design of efficient combustion and gasification reactors, in addition to the influential role of the proposed automated multi-objective design optimization method in this field, creates significant potential for further research on quantitative studies. Defining more accurate thermochemistry and combustion models can definitely help achieving this goal. More powerful computer resources will facilitate implementation of other multi-objective optimization methods such as MOGA (Multi-Objective Genetic Algorithm) in order to search a wider design space.

According to the application of coal combustion and gasification processes in electricity generation, additional objectives such as thermal efficiency of the process and the amount of electricity generation in a combined heat and power system can be added to the environmental objectives in the current study.

Small scale combustion and gasification systems with local alternative fuels in order to generate electricity for local communities have become increasingly important in the last decades. Implementation of automated multi-objective design optimization in order to evaluate the feasibility of different local alternative fuels to build an efficient energy source with regard to the local resource, demands and environmental concerns can be a very suitable application the proposed method of the current study.
Nomenclature

\( \mathbf{v}^p \) particle velocity vectore

\( [c_{mol}] \) molar concentration of species \( k \)

\( \delta_{ij} \) Kronecker delta

\( \dot{c}_{kn} \) rate of changes of the concentration of species \( k \) in reaction \( n \)

\( \epsilon \) dissipation

\( \lambda \) thermal conductivity of the mixture

\( \mu \) dynamic molecular viscosity

\( \mu_t \) dynamic turbulent viscosity

\( \rho^k \) density of species \( k \)

\( \sigma_{ij}^k \) Cartesian stress tensor acting on species \( k \)

\( \tau_e \) characteristic life time

\( \tau_{ij} \) shear stress tensor

\( C_D \) drag coefficient

\( CFD \) Computational Fluid Dynamics

\( DOE \) Design Of Experiments

\( DOE \) Design of Experiment

\( e \) total energy per unit mass

\( f_{i}^{k} \) body force per unit mass of species \( k \) acting on species \( k \)
\( H \) \hspace{1em} \text{total enthalpy per unit mass}

\( h^k \) \hspace{1em} \text{static enthalpy of species } k

\( k \) \hspace{1em} \text{turbulent kinetic energy}

\( l_e \) \hspace{1em} \text{characteristic length}

\( M_k \) \hspace{1em} \text{molecular weight of species } k

\( Nu \) \hspace{1em} \text{The Nusselt number}

\( p^k \) \hspace{1em} \text{static partial pressure of species } k

\( Pr_t \) \hspace{1em} \text{turbulent Prandtl number}

\( Q_c \) \hspace{1em} \text{convective heat transfer}

\( Q_M \) \hspace{1em} \text{latent heat transfer}

\( R \) \hspace{1em} \text{The Universal Gas Constant}

\( Re \) \hspace{1em} \text{specific reaction rate}

\( Sc_t \) \hspace{1em} \text{turbulent Schmidt number}

\( Sh \) \hspace{1em} \text{sherwood number}

\( v_f' \) \hspace{1em} \text{fluctuating velocity}

\( v_i \) \hspace{1em} \text{mass-averaged bulk velocity}

\( V^k_i \) \hspace{1em} \text{Diffusion velocity}

\( v^k_i \) \hspace{1em} \text{Cartesian velocity vector for species } k

\( w^k \) \hspace{1em} \text{Net rate of production of mass of species } k \text{ per unit volume per unit time}
References


