Multiscale CFD Simulations of Entrained Flow Gasification

by

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ABSTRACT

The design of entrained flow gasifiers and their operation has largely been an experience based enterprise. Most, if not all, industrial scale gasifiers were designed before it was practical to apply CFD models. Moreover, gasification CFD models developed over the years may have lacked accuracy or have not been tested over a wide range of operating conditions, gasifier geometries and feedstock compositions. One reason behind this shortcoming is the failure to incorporate detailed physics and chemistry of the coupled non-linear phenomena occurring during solid fuel gasification. In order to accurately predict some of the overall metrics of gasifier performance, like fuel conversion and syngas composition, we need to first gain confidence in the sub-models of the various physical and chemical processes in the gasifier. Moreover, in a multiphysics problem like gasification modeling, one needs to balance the effort expended in any one submodel with its effect on the accuracy of predicting some key output parameters.

Focusing on these considerations, a multiscale CFD gasification model is constructed in this work with special emphasis on the development and validation of key submodels including turbulence, particle turbulent dispersion and char consumption models. The integrated model is validated with experimental data from various pilot-scale and laboratory-scale gasifier designs, further building confidence in the predictive capability of the model. Finally, the validated model is applied to ascertain the impact of changing the values of key operating parameters on the performance of the MHI and GE gasifiers. The model is demonstrated to provide useful quantitative estimates of the expected gain or loss in overall carbon conversion when critical operating parameters such as feedstock grinding size, gasifier mass throughput and pressure are varied.

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NOMENCLATURE

Capital Letters

$A_0$: diffusion constant
$A_i$: pre-exponential factor for $i^{th}$ heterogeneous reaction
$A_0$: particle external surface area ($m^2$)
$C$: fractional char conversion of a particle ($1/s$)
$C_D$: drag coefficient
$C_L$: modeling constant in particle turbulent dispersion model
$E_i$: activation energy for $i^{th}$ heterogeneous reaction ($J/kmol$)
$F_D$: drag force on particle (N)
$G_k, G_\omega, Y_k, Y_\omega, D_\omega$: various generation and depletion terms for $k, \omega$
$G$: net irradiation at the location of particle ($kg/s^3$)
$H_{C, CO2}, H_{C, CO2}, H_{C, H2O}$: enthalpy of reaction for reactions R4, R5, R6 ($J/kg$)
$I$: Radiative Intensity ($W/m^2-Sr$)
$L_e$: eddy length scale (m)
$Nu$: Nusselt number for laminar flow around a spherical particle
$P_i$: total pressure (atm)
$P_\omega$: partial pressure of the species under consideration (atm)
$Pr$: Prandtl number
$Q_G$: heat source in particle energy equation due to reactions R4 - R6 (W)
$R$: universal gas constant ($J/kmol-K$)
$R_p$: initial particle radius in shrinking core model (m)
$Re_p$: particle reynolds number
$S$: internal surface area of a char particle ($m^2/kg$), Swirl Number
$S_0$: initial internal surface area of a char particle ($m^2/kg$)
$S_h$: source term due to homogeneous reactions in gas phase energy equation (W)
$S_{rad}$: radiation source term in gas phase energy equation (W)
$S_{p,m}$, $S_{p,mom}$, $S_{p,h}$, $S_{p,Y}$: inter-phase exchange terms for mass, momentum, enthalpy and species

$S_{yi}$: source term in species equation for $i^{th}$ species due to gas phase reactions

$S_k$, $S_w$: user-defined source terms for $k, \omega$

$T$: gas phase temperature (K)

$T_p$: particle temperature (K)

$T_w$: wall temperature (K)

$Y_i$: mass fraction of the species $i$

**Lowercase Letters**

$a_1, a_2, a_3$: coefficients in expansion of $C_D$

$b$: location of flame front around the particle in MFF model (m)

$c_p$: particle specific heat (J/kg-K)

$d_p$: particle diameter (m)

$dm_{C,CO_2}$, $dm_{C,CO_2}$, $dm_{C,H_2O}$: change in mass of particle due to reactions R4, R5, R6 (kg)

$dm_{devol}$: change in mass of particle due to devolatilization (kg)

$dm_{vapor}$: change in mass of particle due to loss of water vapor (kg)

$h_p$: heat transfer coefficient between spherical particle and gas (W/m$^2$-K)

$h$: gas phase mixture enthalpy (J/kg)

$k$: turbulent kinetic energy (m$^2$/s$^2$)

$k_a$: absorption constant for radiation (1/m)

$k_d$: rate constant for diffusion through boundary layer around particle (kg/atm-s)

$k_{dash}$: rate constant for diffusion through ash layer around particle (kg/atm-s)

$k_g$: gas phase thermal conductivity (W/m-K)

$k_s$: rate constant for heterogeneous kinetics (kg/atm-s), scattering constant for radiation (1/m)

$m_p$: instantaneous mass of a particle (kg)

$m_{po}$: initial char mass of a particle (kg)

$r_p$: instantaneous particle unreacted-core radius in shrinking core model (m)

$u_i$: gas phase velocity components (m/s)
$u$: net gas phase velocity (m/s)
$u'$: fluctuating component of gas phase velocity (m/s)
$ar{u}$: mean gas phase velocity (m/s)
$u_p$: particle velocity (m/s)
$x$: particle char conversion
$x_i$: global coordinates (m)

**Greek Letters**

$\sigma_k, \sigma_\omega$: turbulent prandtl numbers for $k, \omega$
$\psi$: structural parameter for random pore model
$\Theta$: Thiele modulus
$p$: gas phase density (kg/m$^3$)
$p_p$: particle density (kg/m$^3$)
$\alpha'$: damping coefficient for turbulent viscosity
$\mu_t$: turbulent viscosity (kg/m-s)
$\mu$: gas phase viscosity (kg/m-s)
$\epsilon$: turbulent kinetic energy dissipation rate ($m^2/s^3$), voidage of ash layer around particle
$\epsilon_p$: particle emissivity
$\eta$: effectiveness factor for pore diffusion
$\eta_C$: net carbon conversion of a gasifier
$\tau$: average residence time (s)
$\tau_{av}$: average residence time for particles in gasifier (s)
$\sigma$: Stefan-Boltzmann constant (W/m$^2$-K$^4$)
$\omega$: turbulent kinetics energy dissipation rate (1/s)

**Subscripts**

$av$: average
$b$: at the burner
d: diffusion
i: i\textsuperscript{th} species
g: gas-phase
p: particle
s: kinetics
w: wall

Acronyms

ASU: Air Separation Unit
BYU: Brigham Young University
CCS: Carbon dioxide Capture and Storage (or Sequestation)
CPD: Chemical Percolation Devolatilization
CTL: Coal-to-hydrocarbon Liquid
CFD: Computational Fluid Dynamics
CoP: ConocoPhillips
DNS: Direct Numerical Simulation
DOE: United States Department of Energy
ECUST: East China University of Science and Technology
EFG: Entrained Flow Gasifier
FVM: Finite Volume Method
GE: General Electric
HHV: Higher Heating Value
IGCC: Integrated Gasification Combined Cycle
IRZ: Internal Recirculation Zone
LES: Large Eddy Simulation
LH: Langmuir-Hinshelwood
LHV: Lower Heating Value
MFF: Moving Flame Front
MHI: Mitsubishi heavy Industries
NETL: National Energy Technology Laboratory
OMB: Opposed Multi-Burner
PCC: Pulverized Coal Combustion
PCGC: Pulverized Coal Gasification and Combustion
PFR: Plug Flow Reactor
PRENFLO: Pressurized Entrained Flow
RANS: Reynolds-Averaged Navier-Stokes
RMS: Root Mean Square
RNG: Re-Normalization Group
ROM: Reduced Order Model
RPM: Random Pore Model
RSM: Reynolds Stress Model
RTE: Radiative Transport Equation
SC: Super-Critical
SCGP: Shell Coal Gasification Process
SCM: Shrinking Core Model
SCPC: Super-Critical Pulverized Coal
SFG: Solid Fuel Gasification
SST: Shear Stress Transport
TH: Taiheiyo sub-bituminous coal
UNFCCC: United Nations Framework Convention on Climate Change
Chapter 1
INTRODUCTION

1.1 Background and motivation

More than 40% of world’s electricity production comes from utilization of coal. Whereas in the United States, coal accounted for approximately 49% of electric power generated [1], its share is much larger, varying from 65% to 70%, in emerging economies such as China and India. In addition, coal is also used as a source of chemicals such as fertilizers, ammonia, hydrogen, etc., apart from increasingly being utilized for production of liquid fuels like gasoline and diesel in countries with scarcer oil and gas reserves, such as South Africa, China and India. World coal consumption was about 6,743,786,000 tons in 2006 and is expected to increase 48% to 9.98 billion tons by 2030 according to predictions by the Energy Information Administration (EIA) [2]. Figure 1-1 shows EIA’s estimates of how the increasing energy demand over the years will be met by various energy sources. In spite of the invigorated push to renewable sources in various degrees by all major countries in recent years, oil, coal and natural gas are expected to contribute toward meeting bulk of world’s energy demands in the foreseeable future. It should be noted that whereas the supply of oil and gas can vary greatly depending upon regional and political instabilities and conflicts, coal supplies are comparatively secure, at least for countries which are presently major consumers of coal and where demand is expected to grow most significantly.

However, among all fossil fuels, coal also raises special concerns since it leaves the largest environmental footprint owing to the fact that it releases more carbon-dioxide per unit of energy produced than any other energy source. Even on a cumulative basis, coal combustion power plants remain the single largest source of CO₂ emissions, contributing 41% of total
energy-related emissions. Figure 1-2 shows EIA’s predictions on the break-up of projected annual CO₂ emissions between various energy sources. It is evident that any efforts towards mitigation of global warming due to CO₂ emissions need to be directed, in a significant way, toward development of ‘cleaner’ technology and processes for coal-utilization.

Since policy is a primary driver for development of technologies and processes leading to mitigation of CO₂ emissions, United Nations Framework Convention on Climate Change (UNFCCC), informally known as Earth Summit, was first held between sixty-four industrialized as well as developing nations in Rio de Janeiro on 1992. Following several rounds of yearly meetings and negotiations, latest being at Copenhagen in 2010, major countries have set targets on absolute reduction in existing levels of CO₂ emissions, ranging from 25% to 40%, by 2020. These targets can be partially met by increasing the share of renewables in energy production, expanding nuclear energy, enhancing forest cover, encouraging energy conservation and efficiency programs, etc. However, coal-based power generation, being the largest source of CO₂ emissions, will have to contribute significantly to the emissions reduction goals in order to be accepted as a viable energy source moving forward.

1.2 Current practices

Most of present electricity generation from coal employs pulverized coal combustion (PCC) plants. Powdered coal is typically combusted in air-blown industrial boilers operated at atmospheric pressure to raise subcritical steam which is then used to drive a steam cycle. Flue gas from the boiler passes through clean-up units to remove particulates, SOₓ and NOₓ. Flue gas exits the clean-up units at atmospheric pressure, typically contains 10-15% CO₂ and is vented into the atmosphere. On the whole, PCC plants have an efficiency of approximately 35% (HHV).
Figure 1-1: World energy demand to 2030

Figure 1-2: World CO₂ emissions to 2030
1.3 CO₂ capture and sequestration

It is well known that current rate of CO₂ production and emission into the atmosphere far outweighs the CO₂ absorption via natural processes. Estimates by environmental scientists indicate that global average temperatures should not rise by more than 2 °C above pre-industrial times in order to prevent catastrophic consequences on environment. However, it has been argued that the current set of emission cut pledges taken by major countries following the Copenhagen Summit is likely to lead to a rise in global temperatures by 3.2 – 3.5 °C [3]. Clearly, there is a pressing need to limit the amount of CO₂ released into the atmosphere notwithstanding the fact that actual rate of CO₂ production, in all likelihood, will remain above acceptable limits. Therefore, the idea of capturing CO₂ produced from fossil fuel powered power plants and storing it underground, if successfully implemented, can be a game-changer.

Several possibilities exist for underground Carbon capture and storage (CCS). The most probable geological formations for CO₂ are schematically depicted in Figure 1-3 [4] and listed below:

(1) Storage in depleted oil and gas reservoirs
(2) Storage in deep saline formations, offshore and onshore
(3) Use of CO₂ in enhanced oil recovery
(4) Use of CO₂ in enhanced coal bed methane recovery

Several demonstration CCS projects have been undertaken in various part of the world. An exhaustive list of current and plant CCS projects is available on the website of the Carbon Capture and Sequestration Technologies Program at MIT (http://sequestration.mit.edu/). The performance of these projects will be critical to the potential deployment of various clean-coal technologies discussed in this section. It should be kept in mind that various uncertainties exist
in successful scalable implementable of CCS. These uncertainties primarily arise from the high costs involved and absence of robust CO₂ emissions regulations in most countries.

Figure 1-3: Geological storage options for CO₂ [4]

1.4 Alternatives for CO₂ mitigation from coal-based power generation

The problem of addressing CO₂ emissions from coal-fired power plants can be addressed with a combination of broadly three strategies:
(1) Improving plant efficiency in pulverized coal combustion using process or technological enhancements

(2) Developing alternatives to PC combustion offering better efficiencies and pollutant control; for example, coal gasification or oxy-coal combustion

(3) Incorporating carbon capture and sequestration strategies in existing plants and designing newer plants to be ‘capture-ready’

By option (1), designing the PCC plants for operation at higher temperatures and pressures and raising super-critical steam, greater efficiencies can be achieved. Depending upon the operating regime of steam, plants can be classified as super critical pulverized coal (SCPC) or ultra-super critical pulverized coal plants. The increase in efficiency results in greater electric power for same CO₂ emission. A number of supercritical units were built in the US through the 1970’s and early 80’s [5]. However, the roadblock for this technology at that time was availability of suitable materials capable of withstanding high pressures and temperatures. These shortcomings have now been addressed and current state-of-the-art SCPC power generation involves 24.3 MPa and 838 K, resulting in plant efficiency of approximately 38% (HHV).

Plant efficiency can also be improved by switching from conventional PCC operation to Integrated Gasification Combined Cycle (IGCC) or oxy-coal combustion technology. It is useful to discuss these two options along with PCC when coupled with the corresponding CO₂ capture routes as follows:

**Post combustion capture**: With conventional PCC or SCPC plants, complete combustion of coal occurs with air in the boiler. The flue gas contains CO₂ diluted with N₂ and hence separation process is energy intensive. However, this option is also least capital intensive for retrofitting existing PCC plants
(2) **Oxy-fuel capture:** With oxy-fuel combustion plants, complete combustion of coal occurs with oxygen in the boiler. The flue gas is primarily a mixture of CO₂ and H₂O. When flue gas is cooled, steam condenses leaving behind a stream of pure CO₂. Hence, CO₂ capture in this method is very simple. However, there is an energy penalty as well as capital cost associated with the air separation unit (ASU) for generating pure oxygen.

(3) **Pre-combustion capture:** With IGCC plants, coal is not completely combusted within the gasifier, rather converted to syngas, a mixture of CO and H₂, under partial oxidation conditions. After passing through a water-gas shift reactor, a mixture of CO₂ and H₂ is obtained. CO₂ is captured from the gas mixture whereas H₂ is combusted in a gas turbine. Since partial pressure of CO₂ in mixture is higher than that in flue gas of PCC plants, CO₂ capture itself is comparatively economical. However, other capital and energy intensive units are added including gas turbines, ASU, water-gas shift reactor etc. Gasification is the focus of the present work and will be discussed in detail later in this chapter and following chapters.

A plant is said to be designed ‘capture-ready’ if at a future point it can be retrofitted for CO₂ capture and sequestration and still remain economical to operate.

1.5 **Coal gasification and IGCC**

Gasification can be described as the process of converting a carbonaceous fuel into a mixture of carbon monoxide and hydrogen, called syngas. The process typically involves reacting the fuel with a limited amount of oxygen and/or steam at high temperatures and can briefly be described in the following sequence of steps:
(1) Immediately following injection, feedstock heats up and undergoes pyrolysis to release bound moisture and volatiles

(2) Volatiles combust with the injected oxygen generating heat and producing CO₂ and H₂O

(3) Devolatilized feedstock particles react with O₂, CO₂ and H₂O present in the mixture to produce syngas through the following heterogeneous reactions:

\[ C + \frac{1}{2}O_2 \rightarrow CO \]
\[ C + CO_2 \rightarrow 2CO \]
\[ C + H_2O \rightarrow CO + H_2 \]

(4) Water-gas shift reaction proceeds in the gas phase, contributing to the balance between major gas phase species toward the later sections of the gasifier:

\[ CO + H_2O \rightleftharpoons CO_2 + H_2 \]

The sub-processes involved and the corresponding models are described in detail in Chapter 2. It should be mentioned that coal gasification is an old process, having been used to produce 'town gas' for lighting and cooking in Europe and USA in the late nineteenth century. With the advent of natural gas and oil, usage of town gas declined. During both world wars, under shortage of petroleum, gasification was used for the production of liquid fuels. Coal-to-hydrocarbon liquid (CTL) conversion technology continues to be popular in countries with limited supplies of oil and gas. Especially in South Africa, the Sasol Corporation continues to develop CTL technology and collaborates on CTL projects not just in South Africa, but also in China and India [6]. With rising oil prices, it is reasonable to expect that CTL will find increasing usage.
In the current scenario, coal gasification has generated tremendous interest due to its potential to produce cleaner coal-based power using IGCC technology along with carbon capture. A simplified IGCC plant schematic is shown in Figure 1-4. Most of the current gasifier designs for IGCC are employ oxygen feed, thereby necessitating an air separation unit (ASU) within the gasification island. The gasification island also comprises of the gasifier unit, along with the radiant and/or quench cooler, and the syngas clean-up units. Following syngas cooling, particle scrubbers remove ash and unconverted char from the exit stream. Mercury is typically removed using an activated carbon bed. The syngas is then passed through a water-gas shift reactor to yield primarily a mixture of CO₂ and H₂. Subsequently, either selexol or rectisol process is employed to remove H₂S as well as CO₂ from the flue gas.

The power island consists of steam turbines, heat recovery steam generator as well as gas turbines. Pure stream of H₂ obtained from the clean-up units is combusted in gas turbines. Since gas turbines allow higher operating temperatures as compared to steam turbines, plant efficiency in IGCC plants is higher than that in PCC plants. In addition, the process is typically designed for elevated pressures. While higher operating pressure reduces the size of various units and rectors for the same power output and mass flow rates, it also aids in separation of pollutants, including CO₂, since pollutant removal at higher partial pressures is more economical.

As alluded to in the foregoing discussion, IGCC offers a set of unique advantages over competing technologies. These can be point-wise summarized as follows:

1. It has been argued earlier, that a primary driver for considering alternative coal-based energy generation technologies is reduction in CO₂ emission by maintaining high plant efficiencies with CO₂ capture. As shown in Table 1-1, IGCC is predicted to demonstrate better plant efficiency than both SCPC and oxy-coal combustion, for same power output, when CO₂ capture is taken into account. Higher plant efficiency results in lower
cost of electricity (COE) and lower CO₂ emissions per unit of energy generated. The data in Table 1-1 is taken from an interdisciplinary MIT study titled *The Future of Coal* [5].

Figure 1-4: A highly simplified IGCC plant schematic

(2) Since the gas clean-up occurs at higher pressure, emissions control is more effective and economical. Moreover, gasification, being a reducing environment, yields nitrogen and sulfur elements as NH₃ and H₂S respectively, as opposed to the corresponding oxides which are expensive to remove. Mercury and particular emissions from IGCC are generally one-third to one-tenth of those for a PCC plant [7].

(3) IGCC plant can also be used for co-generation, producing chemicals and synthetic fuels from a portion of the syngas.
(4) Gasifiers allow multiple feedstock sources to be co-fired. Hence, IGCC plants can make use of economically accessible refinery residues and biomass as feedstocks along with coal.

Table 1-1: Representative performance and economics for SCPC, super critical oxy-coal (SC Oxy) and IGCC power generation technologies. Basis: 500 MW_e plant net output, Illinois # 6 coal.

<table>
<thead>
<tr>
<th></th>
<th>SCPC</th>
<th>SC Oxy</th>
<th>IGCC</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>w/o Capture</td>
<td>w Capture</td>
<td>w Capture</td>
</tr>
<tr>
<td>Efficiency % (HHV)</td>
<td>38.5</td>
<td>29.3</td>
<td>30.6</td>
</tr>
<tr>
<td>Coal Feed, T/D</td>
<td>4437</td>
<td>5831</td>
<td>5583</td>
</tr>
<tr>
<td>CO₂ emitted, kg/h</td>
<td>414903</td>
<td>54518</td>
<td>52202</td>
</tr>
<tr>
<td>CO₂ captured, kg/h</td>
<td>0</td>
<td>490662</td>
<td>469817</td>
</tr>
<tr>
<td>CO₂ emitted, g/kW_e-h</td>
<td>830</td>
<td>109</td>
<td>104</td>
</tr>
<tr>
<td>Plant Cost, $/kW_e</td>
<td>1330</td>
<td>2140</td>
<td>1900</td>
</tr>
<tr>
<td>COE, ¢/kW_e-h</td>
<td>4.78</td>
<td>7.69</td>
<td>6.98</td>
</tr>
</tbody>
</table>

1.6 Types of gasifiers

Three broad categories of gasifier designs exist, namely fixed bed gasifiers, fluidized bed gasifiers and entrained flow gasifiers (EFGs). According to the DOE/NETL 2007 database, all but one of gasification plants planned worldwide will employ gasifiers of the entrained flow type [8]. The primary advantage of using EFGs, as opposed to the other designs, is their ability to process high mass throughputs, attain high conversions and emit low levels of hydrocarbons.
Accordingly, the present work is focused on modeling and analysis of entrained flow designs only.

Several EFG designs and corresponding gasification processes exist in the market. The characteristics of some popular designs and processes are listed in Table 1-2. Gasifiers can be air-blown or oxygen-blown, single-stage or two-stage, slurry-fed or dry-fed, up-fired or down-fired. Similarly the gasification process might involve a combination of quench and radiant coolers for syngas cooling or a just a quench cooler.

Table 1-2: Characteristics of popular Entrained Flow Gasifier designs and processes

<table>
<thead>
<tr>
<th>Process</th>
<th>Vender</th>
<th>Flow</th>
<th>Feed</th>
<th>Injectors</th>
<th>Oxidant</th>
<th>Stages</th>
<th>Wall Lining</th>
<th>Syngas Cooling</th>
</tr>
</thead>
<tbody>
<tr>
<td>E-GAS</td>
<td>CoP</td>
<td>Up</td>
<td>Slurry</td>
<td>Opposed</td>
<td>O₂</td>
<td>Two</td>
<td>Refractory</td>
<td>Quench</td>
</tr>
<tr>
<td>GE</td>
<td>GE</td>
<td>Down</td>
<td>Slurry</td>
<td>Axial</td>
<td>O₂</td>
<td>One</td>
<td>Refractory</td>
<td>Radiant + Quench</td>
</tr>
<tr>
<td>MHI</td>
<td>MHI</td>
<td>Up</td>
<td>Dry</td>
<td>Radial</td>
<td>Air</td>
<td>Two</td>
<td>Membrane</td>
<td>Quench</td>
</tr>
<tr>
<td>OMB</td>
<td>ECUST</td>
<td>Down</td>
<td>Slurry</td>
<td>Opposed</td>
<td>O₂</td>
<td>One</td>
<td>Refractory</td>
<td>Quench</td>
</tr>
<tr>
<td>PRENFLO</td>
<td>Uhde</td>
<td>Up</td>
<td>Dry</td>
<td>Radial</td>
<td>O₂</td>
<td>One</td>
<td>Membrane</td>
<td>Radiant + Quench</td>
</tr>
<tr>
<td>SCGP</td>
<td>Shell</td>
<td>Up</td>
<td>Dry</td>
<td>Radial</td>
<td>O₂</td>
<td>One</td>
<td>Membrane</td>
<td>Radiant + Quench</td>
</tr>
<tr>
<td>SFG</td>
<td>Siemens</td>
<td>Down</td>
<td>Dry</td>
<td>Axial</td>
<td>O₂</td>
<td>One</td>
<td>Membrane</td>
<td>Quench</td>
</tr>
</tbody>
</table>

Over 90% of planned syngas capacity worldwide is accounted for by three EFG designs: General Electric (GE), Shell Coal Gasification Process (SCGP) and ConocoPhillips E-GAS. Simplified schematics of these designs are shown in Figure 1-5. The choice of gasification technology
Figure 1-5: (a) GE (radiant), (b) CoP E-GAS and (c) SCGP gasifiers
depends on the nature of feedstock, quality and composition of syngas desired, apart from considerations of cost and operational convenience. Coals with high moisture would, for example, yield higher efficiencies with a dry-feed design. Similarly, whether syngas is primarily to be used for electricity generation or production of chemicals and liquid fuels will impact the choice of gasifier design.

1.7 Problems and challenges in commercialization of IGCC

Several challenges remain in way of commercialization of IGCC technology. The most significant issue is of plant availability, i.e., the percentage time during which plant is fully operational. For each of the current IGCC demonstration plants, 3-5 years was required to reach 70-80% availability after commercial operation was initiated in the 90's [7]. By comparison, average availability for a typical PCC plant reaches 90-95% soon after start-up [7]. With regards to the gasifier unit, the primary modes of failure remain injector failure and refractory failure:

**Feed injector failure:** The injectors typically have to withstand high heat fluxes owing to the high temperatures attained by volatile combustion just ahead of injection. It is generally accepted that injector failure is the most significant factor behind low reliability of gasification systems. Based on actual experience, the life of an injector nozzle is between two to six months [9]. A minimum life of one year is desirable in the near term and two years in the long run [9].

**Refractory liner failure:** Refractory liners contribute to a significant amount of downtime and require significant maintenance. Depending upon the operating temperatures and feedstock, refractory liners are reported to last between six to eighteen months [9]. The upper end of this is usually attained by running the gasifier at lower temperatures, invariably with the cost of lower conversion. Costs associated with rebrickling a gasifier involved $1 million of expenditure and three weeks of downtime.
Apart from component failure, there are other challenges to be encountered to make IGCC feasible:

**Poor space utilization:** Gasifier units are massive structures and vastly expensive. The current designs have evolved out of operational experience and are not expected to be optimal in their utilization of available gasifier space.

**High capital costs:** Increasing estimates of capital costs is the most significant factor impacting commercialization of IGCC plants. For example, the DOE FutureGen project on construction of a near-zero emissions power plants with CCS was earlier scheduled to be based on IGCC. Owing to ever increasing cost estimates, the project focus was shifted on retrofitting an existing PCC plant to oxy-fuel combustion with capture [10]. Many IGCC projects are underway throughout the world and their success can lead to dissipation of policy-maker and investor fears.

### 1.8 R&D needs: Development of high fidelity simulations

In order to address the challenges described in the previous section, a multi-pronged instrumentation, experimentation, simulation and validation strategy is needed. The present work focuses on development of a high fidelity CFD modeling tool toward meeting this goal. DOE has identified a list of top twenty R&D needs in order to accelerate sustainable and reliable deployment of IGCC plants [9]. The following items are selections out of that list, which would benefit from high fidelity CFD simulations.

1. Development/improvement of refractory systems
(2) Development/improvement of systems for feeding multiple feedstocks, including coal and biomass feedstocks (in slurry or dry form), to high pressure and other gasifiers

(3) Development of feed injectors that extend life, reduce cost, provide fuel flexibility, and offer effective load following

(4) Assessment/development of novel gasifiers, such as hybrid, high-efficiency, small-scale or low-temperature gasifiers

In addition, DOE recognizes simulations as one of the most important requirements for advancement of gasification technology [9]:

“*The need for more sophisticated advanced gasifier and other process models ranks very high. Needs include: (1) defining what models are clearly needed to benefit the entire industry before developing them; (2) focusing model development on dynamic models that can be used not only to predict the steady-state performance of a gasifier, but also to simulate transient events; and (3) validating the models with actual plant data rather than using theoretical diagnostics or dynamic modeling as substitutes for actual operational experience.*”

1.9 Utility of a validated multiphysics CFD model

High fidelity CFD simulations with elaborate submodels, describing physics of the relevant physical and chemical processes, can be greatly instrumental in understanding gasification process, optimizing gasifier designs and inventing novel gasification processes and concepts. Current gasifier designs have evolved more out of operational expediency rather than rigorous understanding of relevant physical phenomena. While the overall model requires validation at
the level of gasifier input/output data and internal temperature, species measurements, the constituent submodels also need to be validated at the level of individual physical and chemical processes that they describe. The utility of such a validated model can be described in terms of how it addresses the challenges facing IGCC commercialization described in section 1.7:

Resolving injector and refractory liner failure: Analysis based on results of a validated CFD model can be critical in understanding and remedying injector and refractory failure in gasification systems. Experience alone cannot provide an enduring solution, since the components are expected to work not just for one fixed operating condition, but a range of feed rates, feedstocks, particle sizes, etc. Moreover, certain invariably in operating conditions and feedstock quality is unavoidable under practical operation. One could construct a lab scale or a pilot scale test facility to run only a limited number of test cases. Ultimately these test cases need be conducted in parallel with and using information from simulations. An elaborate, validated model can predict the resulting range of temperatures and heat fluxes to the injectors and refractory liners for the complete range of operating conditions. Moreover, the model can be used to numerically test new component designs, configurations and materials.

Efficient space utilization: As results in chapter 4 indicate, some of the current commercial gasifier designs might not be utilizing a large portion of gasifier space, especially towards the end stages of the reactor. In addition, there might be ‘dead zones’ in certain regions where temperatures are too low to guarantee sufficiently fast conversion rates. A CFD model can be used to predict these zones and suggest improvements based on test runs conducted on modified designs.

Addressing high capital costs: The gasifier unit is one of most expensive components in an IGCC plant. As discussed in section 1.7, current gasifier availabilities are lower than ideal. By identifying causes of frequent failure modes including particular feedstocks and corresponding flow rates when the failures occur, design suggestions can be made to improve availability.
Optimization of gasifier operating conditions: As discussed earlier, the current operation of entrained flow gasifiers is based more on experience than actual physical insight. Hence, it is possible that gasifiers might be operating on sub-optimal values of parameters such as gasifier pressure, mass throughput, feedstock grinding size, etc. As results in chapter 5 indicate, a validated model can provide useful quantitative estimates of the gain or loss in net carbon conversion when these operating conditions are varied. Based on such results, one can make an informed decision on the optimal combination of the operating conditions.

1.10 Thesis outline

Chapter 2 describes the component submodels. In Chapter 3, the validation of the cold flow solver and particle turbulent dispersion model using canonical test cases from the literature, are discussed. Chapter 4 discusses validation of the overall model as applied to two gasifiers for which experimental data is available, the MHI gasifier design and an experimental scale gasifier at the Brigham Young University (BYU). Chapter 5 demonstrates the utility of the CFD model in assessing the impact of the variation of key operating parameters on gasifier performance and suggesting optimal values for those parameters. Finally, chapter 6 discusses major conclusions and directions for future work.

References

[6] Sasol Synfuels International (SSI)
(http://www.sasol.com/sasol_internet/frontend/navigation.jsp?navid=16200001&rootid=2)
(http://www.fossil.energy.gov/programs/powersystems/futuregen/)
Chapter 2
MODEL DESCRIPTION

2.1 Background and Motivation

A CFD model of coal gasification attempts to capture the detail of various physical and chemical processes in the gasifier through relevant submodels and their coupling. The modular structure of a CFD model, along with the interactions between various modules, is represented in the block diagram in Figure 2-1. In order to accurately predict some of the overall metrics of gasifier performance, like fuel conversion and syngas composition, we need to carefully construct and validate the most important building blocks of the integrated model. Focusing on such considerations, in this chapter the construction of a multiscale CFD model of entrained flow gasification is described with special emphasis on the development of key submodels including turbulence, particle turbulent dispersion and char consumption models.

Only a limited number of examples of CFD simulations of entrained flow gasification, where adequate attention is provided to the important submodels, exist in the literature. Smoot’s group at the Brigham Young University developed a series of axisymmetric and 3-D CFD models, named PCGC (pulverized coal gasification and combustion) models, since the late 1980’s and tested them on various coals [1][2]. PCGC models were developed following the validation of submodels used in the construction of the overall CFD code, as depicted in figure 2-1. The models were first validated for cold flow, then single-phase reacting flow, followed by independent verification of char kinetics [3]. Beyond the PCGC models, this systematic validation strategy has not been described in literature. With the increase in computational power and steady improvement in modeling sophistication in relevant fields like turbulence, devolatilization and single char particle consumption, there is an exciting opportunity to construct, validate and integrate critical newer submodels and to obtain more accurate
predictions by running the integrated model on sufficiently fine meshes. The meshes used in the present study are several times more refined than those typically used in the gasification CFD literature.

![CFD Modeling Diagram](image)

**Figure 2-1: Block diagram representing components of a CFD model and their interactions**

In this chapter, a general description of the model components is provided along with the relevant transport and constitutive equations. The mode structure and assumptions, along with the list of equations presented in this chapter, will be invoked in Chapters 3, 4 and 5 to explain model predictions.
2.2 Key submodels

Conservation equations for the gas phase and particle phase are listed in Table 1 and Table 2 respectively. As emphasized in the preceding section and depicted in Figure 1, these equations along with the necessary constitutive relations and submodels describe a comprehensive set of physical and chemical processes as described from section 2.2.1 to section 2.2.9.

2.2.1 Gas phase turbulence

Mass and momentum transport for the gas phase are described by equations (2-1) and (2-2), respectively. The closure for the Reynolds stresses, required in equation (2-2), is provided by equation (2-5). The SST k-ω model, described by equations (2-6) – (2-8), is used for modeling turbulence. Accordingly, equations (2-1) – (2-4) for transport of mass, momentum, energy and species are spatially and temporally averaged. The choice of the turbulence model is justified by validating it with experimental data on mean velocities and fluctuations from two canonical turbulent flow test cases, as described in Chapter 3.

Referring to equations (2-6) – (2-8), $\sigma_k$, $\sigma_{\omega}$ are modeling parameters whereas $G_k$, $G_{\omega}$, $Y_k$, $Y_{\omega}$, $D_{\omega}$ represent various generation and depletion terms within the corresponding transport equations. $S_k$, $S_{\omega}$ represent user-defined source terms and $\alpha^*$ is the damping coefficient for turbulent viscosity in the SST k-ω model. The various coefficients and parameters discussed above are defined using a further set of correlations and modeling constants. A comprehensive listing of the SST k-ω equations, parameters and model structure can be found in [4]. It should be noted that the SST k-ω model retains the standard k-ω model formulation in the near-wall region and switches to the standard k-ε model formulation in the far field region using an appropriate blending function. This modification allows the SST model to generate better
Table 2-1. Gas phase conservation equations

<table>
<thead>
<tr>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mass</strong></td>
</tr>
<tr>
<td>[ \frac{\partial}{\partial x_i} (\rho u_i) = S_{p,m} ]</td>
</tr>
</tbody>
</table>

| **Momentum** |
| \[ \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_i}{\partial x_j} \right) \right] + \frac{\partial}{\partial x_j} (-\rho u_i' u_j') + S_{p,\text{mom}} \] |

| **Energy** |
| \[ \frac{\partial}{\partial x_i} (\rho u_i h) = \frac{\partial}{\partial x_i} \left[ \lambda \frac{\partial T}{\partial x_i} \right] + S_{\text{rad}} + S_h + S_{p,h} \] |

| **Species** |
| \[ \frac{\partial}{\partial x_i} (\rho u_i Y_i) = \frac{\partial}{\partial x_i} (\rho D Y_i) + S_{Y_i} + S_{p,Y_i} \] |

| **Reynolds Stresses** |
| \[ -\rho u_i' u_j' = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \left( \rho k + \mu_t \frac{\partial u_i}{\partial x_j} \right) \delta_{ij} \] |

| **Turbulent KE** |
| \[ \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k - Y_k + S_k \] |

| **Specific Dissipation of Turbulent KE** |
| \[ \frac{\partial}{\partial x_i} (\rho \omega u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\omega} \right) \frac{\partial \omega}{\partial x_j} \right] + G_\omega - Y_\omega + D_\omega + S_\omega \] |

| **Turbulent Viscosity** |
| \[ \mu_t = \alpha^* \frac{\rho k}{\omega} \] |
Table 2-2. Particle phase conservation equations

| Mass       | \[
| \frac{dm_p}{dt} = \frac{dm_{C-O_2}}{dt} + \frac{dm_{C-CO_2}}{dt} + \frac{dm_{C-H_2O}}{dt} + \frac{dm_{devol}}{dt} + \frac{dm_{vapor}}{dt} 
| \] |
| Momentum   | \[
| \frac{du_p}{dt} = F_D (u - u_p) + \frac{g_i (\rho_p - \rho)}{\rho_p} + F_i 
| \] |
| Drag       | \[
| C_D = a_1 + \frac{a_2}{Re_p} + \frac{a_3}{Re_p^2}, \quad Re_p = \frac{\rho d_p |u - u_p|}{\mu} 
| \] |
| Energy     | \[
| Q_G = \frac{dm_{C-O_2}}{dt} H_{C-O_2} + \frac{dm_{C-CO_2}}{dt} H_{C-CO_2} + \frac{dm_{C-H_2O}}{dt} H_{C-H_2O} 
| m_p c_p \frac{dT_p}{dt} = h_p A_0 (T - T_p) + \frac{\varepsilon_p A_0}{4} (G - 4 \sigma T_p^4) + Q_G 
| \] |
| Nusselt Number | \[
| Nu = \frac{h_p d_p}{k_g} = 2.0 + 0.6 Re_p Pr^{1/3} 
| \] |

results in adverse pressure gradient flows and swirling flows [4]. These types of flows are observed in many typical gasifiers. The impact of switching from the commonly used standard k-\( \varepsilon \) model to the SST k-\( \omega \) model, on the accuracy of the overall model predictions, is discussed in Chapter 4.
2.2.2 Particle turbulence dispersion

Lagrangian tracking is adopted instead of Eulerian approach owing to the low volume loading of the solid phase in entrained flow gasifiers. In order to simulate turbulent dispersion, particle with each diameter is stochastically tracked several times, the exact number being case-specific, with random fluctuations imposed on the velocity of the surrounding gas-phase. The particle dispersion model is described using equations (2-10) – (2-11) and (2-14) – (2-18).

\[ u = \bar{u} + u' \]  \hspace{1cm} (2-14)

\[ u' = \zeta \sqrt{u'^2} = \zeta \sqrt{2k/3} \]  \hspace{1cm} (2-15)

Equation (2-10) describes the momentum equation for a particle. \( u_p \) is the particle \( x \)-velocity and \( u \) is the local gas phase \( x \)-velocity. \( \rho \) and \( \rho_p \) are the gas phase and particle densities respectively. \( C_D \) is the dimensionless drag coefficient, \( d_p \) is the particle diameter and \( F_x \) is any additional body force. Since a RANS model predicts only the mean values of the field variables, a fluctuation term \( u' \) is added to the predicted RANS mean velocity, \( \bar{u} \), in order to model the effect of gas phase turbulence on particle dispersion, as shown in equation (2-14). By computing the particle trajectory repeatedly using the above dispersion model, we can expect to take the effect of turbulence dispersion on particles into account. Similar models of turbulent particle dispersion have been used in previous studies of coal gasification [5][6][7].

\( u' \) is evaluated using the local value of the turbulent kinetic energy, \( k \), and assuming isotropic turbulence using equation (2-15), where \( \zeta \) is a normally distributed random number. The particle is assumed to interact with a succession of fluid phase eddies during its trajectory and the particle-eddy interaction time is taken to be the smaller of the eddy-traverse time, \( T_{cross} \).
and the eddy lifetime, $T_e$. Once the particle crosses over from one eddy to another, $u'$ is evaluated using a different value of $\zeta$. $T_e$ and $T_{cross}$ are defined as

$$T_e = C_L \frac{k}{\varepsilon}$$  \hspace{1cm} (2-16)

$$T_{cross} = \tau \ln \left[ 1 - \left( \frac{L_e}{\tau |u - u_p|} \right) \right], \quad L_e = C_L \frac{k^{1.5}}{\varepsilon}$$  \hspace{1cm} (2-17)

$$\tau = \frac{\rho_p d_p^2}{18 \mu}$$  \hspace{1cm} (2-18)

where $L_e$ is the eddy length scale, $\tau$ is the particle relaxation time, $\mu$ is the local fluid viscosity and $C_L, C_{Le}$ are modeling constants.

2.2.3 Coupling between gas and particle phase

Particle-source-in-cell approach [8] is used to evaluate the source terms that model the interactions between the gas and the solid phases. These inter-phase exchange terms are denoted by $S_{p,m}, S_{p, mom}, S_{p, h}, S_{p, n}$ in equations (2-1) – (2-4).

2.2.4 Homogeneous and heterogeneous kinetics

Table 3 specifies the reaction kinetics and the reaction rate constants applied in our study. For the homogeneous reactions, the net reaction rate is taken to be the minimum of the Arrhenius rate and turbulent mixing rate as given by the EBU model [9]. The values for both the
homogeneous and the heterogeneous kinetics constants are taken from the literature [10][11][12]. Alternative kinetics mechanisms and expressions for heterogeneous reaction have been suggested in the literature. These are discussed in section 2.2.9.

Table 2-3. Homogeneous [11][10] and heterogeneous [12] reaction rates

<table>
<thead>
<tr>
<th>Homogeneous Reactions</th>
<th>R1</th>
<th>k = 2.24×10^{12} [CO][O_2]^{0.25} [H_2O]^{0.5} \exp(-1.67×10^8 / RT)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R2</td>
<td>k = 6.8×10^{15} T^{-1} [H_2]^{0.25} [O_2]^{1.5} \exp(-1.67×10^8 / RT)</td>
<td></td>
</tr>
<tr>
<td>R3</td>
<td>k_f = 2.75×10^9 [CO][H_2O] \exp(-8.37×10^7 / RT)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Heterogeneous Reactions</th>
<th>R4</th>
<th>k = 2.3T [O_2]^{0.4} \exp(-9.23×10^7 / RT)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R5</td>
<td>k = 4.4T [CO_2]^{0.6} \exp(-1.62×10^8 / RT)</td>
<td></td>
</tr>
<tr>
<td>R6</td>
<td>k = 1.33T [H_2O]^{0.6} \exp(-1.47×10^8 / RT)</td>
<td></td>
</tr>
</tbody>
</table>

2.2.5 Radiative heat transfer

Radiation is the primary mode of heat transport in coal-fired furnaces and gasifiers, where the length scale is of the order of 1 m [13]. For example, the CFD simulations of the MHI gasifier, described in chapter 4, predict that radiation flux is greater than 60% of the total power
received by the wall. In effect, radiation significantly impacts the overall heat transfer process, hence the fluid dynamics and the reaction rates. Accuracy of the radiation heat transfer model is expected to have a considerable impact on the predictive capability of the overall model.

The radiative transport equation (RTE) (2-19) needs to be solved in order to provide the radiative source term, $S_{rad}$, in equation (2-3).

\[
\frac{dI}{ds} = -(k_a + k_s)I + k_a \frac{\sigma T_b^4}{\pi} + k_s \frac{I(\Omega)}{4\pi} \int \Phi(\tilde{s}, \tilde{s}') I(\Omega') d\Omega'
\]

(2-19)

**Figure 2-2: Radiative Transfer Equation**

This equation is derived for a pencil beam of radiation traveling in a direction $\tilde{s}$, with local intensity $I(\tilde{x}, \Omega)$. $k_s$ is the scattering coefficient, $k_a$ is the absorption coefficient, $I_b$ is the black-body intensity and $\Phi(\tilde{s}, \tilde{s}')$ is the scattering phase function from a direction $\tilde{s}'$ to the direction $\tilde{s}$ of the beam of interest. The radiative intensity is defined as the radiative energy passing per unit area normal to the area of cross section per unit solid angle per second with units of W/m²-sr. $I(\tilde{x}, \Omega)$ is a function of position as well as the solid angle $\Omega$ and hence an integral over the complete range of $4\pi$ is warranted in equation (2-19). Hence, the first term on the RHS indicates attenuation in intensity due to scattering and absorption in the medium, second term denotes increase in intensity due to emission and the third term represents increase in intensity due to in-scattering in direction $\tilde{s}$, from other directions $\tilde{s}'$, as shown in figure 2-2. Once the radiative intensity field is evaluated, $S_{rad}$ can be calculated as:
\[ S_{rad} = 4\sigma k_a T^4 - k_a G \]  

(2-20)

where the first term on the right represents local emission and the second term represents local absorption. \( G \) is the local irradiation defined in terms of \( I \) as:

\[ G = \int_{4\pi} I(\Omega') d\Omega' \]  

(2-21)

In a two-phase reacting flow situation like gasification, \( k_a \) and \( k_s \) include contributions from both gas and particle phases. While the weighted-sum-of-gray-gases method is used to evaluate gas phase radiative constants, the particle phase values can be expressed in terms of the number of particles \( N_p \) within a control volume \( (\Delta V) \), particle emissivity, \( \varepsilon_p \), and particle external surface area, \( A_0 \), as follows:

\[ k_p = \sum_p \varepsilon_p A_0 \frac{N_p}{\Delta V} \]  

(2-22)

\[ k_{sp} = \sum_p (1 - \varepsilon_p) A_0 \frac{N_p}{\Delta V} \]  

(2-23)

where the summation is conducted over all the particles present in the control volume.

The 'finite volume method' (FVM), for radiation, is used to solve the radiative transport equation (2-19). In FVM, the RTE, which is fundamentally derived along a beam of radiation, is adapted to the finite volume formulation. The adaptation is achieved by writing the RTE for \( M \) (say) discrete directions for each control volume. Subsequently, we have \( M \) coupled transport equations for the directional radiative intensities \( I'' \). These transport equations are solved through the domain along with the rest of the gas-phase transport equations listed in Table 2-1.
A total of sixteen discrete directions are employed for evaluating the radiative intensity field in the gasifier simulations presented in chapter 4. Further increasing the number of directions produced negligible change in the predictions.

2.2.6 Wall heat transfer

As mentioned in the previous section, radiative heat transport is expected to be a significant portion of the total wall heat flux in entrained flow gasifiers. The incident radiative flux at the wall, \( q_{in} \), is an important output of the RTE solution and is evaluated through a first moment of radiative intensity as follows:

\[
q_{in} = \int_{\vec{s} \cdot \vec{n} > 0} (\vec{s} \cdot \vec{n}) I(\Omega) d\Omega
\]  

(2-24)

where \( \vec{n} \) is the outward wall normal. The emitted heat flux from wall, \( q_{out} \), can be calculated as:

\[
q_{out} = \sigma \varepsilon_w T_w^4 + (1 - \varepsilon_w)q_{in} \quad I_{out} = \frac{q_{out}}{\pi}
\]  

(2-25)

where \( \varepsilon_w \) is the wall emissivity, \( T_w \) is the wall temperature and \( I_{out} \) is the radiative intensity leaving the wall. \( I_{out} \) is used as the boundary condition in the solution of RTE. For a gray wall (\( \varepsilon_w < 1 \)), the emitted radiation depends on the incoming radiation which in turn depends on the calculated intensity field available only after solving the RTE. Hence in the presence of gray walls, the solution is inevitably iterative.
A one-dimensional wall heat resistance boundary condition is used to model heat transfer across the walls [14]. In cases where measures wall temperatures are available, temperature boundary condition is used.

2.2.7 Particle-phase heat transfer

As described by equations (2-12) and (2-13), coal particles exchange heat with the gas phase through convection and radiation. In these equations, $T_p$ is the particle temperature, $h_p$ is the convective heat transfer coefficient between the particle and the gas phase and $H_{c-o_2}$, $H_{c-co_2}$, $H_c$ are the enthalpies of the heterogeneous reactions R4 - R6. The heat lost or gained, $Q_G$, through the char-oxidation and char-gasification reactions R4 - R6 is supplied exclusively to the particle phase since these reactions occur either within or at the surface of the particle. The local irradiation, $G$, required in equation (2-12), at the location of the particle is evaluated using equation (2-21). It should be noted that the same intensity field calculated via equation (2-19) contains all the information of radiation due to the gas phase as well as the particle phase emission, absorption and scattering. This is quite different from the conservation equations of mass, momentum, species and energy which are written separately for the gas phase and the particle phase (with the respective inter-phase source terms describing the impact of one phase on the other).

2.2.8 Devolatilization

As discussed in section 1.5, the coal particle first releases moisture and volatiles as a result of temperature rise following injection in the gasifier. The devolatilization model used in Fluent is a version of the CPD model [15], which predicts devolatilization rates based on the bond-energies and crosslinking in the lattice structure of the parent coal. This model predicts the amount of volatiles released but the volatile species composition is not specified. The same is
true for the traditional CPD model [15] widely used in the literature, and other models such as the two-competing rates Kobayashi model [16], which empirically determines the devolatilization rates through two different relations at high and low temperatures. However, knowledge of the total devolatilization rates is not sufficient in the context of coupled CFD simulations; we also need a quantitative description of the devolatilization product composition. The devolatilization product composition determines the reactions and hence the temperature in the near-burner region and the product composition at the gasifier exit.

Wu and Tomita [17] experimentally determined the pyrolysis product compositions of 17 different coals. The volatile species composition for the coals was specified in terms of oxygen containing gases (CO, CO$_2$, H$_2$O), hydrogen, methane, C2+C3, hydrocarbon liquids (HCL) and tar. The corresponding data for TH coal, which is the feedstock for the MHI gasifier test cases discussed in Chapter 4, taken from [17], is reproduced in Table 2-4. The weight percentage yield of tar, not explicitly mentioned in Table 2-4, is determined as the difference between the total weight loss and the sum of weight percentage yields of other species in the table. Tar yield for TH coal is significant; it amounts to 29.6% of the initial coal mass. We incorporated this experimental data in our model.

Depending on the coal type, (Tar+HCL+C2+C3) constitute 50-75% of the total volatile yield [17]. In the context of incorporating the results of the devolatilization model in the CFD simulations, a major challenge is modeling the reactions which (tar, C2+C3 and HCL) undergo to yield the light gases, that is, CO, CO$_2$, H$_2$, H$_2$O, along with the corresponding reaction rates. While some later versions of the CPD model [18][19] do incorporate the volatile composition data from Table 2-4, the reaction pathways converting tar, C$_2$+C$_3$ and HCL species to the light gases and the corresponding kinetics still remain unknown.
Table 2-4: Pyrolysis products of TH coal, reproduced from [17].

<table>
<thead>
<tr>
<th>Coal Code</th>
<th>Weight Loss (wt%, daf)</th>
<th>Yield (wt%, daf)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>H₂</td>
</tr>
<tr>
<td>TH</td>
<td>53.0</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Column 2 provides the total weight loss (%) due to pyrolysis. The wt % yield of tar (29.6%) is determined as the balance between column 2 and the species yields in columns 3-7.

Not much work has been done on tar reactions, especially at the elevated temperatures and pressures encountered in typical entrained flow gasifiers. As a first step, we model (tar+C₂+C₃+HCL+CH₄) as a hydrocarbon molecule CHₓ. Because tar is the dominant species in these fragments and the oxygen content in tar is only 5-10% by weight [20][21] and <5% by mole, assuming (tar+C₂+C₃+HCL) to be comprised of carbon and hydrogen only is justified. The stoichiometric coefficient x in CHₓ, can be determined from coal mass balance. For TH coal, x≈1.98 and the volatile composition is given by:

\[
\text{Volatile} \rightarrow 0.164CO + 0.394H₂O + 0.104CO₂ + 0.229H₂ \\
+ 2.249CHₓ + 0.056N₂
\quad (R7)
\]

We assume that CHₓ follows reaction kinetics similar to typical light hydrocarbon molecules, e.g. CH₄:

\[
\begin{align*}
CHₓ + \frac{1}{2}O₂ & \rightarrow CO + \frac{x}{2}H₂ \\
CHₓ + H₂O & \rightarrow CO + \left(\frac{x}{2} + 1\right)H₂
\end{align*}
\quad (R8)
\]

where the kinetic rates for these two reactions are given by.
The choice of CH\textsubscript{4} reaction kinetics is justified because the reaction rates with O\textsubscript{2} and H\textsubscript{2}O of many hydrocarbons, including CH\textsubscript{4}, do not vary greatly from each other \cite{11}\cite{10}. We also performed a sensitivity analysis on the kinetic constants of reactions R8 and did not observe significant impact on the final results.

An alternative approach was suggested \cite{22}\cite{23}\cite{7} in which the volatiles are broken up into CH\textsubscript{4}, CO, CO\textsubscript{2}, H\textsubscript{2}, H\textsubscript{2}O and N\textsubscript{2}. This approach may not always yield satisfactory results since the C:H ratio in (Tar+HCL+C2+C3) is sometimes significantly different from 1:4, for example in the case of TH coal.

### 2.2.9 Char consumption

Following devolatilization and vapor loss, coal particles lose mass via the heterogeneous reactions, as described by equation (2-9). This loss of fixed-carbon by the particle via reaction with gas-phase reactants namely O\textsubscript{2}, CO\textsubscript{2}, H\textsubscript{2}O is referred to as ‘char consumption’ in this work. Char consumption is a cumulative effect of three separate physical and chemical processes: diffusion through the boundary layer and char porous structure, heterogeneous kinetics and char structure/surface area evolution. The overall process can be represented as a resistance network comprised of kinetic and diffusion resistances. The resultant char consumption rate, \(\dot{m}_p\), due to heterogeneous reaction with a gas-phase reactant of partial pressure \(P_g\), where \(m_p\) is the particle mass and \(t\) is the time, is given by \cite{24}\cite{25}.

\[
k_{CH_x-O_2} = 4.4 \times 10^{11} \left[CH_x\right]^{0.5} \left[O_2\right]^{1.25} \exp\left(-1.25 \times 10^8 / RT\right)
\]

\[
k_{CH_x-H_2O} = 3 \times 10^8 \left[CH_x\right]\left[H_2O\right] \exp\left(-1.25 \times 10^8 / RT\right)
\]
\[
\dot{m}_p = \frac{P_g}{\frac{1}{k_d} + \frac{1}{k_s}}
\]  
(2-26)

\[
k_d = A_0 \cdot A_d \left( \frac{T_g}{2000} \right)^{0.75} \frac{1}{Pd_p}
\]  
(2-27)

where \(k_d\) and \(k_s\) are the rate constants for diffusion and kinetics respectively. \(P_g\) is the bulk partial pressure of the particular gas phase reactant, such as \(O_2\), \(CO_2\) or \(H_2O\). \(A_0\) is the external surface area of the particle. The diffusion constant \(A_d\) depends on the particular gasification reaction being considered. \(d_p\) is the particle diameter and \(T_g\) is the gas temperature. \(P\) is the total gasifier pressure and \(R\) is the universal gas constant.

Equation (2-26) can be interpreted in a variety of ways, depending upon the particular description of the kinetics coupled with the surface area evolution via the parameter \(k_s\). For example, if heterogeneous reaction is assumed to occur only at the external surface of the particle, equation (2-26) represents a kinetics/diffusion fixed-core model, which is the default char consumption model in Fluent. The model is schematically depicted in figure 2-3. Similar models have been used in CFD simulations of entrained flow gasification [1][2][5][22]. The reaction surface is assumed to be at a fixed radius, coinciding with the original surface area, \(A_0\). The model typically employs \(n^{th}\) order Arrhenius kinetics, with \(n = 1\), to model \(k_s\).

\[
k_s = A_0 \cdot A_s \exp(-E_s / RT)
\]  
(2-28)
The shrinking core model (SCM) [26] is a more accurate alternative that has been used to model char consumption in entrained flow gasification [6][7][27][28]. Apart from the Arrhenius kinetics and the film diffusion effects, the model accounts for the reduction in the char core radius as conversion proceeds. The effect of diffusion through the surrounding ash layer is also incorporated. The reaction occurs at the surface of the inner shrinking core. The resulting char consumption rate is given by

\[
\dot{m}_p = \frac{P_g}{1 + \frac{1}{k_d} + \frac{1}{k_s \left( \frac{r_p}{R} \right)^2 + \frac{1}{k_{dash} \left( \frac{R_p}{r_p} - 1 \right)}}}
\]  

(2-29)
\[ k_{dash} = k_d \varepsilon^{2.5} \]  \hspace{1cm} (2-30)

\( k_{dash} \) is the ash diffusion constant. \( \varepsilon \) is the voidage of the ash layer, defined as the ratio of the void space to the total volume in the ash specimen. \( r_p \) is the instantaneous radius of the shrinking core. \( R_p \) is the fixed radius of the char-ash complex, same as the original radius of shrinking core. A schematic of the SCM is shown in figure 2-4.

![Figure 2-4: Schematic of a shrinking core model (SCM).](image)

The random pore model (RPM) [22] offers a more detailed treatment of the reactive surface area during char conversion than SCM. The evolution of the internal surface area during char conversion is expressed as
\[
\frac{S}{S_0} = (1 - x) \sqrt{1 - \psi \ln(1 - x)}
\]  

(2-31)

where \(x\) is the conversion fraction and \(\psi\) is the structure parameter for the particular coal/char type. \(S\) is the instantaneous total internal reactive area (cm\(^2\)/g) of the porous char particle as opposed to the external surface area used by the previous models. \(S_0\) is the initial internal reactive area. The expression is derived by employing detailed physics of the evolution of the porous structure of a reacting char particle and should be contrasted with the shrinking core model, which gives a surface area evolution of the form \(\frac{A}{A_0} = (1 - x)^{2/3}\), where \(A\) is the instantaneous surface area of the shrinking core. Coupling surface area evolution using RPM with Arrhenius kinetics, the kinetics parameter \(k_s\) can be represented as:

\[
k_s = m_{po}S_A \exp(-E_s / RT)
\]  

(2-32)

where \(m_{po}\) is the original char mass in the particle. In the next section, more accurate descriptions of heterogeneous reaction, than Arrhenius kinetics, are discussed.

### 2.2.9.1 Heterogeneous kinetics

Our review indicates that only one study [23] employed the RPM in detailed CFD simulations of entrained flow gasification. This study used the \(n^{th}\) order Arrhenius rate expression to model the kinetics along with the RPM. It is generally accepted that the \(n^{th}\) order equation may be inaccurate in modeling the pressure-dependence of gasification kinetic rate expressions. Our review indicates that gasification kinetics are better represented by Langmuir-Hinshelwood (LH) type rate expressions for char-\(\text{CO}_2\) and char-\(\text{H}_2\text{O}\) reactions [29][30][31][32][33]. For char-\(\text{CO}_2\) reaction, the LH kinetic rate, \(R_{LH}\), can be expressed as:
\[ R_{LH} = \frac{k_1}{1 + k_2 P_{CO_2} + k_3 P_{CO}} \]  \hspace{1cm} (2-33)

where \( k_1, k_2, k_3 \) are Arrhenius type constants. Similar equations are written for the char-O\(_2\) and char-H\(_2\)O reactions. The LH-type rate is found to be a better fit [34] for the gasification reactions than an \( n^{th} \) order Arrhenius type rate expression. In conjunction with the RPM, the char consumption rate for the char-CO\(_2\) reaction, assuming complete kinetic control, can be written as

\[ \dot{m}_p = k_s P_g = R_{LH} m_{pa} S P_g \]  \hspace{1cm} (2-34)

It is also useful to write the char consumption rate under complete diffusion control.

\[ \dot{m}_p = P_g k_d \]  \hspace{1cm} (2-35)

The formulation in equation (2-33), after extensive derivation [35] is consistent with the following reaction steps:

\[ C_f + CO_2 \rightarrow CO + C(O) \hspace{1cm} C_f: \text{free carbon site} \]
\[ C(O) \rightarrow CO \]  \hspace{1cm} (R9)

Since the LH mechanism accounts for the fundamental heterogeneous kinetic processes of adsorption and desorption, the LH-type rate expression is found to be better for the gasification reactions than an \( n^{th} \) order Arrhenius type rate expression. The gasification rate for char-CO\(_2\) reaction, when experimented upon in the kinetics-limited regime at temperatures up to 1500 K, has been found to increase with the partial pressure of CO\(_2\) up to a point and then remain constant. An LH-type relation models such behavior much better than an \( n^{th} \) order one. The
The $k_3 P_{CO}$ term in (2) pertains to the inhibition in the gasification reaction due to saturation of the char activated surface by CO at high CO partial pressures.

Several variations of the LH mechanism exist in the literature, aimed towards capturing the physics of the heterogeneous reactions better. For example, in one study a modified nth order LH relation was observed to perform better than the first order LH relation [49]:

$$C + O_2 \xrightarrow{ads} C(O)$$

$$C(O) \xrightarrow{des} CO$$

(R10)

$$R_{C-O_2} = \frac{k_{ads} P_{O_2,s}^n}{1 + \left( \frac{k_{ads}}{k_{des}} \right) P_{O_2,s}^n}$$

(2-36)

Here $n$ can be thought of as the order of the adsorption step in reactions R10.

More sophisticated rate expressions are also available [31][30] referred to as the semi-global models, which take into account, to various degrees, the possible adsorption and desorption sub-steps of intermediate complexes for the particular heterogeneous reactions. For example, in [30]:

$$R_{C-CO_2} = -\frac{k_7 k_4 P_{CO_2}}{k_7 + \gamma k_4 P_{CO_2} + \gamma k'_4 P_{CO} + k_4 P_{H_2O} + k'_6 P_{H_2}} \text{ s}^{-1}$$

(2-37)

$$R_{C-H_2O} = -\frac{k_7 k_6 P_{H_2O}}{k_7 + \gamma k_4 P_{CO_2} + \gamma k'_4 P_{CO} + k_4 P_{H_2O} + k'_6 P_{H_2}} \text{ s}^{-1}$$
No work to-date on the CFD modeling of gasification has employed the LH-type relations. The simulations of the MHI and GE gasifiers in Chapter 4 incorporate LH kinetics of the form described by equation (2-33), for which experimental data is available [36][32].

The model still ignores the pore diffusion effects within the particle and assumes a constant reactant concentration inside the particle. The model could be improved to include pore diffusion effects by incorporating an effectiveness factor $\eta$, derived by solving a reaction-diffusion equation within the particle [37] and coming up with a correction factor. In spherical coordinates, $\eta$ can be expressed as:

$$\eta = \frac{1}{\theta} \left( \frac{1}{\tanh(3\theta)} - \frac{1}{3\theta} \right)$$

(2-38)

$$\theta = \frac{r_p}{3} \sqrt{\frac{v_o k_1 k_2 P_g}{2D_e 1+k_2 P_g} (k_2 P_g - \ln(1+k_2 P_g))^{-1/2}}$$

where $k_1$, $k_2$ are the corresponding constants in the LH reaction rate expression (2-33), $v_o$ is the stoichiometric coefficient for the particular gasification reaction and $D_e$ is the internal particle diffusivity.

There are several references in literature to this kind of pore-diffusion correction [38][39] essentially by researchers investigating single particle gasification. To the best of our knowledge, the impact of this effectiveness factor calculation on CFD modeling of entrained flow gasification has not been studied yet. Figure 2-5 shows the variation of $\eta$ for char-CO$_2$ reaction with reaction temperature for a particle of mean diameter in our gasifier. $\eta$ varies from 0.2-1 as generally reported in the literature [38][39]. The present work incorporates the impact of pore diffusion via the effectiveness factor approach described in this section.
2.2.9.2 Single vs double film model

With regards to modeling the transport and homogeneous reactions within the boundary layer of the char particle, broadly two approaches are found in the literature. The first approach, namely the single film model described by equations (2-26) – (2-28), is routinely employed in gasification studies in literature [23][5][40][6][41][7][2][22]. As depicted in figure 2-6(a), the single film model [42] assumes that although CO and O₂ are present simultaneously in the boundary layer around the particle, they do not react with each other. CO and O₂ are allowed to react only after they diffuse out of the boundary layer. To the contrary, the double film model [42], as shown in figure 2-6(b), allows CO and O₂ to react in a diffusion flame in the boundary layer to yield CO₂ which then diffuses on one side towards the particle and on other side into the well-mixed region.
Figure 2-6: (a) Single film and (b) Double film models of char consumption [42]
The most accurate method of predicting char consumption rate would involve solving the complete set of reaction-diffusion equations throughout the particle and into the boundary layer. Efforts within our group to perform such calculations indicate that reality is much closer to the double film than the single film model, as indicated in figure 2-7. The results indicate that homogeneous reactions do occur in the boundary layer and there seems to be a flame-zone outside the particle where both CO and O₂ mole fractions tend to zero and the temperature profile attains a peak. However, the double-film model has not been employed in CFD models of combustion or gasification because, depending on the assumptions, it requires the solution of a system of coupled algebraic equations, if not coupled PDEs. Solving PDEs for each tracked particle can be computationally prohibitive for well-resolved CFD model of any commercial or pilot scale gasifier.

Figure 2-7: Continuous film model
However, using a set of simplifying assumptions, Zhang et al. [43][44] have proposed the moving flame front (MFF) model of char consumption, reducing the set of governing equations such that it can be adapted to CFD model without significant computational expanse. The location of the flame sheet, where oxidation of CO occurs in the boundary layer, and consequently the char consumption rate can be evaluated as explicit functions of various kinetic and diffusion rates involved. The key assumptions involved include neglecting the heterogeneous reaction R5, as referred to in Table 2-3, since in presence of oxygen R4 is proceeds at a much faster rate than R5. Further, the location of flame sheet is allowed to vary based on the instantaneous particle parameters and species mole fractions in the bulk. The flame sheet location is evaluated assuming that it dynamically adjusts so that equilibrium is approached at the fastest possible rate. In the limiting case when R5 is assumed to be much slower than R4, the char consumption rate given by equation (2-26) gets modified by incorporation of MFF model to become:

\[
\frac{dm_p}{dt} = \frac{P_g}{k_d \left( 1 + \frac{d_p}{b} \right) + \frac{1}{k_s}}
\]  

(2-39)

where \( b \) is the location of flame front. It can be inferred from equation (2-39) that as the flame front moves farther away from the particle surface, the diffusion resistance increases and the net burning rate decreases. In the absence of any limiting assumptions, the expressions for the net burning rate and location of the flame front are more complicated [44] and are incorporated into the present Fluent model via a user-defined C subroutine. In Chapter 4, the impact of switching from the single film model to MFF model on the predictions of the MHI pilot-scale gasifier is presented and the corresponding implications are discussed.
References


Chapter 3
VALIDATION OF SUBMODELS

3.1 Chapter Overview

In this paper, two canonical turbulent flow test cases from the literature that exhibit sophisticated flow patterns similar to those found in typical gasifiers, are chosen and the impact of the choice of the turbulence model, on prediction of the flow fields in these cases, is described. Further, the validation and optimization of the particle turbulent dispersion model, generally employed in literature, is discussed.

3.2 Background and Motivation

The turbulent flow solver, including the turbulence closure model, forms the backbone of the structure of any reacting flow model. Unless the underlying flowfield is predicted with acceptable accuracy, errors will invariably propagate through the rest of the model structure. The two-way coupling between flow variables like shear and turbulent fluctuations on one hand and reaction rates and heat release on the other has already been demonstrated in combustion literature [1][2]. In case of a two-phase reacting flow, the flow solver, including the turbulent dispersion model, assumes even greater importance because the location and the extent of predicted large and small scale flow structures play an important role in determining the residence times of particles. Recirculation zones, desirable since they trap particles and enhance char conversion, if predicted accurately lead to improved estimates of not just carbon conversion but also local temperatures and wall heat transfer.
For someone interested in combustion systems modeling, a variety of turbulence models are available to choose from, ranging from the transient, computationally intensive but more accurate DNS/LES methods to the time-averaged, computationally cheap but coarser RANS methods. The various RANS methods developed over the years for turbulence modeling include the standard k-ε model with its multiple variants including the RNG k-ε, Realizable k-ε, non-linear k-ε models. In addition we have the standard k-ω and the SST k-ω models apart from the more computationally expensive Reynolds Stress Models (RSM). It is further possible to have, over and above each of these RANS methods, subtle variations and minor improvements to make the individual models applicable over a variety of flow regimes, including swirling, separating and transitioning flows.

The dependence of predicted flowfield on the particular turbulence model has been aptly demonstrated in the literature of general turbulence modeling [3][4][5] as well as combustion/gasification systems modeling [6][7][8]. Upon analysis of these studies, many of which contain comparisons with experimental data, it becomes clear that while there is an agreement that LES predictions are reasonably accurate, no such consensus exists about the performance of the various RANS models. The standard k-ε model has been adopted in most CFD simulations of gasification [9][10][11][12][13]. However, it has been observed, in several different studies, that the standard k-ε model fares poorly in predicting the mean flow properties in canonical turbulent flow situations, especially when shearing, separating and swirling flows are involved [7][14][15][16]. Such inaccuracy can prove to be severely detrimental while modeling gasification, since one expects to observe high shear and swirling flows in at least some regions of most commercial gasifiers.

The other RANS models used in gasification literature, albeit sparsely, include the Realizable k-ε, non-linear k-ε and the RSM models. The PCGC (pulverized coal gasification and combustion) models [17] developed at Brigham Young University over the 80’s and 90’s employed a non-linear k-ε model, wherein the Reynolds stress tensor is represented as a nonlinear expansion of the Boussinesq hypothesis retaining several nonlinear terms that are neglected in the standard
k-ε model. Wu et. al. [18] employed the Realizable k-ε model in their gasification model of the GE-Texaco design. The choice was based on an earlier study [19] on comparison between various turbulence models with experimental data for cold flow of a co-axial jet stream in a Texaco gasifier testbed. It was observed that although the three tested k-ε models yielded similar predictions, the Realizable k-ε and the RNG k-ε models performed slightly better than the standard k-ε model, with the Realizable k-ε model being marginally better than the RNG counterpart. Fletcher et. al. [20] employed RSM in their CFD model of a pilot scale biomass entrained flow gasifier. The choice was based on an earlier study [21] in which RSM was observed to predict a cold swirling flow pilot scale gasifier test case much better than the standard k-ε model. RSM predicted the existence of the expected recirculation zone whereas the standard k-ε model failed.

Some gasification simulations attempted to overcome the much-observed deficiencies of the standard k-ε model by resorting to ‘improved’ RANS models. However, a larger survey of the fluid mechanics and combustion literature indicates that there is a disagreement over whether these RANS models are the most appropriate choices in predicting swirling and shearing flow fields. For example, it has been observed that both the standard and the non-linear k-ε models suffer from a similar deficiency of poorly predicting mean velocities in confined swirling flows [22]. Menzies [23] observed that the non-linear, realizable and the RNG k-ε models performed worse than the standard k-ε model in predicting swirling isothermal flow inside a gas turbine combustor. Again, Marzouk [3] observed that the standard k-ε model performed better than the realizable and the RNG k-ε models in predicting mean gas phase velocities in simulations of co-axial particle laden swirling air flow in a vertical circular pipe. Generally, RSM produces better predictions of swirling flow than the various k-ε models [22][7][16] since it relaxes the assumption of isotropy used by the Boussinesq approximation. A few studies, though, dispute this conclusion and observed that RSM performs poorly as compared to one or more of the k-ε models [4][24]. Since RSM solves for seven transport equations, instead of two in the eddy viscosity based models, it is argued that more rigorous closure strategies are needed, in turn, for the closure of various terms in those equations [25]. However, a major shortcoming of RSM is its

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higher computational complexity and the concomitant stability issues. Various studies have reported difficulties in obtaining a convergent solution with RSM [26][27], especially when complex flow fields are involved [28]. This difficulty is expected to be compounded at high mesh resolutions. Wu et. al. observed that the RSM had rigorous grid quality requirements in order to predict velocity fields correctly, whereas the k-ε models could predict better numerical solutions based on a reasonable grid [19]. In our own simulations, as discussed in section 3.1, we found that RSM takes too long to converge and experiences numerical instabilities under high mesh resolutions.

Another RANS model, not yet tested in the gasification literature, is the k-ω model [29]. The k-ω model is a two-equation turbulence model, based on eddy viscosity formulation similar to the k-ε models, but with ε replaced by the quantity ω, which is analogous to ε/k. A version this model, called the shear stress transport (SST) k-ω model, which blends the standard k-ε and the k-ω models in appropriate regions [30], has been frequently and successfully applied in the analysis of problems involving swirling and shearing flows [31][32][33], especially in simulations of gas turbine combustors [21][22][23]. Because of its good performance in the authors’ ‘preliminary investigations’ of turbulent swirling free-jets, the SST model has also been employed to simulate combustion of baled biomass [37]. The SST model was also shown to perform better than the standard and the RNG k-ε models [33] and the Realizable k-ε model in swirling flow situations [21]. In another study, the SST model predicted the presence and extent of recirculation zone in a confined swirling flow reasonably well, whereas the standard and non-linear k-ε models failed to predict its presence at higher swirl numbers [38]. Again, using the SST model resulted in better predictions of flame length and turbulence intensity than the standard and non-linear k-ε models in simulations of premixed combustion [31]. Hence, there appears to be a strong case to test and implement the SST k-ω model in gasification studies. In Part I of this paper, we will show that the SST k-ω model yields the most satisfactory predictions of swirling and non-swirling canonical flow cases. In Chapter 4, we will apply the insights from this validation into the construction of the integrated gasification model.
Before describing the validation studies, it should be mentioned that only a few gasification studies in the past have performed extensive flow solver validation as a part of their validation strategy. The PCGC models were based on some cold flow validation studies on laboratory scale gasifier measurements. The conclusion was that the standard k-ε model did a reasonable job of predicting the mean flow fields in both swirling and non-swirling flows, though PCGC-3 later adopted the non-linear k-ε model, probably based on further studies. The cold flow study by Wu et al. was based on a single test case of non-swirling co-axial flow in a Texaco gasifier. The various RANS models tested yielded similar results, apart from the coarser Spalart-Allmaras model, though the Realizable k-ε model was observed to be slightly better than the others [19].

The aim of the present study is to analyze the relative performance of the most popular RANS models, using the CFD package Fluent, through a comprehensive validation framework of canonical flow cases bearing resemblance to the flow patterns expected in typical gasifiers.

The rest of the chapter is organized as follows. Section 3.3 briefly lays out the general turbulence model formulation applicable to all test cases in this study. Section 3.4.1 describes flow solver validation using the swirling and non-swirling flow sudden expansion test cases. In section 3.4.2, flow solver validation using the two-phase flow bluff body test case is described. Section 3.5 uses the same test case to validate the particle turbulent dispersion model. Finally, in section 3.6, the conclusions from the validation studies in this chapter are discussed.

### 3.3 Turbulence model description

Spatially and temporally averaged transport equations for mass and momentum are solved using the finite volume method with a second order upwind scheme on 3-D unstructured meshes for all the cases described in this chapter. For the RANS turbulence models analyzed in this work, two additional transport equations are solved. The formulation of the additional transport equations depends upon the particular turbulence model. For example, while the standard k-ε model solves transport equations for the turbulent kinetic energy, $k$, and its
dissipation rate, $\varepsilon$, the $k$-$\omega$ model solves transport equations for the turbulent kinetic energy and the specific dissipation rate, $\omega$. Equations (3-1) – (3-3) describe the standard $k$-$\varepsilon$ model and equations (3-4) – (3-6) describe the SST $k$-$\omega$ model.

\[
\frac{\partial}{\partial x_i} \rho ku_i = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G - \rho \varepsilon + S_k \tag{3-1}
\]

\[
\frac{\partial}{\partial x_i} \rho \varepsilon u_i = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_1 G - C_2 \rho \frac{\varepsilon^2}{k} + S_\varepsilon \tag{3-2}
\]

\[
\frac{\mu_t}{\sigma_\varepsilon} = \frac{\varepsilon}{C_i} \tag{3-3}
\]

\[
\frac{\partial}{\partial x_i} \rho ku_i = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k - Y_k + S_k \tag{3-4}
\]

\[
\frac{\partial}{\partial x_i} \rho \omega u_i = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\omega} \right) \frac{\partial \omega}{\partial x_j} \right] + G_\omega - Y_\omega + D_\omega + S_\omega \tag{3-5}
\]

\[
\frac{\mu_t}{\sigma_\omega} = \alpha^* \frac{\rho k}{\omega} \tag{3-6}
\]

$C_1$, $C_2$, $C_i$, $\sigma_k$, $\sigma_\varepsilon$, $\sigma_\omega$ are modeling constants whereas $G$, $G_k$, $G_\omega$, $Y_k$, $Y_\omega$, $D_\omega$ represent various generation and depletion terms within the corresponding transport equations. $S_k$, $S_\omega$, $S_\varepsilon$ are user-defined source terms and $\alpha^*$ is the damping coefficient for turbulent viscosity in the $k$-$\omega$ model. Standard values are used for all modeling constants in the transport equations. The SST
k-ω model retains the k-ω model formulation in the near-wall region and switches to the standard k-ε model formulation in the far field region using an appropriate blending function. This modification allows the SST model to generate improved results in adverse pressure gradient flows and swirling flows [30]. The realizable and the RNG k-ε models attempt to improve upon the performance of the standard k-ε model, at least in some target scenarios, by varying their formulation using filtered unsteady equations, as opposed to the time-averaged formulation of the RANS models. LES directly captures the unsteadiness at the larger energetic scales while attempting to model the smaller, lesser energetic scales. Detailed description and formulation of these turbulence models are described in [39].

The particle phase is treated via stochastic Lagrangian tracking. In order to simulate turbulent dispersion, particle of each diameter is stochastically tracked ten times with random fluctuations imposed on the velocity of the surrounding gas-phase. The mesh resolution employed in each of the test cases in section 3.4 is arrived at by corresponding mesh independence study.

### 3.4 Flow solver validation

#### 3.4.1 Axisymmetric sudden expansion

The geometry for the first test case used in the validation of the flow solver is presented in Figure 3-1. The geometry is cylindrical and is used for a non-swirling flow case and a swirling flow case. The flow inlet is located at x=-2D and the flow encounters an axisymmetric sudden expansion downstream at x=0.
The Reynolds number, based on the upstream diameter $D$, is 30000 in both cases. The input parameters are the measured mean axial and tangential velocity profiles at the flow inlet. The swirl number $S$, defined as the ratio of the axial flux of the tangential momentum to the axial flux of the axial momentum times radius, is 0.6 in the swirling case.

$$S = \frac{2 \int \rho uu_\theta r dA}{D \int \rho u^2 dA}$$

(3-7)

where $u$ is the axial velocity and $u_\theta$ is the tangential/swirl velocity. At $S=0.6$, a recirculation zone is formed downstream of the sudden expansion. The test case is utilized to validate the flow solver's capability in predicting the inherent flow structures in the case of (1) sudden expansions/variations in flow geometries observed in some gasifiers and (2) recirculating and swirling flows as observed in other gasifiers, e.g., the MHI and Shell designs.

Measured velocity and velocity fluctuation profiles are provided as inlet boundary conditions at $x=-2D$. Outflow boundary condition is provided on the flow outlet at $x=-10D$. A grid resolution of 800,000 cells is chosen to simulate this case with the RANS models. No difference in results is observed upon switching to a finer grid of 1.6 million cells. However, the grid of 1.6 millions cells...
is found to produce better results than the coarser grid for LES simulations. A time step of 1 ms was chosen for LES simulations, consistent with the CFL criterion. Statistics, for computation of mean and rms values, are gathered for approximately eight to ten flow-through times after attainment of statistically steady state.

The grid with 800,000 cells is depicted in Figures 3-2(a) and 3-2(b). It can be seen that the mesh is finer in the radial and azimuthal directions in all the near-wall regions, as well as in the shear layer formed as flow expands out from the inlet pipe. The mesh is also finer in the axial direction just ahead of the sudden expansion and successively coarsens into the far downstream region. In addition, the inlet pipe is provided with enhanced mesh resolution to guarantee the development of turbulence from imposed velocity boundary conditions at the inlet, especially for LES simulations.

Figures 3-3 and 3-4 show the predicted mean x-velocity along the centerline for swirling and non-swirling flow cases respectively. The standard k-ε model and its variations discussed in Section 3.3 are compared with the SST k-ω and LES models. The blue, green, magenta, red and black lines represent the standard k-ε, Realizable k-ε, RNG k-ε, SST k-ω and LES model predictions respectively. Since the RNG k-ε model performs quite poorly in the swirling flow case, predicting a double-trough in the x-velocity in place of the singular trough suggested by experiments, it is rejected in further case studies discussed in this section. Among the remaining models, LES provides the best predictions for both swirling flow and non-swirling flow cases whereas the standard k-ε model predictions are least satisfactory. This observation is noteworthy since, as mentioned in Section 1, most CFD studies of gasification employ the standard k-ε model to predict turbulence.
Figure 3-2: Axisymmetric sudden expansion geometry mesh along (a) center-plane (b) lateral cross-section
Figure 3-3 and 3-4 demonstrate that Realizable $k$-$\varepsilon$ and SST $k$-$\omega$ deliver the best predictions among the tested RANS models. In the swirling flow case, SST $k$-$\omega$ model outperforms the Realizable $k$-$\varepsilon$ model for most regions upstream and downstream of the sudden expansion except towards the end of the domain where the Realizable $k$-$\varepsilon$ model performs marginally better. In the non-swirling flow case, both models yield similar predictions up to 0.2 m downstream of the sudden expansion beyond which SST $k$-$\omega$ model performs better.

A noteworthy observation from Figure 3-4 is that simulations with both RANS and LES models tend to overpredict axial velocities along the centerline, especially far downstream. The overprediction of mean centerline velocities far downstream is typical in simulations of swirling turbulent flows, especially for the RANS models. The reason appears to be the inability of RANS approaches to accurately model the spanwise momentum transport owing to the simplistic eddy viscosity approximation. It should also be noted that the LES model captures well the location and extent of the central recirculation zone in the swirling flow. Among RANS models, only the SST $k$-$\omega$ model reasonably captures the central recirculation zone, although it overpredicts the axial velocities towards the exit.

Figure 3-5 shows the extent of the recirculation zone predicted by various models in the swirling flow case through contours of axial-velocity. While the standard $k$-$\varepsilon$ model predicts a very weak recirculation zone, the LES and SST $k$-$\omega$ models predict the expected size and extent of the recirculation zone downstream of the sudden expansion. While the LES and SST $k$-$\omega$ model predictions are seen to be qualitatively similar, figure 3-5 also demonstrates out the differences between them. However, keeping in mind the significant benefit in computational expense that RANS modeling offers as compared to LES, the match between LES and SST $k$-$\omega$ model predictions can be considered quite encouraging. Figure 3-6 compares axial velocity contours predicted by the same models for the non-swirling flow case. The three models give very similar results under non-swirling flow conditions.
Centerline x-velocity

Figure 3-3: Centerline mean axial velocity for swirling flow case

Figure 3-4: Centerline mean axial velocity for non-swirling flow case
Figure 3-5: Contours of mean axial velocity (m/s) for swirling flow case
Figure 3-6: Contours of mean axial velocity (m/s) for non-swirling flow case
Figures 3-7(a) – 3-7(d) show mean and RMS axial and tangential velocities at various downstream sections in the flow for the swirl case. The solid lines represent Realizable k-ε model predictions, the dotted lines represent LES predictions and the dash-dot lines represent k-ω model predictions. The comparisons with experimental data for the standard k-ε and the RNG k-ε models are not presented, being much inferior in quality to the rest of the models. Figures 3-7(a) – 3-7(d) further demonstrate that LES offers the best agreements with experimental data for the mean as well as RMS velocities. Figure 3-7(a) shows that the RANS models underpredict the boundary layer close to the wall and overpredict the axial velocity at the centerline. Moreover, as seen from Figures 3-7(a) and 3-7(b), the SST k-ω model predictions are better than those of the Realizable k-ε model at most sections for both mean axial and tangential velocities.

The RMS values are satisfactorily predicted by the LES model, as evident from Figures 3-7(c), 3-7(d). RMS values can also be generated for the RANS models using the turbulent kinetic energy, $k$, although the values so generated are isotropic.

$$u' = v' = w' = \sqrt{2k/3}$$

The RMS values for the SST k-ω and the Realizable k-ε models compare well with experiments considering the fact that they are derived from steady-state rather than transient simulations. In order to understand the success of the SST k-ω model in predicting vortex breakdown, it should be noted that, in general, the k-ω model is observed to predict separating flows and near wall flows quite accurately [29]. Moreover, it has been suggested that the physical mechanism behind vortex breakdown might be similar to that of flow separation [41]. Hence, it is reasonable to assume that the success of the k-ω model in predicting vortex breakdown in a swirling flow is because it was originally formulated to predict separating flows.
Figure 3-7(a) Mean x-velocities, swirl case. Solid line: Realizable k-ε, Dotted line: LES, dot-dashed line: k-ω, symbols: experiments

Figure 3-7(b) Mean tangential velocities, swirl case. Solid line: Realizable k-ε, Dotted line: LES, dot-dashed line: k-ω, symbols: experiments
Figure 3-7(c) RMS x-velocities, swirl case. Solid line: Realizable k-ε, Dotted line: LES, dot-dashed line: k-ω, symbols: experiments

Figure 3-7(d) RMS tangential velocities, swirl case. Solid line: Realizable k-ε, Dotted line: LES, dot-dashed line: k-ω, symbols: experiments
Figures 3-8(a) - 3-8(c) show the radial variation of mean and RMS velocities at various downstream sections in the non-swirl case. Similar to the swirling flow case, only comparisons for the Realizable k-ε, SST k-ω and LES models are presented, being represented by solid, dash-dot and dotted lines respectively. LES predicts the mean x-velocity profiles better as expected, though RANS predictions are also quite good, especially for the SST k-ω model. The RMS x-velocities and tangential velocities shown in Figures 3-8(b) and 3-8(c) are also satisfactorily predicted by LES, though less so by the RANS models. At the distant downstream sections, the RMS x-velocities are slightly underpredicted by the RANS models, indicating faster decay of turbulence in simulations as compared to experiments.

Before closing this section, it should be noted that various studies in the literature have tried to improve the performance of the standard k-ε model in predicting confined swirling flows by either modifying its modeling constants [42] or by adding various source terms to the transport equations for k and ε [43][44]. We tested several of these approaches for the swirling and non-swirling sudden expansion cases as well as the two-phase bluff body case described in the next section. Our results showed that while most modifications had negligible improvement in prediction sudden expansion swirling flow case, a few others caused a more notable improvement only to greatly ill-predict the sudden expansion non-swirling flow case and/or the two-phase bluff body case. In a nutshell, we do not recommend tweaking the standard k-ε model constants or source terms in order to predict complicated flows like those observed in gasifiers.

In summary, the results from the axisymmetric sudden expansion case demonstrate that the SST k-ω model performs best among the RANS models, followed by the Realizable k-ε model. Hence, these two models are selected for the case study in the next section.
Figure 3-8(a) Mean x-velocities, non-swirl case. Solid line: Realizable k-ε , Dotted line: LES, dot-dashed line: k-ω, symbols: experiments

Figure 3-8(b) RMS x-velocities, non-swirl case. Solid line: Realizable k-ε , Dotted line: LES, dot-dashed line: k-ω, symbols: experiments
Figure 3-8(c) RMS tangential velocities, non-swirl case. Solid line: Realizable $k$-$\varepsilon$, Dotted line: LES, dot-dashed line: $k$-$\omega$, symbols: experiments

### 3.4.2 Two-phase bluff body flow

The geometry of the second test case, intended to validate the flow solver as well as the particle turbulent dispersion mode, is presented in Figure 3-9. The test case and experimental data are taken from the work of Boree et. al [45]. The geometry is cylindrical and consists of two flow inlets, at $x=0.1m$, and a single outlet at $x=0.8m$. While glass beads/particles are injected along with air at the inlet of the inner pipe, only air is injected at the inlet of the annular pipe. The mass flow rates in the inner flow and co-flow are such that $\frac{U_i}{U_C} = 0.84$, where $\overline{U_i}$ is the average velocity in the inner flow and $\overline{U_C}$ is the average velocity in the co-flow. The flow regimes in this Bluff-body flow are heavily dependent on the ratio of the mass flow rates in the
inner pipe flow and the co-flow. These aspects have been studied well [46] and the current ratio of 0.84 leads to the formation of internal and external recirculation zones downstream of the bluff body as shown in Figure 3-9.

\[
\frac{U_i}{U_c} = 0.84
\]

\[
\begin{align*}
R_1 &= 0.01 \text{ m} \\
R_{c,1} &= 0.15 \text{ m} \\
R_{c,2} &= 0.075 \text{ m} \\
Re &= 73000 \\
L_1 &= 0.1 \text{ m} \\
L_2 &= 0.8 \text{ m}
\end{align*}
\]

Figure 3-9: Geometry for two-phase bluff body flow case
The ratio of solid-phase mass flux to that of gas-phase in the inner duct is 22%, which results in negligible impact of the particle phase on the gas phase [47]. The particles are injected at the inner pipe inlet with the local gas phase velocity. The utility of the present test case is two-fold: (1) to validate the flow solver for cases where a narrow incoming jet of gas and particles is entrained by a larger stream separated by a bluff body; such situations arise in the radial/tangential injections in several gasifiers, e.g., the MHI, PRENFLO, Shell and E-Gas gasifier designs, and (2) to validate the current particle turbulent dispersion model, once the underlying gas phase flow is reasonably predicted.

A grid resolution of 1 millions cells was chosen to simulate this case with the RANS models. No difference in results was observed upon switching to a finer grid of 2 million cells. Measured velocity and velocity fluctuation profiles are provided as inlet boundary conditions on the inner and outer pipe inlets. Particles are injected with the same velocity as the gas phase at the inner pipe inlet. Outflow boundary condition is provided on the flow outlet at \( x=-0.8 \)m. The grid with 1 million cells is depicted in Figures 3-10(a) and 3-10(b). It can be seen that the mesh is finer in the radial and azimuthal directions in all the near-wall regions, as well as in the two shear layers formed downstream of the bluff body as flow expands out from the inner and outer pipes. Further, as discussed in the next section, the flow undergoes sharp deceleration within a small region just downstream of the bluff body. Hence, the mesh is made finer in the axial direction within a region 0.15m ahead of the bluff body in order to capture the sharp gradients in that region, and then successively coarsens into the far downstream section.

Figure 3-11 shows the mean axial gas velocity along the centerline of the bluff body. The blue, green and red lines represent the predictions from the standard k-\( \epsilon \), Realizable k-\( \epsilon \) and SST k-\( \omega \) models respectively. Comparison with experimental data shows that, similar to the sudden expansion case, SST k-\( \omega \) model performs the best. It is most accurate among the three models in the region just downstream of the bluff body. Although the standard k-\( \epsilon \) model is marginally better than the SST k-\( \omega \) model toward the exit, it greatly overpredicts just downstream of the bluff body. The Realizable k-\( \epsilon \) model also overpredicts the mean axial velocity just downstream
Figure 3-10: Two-phase bluff body case mesh along (a) center-plane (b) lateral cross section
of the bluff body. Moreover, the Realizable $k$-$\varepsilon$ model performs the worst among the three models in the recovery region downstream of the recirculation zone. Owing to the demonstrated superiority of SST $k$-$\omega$ model over other RANS models tested in sudden expansion and two-phase bluff body flow test cases, it will be used for gasifier simulations in Chapter 4.

Figure 3-12 shows the predictions of the particle mean axial velocity along the centerline. Particles are injected uniformly from the inlet surface of the inner pipe. The injection velocity is set equal to the local gas velocity. The solid blue, green and red lines represent predictions with three different numbers of tracked particles, with the blue line representing 5712 tracked particles, green line representing twice as many tracked particles as the blue line and the red line representing four times as many tracked particles as the blue line. The three predictions are quite close indicating convergence with respect to the number of tracked particles. Further, the comparisons with experimental data are encouraging. Although the predicted centerline velocity drops too rapidly compared to experimental data within the recirculation zone, we observe excellent comparison in the downstream region. The discrepancy in predictions in the recirculation zone, just downstream of the bluff body can be attributed to the simplistic RANS model assumption of equilibrium between creation and dissipation of turbulence. This assumption is expected to break down in the complex flow regime established just downstream of the bluff body.
Figure 3-11: Gas mean x-velocities. Solid line: RANS k-\(\varepsilon\), symbols: experiments;

Figure 3-12: Particle mean x-velocities. Solid lines: predictions, symbols: experiments.
Figure 3-13: Contours of mean gas-phase axial velocity (m/s)

Figure 3-13 shows the contours of mean gas-phase axial velocity. The recirculation zone formed downstream of the bluff body as well the mixing layer formed between the bulk flow and the outer inlet are clearly observable. Moreover, the high gradients observed in the region just downstream of the bluff body as well as in the mixing layer justify the enhanced mesh resolution in those regions as depicted in figures 3-10(a) and 3-10(b). Figures 3-14(a) and 3-14(b) show a comparison between the predicted and experimental gas mean x-velocities and radial velocities respectively at various sections downstream of the bluff body. The predicted x-velocities are in good comparison with the experimental data. The predicted radial velocities also compare reasonably well with the experimental data except for slight discrepancies in the sections within the recirculation zone. Figures 3-15(a) and 3-15(b) show a comparison between the predicted and experimental gas RMS x-velocities and radial velocities respectively. Again,
Figure 3-14(a) Gas mean x-velocities. Solid line: SST k-ω, symbols: experiments

Figure 3-14(b) Gas mean radial-velocities. Solid line: SST k-ω, symbols: experiments
Figure 3-15(a) Gas RMS x-velocities. Solid line: SST $k$-$\omega$, symbols: experiments

Figure 3-15(b) Gas RMS radial-velocities. Solid line: SST $k$-$\omega$, symbols: experiments
predicted RMS values are evaluated assuming isotropic turbulence, as is the practice in eddy viscosity turbulence models, using the relation $u' = v' = w' = \sqrt{2k/3}$ where $k$ is the turbulent kinetic energy. The assumption of isotropic turbulence seems reasonable in the bluff body case, judging from the good comparisons with experimental data in Figures 3-15(a) and 3-15(b), although slight overprediction is observed radially outwards of the second shear layer and towards the bounding wall in most sections. The RANS model does not seem to capture well the damping effect of bounding wall on turbulence.

The predictions for this two-phase bluff body flow, shown in Figures 3-11, 3-12, 3-14 and 3-15, are encouraging. The RANS approach is much cheaper than the LES simulations; the latter was reported in [47]. It should be noted that comparisons with experimental data are better for the RANS models in the two-phase bluff body case than in the sudden expansion case notwithstanding the fact that the former also involves significantly more complicated flow structures including formation of an internal recirculation zone along the axis and an external recirculation zone just ahead of the bluff body. This observation suggests that although the RANS models leave out the unsteady phenomena intrinsic to turbulence, they can also yield surprisingly close match with experimental data in many practical applications.

We also performed LES simulations for this case using a second order upwind scheme. The LES results yielded poor comparisons with experimental data as compared to the RANS models. It has been reported that second order schemes yield unsatisfactory results in the LES of two-phase bluff body case and a third order finite element scheme performs significantly better [47]. Our work on comparing LES, incorporated with higher order differencing and well-resolved initial conditions, with RANS for this test case will be presented in a future study.
3.5 Particle Turbulent Dispersion Model Validation: Two-phase bluff body flow

Since the mean flow is well predicted by the RANS model, the bluff body case is a suitable candidate for the validation of the particle dispersion model. A good agreement with particle mean velocity experimental data would suggest that the current dispersion model satisfactorily describes the effect of fluid turbulence on the particle trajectory. The particle dispersion model incorporated in these simulations has been described in Chapter 2 using equations (2-10), (2-11) and (2-14) – (2-18). By computing the particle trajectory repeatedly using this dispersion model, we can expect to take the effect of turbulence dispersion on particles into account. Similar models of turbulent particle dispersion have been used in previous studies of coal gasification [10][11][13].

c, a normally distributed random number, imparts a stochastic nature to the particle dispersion. Before presenting the prediction of the particle mean and rms velocities, it is useful to describe the sampling and averaging procedure employed to obtain these values from the lagrangian tracking methodology. A total of 17208 particles, as justified based on trends observed in figure 3-12, were tracked to gather statistics. Owing to the stochastic nature of particle dispersion, the particles sampled at any section would arrive with a distribution of velocities.

Figures 3-16(a) and 3-16(b) show the particle axial velocities sampled along the geometry centerline and a sample plane at x = 8cm respectively. Red line represents the sampled axial velocity whereas black line represents the velocity profile obtained following the averaging procedure. The averaging or smoothing procedure involves local regression using weighted linear least squares and a second degree polynomial model. A lower weight is assigned to the outliers for better smoothing. Local rms values are evaluated using the local averaged value thus calculated and twenty sample points on either side of the data point under consideration.
Figure 3-16: Particle velocity data sampling procedure at (a) geometry centerline (b) sample plane $x = 8$cm
Figures 3-17(a) and 3-17(b) show a comparison between the predicted and experimental data for particle mean axial and radial velocities respectively at various sections downstream of the bluff body. The comparisons are good at most sections except at a couple of sections within the recirculation zone. The underprediction of x-velocity close to the axis within the recirculation zone, e.g., at section at x=16 cm in Figure 3-17(a), was also observed in Figure 3-12. But largely, the predicted radial variations of x-velocities at all sections are observed to be faithful to the experimental data.

Again, discrepancies are observed in the radial velocity predictions within the recirculation zone, at sections x=16 cm and x=20 cm. These discrepancies can be attributed to the difficulty in predicting the characteristics of the recirculation zone itself in such complicated flows. For example, the gas-phase mean radial velocities have similar discrepancies at the same sections in Figure 3-14(b). Since the magnitude of the radial velocities is much smaller compared to the axial velocities, the corresponding discrepancies can be assumed to be of minor importance.

It should be noted that the predicted mean values in Figures 3-17(a), 3-17(b) have been evaluated by sampling a large number of particles that cross each section. The mean values were observed to be independent of the number of tracked particles if the total number of tracked particles was in excess of approximately 6000, as seen from Figure 3-12.
Figure 3-17(a) Particle mean x-velocities. Solid line: predictions, symbols: experiments

Figure 3-17(b) Particle mean radial-velocities. Solid line: predictions, symbols: experiments
The particle dispersion model ensures that we can also obtain velocity fluctuations apart from mean values. Hence, the results in this section are obtained by tracking a total of 20000 particles through the domain to obtain statistically meaningful values of velocity fluctuations. Figures 3-18(a) and 3-18(b) show the comparisons between the predicted and experimental data for particle axial and radial fluctuation velocities respectively, with sensitivity analysis on the modeling constant, $C_l$, in equation 2-16. The blue, red and green lines represent $C_l$ values of 0.15, 0.4 and 0.6 respectively. The default value of $C_l$ is generally taken as 0.15 and our literature survey indicated that no study has focused on validating this choice. Figures 3-18(a) and 3-18(b) show that simulation results with this default value underpredict the particle fluctuation velocities up to 40-50%. The best fit with experiments is observed with a $C_l$ value of 0.6, though some underprediction is still observed for RMS axial velocities in the downstream sections. Beyond a value of 0.6, results do not vary with changing $C_l$. Hence, $C_l=0.6$ is chosen for all gasifier simulations in Chapter 4.

The underprediction of particle fluctuation velocities in Figure 3-18(a) occurs in spite of the fact that the gas phase velocity fluctuations are well predicted for the most part and overpredicted in some regions, as observed from Figures 3-15(a) and 3-15(b). This result is contrary to that obtained by Sommerfield et. al [48] where it was observed that the underprediction of particle fluctuation velocities was a direct consequence of the underprediction of the gas fluctuation velocities, for swirling two-phase flow through a pipe expansion. In our case, the underprediction seems to occur as a result of the inadequate modeling of the coupling between the flow solver and the particle dispersion model. Tracking the particles through an unsteady field, generated by an unsteady model like LES, may be required for the accurate prediction of the particle fluctuation velocity. In the context of gasification modeling using RANS models, predicting mean velocities accurately at critical locations within the gasifier, specially the recirculation zones, is expected to be good enough for reasonable predictions of carbon conversion and species compositions. However, underpredicting the fluctuation velocities might lead to further inaccuracies in a coupled reacting flow scenario as compared to the cold flow.
Figure 3-18(a) Particle RMS x-velocities. Blue line: $C_L = 0.15$, Red line: $C_L = 0.4$, Green line: $C_L = 0.6$, symbols: experiments

Figure 3-18(b) Particle RMS radial velocities. Blue line: $C_L = 0.15$, Red line: $C_L = 0.4$, Green line: $C_L = 0.6$, symbols: experiments
situation considered here. Hence, future research needs to focus on better prediction of particle fluctuation velocities, apart from particle mean velocities.

Summarizing the results of this section, we can safely conclude that the current particle dispersion model embedded in the RANS simulations describes the mean particle motion in a reasonably accurate fashion. Better prediction of particle fluctuation velocities can be achieved by either switching to a dynamic solver, or probably an intelligent modification of the turbulent dispersion model.

3.6 Conclusions

1) The sudden expansion swirling and non-swirling flow cases demonstrates that LES yields better predictions than RANS models and SST k-ω model performs best among the tested RANS models. The two-phase bluff body flow case demonstrates the ability of SST k-ω model to reasonably predict complex flow structures. Hence, it is taken as the model of choice for gasifier simulations in Chapter 4.

2) The particle dispersion model embedded in the RANS simulations predicts the mean particle velocities well. The particle fluctuation velocities are slightly underpredicted by the current particle dispersion model although mean and RMS flow values are reasonably predicted. An optimal value of 0.6 is suggested for the modeling constant, $C_L$, for use in Chapter 4.
References


Chapter 4

VALIDATION OF THE OVERALL MODEL

4.1 Chapter Overview

In Chapter 3, the validation of the turbulence and particle turbulent dispersion submodels was shown. In this chapter, the impact of suggested improvements in these submodels on the predictions of key output parameters is analyzed through appropriate sensitivity analyses. In addition, the impact of adapting the moving flame front (MFF) model of char consumption to gasification CFD on the overall predictions is presented. The accuracy of the integrated gasifier model is demonstrated by comparing its predictions with experimental data from pilot and research-scale Mitsubishi Heavy Industries (MHI) gasifiers and a laboratory scale gasifier from Brigham Young University (BYU). The model is also applied to analyze the performance of the pilot-scale GE gasifier. Finally, a practical limit on mesh refinement for RANS simulations of two-phase reacting flows, governed by solution stability, is discussed.

4.2 Background and Motivation

Integrated CFD models of gasification are generally validated using data from a single type of gasifier. Such limited validation leaves room for uncertainty since commercial gasifiers vary from air-blown to oxygen blown, atmospheric pressure to pressurized, single-stage to multiple-stage, dry-fed to slurry-fed, involving swirling to non-swirling flows and having refractory insulation to having membrane walls. Keeping these considerations in mind, the present study aims to validate the integrated model against experimental data from three different set of gasifier designs, namely 1) 200 tons/day pilot-scale MHI gasifier, 2) 2 tons/day research-scale
MHI gasifier and 3) laboratory-scale BYU gasifier. While the MHI gasifier is air-blown, two-stage, pressurized and involves swirling flow, the BYU gasifier is oxygen-blown, single-stage, operating at atmospheric pressure and involving non-swirling flow. The gasifiers used for validation in this work cover a reasonably comprehensive range of operating conditions for model evaluation.

The gas phase equations are solved using the finite volume method with a second order upwind scheme on 3-D unstructured meshes for the MHI and BYU gasifiers and on 2-D unstructured mesh for the GE gasifier. Modifications in the submodels, such as those suggested in section 2.2.9, are incorporated in the Fluent model through user-defined C subroutines.

The rest of this chapter is arranged as follows. Section 4.3 describes the pilot-scale MHI gasifier test case which is also used as the base case to perform sensitivity analysis on important submodels. Since the pilot scale design operates on 200 tons/day of feedstock, it is closer to the commercial scale gasifiers which typically operate on 2000 tons/day than the laboratory and research-scale designs. Hence, this design is chosen to perform sensitivity analysis on the turbulence, particle turbulent dispersion and char consumption models in sections 4.3.2, 4.3.3 and 4.3.4, respectively. In sections 4.4 and 4.5, integrated model validation studies against corresponding experimental data-sets from the MHI research scale gasifier and BYU lab scale gasifier are described. Section 4.6 presents the application of the CFD model to a pilot-scale GE gasifier. Section 4.7 describes the impact of mesh refinement on solution accuracy and stability, as learned from the MHI gasifier test cases. Finally, in Section 4.8 the major conclusions drawn from this chapter are discussed.
4.3 MHI pilot-scale gasifier test case

4.3.1 Case description for validation of Submodels

The 200 tons/day pilot scale two-stage dry-fed MHI gasifier is used in this work as a test case for the construction and refinement of different submodels. The gasifier geometry has previously been employed in several studies [1][2][3] and depicted here in Figure 4-1.

Figure 4-1: MHI pilot-scale gasifier geometry along with swirl injector configurations: (1), (2) and (3) indicate the locations of the coal and recycled char injectors
The MHI gasifier incorporates three different dry-feed injectors. The first two are within the combustor region, where oxygen is available for reaction with the volatiles and the char. The third injector is in the diffuser section where more than 50% of the total coal in injected. Our numerical analysis and the experimental data reported in [1] indicate that this gasifier typically produces lower carbon conversions, 70-90%, and char recycling is required. Recycled char is injected through the combustor char burner (injector 2 in Figure 4-1). Taiheiyo bituminous coal (TH) is used in the experiments [1][2] and modeled in our work. The coal properties and the gasifier operating parameters used in this work are listed in Table 4-1 and Table 4-2, respectively. It should be noted that no steam is injected in the MHI gasifier.

Table 4-1. Properties for the coal (Taiheiyo sub-bituminous)

<table>
<thead>
<tr>
<th>Proximate Analysis (wt%)</th>
<th>Ultimate Analysis (wt%)</th>
</tr>
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<tbody>
<tr>
<td>Fixed Carbon</td>
<td>35.8</td>
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<tr>
<td>Volatile Matter</td>
<td>46.8</td>
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<td>Ash</td>
<td>12.1</td>
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<td>Moisture</td>
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</tr>
<tr>
<td>HHV</td>
<td>2.74x10^7 J/kg</td>
</tr>
<tr>
<td></td>
<td>C</td>
</tr>
<tr>
<td></td>
<td>H</td>
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<td>O</td>
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<td>N</td>
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<td>1.13</td>
</tr>
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<td></td>
<td>0.22</td>
</tr>
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</table>

Table 4-2. Inlet and operating conditions

<table>
<thead>
<tr>
<th>Pressure</th>
<th>2.7 MPa</th>
<th>Coal Flow Rates (kg/s)</th>
<th>Air Flow Rates (kg/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal Inlet Temperature</td>
<td>300 K</td>
<td>Combustor Coal Burner</td>
<td>0.472</td>
</tr>
<tr>
<td>Air Inlet Temperature</td>
<td>450 K</td>
<td>Combustor Char Burner</td>
<td>1.112</td>
</tr>
<tr>
<td>Equivalence Ratio</td>
<td>2.5</td>
<td>Reductor Burner</td>
<td>1.832</td>
</tr>
</tbody>
</table>
208000 cells are used in order to discretize the computational domain of this gasifier. Section 4-7 discusses the mesh independence study performed for the pilot scale gasifier in detail. A total of 1200 computational particles are tracked. No significant changes were observed when the number of tracked particles was doubled. Particles of ten different diameters, extracted using a Rosin-Rammler distribution around a mean diameter of 40 μm, are considered.

4.3.2 Turbulence Model

As discussed in Chapter 3, the flow solver provides the fundamental substructure of a CFD model. Moreover, many gasifiers have complicated geometries, multiple injections, and high levels of turbulence apart from the homogeneous and heterogeneous reactions, all contributing to formation of complicated flow structures. Accurate modeling of turbulent flow is paramount toward gaining predictive accuracy of the overall model. As demonstrated in Chapter 3 through extensive flow solver validation studies, SST k-ω model is the best choice among the commonly used RANS models for the type of flows observed in typical entrained flow gasifiers. Here we demonstrate the impact of incorporating the SST k-ω model, vis-à-vis the standard k-ε model, through analysis of overall model predictions of species, velocity and temperature fields in the gasifier and relevant comparisons with experimental data. Comparisons with the standard k-ε model are interesting because it is the most frequently employed turbulence model in gasification CFD studies [1][2][4][5][6].

Figure 4-2 compares the predictions of major species at the gasifier exit with experimental data using the standard k-ε and the SST k-ω models. The exit species are well predicted using both models though the SST k-ω model predictions are more accurate. It should be noted that the exit species are predicted to be in equilibrium, as also indicated by experimental measurements [2]. Figure 4-3 shows the carbon conversion along the length of the gasifier, starting from the location of the diffuser injector. Carbon conversion is governed by transport and kinetics. The
red and blue lines represent predictions using the standard k-ε and the SST k-ω models respectively. The experimental value of 83% conversion is well predicted using both models with the SST k-ω model performing marginally better. Interestingly, most of the carbon conversion happening in the pilot-scale MHI design is predicted to be completed within approximately six meters of the gasifier length. The remaining 7 meters account for 1-2% of additional conversion only. The results thus indicate the possibility of designing a more compact gasifier in order to increase space efficiency.

It should be noted that apart from the turbulence model, accurate char reaction kinetics extracted for the appropriate range of operating pressures are also essential for accurate prediction of exit species and carbon conversion, as further discussed in section 4.5. In this case, the kinetics for TH coal have been taken from a study conducted at pressures up to 2 MPa [7] and hence are suitable to simulate the pressurized MHI gasifier.

In figures 4-4 to 4-9, the red and blue lines show predictions along the gasifier centerline using the standard k-ε and the SST k-ω models respectively. Figure 4-4 shows that the SST k-ω model predicts temperature in the combustor section much better than the standard k-ε model, as indicated by the comparisons with available experimental data. Whereas the SST k-ω model predicts a larger peak in temperature in the combustor section and a relatively smaller peak at the location of the diffuser injector, the standard k-ε predicts just the opposite trend. Figure 4-5 demonstrates a crucial shortcoming of the standard k-ε model in its failure to predict the recirculation zone formed in the combustor section. The recirculation zone is created as a result of the tangential injectors creating a swirling flow in that region. As also done in gas turbine combustors, the aim of having swirling flows is to precisely create such recirculation zones which create a well-mixed region leading to faster fuel conversion and hence a shorter reactor. Moreover, existence of a recirculation in this MHI design is indirectly confirmed by the accurate prediction of temperature by the SST k-ω model.
Further, figure 4-4 shows that the SST k-ω model predicts a minimum in temperature following the injection at the diffuser, whereas the standard k-ε shows a monotonic temperature drop from the location of the diffuser injector up to the gasifier exit. Regardless of the turbulence model used, the sharp temperature drop at the diffuser injector occurs because more than 50% of the total coal injected in this gasifier is injected at that location along with minimal quantity of air as compared to the combustor injectors. Hence, the high temperature gas undergoes a very rapid quench owing to its reduction via gasification of the injected coal. The SST k-ω model differs from the standard k-ε model in predicting a minor enhancement, around the diffuser, of the central recirculation zone that was formed in the combustor section, as indicated by figure 4-5. The recirculation zone, thus formed, leads to enhanced mixing and hence the endothermic gasification reactions, as compared to the predictions of the standard k-ε model. The exit temperature is approximately predicted to be 1400 K by both models.

![Species Mole Fractions @ Exit](image)

**Figure 4-2:** Exit species mole fractions in pilot-scale MHI gasifier
Figure 4-3: Carbon conversion along the gasifier length in pilot-scale MHI gasifier

Figure 4-4: Temperature along the MHI gasifier centerline
Figure 4-6 to 4-9 show the CO, H₂, H₂O and CO₂ mole fraction respectively along the gasifier centerline. Again, significant differences in predictions of the two turbulence models are observed. The CO mole fraction is predicted to reach a minimum just prior to the diffuser injection using both models but the minimum predicted by the standard k-ε model is much more pronounced. As observed in figure 4-6, this minimum can be correlated to the similarly pronounced peak in temperature predicted by the standard k-ε model at the same location. The prediction of higher temperature by the standard k-ε model as compared to SST k-ω model leads to lower prediction of CO, as dictated by water-gas shift equilibrium.

Another significant difference, observed from figures 4-6 to 4-9, is the prediction of peaks in CO and H₂ profiles and minimum in CO₂ and H₂O profiles just ahead of the diffuser injector using the SST k-ω model whereas no such peaks or minimum are predicted by the standard k-ε model. The SST k-ω model predicts entrainment within central recirculation zone of some of the
coal injected at the diffuser burner. This entrapment leads to higher rate of endothermic gasification reactions within the recirculation zone resulting in a local maximum in CO and H₂ profiles.

Figures 4-10(a) to 4-10(f) show contours of temperature, axial velocity and species mole fractions for the first 4.5m of MHI gasifier using the standard k-ε and the SST k-ω models. The initial one-third of the gasifier is chosen since most of the carbon conversion and the presence of critical flow structures occur in this region of the gasifier. The figures clearly demonstrate the stark difference in the predictions by the two turbulence models. Figure 4-10(a) shows that while the standard k-ε model predicts high temperatures close to the wall in the diffuser section, the SST k-ω model predicts lower temperatures and hence lower heat transfer through the wall. It is because of this reason that the SST k-ω model predicts marginally lower exit temperature compared to the standard k-ε model, as seen also from figure 4-4. Figure 4-10(b) shows the existence of a central recirculation zone for the SST k-ω model whereas the standard k-ε model predicts largely positive axial velocities along the center. Furthermore, there are pronounced differences in the predictions of all the major species between the two models, as described earlier. Prediction of high temperatures close to the walls can also be attributed to the fact that while some of the inlet charge gets trapped into the central recirculation zone, the rest travels with high axial velocity, as seen in Figure 4-10(b), and gets combusted along the gasifier walls. This is a direct consequence of the re-distribution of residence times arising from the formation of a central recirculation zone.
Figure 4-6: CO mole fraction along the MHI gasifier centerline

Figure 4-7: H₂ mole fraction along the MHI gasifier centerline
Figure 4-8: H$_2$O mole fraction along the MHI gasifier centerline

Figure 4-9: CO$_2$ mole fraction along the MHI gasifier centerline
a) Temperature (K)

b) X-velocity (m/s), velocity vectors

c) Char concentration (10^-6 kg/m^3)

d) CO mole fraction
4.3.3 Particle turbulence dispersion model

In Chapter 3, validation of the particle turbulent dispersion model in a non-reacting flow was presented. Using comparison of model predictions with experimental data on particle rms velocities in the two-phase flow bluff body case, the modeling parameter, $C_L$, was found to have an optimal value of 0.6. In this section, the impact of varying $C_L$ on the continuum-scale quantities like temperature and species mole fractions is investigated. Figures 4-11 to 4-13 show that changing the value of $C_L$ from 0.15, the default value popularly used, to the optimal value of 0.6 has a noticeable effect on the temperature and species mole fraction predictions, especially in the combustor and early diffuser section. This is expected, since most char conversion happens in the combustor and diffuser sections and variation in the modeling of...
particle turbulent dispersion, brought about by change in the value of $C_L$, is expected to impact the trajectory of particles as they cross these regions.

Figure 4-11: Impact of $C_L$ on temperature profile

Figure 4-12: Impact of $C_L$ on CO mole fraction profile
4.3.4 Char consumption model

In Chapter 2, the moving flame front (MFF) model of char consumption was contrasted with the typically used single-film model. In this section, the impact of adapting the MFF model to gasification CFD on the predictions of MHI gasifier is presented. Experimentally measured $n^{\text{th}}$ order Arrhenius kinetics for TH coal are employed [7]. Alternatively, Langmuir-Hinshelwood kinetics, extracted for a bituminous coal [8], were also employed and found to give similar results.
In figure 4-14, the solid and the dotted lines represent predictions of the single film model and the MFF model, respectively, for the CO and CO$_2$ mole fractions along the gasifier centerline. Negligible difference in predictions between the two models was observed for the H$_2$ and H$_2$O mole fractions and temperature. Figure 4-14 shows that predictions of the more accurate MFF model differ from single film model predictions in the combustor section owing to the presence of oxygen in that section. It should be pointed out that MFF is 'switched on' only in the combustor section of the MHI gasifier since it is expected to make a difference in predictions only when O$_2$ is available. In the reductor section, the model reverts to the single film model implementation since no oxygen is available to form a CO-O$_2$ flame around the particles.

Moreover, in a single stage gasifier, the difference between single film model and MFF predictions is expected to be minimal. Our results indicate that both models yield identical
results for the single stage laboratory scale BYU gasifier, described in section 4.5, and the GE gasifier, described in section 4.6. The results also demonstrate that the particle char consumption model needs to be resolved accurately since it has a noticeable effect of model predictions at the bulk level.

4.4 MHI research-scale gasifier

The research-scale MHI gasifier operates at 2 tons/day as opposed to the 200 tons/day operation of the pilot-scale gasifier. The length of the gasifier is 5.85 m, as opposed to 13 m for the pilot-scale design, and the reductor diameter is 0.24 m as opposed to 0.6 m for the pilot-scale. Here comparisons with experimental data for an Australian black coal, coal M, are presented for the integrated gasifier model developed in this work. Properties of coal M and the mass flow rates of coal, recycled char and air through the gasifier are given in Table 4-3 and Table 4-4 respectively. Four test cases with varying flow rates of coal, recycled char and air are available, characterized on the basis on a parameter called the gasifier air ratio, which is ratio of net air input in the gasifier to the amount of stoichiometric air needed for complete combustion of the coal and char. The gasifier configuration and rest of the operating conditions including reactor pressure and swirling injections are similar to the pilot scale MHI design.

Table 4-3: Properties for Coal M (Australian black coal)

<table>
<thead>
<tr>
<th>Proximate Analysis (wt%)</th>
<th>Ultimate Analysis (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed Carbon</td>
<td>C</td>
</tr>
<tr>
<td>Volatile Matter</td>
<td>H</td>
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<tr>
<td>Ash</td>
<td>O</td>
</tr>
<tr>
<td>Moisture</td>
<td>N</td>
</tr>
<tr>
<td>HHV</td>
<td>S</td>
</tr>
</tbody>
</table>

| Fixed Carbon | 56.2 | C | 76.3 |
| Volatile Matter | 30.9  | H | 5.31 |
| Ash | 8.7 | O | 7.31 |
| Moisture | 4.2 | N | 1.54 |
| HHV | 3.0x10^7 J/kg | S | 0.46 |
A hexahedral mesh with 670000 cells is used. The mesh is finer in the combustor, throat and diffuser sections, with average grid size of 7.5 mm, and courser in the reductor section, with average mesh size of 20 mm. The mesh is also sufficiently fine close to the walls. The SST k-ω model is used for turbulence. Figures 4-15 and 4-16 show the comparison between the experimental data and the model predictions for net carbon conversion and exit species mole fractions respectively. Comparisons with experimental data are satisfactory. The exit species are in equilibrium, similar to the pilot scale case. Figure 4-17 shows the variation of the gasifier temperature along the centerline for the four test cases, along with comparisons with experimental data at one point in the combustor section and four points in the reductor section. The comparison with experiments is satisfactory. The temperature distribution along the axis of the research-scale design looks similar to that of the pilot scale design, as predicted by the SST k-ω model in figure 4-4. The only difference is that twin peaks in the combustor section observed in the pilot scale predictions are not seen in the research-scale gasifier. This probably arises due to the difference in scale between to the two designs, leading to the smearing of the second peak in the research-scale design.

<table>
<thead>
<tr>
<th></th>
<th>M1</th>
<th>M2</th>
<th>M3</th>
<th>M4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Combustor Coal (kg/hr)</td>
<td>40.7</td>
<td>41.4</td>
<td>40.6</td>
<td>41.2</td>
</tr>
<tr>
<td>Reductor Coal (kg/hr)</td>
<td>60.3</td>
<td>59.3</td>
<td>58.3</td>
<td>61.3</td>
</tr>
<tr>
<td>Recycled Char (kg/hr)</td>
<td>38.1</td>
<td>36.3</td>
<td>34.8</td>
<td>37.8</td>
</tr>
<tr>
<td>Combustor Air (kg/hr)</td>
<td>391.7</td>
<td>418.4</td>
<td>436.6</td>
<td>409.7</td>
</tr>
<tr>
<td>Reductor Air (kg/hr)</td>
<td>66.96</td>
<td>66.58</td>
<td>66.49</td>
<td>66.68</td>
</tr>
<tr>
<td>Gasifier Air Ratio</td>
<td>0.358</td>
<td>0.381</td>
<td>0.409</td>
<td>0.367</td>
</tr>
</tbody>
</table>

Table 4-4: Mass flow rates of coal, recycled char and air
Figure 4-15: Comparisons with experiments of carbon conversion

Figure 4-16: Comparisons with experiments of exit species mole fractions
Figure 4-17: Comparisons with experiments of temperature along the gasifier centerline

4.5 BYU laboratory-scale gasifier

The validation of integrated gasifier model against experimental data from an atmospheric pressure, oxygen-fed gasifier from the Brigham and Young University (BYU) is described here. Several coal combustion and gasification experiments were conducted [9] at BYU test facilities in the 1980’s. The experimental data presented in this section comes from the test setup shown in figure 4-18 [10]. Although in the original work four cases were presented with four different coals, only two of those cases have been chosen for comparisons with model predictions.
because: 1) the coal properties, namely the ultimate and proximate analyses, were found to contain inconsistent values and 2) the experimental data for one of the cases left out had large differences between repeated experiments due to uncertainties, as reported by the authors [10]. The relevant coal properties and experimental conditions are reported in Table 4-5. The primary stream consists mainly of $O_2$, along with some $H_2O$ and Ar, which is used as a carrier gas for coal. Coal is also injected into the domain through the primary stream. The secondary stream consists of steam. The setup is laboratory scale, with a length of 1.8 m and a diameter of 0.2 m. Although the reactor is equipped with a swirl block, non-swirling flows were used for all the gasification experiments [9][10].

![BYU gasifier schematic and operating conditions](image)

**Figure 4-18: BYU gasifier schematic and operating conditions**
The BYU gasifier operates on different conditions as compared to the MHI gasifier. The MHI gasifier involves swirling flows whereas the BYU gasifier operates with non-swirling flows. While the MHI gasifier is air-fed and pressurized, the BYU gasifier is oxygen-fed and operates at atmospheric pressure. In this regards, figure 4-19 demonstrates the importance of incorporating char kinetics extracted at the appropriate pressure range for the gasifier studied. It can be observed that kinetics extracted at atmospheric pressure can be a couple of orders of magnitude faster than those obtained at higher pressures. Figure 4-19 also implies that kinetics extracted at atmospheric pressure cannot be extrapolated to higher pressures and vice-versa, as was also pointed out Liu et al. [11][8] in their studies on Australian coals. Similarly, in a previous CFD study on pressurized MHI gasifier [12], it was observed that using atmospheric pressure kinetics with Wen's shrinking core model [13] predicted carbon conversion of 100% as compared to more accurate value of 83% predicted using kinetics extracted at higher pressures. In the BYU gasifier case, we have accordingly incorporated kinetics extracted at atmospheric pressure [10] for the coals considered.

Figure 4-20 shows the distribution of the axial velocity along the centerline for the two coals. The solid and the dotted lines represent predictions using the standard k-ε and the SST k-ω models, respectively. Two noteworthy observations: there is no central recirculation zone in this case because of the absence of swirling flow, and the standard k-ε and the SST k-ω models predict similar flow behavior. The latter implies that while the SST k-ω model successfully predicts the existence of a recirculation zone in appropriately swirling flows as opposed to the standard k-ε model, it collapses onto the standard k-ε model in case of non-swirling cases. This is expected, since the SST k-ω model adheres to the k-ω formulation of turbulence only in the near-wall regions and switches to the k-ε description far away from the walls [14].
Table 4-5: Coal properties and experimental test conditions

<table>
<thead>
<tr>
<th></th>
<th>Utah Bit</th>
<th>Illinois No. 6</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Proximate Analysis</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Moisture</td>
<td>2.4</td>
<td>6.7</td>
</tr>
<tr>
<td>Ash</td>
<td>8.3</td>
<td>10.4</td>
</tr>
<tr>
<td>Volatiles</td>
<td>45.6</td>
<td>39.4</td>
</tr>
<tr>
<td>Fixed Carbon</td>
<td>43.7</td>
<td>43.5</td>
</tr>
<tr>
<td>HHV (MJ/kg, dry)</td>
<td>29.8</td>
<td>27.4</td>
</tr>
<tr>
<td><strong>Ultimate Analysis</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ash</td>
<td>8.5</td>
<td>11.2</td>
</tr>
<tr>
<td>H</td>
<td>6.0</td>
<td>4.7</td>
</tr>
<tr>
<td>C</td>
<td>71.0</td>
<td>66.9</td>
</tr>
<tr>
<td>N</td>
<td>1.3</td>
<td>1.4</td>
</tr>
<tr>
<td>S</td>
<td>0.5</td>
<td>4.3</td>
</tr>
<tr>
<td>O</td>
<td>12.7</td>
<td>11.5</td>
</tr>
<tr>
<td><strong>Test Conditions</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Primary Flow Rate (Kg/s)</td>
<td>0.00729</td>
<td>0.00922</td>
</tr>
<tr>
<td>Primary Components, mole fractions</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O$_2$</td>
<td>0.850</td>
<td>0.814</td>
</tr>
<tr>
<td>Ar</td>
<td>0.126</td>
<td>0.122</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>0.024</td>
<td>0.064</td>
</tr>
<tr>
<td>Sec. Flow Rate (H$_2$O, Kg/s)</td>
<td>0.00184</td>
<td>0.00066</td>
</tr>
<tr>
<td>Primary Particle Loading</td>
<td>0.910</td>
<td>0.892</td>
</tr>
<tr>
<td>Primary size dist., μm, approx. from measured dist.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20%</td>
<td>3</td>
<td>8</td>
</tr>
<tr>
<td>20%</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>20%</td>
<td>28</td>
<td>40</td>
</tr>
<tr>
<td>20%</td>
<td>50</td>
<td>63</td>
</tr>
<tr>
<td>20%</td>
<td>80</td>
<td>126</td>
</tr>
<tr>
<td>Mass mean diameter (μm)</td>
<td>36</td>
<td>51</td>
</tr>
</tbody>
</table>
Figure 4-19: Comparing kinetics extracted at atmospheric and high (20 MPa) pressure

Figure 4-20: Comparing predictions of standard k-ε and SST k-ω models along the centerline in BYU design
The SST k-ω model is employed for comparisons with experiments. A grid resolution of 320000 cells is chosen. The mesh was confirmed to be sufficiently fine through a mesh sensitivity study where adaptive refinement of the original mesh in regions of highest temperature gradients did not change predictions. Further considerations on mesh refinement are discussed in section 4.7. Figures 4-21(a) to 4-21(d) and figures 4-22(a) to 4-22(d) depict the comparisons with experimental data of the integrated gasifier model predictions for the Utah bituminous and Illinois No. 6 coals respectively. Agreement with experiments is satisfactory for both coals, considering the fact that a RANS model was used. The Illinois No. 6 case shows much more fluctuations along the centerline than the Utah bituminous case, both in predictions and experimental data. While the model may not sufficiently capture all the variations along the length of the gasifier, the exit mole fractions are well-predicted in all cases. The mismatch with experimental data for some species close to the injector may be attributed to the unsteady large scale unsteadiness of the flow in that region. Preliminary LES studies on the BYU gasifier within our group indicate the existence of highly transient large scale structures close to the injector. The impact of such structures on the dynamics and mixing is not captured by RANS. Our preliminary LES results yield better comparisons with experimental data close to the injector and indicate that RANS solution methods may not accurately capture mean values in the presence of such transients.
Figure 4-21: Species predictions along centerline for Utah bituminous coal
Figure 4-22: Species predictions along centerline for Illinois No. 6 bituminous coal.
Figures 4-23(a) to 4-23(f) show the contours of temperature, axial-velocity and major species within the first 0.5 m of BYU gasifier, where the highest gradients are observed. It can be seen that the highest temperature occurs away from the centerline. These high temperatures are achieved because of the combustion of volatiles as they are released and transported radially outward from the colder central jet. Accordingly, CO$_2$ and H$_2$O profiles also show similar variations as the temperature in that region, because of the oxidation of C and H released from volatiles to CO$_2$ and H$_2$O, respectively. Figure 4-24 and 4-25 show the evolution of conversion along the gasifier and the temperature distribution along the gasifier centerline, respectively. The black and the red lines represent predictions for Utah bituminous and Illinois No. 6, respectively, whereas the corresponding dots represent the experimental carbon conversion and temperature values at the exit. Similar to the MHI gasifier, figure 4-24 shows that most of the conversion occurs in the initial one-third of length of the gasifier. The exit conversion is satisfactorily predicted for both coals. Figure 4-25 shows that temperature peak in the initial part of the reactor is higher for Illinois No. 6 than the Utah bituminous coal because of the higher throughput of oxidant and coal through the reactor for the Illinois No. 6 coal. Prediction of the exit temperature is satisfactory for both coals.
Figure 4-23: Temperature, velocity and species contours within the first 0.5 m of BYU gasifier
Figure 4-24: Carbon conversion along the BYU gasifier

Figure 4-25: Temperature along the gasifier centerline.
4.6 Texaco (GE) pilot-scale gasifier

The CFD model is next applied to the GE 1000 tons/day gasifier. Limited input-output data is available from the operation of this gasifier at the Cool Water IGCC project over the period 1980-1990. Despite the fact that this gasifier was referred to as ‘pilot-scale’ during Cool Water operation, it is really a commercial scale unit and since the mid 1990s had been in commercial operation at the Coffeyville Resources plant in Coffeyville, Kansas. It, along with a second GE gasifier, is used to produce ammonia from petroleum coke.

Figure 4-26 shows the gasifier layout along with a listing of the dimensions and some operational characteristics. The GE gasifier is pressurized, down-fired, slurry-fed, oxygen-blown, one-stage, refractory-lined and radiant-cooled. These operating conditions should be contrasted with those of the MHI gasifier, discussed in the previous section, in table [ ]. In particular, the GE gasifier operates at higher temperatures and yields higher conversions. However, it offers lower plant efficiencies primarily because it needs extra oxidant in order to vaporize the steam injected in the slurry feed. The minimum water fraction in the slurry feed, required for blockage-free transportation, is typically in excess of the amount needed for gasification of the coal fraction in the slurry.

Table 4-6 shows a list of operating parameters and feed rates for the test case presented in this section. Illinois #6 bituminous coal is the feedstock. The corresponding coal properties are shown in table 4-5. A layout of the mesh used for the simulation of the GE gasifier is shown in figure 4-27. The volume of the GE gasifier is approximately ten times that of the pilot-scale MHI design and a 3-D simulation would have required at least a million grid points for sufficient resolution. However, as discussed later in section 4.8, the Fluent solver suffers from numerical instability and convergence issues when solving two-phase reacting flows with mesh resolutions of over 200,000 grid points. Hence, a 2-D axisymmetric geometry is chosen to simulate the GE gasifier in the present work. The corresponding mesh consists of 30,000 grid points.
points. As shown in figure 4-27, the mesh is finer close to the gasifier axis, especially just
downstream of the injection. This region has the sharpest gradients in temperature and species
mole fractions as seen from the corresponding contours in figures 4-30(a) to 4-30(h).

Figure 4-26: GE gasifier layout, dimensions and characteristics
Table 4-6: Comparison of the MHI gasifier with the GE gasifier

<table>
<thead>
<tr>
<th></th>
<th>MHI</th>
<th>GE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exit Temperature</td>
<td>~ 1400K</td>
<td>~ 1650 K</td>
</tr>
<tr>
<td>Carbon Conversion</td>
<td>~ 80%</td>
<td>~ 98%</td>
</tr>
<tr>
<td>Char Recycling?</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>Wall Insulation</td>
<td>Membrane Lining</td>
<td>Refractory Lining</td>
</tr>
<tr>
<td>Tars in outlet stream?</td>
<td>Present, in low amounts</td>
<td>Negligible</td>
</tr>
<tr>
<td>Syngas Cooling</td>
<td>Gas quench</td>
<td>Radiant Quench</td>
</tr>
<tr>
<td>Plant Efficiency</td>
<td>Higher (~42%)</td>
<td>Lower (~38%)</td>
</tr>
</tbody>
</table>

Table 4-7: Operating conditions and Feed rates for the GE gasifier

<table>
<thead>
<tr>
<th>Operating Parameters</th>
<th>Feed Rates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure (bar)</td>
<td>Coal (kg/h)</td>
</tr>
<tr>
<td>Reactor Size (m³)</td>
<td>Slurry Loading (63.4%)</td>
</tr>
<tr>
<td>Coal throughput (TPD)</td>
<td>Slurry flow (kg/h)</td>
</tr>
<tr>
<td>Syngas Production (MWth)</td>
<td>O₂ (kg/h)</td>
</tr>
</tbody>
</table>

Slurry Loading | 63.4 %
Coal (kg/h)    | 42871
Slurry flow (kg/h) | 21821
O₂ (kg/h) | 33483

Figure 4-27: The 2-D axisymmetric mesh used for simulation of the GE gasifier
Figure 4-28 shows the carbon conversion along the length of the gasifier. The exit conversion matches well with the experimental value. The trends in figure 4-28 should be compared with those for the MHI pilot-scale design in figure 4-3. The results indicate that the GE gasifier utilizes a larger fraction of its length for carbon conversion than the MHI pilot-scale design. Nevertheless, it should be noted that a large fraction, close to 85%, of the overall conversion achieved within the GE gasifier occurs with the initial one-third of its length. Figure 4-29 shows the comparison between the predicted and experimental values of exit mole fractions for CO, H₂ and CO₂. The predictions satisfy water-gas equilibrium and match satisfactorily with the experimental data.

Figures 4-30(a) to 4-30(h) show the contours of temperature, axial-velocity and various species mole fractions in the gasifier. Figure 4-30(a) shows that the highest temperatures occur slightly away from the centerline within a region ~ 1.5 m downstream of the injector. These high temperatures are achieved due to combustion of volatiles as they are released and transported radially outward from the colder central jet. Accordingly, CO₂ profile also shows similar variations as temperature in that region, owing to the oxidation of C released from volatiles to CO₂. Similar trends were reported in section 4.5 for the BYU gasifier, which also involves axial firing from a small diameter nozzle into a larger reactor. The contours of axial-velocity in figure 4-30(b) show that an external recirculation zone exists close to the peripheral gasifier wall, similar to the BYU gasifier.
Figure 4-28: Carbon conversion along the gasifier length (m)

Figure 4-29: Comparison of predicted and experimental species mole fractions at gasifier exit
Figures 4-30(c) and 4-30(d) indicate that oxygen and volatiles, respectively, are consumed within a small distance, approximately ~ 1m, downstream of the injector. Figure 4-30(h) shows that variation in the H$_2$O fraction continues to occur far downstream from the injector, since steam is the primary gasification agent in this gasifier. It should be noted that most contours in figures 4-30(a) to 4-30(h) show fluctuations close to the centerline just downstream of the injector. Similar fluctuations were predicted for the BYU gasifier. As mentioned earlier in section 4.5, highly transient large scale structures, present close to the injector in such axially-fired reactors involving turbulent flow, are expected to be captured more accurately by LES simulations rather than RANS.

(a) Temperature (K)  (b) Axial-velocity (m/s)  (c) O$_2$ mole fraction
Figure 4-30: Temperature, velocity and species mole fraction contours for the GE gasifier
4.7 Considerations on mesh resolution

Grid independence study is necessary in a CFD analysis in order to attain the best possible results from a given set of models, parameters and numerics. However, for large scale commercial systems like gasifiers, the grid points might reach daunting numbers before grid independence is attained. Here we present our study on grid independence for the MHI pilot scale design starting from a reasonably fine mesh of 208000 cells. The mesh was first refined by roughly a factor of two only in regions of the highest temperature gradients as shown in Figure 4-31. The cut-off value of temperature gradient for refinement was taken as 80 and the number of cells in the refined mesh was 430000. Figures 4-32 to 4-34 show that grid independence was not reached at 208000 cells and further refinement was necessary. However, it was also found that the refined mesh case became increasingly unstable and difficult to converge. Further, if the coarser mesh is uniformly refined by a factor of 2 to final resolution of 1.6 million cells, the correspondingly refined mesh does not converge and the solution keeps oscillating or blows up in spite of the most conservative relaxation factors.

![Figure 4-31: Contours of temperature gradient for adaptive mesh refinement.](image)
Figure 4-32: Mesh refinement - Temperature along the gasifier centerline

Figure 4-33: Mesh refinement – CO mole fraction along the gasifier centerline
A possible explanation for this observation is that it becomes increasingly difficult to find a steady-state solution to the inherently transient problem of turbulent two-phase reacting flows in gasifiers as increasingly finer structures are captured through mesh refinement. Moreover, the stochastic nature of the particle turbulent dispersion model enhances the unsteadiness of the problem. Hence, unsteady RANS and ultimately LES should be attempted with increasing computational power for such inherently transient processes.
4.8 Conclusions

1) The SST k-ω model provides better comparisons with experimental data for the pilot-scale MHI design than the standard k-ε model. The SST k-ω model predicts the formation of the central recirculation zone for the swirling flow scenario established in the MHI gasifier, whereas the standard k-ε model fails to predict this complex flow.

2) Varying the particle turbulent dispersion modeling parameter, $C_L$, has a noticeable impact on the prediction of continuum-scale quantities such as the temperature and mole fraction. An optimal value of 0.6, as suggested in Chapter 3, should be used.

3) MFF model describes char consumption more accurately than the popularly used single flame model. The present implementation of MFF model in gasification CFD shows that it yields noticeably different predictions of key species in the combustor section.

4) Predictions from the integrated gasifier model compare well with experimental data for the lab and research-scale MHI gasifiers and the laboratory-scale BYU gasifier. Predictions of exit carbon conversion and species mole fractions compare well with experimental values for the GE Cool Water gasifier.

5) Mesh sensitivity analysis indicates that beyond a certain level of refinement, the two-phase reacting flow CFD model becomes increasingly unstable. If such fine scales need to be resolved, then an unsteady solution methodology like unsteady RANS or LES is recommended.

6) The present model, having undergone extensive validation both at the level of the critical submodels as well as the integrated model, can be used as an analysis and
potentially preliminary design tool to predict improved and optimal gasifier designs and operating conditions

References


Chapter 5
APPLICATION OF THE OVERALL MODEL

5.1 Chapter overview

Following the construction and validation of the CFD model in the earlier chapters, it is employed to analyze the performance of the pilot-scale MHI and the pilot-scale GE gasifiers in this chapter. In particular, the model is used to study the impact of feedstock particle size, reactor pressure and mass throughput on the gasifier performance.

5.2 Background and motivation

The design of coal gasifiers has been largely an experience-based enterprise. Consequently, many of the present gasifiers are susceptible to several failure modes including refractory damage, injector blockage or burn-out and slag port blockage. Moreover, it is unclear whether the accepted operational practices are optimal with respect to parameters such as the reactor pressure, mass throughput, injection swirl, angle of injection in case of tangential injection, dimensions of critical regions, extent of feedstock grinding, etc. A comprehensive and validated CFD model is instrumental in ascertaining whether important gasifier performance metrics like carbon conversion and cold gas efficiency are optimized with respect to the relevant parameters.

The multiscale model of entrained flow gasification developed in this work has been validated at the level of individual critical submodels including the turbulence model and the particle turbulent dispersion model. In addition, the overall model has been validated for a variety of gasifiers operating under conditions including air-blown to oxygen-blown, atmospheric pressure
to pressurized, pilot-scale to lab-scale, tangentially-injected to axially injected conditions. In the present chapter, the validated model is applied to ascertain the impact of changing the values for particle grinding sizes, operating pressure and reactor throughput on the performance of the MHI and GE gasifiers.

5.3 Particle size

Determining the impact of particle size on carbon conversion is critical for two important reasons:

(1) Depending on the particular gasifier design and stoichiometric ratio within specific regions of the gasifier, as discussed in the next section, fine grinding of coal may or may not have a significant impact on carbon conversion rate. Accurate modeling can reveal this dependence and help make informed decisions.

(2) There have been studies indicating that there is a premium in fine grinding of coal. Although the grinding energy itself might remain a miniscule fraction of the heating value, a more stringent requirement on grinding leads to a reduction in the mill capacity. The extent of reduction depends on the particular grinding mill employed and the grindability index of the coal used [1].

5.3.1 Char consumption model

In order to explain the results on the impact of particle size on char conversion, we need to invoke certain aspects of the char consumption model developed in section 2.2.9. In particular, equations (2-34) and (2-35) determining char consumption rate under complete kinetic control
and complete diffusion control, respectively, will be useful in this chapter and are re-stated below.

The char consumption rate via C-CO\textsubscript{2} reaction, in the regime where kinetic control can be assumed, is written as [2]:

$$
\dot{m}_p = k_s P_g = m_{po} S_0 (1-x) \sqrt{1-\psi \ln(1-x)} \frac{k_{11} P_{CO_2}}{1 + k_{12} P_{CO_2} + k_{13} P_{CO}}
$$

(5-1a)

where $m_{po}$ is the initial char mass of the particle, $S_0$ is initial internal surface area ($m^2$/kg), $x$ is the instantaneous particle char conversion, $\psi$ is the structural parameter for the random pore model, $k_1$'s are Arrhenius constants, and $P_{CO_2}$ and $P_{CO}$ are the free stream partial pressures of CO\textsubscript{2} and CO, respectively, in the vicinity of the particle. This rate expression is 'intrinsic', since it depends on $S_0$. Similar expression for the C-H\textsubscript{2}O reaction, in the kinetics-controlled regime, is written as [3]:

$$
\dot{m}_p = k_s P_g = m_{po} S_0 (1-x) \sqrt{1-\psi \ln(1-x)} \frac{k_{21} P_{H_2O}}{1 + k_{22} P_{H_2O} + k_{23} \sqrt{P_{H_2}}}
$$

(5-1b)

where $k_2$'s are Arrhenius constants, and $P_{H2O}$ and $P_{H2}$ are the free stream partial pressures of H\textsubscript{2}O and H\textsubscript{2}, respectively, in the vicinity of the particle. An n\textsuperscript{th} order extrinsic rate expression is used for the C-O\textsubscript{2} reaction [4]:

$$
\dot{m}_p = k_s P^o = m_{po} (1-x) \sqrt{1-\psi \ln(1-x)} k_{31} P_{O_2}^o
$$

(5-2)

where $k_{31}$ is an Arrhenius constant, and $P_{O2}$ is the free stream partial pressure O\textsubscript{2} in the vicinity of the particle. As shown later in this chapter, the C-O\textsubscript{2} reaction is typically limited by diffusion through the boundary layer. Under complete diffusion control, the char consumption rate is given as
\[ \dot{m}_p = P_g k_d = A_0 P_g \frac{A_d}{P d_p} \left( \frac{T_g}{2000} \right)^{0.75} \] (5-3)

where \( A_0 \) is the external surface area of the particle (m\(^2\)), \( A_d \) is a constant and depends on the corresponding gas-phase reactant, \( P_g \) is the free stream partial pressure of the gas-phase reactant, \( T_g \) is the gas-phase temperature in the vicinity of the particle, \( P \) is the total pressure and \( d_p \) is the particle diameter. Relations (5-1) – (5-3) will be employed in the following sections to develop scaling relations for the dependence of particle conversion rate on the relevant physical quantities such as reactor pressure and particle diameter.

### 5.3.2 Results for MHI pilot-scale gasifier

Before presenting the impact of particle size on carbon conversion in the MHI gasifier, it is useful to emphasize that the generation of the primary gasification products, CO and H\(_2\), is accomplished by partitioning the net coal feed between two stages in this design. Referring to figure 4-1, the combustor section is much richer in oxygen as compared to the diffuser section by design. Approximately 55% of the total coal is injected at the diffuser burner and the rest at the combustor burners, whereas only 15% of the total air is injected at the diffuser burner with the remaining 85% being injected at the two combustor burners.

Figure 5-1(a) shows the variation of the oxygen mole fraction within the gasifier. Oxygen is available within the lower combustor section and only close to the injectors near the char combustor burner. Oxygen concentration is negligible in the diffuser burner, especially compared to the amount of coal injected at that location. The combustor stage primarily produces CO\(_2\) and H\(_2\)O, and thermal energy through the combustion of volatiles, recycled char and some of the coal with O\(_2\), which are then used to gasify the coal injected within the diffuser and reductor regions to yield CO and H\(_2\) as the final products.
Figure 5-1: Contours of (a) O$_2$ mole fraction, (b) Temperature (c) Char concentration and (d) Axial velocity contours (m/s)

Axial velocity, within the initial one-third section of MHI gasifier
It should be noted that even in a single stage gasifier, such as the GE design discussed in the next section, the zone where temperature rises is where combustion occurs, otherwise it is where gasification takes place. The temperature rise is primarily due to the combustion of volatiles, followed by combustion of some of the char.

In figures 5-2 to 5-4, the bars depict the average particle char conversion, the time taken for a certain fraction of conversion and the corresponding axial location at that fraction of conversion at the two combustor burners and the diffuser burner respectively, whereas the error bars depict the standard deviation over the mean values. The values are presented for ten classes of diameter sizes from 4 µm to 150 µm, as determined from measurements on the coal feed sample in the MHI pilot scale case [5]. Because of the stochastic nature of particle tracking, a statistically significant number of particles are tracked through the gasifier domain to collect data for figures 5-2 to 5-4. We found that tracking 350 particles provided statistically convergent results.

Figures 5-2(a) and 5-3(a) show the time taken for 95% char conversion for particles injected at the combustor coal burner and the combustor char burner, respectively. Average carbon conversion at the gasifier exit for particles injected at both these burners is 99.9%. Results show that the time taken for conversion increases with particle diameter. Beyond ~ 115 µm for the coal particles injected at the combustor burner, and ~ 30 µm for the char particles injected at the char burner, the conversion time is independent of the particle diameter for the range of particle sizes analyzed in this work. As argued later, this transition occurs because the char consumption switches from being primarily diffusion-limited to kinetics-limited.

Moreover, figures 5-2(b) and 5-3(b) show the axial location at 95% char conversion for particles injected at the combustor coal burner and the combustor char burner, respectively. The axial location in these figures is measured from the base of the gasifier. It should be noted that the two combustor burners are located at axial locations of 0.4m and 0.7m, respectively. The trends in figures 5-2(b) and 5-3(b) are similar to the trends observed in figures 5-2(a) and 5-2(b). The
 axial location for 95% conversion increases with particle diameter. Beyond ~ 115 μm for the coal particles injected at the combustor burner, and ~ 30 μm for the char particles injected at the char burner, the axial location is independent of particle diameter for the range of particle sizes analyzed in this work. Another important observation from figures 5-2(b) and 5-3(b) is that particles injected at the two combus tor burners undergo most of their conversion within the combustor section itself.

Figures 5-4(a) to 5-4(c) show that particle char conversion at the gasifier exit, time taken for 20% conversion and the axial location at 20% conversion are independent of particle size for the range of particle sizes injected at the diffuser burner. A value of 20% conversion was chosen since nearly all tracked particles injected at the diffuser burner attain a minimum of 20% conversion by the time they leave the gasifier. The average char conversion at the gasifier exit for particles injected at this burner is 41%.
Figure 5-2(a): Dependence of time for conversion on particle diameter at the combustor coal burner for the MHI gasifier

Figure 5-2(b): Dependence of axial location for conversion on particle diameter at the combustor coal burner for the MHI gasifier
Figure 5-3(a): Dependence of time for conversion on particle diameter at the combustor char burner for the MHI gasifier.
Figure 5-4 (a): Dependence of particle char conversion on particle diameter at the diffuser burner for the MHI gasifier

Figure 5-4 (b): Dependence of time for 20% conversion on particle diameter at the diffuser burner for the MHI gasifier
Particles injected at Diffuser Burner

![Graph showing dependence of axial location at 20% conversion on particle diameter at the diffuser burner for the MHI gasifier.]

**Figure 5-4 (c): Dependence of axial location at 20% conversion on particle diameter at the diffuser burner for the MHI gasifier**

The trends observed in figures 5-2 to 5-4 can be explained by identifying the respective limiting mechanism of char consumption, whether heterogeneous kinetics or diffusive transport to the particle surface, applicable to particles injected at the two different gasifier stages. The limiting mechanism, in turn, depends on the temperature in the vicinity of the particle, availability of the respective gasification/combustion agents, O$_2$ or CO$_2$ and H$_2$O, and the particle diameter. In figures 5-5(a) and 5-5(b), the solid and dotted lines represent the diffusion and kinetics conductances respectively, evaluated according to the definitions used along with the resistance network model represented by equation (2-26). These figures show the variation of the individual conductances during char conversion along the trajectory of a particle of 40 μm diameter injected at the combustor coal burner. It should be noted 40 μm is the mean value of the diameter distribution of particles injected in this gasifier.
The kinetic conductance in these figures is evaluated for the corresponding heterogeneous reaction. In figure 5-5(a), the black line represents data for C-O\textsubscript{2} reaction whereas in figure 5-5(b), the red line represents data for C-CO\textsubscript{2} reaction and the black line represents data for C-H\textsubscript{2}O reaction for the same particle. Figure 5-5(c) shows the temperature variation along the trajectory of the same particle. Figure 5-5(a) shows that the diffusion conductances have much lower values than the kinetics conductances for the C-O\textsubscript{2} reaction. This is expected, because of the high temperatures and faster oxidation reaction in the combustor section. However, figure 5-5(b) shows that the diffusion conductances have higher values than the kinetics conductances for both the C-CO\textsubscript{2} and C-H\textsubscript{2}O reactions. This is because the temperatures are lower in the diffuser and reductor regions leading to slower kinetics, and the conversion rate becomes kinetics-limited. Moreover, the kinetics of C-CO\textsubscript{2} and C-H\textsubscript{2}O reactions are typically much slower than the char oxidation reaction, further adding to the kinetics limitation on the overall conversion rate.

Figures 5-5(a) and 5-5(b) establish that whereas the C-O\textsubscript{2} reaction is limited by diffusion, the C-CO\textsubscript{2} and C-H\textsubscript{2}O reactions are limited by kinetics. Although these figures represent data extracted for a mean particle diameter of 40 µm, these trends were confirmed across the range of particle sizes tested in this work. While the diffusion limitation of the C-O\textsubscript{2} reaction becomes stronger with increasing particle size, the kinetics limitation of C-CO\textsubscript{2} and C-H\textsubscript{2}O reactions becomes weaker with increasing particle size. Nonetheless, kinetics limitation still applies for the particles of largest diameter tracked in this study, as shown later in figure 5-8.
Particles injected at Combustor Coal Injection, $d_p = 40\mu m$

Figure 5-5 (a): Diffusion and kinetics conductance for C-O$_2$ reaction along particle trajectory shown as function of char conversion for a particle injected at combustor coal burner

Figure 5-5 (b): Diffusion and kinetics conductance C-CO$_2$, C-H$_2$O reactions, along particle trajectory shown as function of char conversion for a particle injected at combustor coal burner
Fig. 5-5 (c): Temperature along particle trajectory shown as function of char conversion for the same particle.

In light of these observations, we explain the trends seen in figures 5-2 to 5-4 by developing a set of scaling rules for the variation of conversion time under diffusion limitation and kinetics limitation respectively. The char consumption model is invoked in order to construct the scaling relations.

Equations (5-1) – (5-3) indicate that the char consumption rate is a function of several parameters such as the initial char mass, $m_{p0}$, initial reactive surface area, $S_0$, initial particle diameter, $d_p$, external surface area, $A_0$, instantaneous char conversion, $x$, local reactant partial pressure, $P_g$, local gas temperature, $T_g$, instantaneous particle temperature, $T_p$, etc. Several of these parameters vary along the particle trajectory, i.e., are functions of time:

$$\dot{m}_p = f_1(A_0, S_0, m_{p0}, d_p) \cdot f_2(x(t), P_g(t), T_g(t), T_p(t))$$  \hspace{1cm} (5-4a)
In order to develop approximate scaling relations for conversion time, we assume time-averaged values for these variable parameters.

\[
\dot{m}_{p,av} = f_1(A_0, S_0, m_{p0}, d_p) \left| f_2(x(t) P_g(t) T_g(t) T_p(t))_a v\right.
\]  \hspace{1cm} (5-4b)

Conversion time can be approximated as:

\[
\dot{m}_{p,av} \approx \frac{m_{p0}}{t_{conver}} \Rightarrow t_{conver} \propto \frac{m_{p0}}{\dot{m}_{p,av}} \propto \frac{d_p^3}{\dot{m}_{p,av}}
\]  \hspace{1cm} (5-4c)

The scaling of \( \dot{m}_{p,av} \) with particle diameter depends on the corresponding limiting mechanism for char consumption. Under diffusion limited conversion, using equations (5-3) and (5-4c), the time for char conversion varies with the square of particle diameter:

\[
t_{conver} \propto \frac{d_p^3}{A_0} \propto \frac{d_p^3}{d_p^2} \propto d_p^2
\]  \hspace{1cm} (5-5)

However, under kinetics limited conversion, using equations (5-1) and (5-4c),

\[
t_{conver} \propto \frac{d_p^3}{m_{p0} S_0} \propto \frac{1}{S_0}
\]  \hspace{1cm} (5-6)

and hence time for conversion is “nearly” independent of diameter. It should be emphasized that the scaling relations (5-5) and (5-6) are limited by the approximation brought about by the time-averaging in equation (5-4b) and are not applicable in the limit of the particle size going to zero or during the very last stages of char conversion.
We can now interpret the trends observed in figures 5-2 to 5-4 with the aid of these scaling relations and the knowledge of the corresponding limiting mechanisms for particles injected at the three sets of burners. At the diffuser burner, CO$_2$ and H$_2$O are the primary gasification agents since the fraction of O$_2$ available for heterogeneous reaction is negligible. C-CO$_2$ and C-H$_2$O reactions are limited by the corresponding slow kinetics and the relatively low temperature in the reductor. Hence, the average char conversion and time for conversion at the diffuser burner are predicted to be independent of particle diameter for the range of particle sizes analyzed in this work, as observed in figures 5-4(a) to 5-4(c). It should be noted that as particle diameter increases beyond 150 µm, the largest size analyzed in our work, diffusion limitation will increasingly become important vis-à-vis the kinetics limitation. Hence, the trend of independence of the conversion time on particle diameter cannot be indefinitely extended to larger particle sizes beyond 150 µm. When diffusion limitation becomes comparable to kinetics limitation, conversion time is expected to increase with particle diameter, as dictated by relation (5-5).

It is important to point out that although the kinetics limitation of C-CO$_2$ and C-H$_2$O reactions weakens with increasing particle size, it still applies for the largest particle size of 150 µm analyzed in this work, as observed in figure 5-6(a). Figure 5-6(b) shows the temperature variation along the trajectory of the same particle. It should be noted that the particle represented in figures 5-6(a) and 5-6(b) undergoes incomplete char conversion.
Particle injected at Diffuser Injection, \( d_p = 150\mu m \)

**Figure 5-6 (a):** Diffusion and kinetics conductance \( \text{C-CO}_2, \text{C-H}_2\text{O} \) reactions, along particle trajectory shown as function of char conversion, for a particle of 150 \( \mu m \) diameter injected at diffuser burner.

**Figure 5-6 (b):** Temperature along particle trajectory shown as function of char conversion for the same particle.

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Contrary to the diffuser and reductor sections, \( \text{O}_2 \) is available for the heterogeneous reactions in the lower combustor section, as observed in figure 5-1(a). In the high temperature environment of the combustor, the C-O\(_2\) reaction is limited by diffusion and hence time for char conversion increases with particle diameter, but only up to a point. This is because the larger particles take longer to burn in the combustor section; they flow out of the oxygen-rich regions, before complete conversion, into the diffuser section or oxygen starved regions within the combustor section. The particle trajectory plots, shown later in section 5.3.2.1, confirm that the larger particles injected at the two combustor burners have limited availability to oxygen. In the oxygen-starved regions, the primary gasification agents are \( \text{CO}_2 \) and \( \text{H}_2\text{O} \), and the dependence on particle diameter vanishes. Since most of the oxygen within the combustor is available in the lower combustor region, the dependence on diameter vanishes sooner at the higher located combustor char burner than the combustor coal burner, as observed in figures 5-2 and 5-3.

Figures 5-7(a) and 5-7 (b) show the availability of oxygen for heterogeneous reaction and the overall fractional conversion rate, respectively, as functions of char conversion for particles of two different diameters, 4 \( \mu \text{m} \) and 50 \( \mu \text{m} \), injected at the combustor char burner. Figure 5-7(c) shows the temperature variation along the trajectory of the same particles. The fractional conversion rate, \( C \), plotted on the y-axis in figure 5-7(b), is defined as the ratio of the instantaneous particle conversion rate to the initial char mass in the particle:

\[
C = \frac{\dot{m}_p}{m_{p0}}
\]  

These figures support the claim made in the preceding paragraph that larger particles, above 36 \( \mu \text{m} \), convert largely in oxygen-starved environments. Consequently, they experience slower conversion rates than the smaller particles since the gasification reactions are much slower than the oxidation reaction.
Tables 5-1(a) to 5-1(c) present a summary of the trends observed in figures 5-2 to 5-4 for the three different burners in the MHI gasifier. Results and analysis presented above indicate that fine-ground coal would convert faster than coarse-ground coal in the oxygen-rich combustor section of the two-stage MHI gasifier. We observe however that because of the higher temperature and the higher oxygen concentration, even the larger particles are predicted to convert completely and the penalty associated with injecting larger particles in the combustor section is likely to be small. On the other hand, fine-grinding the coal beyond 150 \( \mu m \) is not predicted to offer any advantage with respect to carbon conversion for particles injected at the diffuser burner.
Table 5-1(a). Summary of trends observed in figures 5-2(a) and 5-2(b) on the diameter dependence of particle char conversion at the combustor coal burner in MHI gasifier

<table>
<thead>
<tr>
<th>Diameter Class</th>
<th>4 μm – 101 μm</th>
<th>118 μm – 150 μm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conversion time * (s)</td>
<td>~0.2 – ~0.6</td>
<td>~0.6</td>
</tr>
<tr>
<td>Axial location ** (m)</td>
<td>~0.45 – ~0.55</td>
<td>~0.55</td>
</tr>
<tr>
<td>Average conversion</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Gasification agent</td>
<td>primarily O₂, some H₂O, CO₂</td>
<td>some O₂, primarily H₂O, CO₂</td>
</tr>
<tr>
<td>Limiting Mechanism</td>
<td>primarily diffusion</td>
<td>primarily kinetics</td>
</tr>
</tbody>
</table>

*: time for 95% char conversion. **: axial location at 95% char conversion

Table 5-1(b). Summary of trends observed in figures 5-3(a) and 5-3(b) on the diameter dependence of particle char conversion at the combustor char burner in MHI gasifier

<table>
<thead>
<tr>
<th>Diameter Class</th>
<th>4 μm – 36 μm</th>
<th>53 μm – 150 μm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conversion time * (s)</td>
<td>~0.1 – ~0.35</td>
<td>~0.35</td>
</tr>
<tr>
<td>Axial location ** (m)</td>
<td>~0.8 – ~1.5</td>
<td>~1.5</td>
</tr>
<tr>
<td>Average conversion</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Gasification agent</td>
<td>primarily O₂, some H₂O, CO₂</td>
<td>some O₂, primarily H₂O, CO₂</td>
</tr>
<tr>
<td>Limiting Mechanism</td>
<td>primarily diffusion</td>
<td>primarily kinetics</td>
</tr>
</tbody>
</table>

*: time for 95% char conversion. **: axial location at 95% char conversion
Table 5-1(c). Summary of trends observed in figures 5-4(a) to 5-4(c) on the diameter dependence of particle char conversion at the diffuser burner in MHI gasifier

<table>
<thead>
<tr>
<th>Diameter Class</th>
<th>4 μm – 150 μm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conversion time</td>
<td>~ 1.4</td>
</tr>
<tr>
<td>Axial location</td>
<td>~5.5 - ~6.5</td>
</tr>
<tr>
<td>Average conversion</td>
<td>0.41</td>
</tr>
<tr>
<td>Gasification agent</td>
<td>H₂O, CO₂</td>
</tr>
<tr>
<td>Limiting Mechanism</td>
<td>primarily kinetics</td>
</tr>
</tbody>
</table>

*: time for 20% char conversion. **: axial location at 20% char conversion

5.3.2.1 Reactant availability vs particle size

Certain trends in the preceding section, especially the impact of particle size on conversion time within the combustor section, have been explained on the basis of the availability of particular gasification agents, whether O₂ or CO₂ and H₂. In this section, the availability of various gasification agents and the corresponding char consumption rates are presented along the trajectory for particles of different diameters, injected at the three burners in the MHI gasifier. Data along the trajectories is presented for three different particle sizes: a ‘small’ size of 20 μm diameter, a ‘medium’ size of 69 μm diameter and a ‘large’ size of 134 μm diameter.

Figures 5-8 to 5-10 present data along the trajectory for particles injected at the combustor coal burner, figures 5-11 to 5-13 present data along the trajectory for particles injected at the combustor char burner whereas figures 5-14 to 5-16 present the corresponding data for particles injected at the diffuser burner. Moreover, figures 5-8, 5-11 and 5-14 show plots for the ‘small’ particles, figures 5-9, 5-12 and 5-15 show plots for the ‘medium’ particles, whereas figures 5-10, 5-13 and 5-16 show corresponding plots for the ‘large’ particles injected at the respective burners.
In each of the figures from figure 5-8 to figure 5-16, respective data along the trajectory is presented in three different plots. The plot (a) in each figure shows the variation of the partial pressure of O₂, CO₂ and H₂O with time elapsed since injection. The plot (b) shows the variation of the consumption rates due to C-O₂, C-CO₂ and C-H₂O reactions with the time elapsed since injection. Finally, the plot (c) shows the variation of the consumption rates due to C-O₂, C-CO₂ and C-H₂O reactions with the particle char conversion. In the (a) plots, the black line, blue and red lines represents partial pressures of O₂, CO₂ and H₂O, respectively. In the (b) and (c) plots, the black, blue and red lines represent consumption rates due to C-O₂, C-CO₂ and C-H₂O reactions, respectively.

Most of the (a) plots in these figures show that oxygen is available only in small regions, mostly as sharp spikes, along the particle trajectories. CO₂ and H₂O are available in much more abundance, not just at the diffuser burner, but also at the two combustor burners. The (b) plots in these figures show that the presence of oxygen, as indicated by the (a) plots, corresponds with a peak in the consumption rate due to the C-O₂ reaction. The peak value of the consumption rate due to the C-O₂ reaction is typically at least an order of magnitude larger than the consumption rates, along the same trajectory, due to the C-CO₂ and C-H₂O reactions. This is expected since the kinetics of the C-O₂ reaction is much faster than the kinetics of the C-CO₂ and C-H₂O reactions.

Figures 5-8(c) and 5-11(c), for small-sized particles injected at the combustor coal burner and combustor char burner, respectively, show that the consumption rate due to C-O₂ reaction dominates over the other two reactions during char conversion. Although oxygen is available for only a small part of the particle trajectories, as seen in the corresponding (a) and (b) plots, it is sufficient to completely convert the small particles during the span of its availability.

Figures 5-9(c) and 5-12(c), for medium-sized particles injected at the combustor coal burner and combustor char burner, respectively, show that the consumption rate due to C-O₂ reaction
dominates only during the initial part of the conversion regime. Moreover, figures 5-10(c) and 5-13(c), for large-sized particles injected at the combustor coal burner and combustor char burner, respectively, show that the consumption rates due to \( \text{C-CO}_2 \) and \( \text{C-H}_2\text{O} \) reactions dominate during most part of char conversion. These observations support our analysis, in the preceding section, on the transition in rate-determining step for char consumption from diffusive transport to reaction kinetics as the particle size increases beyond a critical value at the two combustor burners. With increasing particle size, the gasification medium changes from being \( \text{O}_2 \)-dominated to that dominated by \( \text{H}_2\text{O} \) and \( \text{CO}_2 \). Hence, the consumption rates due to \( \text{C-CO}_2 \) and \( \text{C-H}_2\text{O} \) reactions dominate over the \( \text{C-O}_2 \) reaction for the larger particles. Since char consumption due to the \( \text{C-CO}_2 \) and \( \text{C-H}_2\text{O} \) reactions is primarily kinetics-limited, the dependence of conversion time on particle diameter weakens with increasing particle size at the two combustor burners.

The (b) and (c) plots in figures 5-14 to 5-16, for particles injected at the diffuser burner, show that the consumption rate due to \( \text{C-H}_2\text{O} \) reaction is several times faster than that due to \( \text{C-CO}_2 \) reaction. This is because steam gasification kinetics is faster than the kinetics of gasification with \( \text{CO}_2 \). It should be noted that the \( \text{CO}_2 \) and \( \text{H}_2\text{O} \) partial pressures in the vicinity of the particles are similar, as seen from the corresponding (a) plots in these figures.
Figure 5-8: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 20 μm diameter injected at the combustor coal burner.
Figure 5-9: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 69 μm diameter injected at the combustor coal burner.
Figure 5-10: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 134 μm diameter injected at the combustor coal burner.
Figure 5-11: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 20 μm diameter injected at the combustor char burner.
Figure 5-12: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 69 μm diameter injected at the combustor char burner.
Figure 5-13: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 134 μm diameter injected at the combustor char burner.
Figure 5-14: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 20 μm diameter injected at the diffuser burner.
Figure 5-15: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 69 μm diameter injected at the diffuser burner.
Figure 5-16: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 134 \mu m diameter injected at the diffuser burner.
5.3.2.2 Radial dispersion vs particle size

The transport and dispersion of particles through the gasifier is modeled by the turbulent dispersion model described in chapter 2. The impact of the swirling flow in the MHI gasifier should lead to an interesting radial dispersion of particles during their respective trajectories. Figures 5-17(a), 5-17(b) and 5-17(c) show the variation of the mean radial-coordinate of a particle trajectory with particle diameter. The mean is taken over the complete trajectory of an individual particle tracked through the gasifier. Moreover, the data used for figures 5-17(a) to 5-17(c) is generated by evaluating the mean and standard deviation of this mean radial coordinate value over 350 particles for each diameter class.

The figures show that the heavier particles tend to reside at slightly larger radial distances, on an average. However, the difference between the average value of the mean radial coordinate varies only modestly from ~0.4 m to ~0.5 between the lightest and the heaviest particles.

![Particles injected at Combustor Coal Burner](image)
Figure 5-17: Mean radial coordinate of trajectory vs particle diameter for particles injected at (a) combustor coal burner, (b) combustor char burner, and (c) diffuser burner.
5.3.3 Results for Texaco (GE) pilot-scale gasifier

In this section, the GE Cool Water gasifier is analyzed for the impact of particle size on char conversion. Figures 5-18(a), 5-18(b) and 5-18(c) depict average particle char conversion, time taken for 75% char conversion and axial location at 75% conversion, respectively, for ten classes of diameter sizes from 4 µm to 150 µm. A value of 75% conversion was chosen since nearly all tracked particles attain a minimum of 75% conversion by the time they leave the gasifier. 350 particles are tracked, similar to previous section, to yield statistically significant results. Figure 5-18(a) shows that average particle char conversion drops gradually from ~100%, for the particles of smallest diameter, to ~90%, for the particles of largest diameter. Figure 5-18(b) shows that the time taken for 75% conversion increases with particle diameter. Beyond ~ 134 µm, the conversion time is very weakly dependent on the particle diameter, for the range of particle sizes analyzed in this work. Similarly, figure 18(c) shows that the axial location at 75% conversion increases with particle diameter for smaller particles but the impact of particle size is minimal beyond ~ 85 µm.

The trends in the figures 5-18(b) and 5-18(c) are similar to those observed in figure 5-2 for particles injected at the combustor coal burner in the MHI gasifier. Those particles have access to O₂, in regions close to the injector, and to CO₂ and H₂O, in the far downstream regions. Similar distribution of gasification agents, with respect to the injector, is observed in the GE gasifier. Figure 5-19(a) and 5-19(b) show that O₂ is available up to ~ 1m downstream of the injector beyond which H₂O is the primary gasification agent. Hence, particles convert under diffusion-limitation in the presence of oxygen, with a dependence on diameter as dictated by equation (5-5): \( t_{\text{conversion}} \propto d_p^2 \). The dependence on diameter successively weakens as particles move toward oxygen-starved regions of the gasifier. It should be noted that the near-injector region, apart from being rich in oxygen, also has high temperatures. This contributes to the high conversion rates close to the injector as shown later in figure 5-20.
Figure 5-18(b) shows that the conversion time is of the order of 0.1 s for the smallest particles up to 20 μm. For the larger particles, the conversion time ranges from 1 - 3s. Moreover, as seen in figure 5-18(c) the smallest particles convert completely within ~0.7m of the injector whereas the larger particles convert completely only beyond ~2m. It is also observed that the dependence of conversion time on particle diameter greatly weakens for the larger particles beyond 118 μm. These two transitions are explained by the corresponding changes in the availability of O₂, as opposed to H₂O and CO₂, as the primary gasification agent and the temperature. Figures 5-20(a) and 5-20(b) show the availability of oxygen for heterogeneous reaction and the overall fractional conversion rate, respectively, as functions of char conversion for particles of three different diameters, 20 μm, 35 μm and 135 μm. Figure 5-20(c) shows the temperature variation along the trajectories of the three particles. Oxygen is available for the 20 μm diameter particle during most of its lifetime. Moreover, it has access to the highest temperatures. It consequently experiences the fastest fractional conversion rates. The 35 μm diameter particle takes longer to convert under diffusion limitation, than the 20 μm diameter particle, and oxygen is its primary gasification agent for roughly half of its lifetime, during which the conversion rate is high. However, the fractional conversion rate drops by almost two orders of magnitude in the latter half of its lifetime where H₂O becomes its primary gasification agent. Finally, the 150 μm diameter particle practically undergoes all of its conversion in the oxygen-starved regions and experiences lower fractional conversion rates than the two smaller particles.

Table 5-2 presents a summary of the trends observed in figures 5-18(a) to 5-18(c). It differentiates the three ranges of particle sizes, i.e. 4-20 μm, 36-101 μm and 118-150 μm, on the basis of the availability of various gasification agents and the rate-determining step for char consumption. The availability of various gasification agents for particles of different diameters in the GE gasifier is further analyzed in section 5.3.3.1.
Figure 5-18: Dependence of (a) particle char conversion and (b) time for 75% conversion on particle diameter, for the GE gasifier.
Figure 5-18 (c): Dependence of axial location for 75% conversion on particle diameter for the GE gasifier

(a) O₂ mole fraction  
(b) H₂O mole fraction
Figure 5-19: Temperature and species mole fraction contours in the GE gasifier
(a) 

(b)
Figure 5-20: (a) Oxygen partial pressure in the vicinity and (b) fractional conversion rate, and (c) temperature of particles of three different diameters injected in the GE gasifier

Table 5-2. Summary of trends observed in figures 5-10 and 5-11 on the diameter dependence of particle char conversion in GE gasifier

<table>
<thead>
<tr>
<th>Diameter Class</th>
<th>4 µm - 20 µm</th>
<th>20 µm - 101 µm</th>
<th>101 µm - 150 µm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conversion time * (s)</td>
<td>~ 0.1</td>
<td>1 - 3</td>
<td>&gt; 3</td>
</tr>
<tr>
<td>Axial location ** (m)</td>
<td>~ 0.8</td>
<td>2.2 - 3</td>
<td>~3</td>
</tr>
<tr>
<td>Average conversion</td>
<td>1.0</td>
<td>~ 0.95</td>
<td>~ 0.91</td>
</tr>
<tr>
<td>Gasification agent</td>
<td>O₂</td>
<td>partly O₂, partly H₂O, CO₂</td>
<td>primarily H₂O, CO₂</td>
</tr>
<tr>
<td>Limiting Mechanism</td>
<td>diffusion</td>
<td>diffusion, then kinetics</td>
<td>primarily kinetics</td>
</tr>
</tbody>
</table>

*: time for 75% char conversion. **: axial location at 75% char conversion
It is tempting to infer from figure 5-18(b) that if all of the injected feedstock is ground to sizes below 20 μm then average conversion time can be brought down to ~ 0.1s. However, it should be noted that only limited amount of oxygen is available for reacting with char. In case all of the injected coal particles were ground to a size below 20 μm, then oxygen would be available for only a small fraction of the overall conversion of those particles.

Before closing the discussion on the dependence of char conversion in the GE gasifier on particle size, it is useful to emphasize that the limiting mechanisms for the various oxidation and gasification reactions remain the same as discussed in section 5.3.2. Figures 5-21(a) and 5-21(b) show the variation of the diffusion and kinetics conductances for the C-O₂ and C-H₂O reactions respectively, evaluated in the same manner as described in section 5.3.2, during char conversion. The solid and dotted lines represent the diffusion and kinetics conductances, respectively, along the trajectory of a particle of 40 μm diameter. Figure 5-21(c) shows the temperature variation along the trajectory for the same particle.

Figure 5-21(a) shows that the kinetics conductances have higher values than the diffusion conductances for the C-O₂ reaction. Figure 5-21(b) shows that the diffusion conductances have higher values than the kinetics conductances for the C-H₂O reaction. Figures 5-21(a) and 5-21(b) confirm our assumptions in the foregoing analysis that the C-O₂ reaction proceeds under diffusion-limitation and the C-H₂O reaction proceeds under kinetics-limitation in the GE gasifier.
Figure 5-21(a): Diffusion and kinetics conductance for C-O₂ as function of char conversion for a particle tracked through the GE gasifier.

Figure 5-21(b): Diffusion and kinetics conductance for C-H₂O reactions, as function of char conversion for a particle tracked through the GE gasifier.
5.3.3.1 Reactant availability vs particle size

In this section, the availability of various gasification agents and the corresponding char consumption rates are presented along the trajectory for particles of different diameters tracked through the GE gasifier. As done in section 5.3.2.1, data along the trajectories is presented for three different particle sizes: a ‘small’ size of 20 μm diameter, a ‘medium’ size of 69 μm diameter and a ‘large’ size of 134 μm diameter.

Figure 5-22 shows plots for the ‘small’ particles, figure 5-23 shows plots for the ‘medium’ particles, whereas figure 5-24 shows plots for the ‘large’ particles. In each of the figures from 5-22 to 5-24, the respective trajectory data is presented as three different plots. The plot (a) in each figure shows the variation of the partial pressure of O₂, CO₂ and H₂O with time elapsed since injection. The plot (b) shows the variation of the consumption rates due to C-O₂, C-CO₂.
and C-H₂O reactions with the time elapsed since injection. Finally, the plot (c) shows the variation of the consumption rates due to C-O₂, C-CO₂ and C-H₂O reactions with the particle char conversion. In the (a) plots, the black line, blue and red lines represent partial pressures of O₂, CO₂ and H₂O, respectively. In the (b) and (c) plots, the black, blue and red lines represent consumption rates due to C-O₂, C-CO₂ and C-H₂O reactions, respectively.

Most of the (a) plots in these figures show that oxygen is available, if at all, as sharp spikes close to the injection. Steam is available in abundance throughout the gasifier, followed by some CO₂. Figure 5-22(c), for small-size particles, shows that the consumption rate due to C-O₂ reaction dominates over the other two reactions during char conversion. This occurs in spite of the fact that oxygen is available for only a small part of the particle trajectory. The reason, as mentioned earlier, is the much faster kinetics of the C-O₂ reaction as compared to the C-CO₂ and C-H₂O reactions.

Figures 5-23(c) and 5-24(c), for medium-size and large-size particles, respectively, show that the consumption rate due to steam gasification dominates during the conversion regime. Moreover, the contribution to the consumption rate from C-O₂ reaction is small for the medium size particle and negligible for the large-size particle. The reason why the consumption rate is dominated by the C-CO₂ reaction is due to the fact that the C-H₂O kinetics is much faster than the C-CO₂ kinetics and the higher concentration of H₂O in the GE gasifier.
Figure 5-22: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 20 μm diameter for the GE gasifier.
Figure 5-23: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 69 μm diameter for the GE gasifier.
Figure 5-24: (a) Reactant partial pressure vs time since injection, (b) consumption rates vs time since injection, and (c) consumption rates vs particle char conversion, along the trajectory of a particle of 134 μm diameter for the GE gasifier.
5.3.3.2 Radial dispersion vs particle size

Figure 5-25 shows the variation of the mean radial-coordinate of a particle trajectory as function of the particle diameter for the GE gasifier. The data for this figure is extracted in the same manner as described in section 5.3.2.2 for the MHI gasifier. The mean radial coordinate varies only from ~0.51 to ~0.54 across the range of particle sizes. The difference, in this regard, from the MHI gasifier can be attributed to the absence of swirl in the GE gasifier.

Figure 5-25: Mean radial coordinate of trajectory vs particle diameter in the GE gasifier
5.4 Gasifier operating pressure and mass throughput

In this section, we investigate the impact of varying two key parameters, the mass throughput and the reactor operating pressure, on the gasifier performance. Such a study is useful for two reasons. First, it is not uncommon for commercial gasifiers to be operated at off-design values of these two parameters in order to extract more output than the vendor’s specification. Hence, it is useful to have a quantitative estimate of the corresponding impact on overall carbon conversion. Second, such an analysis can be used to inform innovative gasifier design and provide an estimate of the combination of design parameters required for optimal performance. The CFD tool offers an opportunity to analyze the impact of these operating parameters on fluid mechanics, heat fluxes, temperature distributions and most importantly, the net carbon conversion.

5.4.1 Results for MHI pilot-scale gasifier

Figures 5-26(a), 5-26(b) and 5-26(c) show the response of the net carbon conversion, gasifier exit temperature and cold gas efficiency to the changes in two operating parameters: the gasifier pressure, $P$, and mass throughput, $\dot{m}$. A mass throughput of 1X and pressure of 27 bar represent the base case as shown in Table 4-2. While varying the mass throughput, both coal feedstock and air flow rates are adjusted so that the net equivalence ratio of 2.5 is maintained. Note that $\dot{m} = \dot{m}_{air} + \dot{m}_{coal}$, where $\dot{m}_{air}$ is the mass throughput of injected air and $\dot{m}_{coal}$ is the mass throughput of injected coal. Moreover, 0.5X, 2X and 4X represent cases where the gasifier mass throughput, $\dot{m}$, is halved, doubled and quadrupled respectively. All the four mass throughput cases are run at the base pressure of 27 bar and an elevated pressure of 54 bar. For the sake of convenience, the test cases at 27 bar pressure are labeled $P_a0$, $P_a1$, $P_a2$, $P_a3$ whereas those at 54 bar pressure are labeled $P_b1$, $P_b2$, $P_b3$ in figure 5-26(a).
Feedstock, Air = 0.5X
Feedstock, Air = 1X
Feedstock, Air = 2X
Feedstock, Air = 4X

LIFeedstock, Air = 2X
tFeedstock, Ar = 4X

P = 27bar
P = 54bar

IRZ not formed

Exit Temperature (K)
P = 27bar
P = 54bar
Figure 5-26: Dependence of (a) net carbon conversion, (b) exit temperature, (c) cold gas efficiency, on operating pressure and gasifier mass throughput in the MHI gasifier. The ovals in (a) indicate cases where an internal recirculation zone is not formed.

It should be noted that the exit velocity from the burners changes accordingly when the pressure and mass throughput are varied, because the burner size is kept fixed in these simulations. The impact on the burner exit velocity can be assessed using the relation $\dot{\mathbf{m}}_{\text{air}} = \rho_b A_b V_b$, where $\rho_b$ and $V_b$ are the gas-phase density and velocity at the burner exit, respectively, and $A_b$ is the burner area:

- a) Increasing the reactor pressure reduces $\rho_b$ when $\dot{\mathbf{m}}_{\text{air}}$ is fixed reduces $V_b$ and increases $\tau_{\text{res}}$, the average residence time (for fixed gasifier size)
- b) Increasing $\dot{\mathbf{m}}_{\text{air}}$, when reactor pressure is fixed, increases $V_b$ and reduces $\tau_{\text{res}}$ (for fixed gasifier size)
It can be seen from Figure 5-26(a) that at the same mass throughput, carbon conversion across the gasifier is higher at higher pressure. Moreover, the exit temperature decreases with increasing the pressure, as shown in figure 5-26(b). Another observation from figure 5-26(a) is that at a fixed operating pressure, increasing the mass throughput lowers carbon conversion through the gasifier in most cases. In addition, figure 5-26(b) shows that the gasifier exit temperature increases with increasing mass throughput. The variation in the cold gas efficiency in figure 5-26(c) mirrors the corresponding variation in the net carbon conversion. This is expected, because higher conversion leads to greater amount of CO and H₂ in the syngas.

Results shown in figure 5-26(a) indicate that doubling the gasifier mass throughput at constant pressure results in a drop in carbon conversion of only 2-3 percentage points. These predictions certainly seem optimistic! It should be noted that the accuracy of model predictions is dependent on the accuracy of the reaction kinetics expressed in equations (5-1) and (5-2), especially at higher pressures. It also depends on the accuracy of the turbulence chemistry interaction model used in this work, i.e. the finite rate/EBU model, which may not hold as well throughout the range of conditions analyzed in this work. While the present model predicts 100% conversion under all test cases for coal particles injected at the two combustor burners, incomplete mixing at higher flow rates will give rise to incomplete conversion in the combustor section. While the trends in figures 5-26(a) to 5-26(c) are useful in evaluating gasifier performance under varying reactor pressure and mass throughput, the corresponding quantitative estimates need to taken with caution.

As mentioned in Section 5.3.2, carbon conversion is 100% for particles injected in the combustor section of the MHI gasifier. Moreover, volatiles released from coal injected at the diffuser burner react and are likely to get converted (combusted or gasified) completely before leaving the gasifier, because of the much faster rate of gas mixing and homogeneous kinetics. The reason we observe incomplete carbon conversion for all the test cases in figure 5-26(a) is that the average conversion of fixed carbon from coal injected at the diffuser burner is low, varying from 30% to 45% depending on the particular test case. As pointed out in section 5.3.2,
char conversion at the diffuser burner occurs primarily under kinetics limitation via the C-CO$_2$ and C-H$_2$O reactions.

It is possible to draw an analogy between the reductor region of this design and a plug-flow reactor (PFR). The PFR is a reduced order model of a continuous flowing system in which the fluid is assumed to be well-mixed in the spanwise direction, but not in the streamwise direction, and streamwise mixing is neglected. In the reductor section, the heterogeneous reactions, occurring on the char resulting from coal injected at the diffuser burner, satisfy this assumption due to their kinetics limitation. The average char conversion through a PFR can be written as [6]:

$$x_{av} = 1 - \exp(-C_{av} \tau_{av})$$

(5-8)

where $C_{av}$ is the averaged value of the fractional conversion rate, $C$, expressed in equation (5-7). $\tau_{av}$ is the average residence time and $x_{av}$ is the average char conversion for all particles injected at the diffuser burner. Using equation (2-26), $C$ can be expressed as

$$C = \frac{\dot{m}_p}{m_{p0}} = \frac{P_g}{\frac{m_{p0} + m_{p0}}{k_s + k_d}} = \frac{1}{C_d + \frac{1}{C_k}}$$

(5-9)

where $C_d$ is the contribution from diffusion and $C_k$ is the contribution from kinetics. Equation (5-9) allows us to develop scaling laws for the dependence of $C$ on reactor pressure under both kinetics and diffusion limitation. Using equation (5-1), $C_k$ can be scaled to first order for dependence on reactor pressure as:

$$C_k \propto P_g \propto P$$

(5-10)

Using equation (5-3), $C_d$ can be scaled as:
Hence, the diffusive component of $C$ is not impacted by the reactor pressure. However, increasing reactor pressure leads to an increase in the fractional conversion rate due to a speed up in the kinetics, as indicated by relation (5-10). With the aid of relations (5-8) to (5-11), we can analyze the trends observed in figure 5-26(a). First, it is important to identify the three physical quantities, relevant to the PFR analogy in equation (5-8), that impact char conversion and are impacted by the reactor pressure or mass throughput:

(a) Residence time: $\tau_{av}$ doubles with halving the mass throughput and doubles with doubling the reactor pressure. Increasing $\tau_{av}$ increases $x_{av}$ through equation (5-8).

(b) Fractional conversion rate: $C_{av}$ increases with increasing reactor pressure but is unaffected by the variation in mass throughput alone. Increasing $C_{av}$ increases $x_{av}$ through equation (5-8).

(c) Particle temperature: $T_{p,av}$, the average particle temperature, during char conversion in the reductor, increases with decreasing $x_{av}$ and decreases with increasing $x_{av}$. This is because the heterogeneous reactions occurring in the reductor section are endothermic. The variation in $T_{p,av}$, in turn, impacts $C_{av}$ because both the kinetics and diffusive transport are enhanced by increasing temperature.

In effect, the temperature acts as a restoring force to temper the impact on carbon conversion due to variation of either $\tau_{av}$ or $C_{av}$. This can be illustrated through the following example. Assume that mass throughput is doubled while keeping reactor pressure constant. $\tau_{av}$ is halved, thereby decreasing $x_{av}$. However, decreasing $x_{av}$ results in a rise in $T_{p,av}$, as argued in point (c) above. Increasing $T_{p,av}$ increases $C_{av}$. Increasing $C_{av}$ increases $x_{av}$, thereby tempering the original impact.
The prediction of the CFD model is a cumulative effect of the coupled variations in all the relevant physical quantities involved. Table 5-3 lists the variation in $T_{p,av}$, $C_{av}$ and $\tau_{av}$ for the cases presented in figures 5-26(a) to 5-26(c). As expected, there is a noticeable variation in $T_{p,av}$ across all the cases. The values of $T_{p,av}$, $C_{av}$ and $\tau_{av}$ are extracted from the particle tracking data of the CFD model executed for the various test cases. The $x_{av}$ values are generated using equation (5-8). The overall estimated carbon conversion in the gasifier, $\eta_C$ (estimated), is generated using the $x_{av}$ values. The $\eta_C$ (predicted) values are outputs from the CFD model.

Table 5-3. Estimation of carbon conversion via analysis of particle tracking data, and comparison with carbon conversion predicted by the CFD model for the MHI gasifier

<table>
<thead>
<tr>
<th>Cases</th>
<th>$P_a0$</th>
<th>$P_a1$</th>
<th>$P_a2$</th>
<th>$P_a3$</th>
<th>$P_b1$</th>
<th>$P_b2$</th>
<th>$P_b3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P=27\text{bar}$</td>
<td>$P=27\text{bar}$</td>
<td>$P=27\text{bar}$</td>
<td>$P=27\text{bar}$</td>
<td>$P=54\text{bar}$</td>
<td>$P=54\text{bar}$</td>
<td>$P=54\text{bar}$</td>
<td></td>
</tr>
<tr>
<td>$\dot{m} = 0.5\text{X}$</td>
<td>$\dot{m} = 1\text{X}$</td>
<td>$\dot{m} = 2\text{X}$</td>
<td>$\dot{m} = 4\text{X}$</td>
<td>$\dot{m} = 1\text{X}$</td>
<td>$\dot{m} = 2\text{X}$</td>
<td>$\dot{m} = 4\text{X}$</td>
<td></td>
</tr>
<tr>
<td>$T_{p,av}$ ($K$)</td>
<td>1615</td>
<td>1661</td>
<td>1708</td>
<td>1736</td>
<td>1614</td>
<td>1677</td>
<td>1705</td>
</tr>
<tr>
<td>$C_{av}$ (1/s)</td>
<td>0.0492</td>
<td>0.0865</td>
<td>0.1477</td>
<td>0.1908</td>
<td>0.0562</td>
<td>0.1113</td>
<td>0.1538</td>
</tr>
<tr>
<td>$\tau_{av}$ (s)</td>
<td>10.4</td>
<td>5.2</td>
<td>2.6</td>
<td>1.3</td>
<td>10.4</td>
<td>5.2</td>
<td>2.6</td>
</tr>
<tr>
<td>$x_{av}$</td>
<td>0.446</td>
<td>0.405</td>
<td>0.358</td>
<td>0.249</td>
<td>0.491</td>
<td>0.487</td>
<td>0.370</td>
</tr>
<tr>
<td>$\eta_C$ (estimated) %</td>
<td>83.6</td>
<td>82.5</td>
<td>81.1</td>
<td>77.9</td>
<td>85.0</td>
<td>84.9</td>
<td>81.4</td>
</tr>
<tr>
<td>$\eta_C$ (predicted) %</td>
<td>84.0</td>
<td>82.9</td>
<td>80.0</td>
<td>77.8</td>
<td>86.6</td>
<td>86.7</td>
<td>83.5</td>
</tr>
</tbody>
</table>

The variations between various test cases can be further explored by analyzing the transitions between individual test cases as follows. Note that the cases where a recirculation zone is formed, as indicated in figure 5-26(a) are deliberately omitted from this analysis and are analyzed in the next section instead.

(1) $P_a2 - P_a3$: Mass throughput is doubled while keeping reactor pressure constant. As shown in Table 5-3, $\tau_{av}$ is halved. $T_{p,av}$ increases as a tempering effect. $C_{av}$ increases due to an increase
in $T_{p,av}$. Net impact is a decrease in $x_{av}$. This explains the drop in $\eta_c$ from 80.0% to 77.8% as observed in figure 5-26(a).

(2) $P_2 - P_3$: Mass throughput and reactor pressure are doubled. As shown in Table 5-3, $\tau_{av}$ remains constant. $T_{p,av}$ slightly decreases. $C_{av}$ increases due to speed up of kinetics at the higher pressure. Net impact is an increase in $x_{av}$. This explains the rise in $\eta_c$ from 80.0% to 83.5% as observed in figure 5-26(a).

(3) $P_2 - P_2$: Reactor pressure is doubled while keeping the mass throughput constant. As shown in Table 5-3, $\tau_{av}$ is doubled. $T_{p,av}$ is decreased and this acts as a tempering effect. $C_{av}$ increases due to speed up of kinetics at the higher pressure, the drop in $T_{p,av}$ notwithstanding. Net impact is a decrease in $x_{av}$. This explains the rise in $\eta_c$ from 80.0% to 86.7% as observed in figure 5-26(a).

The analysis above, on case transitions (1), (2) and (3), can be described in another manner. Case transition (1) incorporates the impact of changing the residence time only, not the reactor pressure. Case transition (2) incorporates the impact of changing the reactor pressure only, not the residence time. Case transition (3) incorporates the impact of changing the reactor pressure as well as the residence time. Consequently, the rise in overall carbon conversion is greater in case transition (3) as compared to case transition (2). It should be reiterated that the balancing impact of temperature is present, to a varying degree, in all the transitions.

5.4.2 Characterizing the formation of an internal recirculation zone in the MHI design

The pilot scale MHI gasifier analyzed in this work incorporates tangential injection in the combustor section, as seen in Figure 4-1, in order to create a swirling flow region. As previously demonstrated [7], the swirling flow leads to formation of an internal circulation zone (IRZ) near
the gasifier axis. The recirculation zone traps hot gases and keeps them in contact with the incoming fresh gases, raising their temperature and leading to early ignition. Our results indicate that the recirculation zone is formed only under a certain combination of operating conditions. In this section, we discuss this specific combination of operating conditions and present the impact of the recirculation zone on the overall carbon conversion from the data presented in figures 5-26(a) – 5-26(c).

Figure 5-26(a) shows that increasing mass throughput does not result in the expected drop in carbon conversion when

(a) at 27 bar, the mass throughput is increased from 0.5X to 1X and
(b) at 54 bar, the mass throughput is increased from 1X to 2X.

Further analysis of the results shows that this anomaly can be attributed to the fact that at any operating pressure, a central recirculation zone forms only above a critical value of mass throughput, \( \dot{m}_{cr} \). At 27 bar, \( \dot{m}_{cr} \) lies between 0.5X and 1X, i.e., a recirculation zone does not form for 0.5X and forms for 1X, whereas at 54 bar, \( \dot{m}_{cr} \) lies between 1X and 2X. More work needs to be done in order to include the effects of the formation of recirculation zone within the theoretical framework discussed in the preceding section. Nevertheless, these results indicate that, just based on the optimization of the net carbon conversion, the gasifier should be operated at a value of mass throughput higher than \( \dot{m}_{cr} \) since the formation of a recirculation zone at \( \dot{m}_{cr} \) improves the overall carbon conversion (not forming an IRZ may lead to extinction or make it impossible to achieve ignition).

Figures 5-27(a) – 5-27(e) shows the axial velocity contours for some of the runs conducted at the two different pressures for different values of the mass throughput. The double-headed arrows between figures indicate cases where the axial-velocity magnitudes shown by the color-maps are similar. The most noteworthy observation is the difference between cases
represented by figures 5-27(a), 5-27(d), where the central recirculation zone is absent, and figures 5-27(b), 5-27(c), 5-27(e), where the central recirculation is present. While figures 5-27(b), 5-27(c), 5-27(e) show negative axial velocities close to the axis and higher axial velocities along the periphery, figures 5-27(a), 5-27(d) show positive velocities along the gasifier axis and comparatively lower velocities along the periphery.

In order to further explore the formation of a recirculation zone in this gasifier, it is useful to look at the magnitudes of the axial velocities for different cases along the gasifier centerline. Figures 5-28(a) shows the centerline axial velocity for different values of the mass throughput at 27 bar whereas figure 5-28(b) shows the corresponding values at 54 bar. Beyond \( \dot{m}_{cr} \), increasing the mass throughput leads to higher negative velocities in the central recirculation zone. Moreover, there is a similarity in the magnitude of the axial velocity across the two pressures with respect to onset of recirculation zone formation. At 27 bar and 54 bar, the cases where a recirculation zone is not observed correspond to an exit axial velocity of approximately 2 m/s. Similarly, the cases where \( \dot{m}_{cr} \) is first crossed correspond to exit axial velocities of approximately 4 m/s at both pressures.
Figure 5-27: Contours of axial velocity in the MHI gasifier at different values of gasifier pressure and mass throughput
Figure 5.28: Axial velocities at different values of mass throughput along the gasifier centerline for operating pressure of (a) 27 bar and (b) 54 bar for the MHI gasifier
In order to define a criterion for onset of recirculation zone in this tangentially fired gasifier, we start with the often used definition of the swirl number, $S$, as the ratio of the axial flux of angular momentum to the axial flux of linear momentum. This definition has been applied to characterize swirling flows in combustors equipped with swirl vanes to create a tangential flow component starting with purely axial flow [8]:

$$ S = \frac{2 \int \rho u r dA}{D \int \rho u^2 dA} $$

(5-12)

where $D$ is the reactor diameter, $\rho$ is the mixture density, $r$ is the radial coordinate and $u$, $u_\theta$ are local axial and tangential velocities respectively. A central recirculation zone is observed to form when $S$ crosses a threshold value. However, as shown in Table 5-4, this definition fails to capture the onset of recirculation zone in the gasifier case. Moreover, $S$ remains almost constant, ranging from 1.8 to 2.0, and does not show a monotonic trend as the mass throughput and pressure are varied.

<p>| Table 5-4. Variation of swirl number, $S$, with reactor pressure and mass throughput for the MHI gasifier |
|-------------------------------------------------|------|------|------|------|</p>
<table>
<thead>
<tr>
<th>Mass Throughput</th>
<th>0.5X</th>
<th>1X</th>
<th>2X</th>
<th>4X</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P = 27$ bar</td>
<td>2.04</td>
<td>1.81</td>
<td>1.99</td>
<td>1.94</td>
</tr>
<tr>
<td>$P = 54$ bar</td>
<td>-</td>
<td>1.82</td>
<td>1.78</td>
<td>1.80</td>
</tr>
</tbody>
</table>

For the case analyzed here in which a purely tangential flow is injected from the combustor burners at the bottom of the reactor, both the axial and tangential velocities in equation (5-12) are expected to scale linearly when either the mass throughput or the reactor pressure is varied. Because of this similar scaling of the numerator and denominator, $S$ is observed to be almost constant in Table 5-4 across the range of tested parameters. Consequently, the observation that recirculation zone gets formed above a constant threshold velocity is not
A modified swirl number, $S'$, is proposed in order to characterize the onset of recirculation zone with variable mass throughput and operating pressure in the MHI gasifier:

$$S' = \frac{8\int \rho uu_g r dA}{PD^3} \approx \frac{8\int uu_g r dA}{RT_{av} D^3}$$

where $R$ is the universal gas constant, $\rho_{av}$ is the average mixture density. $T_{av}$ is the average temperature, not observed to vary significantly across various test cases in this study. However, $T_{av}$ will depend on the overall equivalence ratio, coal type and inlet temperatures. In this definition, velocities are only present in the numerator. Hence, $S'$ can be used to characterize the kind of flows analyzed in this study where the onset of recirculation zone correlates with magnitude of axial velocity, as observed in figures 5-28(a) and 5-28(b). Table 5-5 shows that the recirculation zone forms when $S'$ exceeds $2.0 \times 10^{-4}$ for both values of the pressure tested here. In fact, the transition value of $S'$ is expected to lie between $2.0 \times 10^{-4}$ and $7.0 \times 10^{-4}$. Further research is needed to ascertain the scope of applicability of the modified swirl number across an exhaustive set of relevant operating parameters. In addition, suitable experimental investigation on recirculation zone formation in reactors similar to the MHI design will be instrumental in further exploring the relevant physics.

<table>
<thead>
<tr>
<th>Table 5-5. Variation of $S'(x10^4)$ with reactor pressure and mass throughput for the MHI gasifier</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Throughput &amp; 0.5X &amp; 1X &amp; 2X &amp; 4X</td>
</tr>
<tr>
<td>P = 27 bar</td>
</tr>
<tr>
<td>P = 54 bar</td>
</tr>
</tbody>
</table>
5.4.3 Results for Texaco (GE) pilot-scale gasifier

In this section, the GE Cool Water gasifier is analyzed for the impact of gasifier pressure and mass throughput on carbon conversion, exit temperature and cold gas efficiency. Referring to figures 5-29(a) to 5-29(c), a mass throughput of 1X and pressure of 42 bar represent the base case as shown in Table 4-7. The 2X and 4X represent cases where the mass throughput is doubled and quadrupled respectively. All the three mass throughput cases are run at the base pressure of 42 bar and an elevated pressure of 84 bar. For the sake of convenience, the test cases at 42 bar pressure are labeled P_a1, P_a2, P_a3 whereas those at 54 bar pressure are labeled P_b1, P_b2, P_b3 in figure 5-29(a).

Despite the limited similarities between GE and MHI designs, the overall trends observed in figures 5-29(a) to 5-29(c) are similar to those observed in figures 5-26(a) to 5-26(c). The carbon conversion decreases with increasing mass throughput and increases with increasing reactor pressure. The exit temperature increases with increasing mass throughput and decreases with increasing pressure. The reason, as in the MHI gasifier, is the endothermicity of the C-H_2O and C-CO_2 gasification reactions which dominate away from the near-nozzle region. The cold gas efficiency follows the same trends as the carbon conversion since greater conversion implies greater amounts of CO and H_2 in the exit stream.

It should be noted that the added complication of the presence of a central recirculation zone, under specific conditions, is not present in the GE gasifier. However, in the GE gasifier, an external recirculation zone invariably forms close to the side wall near the injector and negative velocities are observed near the top dome-shaped wall, as observed in figure 5-19(d).
Table 5-6 lists the variation in $T_{p,av}$, $C_{av}$ and $\tau_{av}$ for the cases presented in figures 5-29(a) to 5-29(c). The values of $T_{p,av}$, $C_{av}$ and $\tau_{av}$ are extracted from the particle tracking data of the CFD model executed for the various test cases. The $x_{av}$ values are generated using the PFR output conversion relation (5-8). The overall estimated carbon conversion in the gasifier, $\eta_C$ (estimated), is generated using the $x_{av}$ values. The $\eta_C$ (predicted) values are outputs from the CFD model. As done for the MHI gasifier in section 5.4.1, the variations between various test cases are explored by analyzing the transitions between a set of individual test cases.

(1) $P_a2 - P_a3$: Mass throughput is doubled while keeping reactor pressure constant. As shown in Table 5-6, $\tau_{av}$ is halved. $T_{p,av}$ increases as a tempering effect. $C_{av}$ increases due to an increase
in $T_{p,av}$. Net impact is a decrease in $x_{av}$. This explains the drop in $\eta_c$ from 94.2% to 92.4% as observed in figure 5-29(a).

(2) $P_a2 - P_b3$: Mass throughput and reactor pressure are doubled. As shown in Table 5-6, $\tau_{av}$ remains constant. $T_{p,av}$ slightly increases. $C_{av}$ increases due to speed up of kinetics at the higher pressure. Net impact is an increase in $x_{av}$. This explains the rise in $\eta_c$ from 94.2% to 98.1% as observed in figure 5-29(a).

(3) $P_a2 - P_b2$: Reactor pressure is doubled while keeping mass throughput constant. As shown in Table 5-6, $\tau_{av}$ is doubled. $T_{p,av}$ decreases as a tempering effect. $C_{av}$ increases due to speed up of kinetics at the higher pressure, the drop in $T_{p,av}$ notwithstanding. Net impact is a decrease in $x_{av}$. This explains the rise in $\eta_c$ from 94.2% to 99.3% as observed in figure 5-29(a).

The match between $\eta_c$ (estimated) and $\eta_c$ (predicted), as observed in Table 5-6, is not as good for the GE gasifier as it is for the MHI gasifier. The reason is that due to the prominent external recirculation zone, a PFR analogy is not completely applicable to the GE gasifier. Nonetheless, the data in Table 5-6 does provide useful qualitative trends. It should be noted that overall conversions in the GE gasifier are reasonably high across the range of test cases presented here. This is primarily due to the excess oxygen injected and the high temperatures attained, as observed in figure 5-19(e). The peak temperatures in the GE gasifier are about 500K higher than those in the MHI gasifier, while the exit temperatures are about 200K higher than the corresponding values for the MHI design.
Table 5-6. Estimation of carbon conversion via analysis of particle tracking data, and comparison with carbon conversion predicted by the CFD model for the GE gasifier

<table>
<thead>
<tr>
<th>Cases</th>
<th>( P_{a1} ) (bar)</th>
<th>( P_{a2} ) (bar)</th>
<th>( P_{a3} ) (bar)</th>
<th>( P_{b1} ) (bar)</th>
<th>( P_{b2} ) (bar)</th>
<th>( P_{b3} ) (bar)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( m = 1X )</td>
<td>( m = 2X )</td>
<td>( m = 4X )</td>
<td>( m = 1X )</td>
<td>( m = 2X )</td>
<td>( m = 4X )</td>
</tr>
<tr>
<td>( T_{p,av} ) (K)</td>
<td>1798</td>
<td>1853</td>
<td>1890</td>
<td>1765</td>
<td>1816</td>
<td>1874</td>
</tr>
<tr>
<td>( C_{av} ) (1/s)</td>
<td>1.769</td>
<td>2.483</td>
<td>3.212</td>
<td>1.427</td>
<td>2.026</td>
<td>3.009</td>
</tr>
<tr>
<td>( t_{av} ) (s)</td>
<td>4.8</td>
<td>2.4</td>
<td>1.2</td>
<td>9.6</td>
<td>4.8</td>
<td>2.4</td>
</tr>
<tr>
<td>( x_{av} )</td>
<td>1.0</td>
<td>0.997</td>
<td>0.979</td>
<td>1.0</td>
<td>1.0</td>
<td>0.999</td>
</tr>
<tr>
<td>( \eta_{C} ) (estimated) %</td>
<td>100.0</td>
<td>99.8</td>
<td>98.6</td>
<td>100.0</td>
<td>100.0</td>
<td>99.9</td>
</tr>
<tr>
<td>( \eta_{C} ) (predicted) %</td>
<td>95.9</td>
<td>94.2</td>
<td>92.4</td>
<td>99.9</td>
<td>99.3</td>
<td>98.1</td>
</tr>
</tbody>
</table>

5.5 Conclusions

The following conclusions can be drawn from this work:

1) Fine grinding helps accelerate carbon conversion in reactors where conversion is diffusion-limited, for example within the oxygen-rich combustor section of the MHI gasifier. The impact is not as noticeable where conversion is kinetics-limited, for example in the low temperature reductor section of MHI gasifier.

2) Fine grinding speeds up conversion in the GE gasifier, in particular, in the oxygen-rich near-nozzle region where diffusion limited conversion takes place. The smallest particles convert completely in the near-nozzle region. The larger particles convert farther downstream in the \( H_2O \)-dominated regions.
3) The onset of recirculation zone formation in MHI gasifier, at a given operating pressure, occurs beyond a critical value of gasifier mass throughput, \( \dot{m}_{cr} \). Across operating pressures, the onset is observed to occur above a critical value of average axial velocity. The modified swirl number, \( S' \), takes this aspect into account.

4) Formation of internal recirculation zone at \( \dot{m}_{cr} \) boosts carbon conversion in the MHI gasifier. It is recommended that gasifier mass throughput be in excess of \( \dot{m}_{cr} \) in order to optimize carbon conversion.

5) Higher operating pressure lead to higher carbon conversion, increasing the gasifier mass throughput reduces carbon conversion. The average residence time, average particle temperature during conversion and pressure effect on kinetics are the key factors that influence the overall carbon conversion when the operating pressure and gasifier mass throughput are varied.

References


Chapter 6

CONCLUSIONS AND FUTURE WORK

6.1 Conclusions

A multiscale model of entrained flow gasification has been developed and comprehensively validated. Validation was performed at the level of individual critical submodels including the turbulence model and the particle turbulent dispersion model. Special consideration was given to the construction of the char consumption model since it affects the prediction of carbon conversion most directly. In addition, the overall CFD model was validated for a variety of the gasifier operating conditions including air-blown to oxygen-blown, atmospheric pressure to pressurized, pilot-scale to lab-scale, tangentially-injected to axially injected conditions. The validated model is then used to study the impact of key operating parameters such as feedstock particle size, reactor pressure and mass throughput, via sensitivity analysis, on the performance of the pilot-scale MHI gasifier and the GE Cool Water gasifier. The sensitivity analysis yielded interesting results on the conditions under which fine grinding is helpful in the two gasifiers. Moreover, the model gave quantitative estimates of the expected gain or loss in overall carbon conversion when critical operating parameters such as gasifier mass throughput and pressure are varied.

Finally, it is concluded that the validated CFD model is a useful tool for optimization of gasifier operating conditions and for understanding of various physico-chemical phenomena occurring within the gasifier and affecting its performance.
6.2 Directions for future work

The validated CFD model can be used to perform sensitivity analyses on the impact of more critical design and operating parameters such as injection angle, burner diameter, slurry loading, gasifier length and diameter. In addition, it can be used as a design tool to investigate innovative design ideas.

The CFD model developed in this work takes \(\sim\) two days to converge under a typical mesh resolution of 200,000 grid points, provided that a reasonable starting solution is available. However, arriving at a converged solution from scratch typically takes 4-5 days. A reduced order model (ROM) can be very helpful to run test cases with a much shorter turnaround time, of the order several minutes. The shortcoming of a ROM is that it compromises predictive accuracy by assuming lumped-parameter estimates for complex physical phenomena, including recirculation zones, and involves coarse-grained modeling of physical processes demanding large computational expense, such as radiative heat transport.

Apart from the demonstrated utility of the CFD model in analyzing and predicting gasifier performance, it is also useful as a tool to provide reasonably accurate estimates of relevant lumped parameters to a ROM. For example, the present model has been applied to inform the in-house ROM in our group on the amount of mass flow in the external recirculation zone within the GE gasifier. The CFD model can also be used to check and inform the values of radiative heat transfer, wall heat transfer and conversion rates predicted by ROM. In short, a comprehensively validated CFD model can be used to validate coarse-grained submodels within a ROM.