**“Exergy analysis and CFD modeling of Downdraft Gasifier for Biomass Gasification”**

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By

**AKASH MISHRA [01/THR/09]**

Under the guidance of

**Asst. Prof. RAJ KUMAR SINGH**



**Department of Mechanical Engineering,**

**Delhi College of Engineering, University of Delhi, Delhi**

**Session 2007-11**

**CERTIFICATE**

This is to certify that the thesis entitled **“Exergy analysis and CFD modeling OF Downdraft Gasifier for Biomass Gasification”** by **Akash Mishra**, University Roll No. 8571, College Roll No. 01/THR/09 in partial fulfilment of the requirement for the award of the degree of Master of Engineering in Structural Engineering, Delhi College of Engineering, Delhi, is an authentic. The work is being carried out by him under our guidance and supervision in the academic year 2010-2011. This is to our knowledge has reached requisite standards.

Also, I do hereby state that I have not submitted the matter embodied in this thesis for the award of any degree.

**AKASH MISHRA**

**College Roll No. ME/THR/01**

**University Roll NO. 8571**

This is to certify that the above statements made by Akash Mishra are correct to the best of our knowledge.

**Raj Kumar Singh**

**Asst. Professor**

**Department of Mechanical Engineering**

**Project Guide**

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**Akash Mishra**

M. E. (Thermal Engineering)

College Roll No. ME/THR/01

University Roll No. 8571

Department of Mechanical Engineering

Delhi College of Engineering

Delhi-110042

ABSTRACT



Biomass energy combined with computational fluid dynamics (CFD) software has been described in some detail in the following study. The aspect of biomass gasifier has been investigated with regard to the potential of designing future gasifier using simulation in FLUENT software.

The project is about the study and CFD modeling of fluid flow of biomass fuel inside biomass downdraft gasifier. Gasifier is divided in to three different zones viz.

1.Drying and Pyrolysis Zone.

2.Oxidation Zone.

3.Reduction Zone.

Firstly the study of gasification process is undertaken by means of thermodynamic equilibrium modeling in each zones with the help of EES software and the effect of moisture content on model is evaluated.

Then using the typical design of gasifier, a 2-D model is produced for easier iterations and simulations. The type of gasifier modeled is atmospheric Downdraft gasifier. The gasifier model is set to have initial temperature at 400 K and operating pressure of 1 atmosphere. After iterating in FLUENT with first-order discretization, the results obtained are convergent and show that using second-order discretization is not suitable for 2-Dimensional model. Finally performance evaluation of gasification process is undertaken and future investigations are also suggested in this study for more accurate result using computational fluid dynamic (CFD) software.

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**CHAPTER 1**

**ENERGY SCENARIO**



* 1. **Introduction**

Energy is one of the major inputs for the economic development of any Country. In the case of the developing countries, the energy sector assumes a Critical importance in view of the ever increasing energy needs requiring huge investments. Energy can be classified into several types based on the following criteria:

* Primary and Secondary energy
* Commercial and Non commercial energy
* Renewable and Non-Renewable energy
  + 1. **Primary and Secondary Energy**

Primary energy sources are those that are either found or stored in nature. Common primary energy sources are coal, oil, natural gas, and biomass (such as wood). Other primary energy sources available include nuclear energy from radioactive substances, thermal energy stored in earth's interior, and potential energy due to earth's gravity. Primary energy sources are mostly converted in industrial utilities into secondary energy sources; for example coal, oil or gas converted into steam and electricity.

**1.1.2 Commercial Energy and Non Commercial Energy**

The energy sources that are available in the market for a definite price are known as commercial energy. By far the most important forms of commercial energy are electricity, coal and refined petroleum products. Commercial energy forms the basis of industrial, agricultural, transport and commercial development in the modern world. In the industrialized countries, commercialized fuels are predominant source not only for economic production, but also for many household tasks of general population. Examples: Electricity, coal, oil, natural gas etc.

The energy sources that are not available in the commercial market for a price are classified as non-commercial energy. Non-commercial energy sources include fuels such as firewood, cattle dung and agricultural wastes, which are traditionally gathered, and not bought at a price used especially in rural households. These are also called traditional fuels. Non-commercial energy is often ignored in energy accounting. Example: Firewood, agro waste in rural areas; solar energy for water heating, energy for lifting water and electricity generation, biomass etc.

**1.1.3 Renewable and Non-Renewable Energy**

Renewable energy is energy obtained from sources that are essentially inexhaustible. Examples of renewable resources include wind power, solar power, geothermal energy, tidal power and hydroelectric power. The most important feature of renewable energy is that it can be harnessed without the release of harmful pollutants. Non-renewable energy is the conventional fossil fuels such as coal, oil and gas, which are likely to deplete with time.

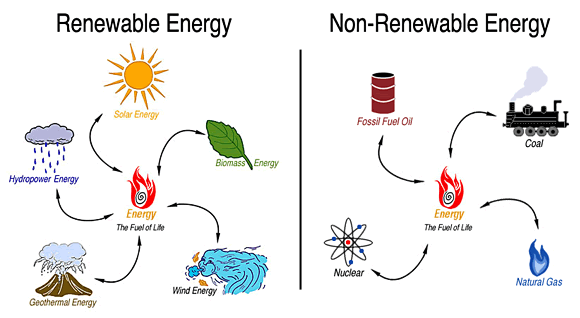


Figure 1: Renewable and Non renewable energy sources [36]

* 1. **GLOBAL Primary Energy Consumption**

In 2009, world energy consumption decreased for the first time in 30 years (-1.1%) or 130 Megaton oil equivalent, as a result of the financial and economic crisis (GDP drop by 0.6% in 2009). This evolution is the result of two contrasting trends. Energy consumption growth remained vigorous in several developing countries, specifically in Asia (+4%).In North America, Europe and CIS, consumptions shrank by 4.5%, 5% and 8.5% respectively due to the slowdown in economic activity. China became the world's largest energy consumer (18% of the total) since its consumption surged by 8% during 2009 (from 4% in 2008). Oil remained the largest energy source (33%) despite the fact that its share has been decreasing over time. Coal posted a growing role in the world's energy consumption: in 2009, it accounted for 27% of the total.

Energy consumption is loosely correlated with gross national product and climate, but there is a large difference even between the most highly developed countries, such as Japan and Germany with 6 kWh per person and United States with 11.4 kWh per person. In developing countries, particularly those that are sub-tropical or tropical such as India, the per person energy use is closer to 0.7 kWh.

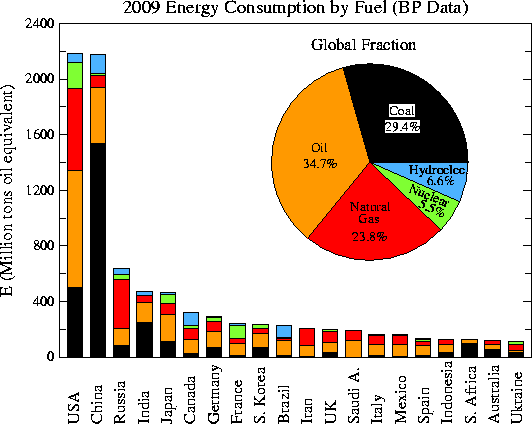


Figure 2: World’s energy consumption, 2009 [36]

* 1. **India’s Energy scenario**

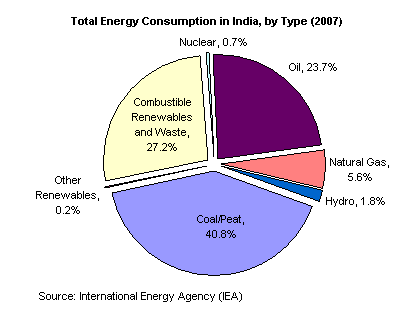
India ranks fifth in the world in terms of primary energy consumption, accounting for about 3.5% of the world commercial energy demand in the year 2003. Despite the overall increase in energy demand, per capita energy consumption in India is still very low compared to other developing countries. India is well-endowed with both exhaustible and renewable energy resources. Coal, oil, and natural gas are the three primary commercial energy sources. India is, however, poorly endowed with oil assets and has to depend on crude imports to meet a major share of its needs (around 70 percent). India’s primary energy mix has been changing over a period of time. Despite increasing dependency on commercial fuels, a sizeable quantum of energy requirements (40% of total energy requirement), especially in the rural household sector, is met by non-commercial and traditional energy sources, which include fuel wood, crop residue, biomass and animal waste, including human and draught animal power. The usage of such sources of energy is estimated at around 155 Mtoe per annum. However, other forms of commercial energy of a much higher quality and efficiency are steadily replacing the traditional energy resources being consumed in the rural sector.

Coal is the most important & abundant fossil fuel in India and accounts for 55% of India's energy need. India's industrial heritage was built upon indigenous coal, largely mined in the eastern and the central regions of the country. Thirty per cent of commercial energy requirements are met by petroleum products, nearly 7.5 per cent by natural gas and 3.5 per cent by primary electricity. India faces coal shortage of 24 MT. Production of petroleum reserves has been stretched from 5.7 MT during 1970/ 71 to 110 MT in 2003/ 04. Natural gas demand too has been steadily growing at the rate of about 6.5% during the last 10 years.

* + 1. **India’s Renewable Energy Sources**

Renewable energy sources offer viable option to address the energy security concerns of a country. Today, India has one of the highest potentials for the effective use of renewable energy. India is the world’s fifth largest producer of wind power after Denmark, Germany, Spain, and the USA. There is a significant potential in India for generation of power from renewable energy sources— wind, small hydro, biomass, and solar energy. The country has an estimated SHP (small-hydro power) potential of about 15000 MW. Installed combined electricity generation capacity of hydro and wind has increased from 19194 MW in 1991/ 92 to 31995 MW in 2003/ 04, with a compound growth rate of 4.35% during this period.

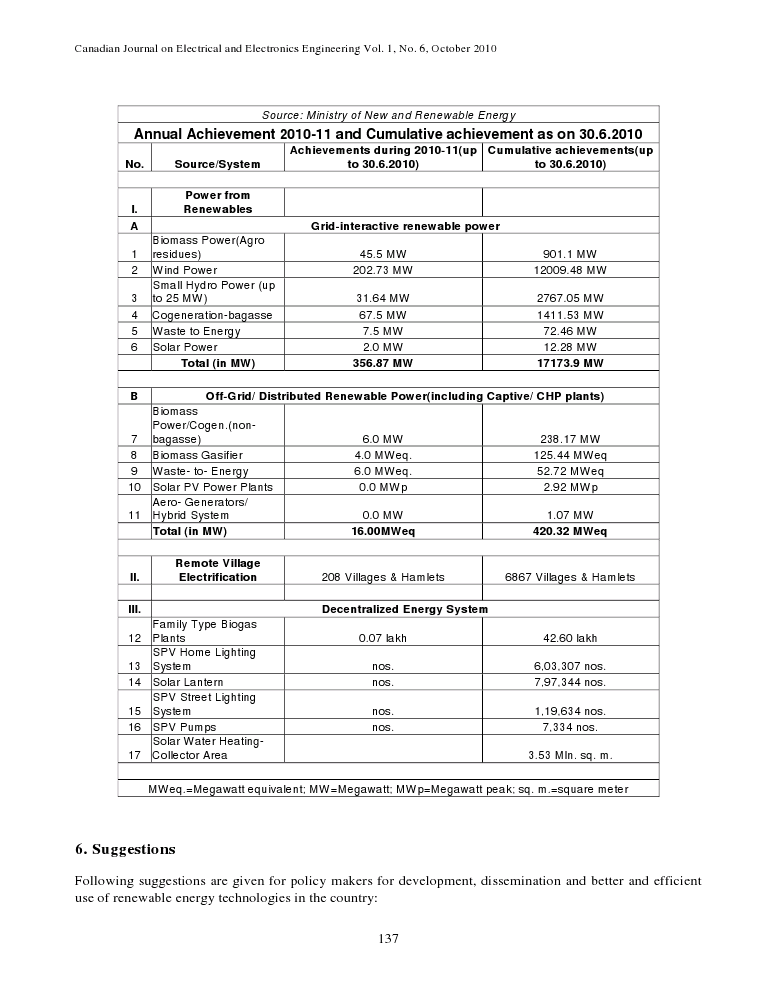
Other renewable energy technologies, including solar photovoltaic, solar thermal, small hydro and biomass power are also spreading. Greater reliance on renewable energy sources offers enormous economic, social, and environmental benefits. The potential for power production from captive and field-based biomass resources, using technologies for distributed power generation, is currently assessed at 19500 MW including 3500 MW of exportable surplus power from bagasse-based cogeneration in sugar mills.



**Figure 3: Total energy consumption of India [36]**

The Table 1 shows the magnitude of power generation from various renewable energy sources of India for the year of 2010-2011.From this point onwards focus will be towards biomass gasification as an alternative energy source against fossil fuels.

Table 1: power generation assessment of india, 2010-2011.



**GASIFICATION**

Gasification is the thermal upgrading process (Figure 2.1), in which the majority of carbon is converted into synthesis gas commonly known as syngas (consisting of carbon monoxide, methane and hydrogen), leaving an inert residue, by partial combustion of waste in the reactor with air or with pure oxygen or with oxygen enriched air or by counter current reaction with steam. Relatively high temperatures are employed, 900-1100 oC with air and 1100-1400 oC with oxygen.

GASIFICATION and PYROLYSIS are similar processes. Both decomposes organic and inorganic wastes by exposing it high temperatures.Both processes limit the amount of oxygenpresent during decomposition; Gasification allows a small amount of oxygen, pyrolysis allows none.In other words both prevents oxygen.

* 1. **Significance of current work**

There are several types of gasifier that are normally used for converting biomass fuel to get power. For example, updraft gasifier, downdraft gasifier and fluidised bed gasifier.

In the dissertation, biomass gasification is modelled in downdraft gasifier. This study has shown that the quality of the product gas is found to be dependent on the smooth flow of the fuel and the uniformity of the pyrolysis process. Various authors have also suggested that gasification of biomass products is a clean alternative to fossil fuels and this product gas can be directly used in internal gas combustion engines or after suitable modification in CHP plants. This model can provide useful predictions of operating other downdraft gasifier using diverse biomass feeds as fuel.

* 1. **Aim & objectives of the study**

Firstly the gasification process is analyzed from thermodynamic equilibrium point of view (1-D Modeling) and effect of moisture content on reaction temperature, lower heating value of fuel and mole fractions of components of producer gas was also undertaken and the results so obtained are compared with experimental work carried out by J.K. Ratnadhariya and S.A. Channiwala.

In the simulation part of the project, a 2-D model of downdraft gasifier consistent with main observed phenomena is proposed and designed and meshed in GAMBIT. To adapt the model for numerical analysis, the Non – premixed combustion model was utilized to simulate the process of gasification in the biomass gasifier in FLUENT 6.3Some results obtained from numerical methods are analyzed and also effect of some operating parameters was seen on gasification phenomenon. On this basis, the validity of proposed model is being discussed.

**Chapter 2**

**gasification**

**2.1 Historical background**

The process of gasification to produce combustible from organic feeds was used in blast furnaces over 180 years ago. The possibility of using this gas for heating and power generation was soon realized and there emerged in Europe producer gas systems, which used charcoal and peat as feed material. By 1945 the gas was being used to power trucks, buses and agricultural and industrial machines. It is estimated that there were close to 9000,000 Vehicles running on producer gas all over the world.

After World War II the lack of strategic impetus and the availability of cheap fossil fuels led to general decline in the producer gas industry. However Sweden continued to work on producer gas technology and the work was accelerated after 1956 Suez Canal crisis. Research into suitable designs of wood gasifier, essentially for transport use, was carried out at the National Swedish Institute for Agricultural Machinery Testing and is still in progress.

Historically, emphasis has been placed on small-scale gasifier, and numerous designs have been built and tested. Over the past two decades, there has been increasing interest in the use of larger-scale gasifier to provide fuel for advanced power generation concepts such as gas turbines, or for use where strict environmental emission regulations exist. In these cases, the raw product gas must be cleaned and conditioned prior to use. The ability to produce clean energy potentially allows gasification to be used in other situations where combustion is unsuitable including:

* Facilities where stringent emission standards are enforced.

Locations where public perception of combustors is negative.

**2.2 Biomass conversion technologies**

There are a number of technological options available to make use of a wide variety of biomass types as a renewable energy source. Conversion technologies may release the energy directly, in the form of heat or electricity, or may convert it to another form, such as liquid biofuel or combustible biogas. While for some classes of biomass resource there may be a number of usage options, for others there may only one appropriate technology. In Thermo-chemical processing, the equivalence ratio Φ is an important parameter and is given by

**Φ = (actual fuel-air ratio):(stoichiometric fuel air ratio )**

The stoichiometric oxygen to fuel ratio is the theoretical amount of oxygen needed to completely combust the fuel. Based on the equivalence ratio, different types of thermal processes of biomass fuels are characterized as follows.

I) Pyrolysis: 0≤ Φ ≤ 0.2

II) Combustion: Φ ≥ 0.4

III) Gasification: 0.2≤Φ≤ 0.40

The various biomass conversion processes consist of:-

**2.2.1 Thermal conversion**

These are processes in which heat is the dominant mechanism to convert the biomass into another chemical form. The basic alternatives are separated principally by the extent to which the chemical reactions involved are allowed to proceed:

1. **Combustion** means oxidation of biomass to release energy. This heat can itself be used in a number of ways:

* Space heating
* Water heating for central or district heating or process heat
* Steam for electricity generation in co-firing and combined heat and power plants (CHP).

1. **Gasification** is a partial oxidation process whereby a carbon source such as coal, natural gas or biomass, is broken down into carbon monoxide (CO) and hydrogen (H2), carbon dioxide (CO2) and methane (CH4). The oxidizer may be air, in which case the producer gas will also contain nitrogen (N2), or steam or oxygen.

It is classified further depending on Operating Temperature regime:-

**Low temperature gasification**

If the gasification takes place at a relatively low temperature, such as 700ºC to 1000ºC, the product gas will have a relatively high level of hydrocarbons compared to high temperature gasification.



**High temperature gasification**

Higher temperature gasification (1200ºC to 1600ºC) leads to few hydrocarbons in the product gas, and a higher proportion of CO and H2.This is known as synthesis gas (syngas or biosyngas) as it can be used to synthesize longer chain hydrocarbons using techniques such as Fischer-Tropsch (FT) synthesis.

If the ratio of H2 to CO is correct (2:1) FT synthesis can be used to convert syngas into high quality synthetic diesel biofuel which is completely compatible with conventional fossil diesel and diesel engines.

Gasification technology can be used for:

* Heating water in central heating, district heating or process heating applications
* Steam for electricity generation or motive force
* As part of systems producing electricity or motive force
* Transport using an internal combustion engine.

1. **Pyrolysis**is the precursor to gasification, and takes place as part of both gasification and combustion.  It consists of thermal decomposition in the absence of oxygen. The products of pyrolysis include gas, liquid and a sold char, with the proportions of each depending upon the parameters of the process. Lower temperatures (around 400ºC) tend to produce more solid char (slow pyrolysis), whereas somewhat higher temperatures (around 500ºC) produce a much higher proportion of liquid (bio-oil), provided the vapor residence time is kept down to around 1s or less.  After this, secondary reactions take place and increase the gas yield.



Applications for pyrolysis include:

* Biomass energy densification for transport or storage
* Co-firing for heat or power
* Feedstock for gasification.

1. **Hydrothermal upgrading (HTU)** is a liquefaction process that has been developed specifically to convert high moisture content biomass into a product with higher energy density. Many forms of biomass in the waste stream have very high moisture content, which makes them both inefficient to store or transport, and difficult to process by most conventional technologies.  They do potentially offer a very cheap feedstock, however, as there may often be a charge to dispose of such putrescible waste, rendering it either very low, or even negative cost. HTU makes use of biomass, typically in 25% slurry in water, and subjects it to pressures up to of 120-180 bar, and temperatures of 300 to 350ºC for 5-20 minutes to yield a mixture of liquid 'bio-crude', gas (mainly CO2) and water.

**2.2.2. Chemical conversion**

A range of chemical processes may be used to convert biomass into other forms, such as to produce a fuel that is more conveniently used, transported or stored, or to exploit some property of the process itself.

**2.2.3 Biochemical conversion**

As biomass is a natural material, many highly efficient biochemical processes have developed in nature to break down the molecules of which biomass is composed, and many of these biochemical conversion processes can be harnessed. Biochemical conversion makes use of the enzymes of bacteria and other micro-organisms to break down biomass. In most cases micro-organisms are used to perform the conversion process:

1. Fermentation
2. Composting
3. Anaerobic digestion

**2.3 Basics of Biomass Gasification**

The biomass gasification is an environment-friendly and sustainable technology that can fight against energy crisis in the world. It can reduce the dependence on fossil fuels to a great extent. The technology can recycle bio-waste and can be made available on demand without the need for separate storage. The electricity produced from biomass gasification can be used for lighting houses, powering irrigation pumps and operating machines such as chiller.

There are different options for converting biomass energy to electricity, these are:-

1. Conventional steam cycle –In this biomass is combusted to produce steam that is then used to drive a steam turbine
2. Gasification – In this case, biomass is converted to a mixture of gas in presence of high temperature and partial oxidizing agent.
3. Pyrolysis – In this, biomass is converted to a liquid rather than a mixture of gases.
4. Anaerobic digestion – In this the sewage waste is digested in digester to produce methane
5. Landfill gas – It’s a collection of gas from landfill sites.

The production of generator gas (producer gas) called gasification, is partial combustion of solid fuel (biomass) and takes place at temperatures of about 10000C. The reactor is called gasifier. The combustion products from complete combustion of biomass generally contain nitrogen, water vapor, carbon dioxide and surplus of oxygen. However in gasification where there is a surplus of solid fuel (incomplete combustion) the products of combustion are combustible gases like Carbon monoxide (CO), Hydrogen (H2) and traces of Methane and non useful products like tar and dust. The production of these gases is by reaction of water vapor and carbon dioxide through a glowing layer of charcoal. Thus the key to gasifier design is to create conditions such that a) biomass is reduced to charcoal and, b) charcoal is converted at suitable temperature to produce CO and H2.

The following Table shows the typical product gas composition in presence of different gasification agents:-

**Table 2: Syngas Composition (mol fraction. %)**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Gasification agent** | **Hydrogen** | **Carbon monoxide** | **Methane** | **Carbon dioxide** | **Nitrogen** |
| **Steam** | **40%** | **25%** | **8%** | **25%** | **2%** |
| **Air** | **15%** | **20%** | **2%** | **15%** | **48%** |

**2.4 FUELS FOR GASIFICATION**

Almost any carbonaceous or biomass fuel can be gasified under experimental or laboratory conditions19. However the real test for a good gasifier is not whether a combustible gas can be generated by burning a biomass fuel with 20-40% stoichiometric air but that a reliable gas producer can be made which can also be economically attractive to the customer. Towards this goal the fuel characteristics have to be evaluated and fuel processing done. A gasifier is very fuel specific and it is tailored around a fuel rather than the other way round. Thus a gasifier fuel can be classified as good or bad according to the following parameters:

**2.4.1 Energy content and Bulk Density of fuel**

The higher the energy content and bulk density of fuel, the similar is the gasifier volume since for one charge one can get power for longer time.

**2.4.2 Moisture content**

In most fuels there is very little choice in moisture content since it is determined by the type of fuel, its origin and treatment. It is desirable to use fuel with low moisture content because heat loss due to its evaporation before gasification is considerable and the heat budget of the gasification reaction is impaired. For example, for fuel at 250C and raw gas exit temperature from gasifier at 3000C, 2875 KJ/kg moisture must be supplied by fuel to heat and evaporate moisture.

Besides impairing the gasifier heat budget, high moisture content also puts load on cooling and filtering equipment by increasing the pressure drop across these units because of condensing liquid. Thus in order to reduce the moisture content of fuel some pretreatment of fuel is required. Generally desirable moisture content for fuel should be less than 20%.

**2.4.3 Dust content**

All gasifier fuels produce dust. This dust is a nuisance since it can clog the internal combustion engine and hence has to be removed. The gasifier design should be such that it should not produce more than 2-6 g/m3 of dust .The higher the dust produced, more load is put on filters necessitating their frequent flushing and increased maintenance.

**2.4.4 Tar**

Tar is one of the most unpleasant constituents of the gas as it tends to deposit in the carburetor and intake valves causing sticking and troublesome operations. It is a product of highly irreversible process taking place in the pyrolysis zone. The physical property of tar depends upon temperature and heat rate and the appearance ranges from brown and watery (60% water) to black and highly viscous (7% water content).there are approx 200 constituents that have been identified in tar.

Very little research work has been done in the area of removing or burning tar in the gasifier so that relatively tar free gas comes out. Thus the major effort has been devoted to cleaning this tar by filters and coolers. A well-designed gasifier should put out less than 1 g/m3 of tar. Usually it is assumed that a downdraft gasifier produces less tar than other gasifiers25. However because of localized inefficient processes taking place in the throat of the downdraft gasifier it does not allow the complete dissociation of tar

**2.4.5** **Ash and Slagging Characteristics**

The mineral content in the fuel that remains in oxidized form after complete combustion is usually called ash. The ash content of a fuel and the ash composition has a major impact on trouble free operation of gasifier. Ash basically interferes with gasification process in two ways

1. It fuses together to form slag and this clinker stops or inhibits the downward flow of biomass feed.
2. Even if it does not fuse together it shelters the points in fuel where ignition is initiated and thus lowers the fuel’s reaction response.

Ash and tar removal are the two most important processes in gasification system for its smooth running. Various systems have been devised for ash removal. Slagging, however, can be overcome by two types of operation of gasifier:

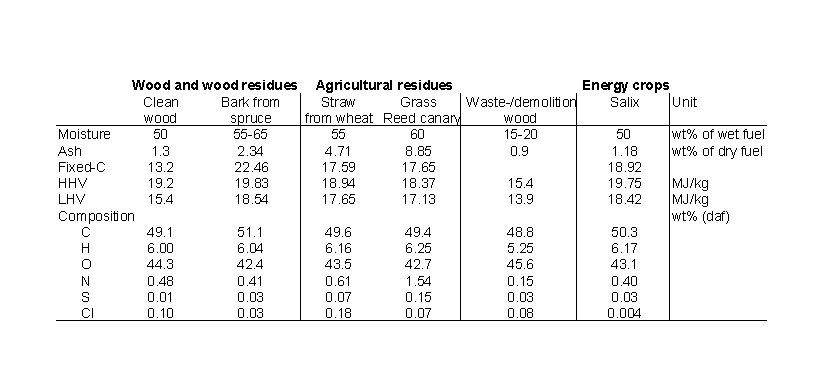
1. Low temperature operation that keeps the temperature well below the flow temperature of the ash.
2. High temperature operation that keeps the temperature above the melting point of ash.

Thus not every fuel can undergo successful gasification. Most of the development work is carried out with common fuels such as coal, charcoal and wood. It was recognized that fuel properties such as surface, size, shape as well as moisture content, volatile matter and carbon content influence gasification. The Main Biomass sources are:

* **Virgin wood**, from forestry, arboricultural activities or from wood processing
* **Energy crops**: high yield crops grown specifically for energy applications
* **Agricultural residues**: residues from agriculture harvesting or processing
* **Food waste**, from food and drink manufacture, preparation and processing, and post-consumer waste
* **Industrial waste and co-products** from manufacturing and industrial processes.

Here are examples of ultimate analyses of different types of biomass fuel. They have very low value of sulfur & low carbon that are more favorable from coal.

Table 3: Ultimate and proximate analysis of fuels for gasification.



**2.5 Gasification Approaches**

While the characteristics of the product gases from different concepts varies significantly, gasification approaches can be grouped into two general types based on the energy content of the product. The energy content of the gas depends on the approach used to supply heat to drive the gasification reactions. Most designs use oxygen, either in air or in its separated form, as an oxidizing agent to generate heat by partially combusting the biomass feedstock.

* 1. **Types of Gasification**
     1. **Direct gasification**

In direct gasification, Oxygen or Air is used as blast. Gasification can be accomplished by using the principal of partial oxidation. In this case exothermic gasification occurs by supplying sub-stoichiometric blast to the process. The equivalence ratio (ER) is the amount of oxidant supplied relative to the stoichiometric requirement. Optimum gasification efficiency occurs near an equivalence ratio of 0.26 in purely direct biomass gasification. In practical reality, incomplete conversion will occur due to kinetic limitations of volatile matter conversion and heat and mass transfer limitations of fixed carbon conversion. These effects relate to reactor design constraints and system configuration effects. The amount of tar in the generated gas often depends on reactor design. Minimizing tar with creative equipment design is a principal goal for gasification engineers.

**2.6.2 Indirect Gasification**

Indirect gasification is accomplished using steam as an oxidant. However, steam reforming of biomass is endothermic and often heat transfer limited. Endothermic gasification generates more methane than direct gasification per volume of gas, so the energy density may be higher. The thermal input required for steam reforming of biomass means that some clever method of high rate heat transfer must be devised.

Steam gasification is thermodynamically more efficient than direct gasification, but practical heat transfer limitations and thermodynamic availability requirements for high temperature heat exchange often makes reality a bit different.

**2.7 TYPES of reactors**

Based on the design of gasifier and type of fuels used, there exists different kinds of gasifier. A technology such as biomass gasification that allows utilization of biomass fuel is of great importance. Hence for various fuels and output gas applications, different types of gasifier are used. Some of the commonly used gasifiers are:

**2.7.1 Updraft or Counter-current Gasifier**

It is one of the oldest and most simplified types of gasifier. In an updraft gasifier, the flow of the biomass particles and the gasification agent (i.e. air/oxygen/steam) is in opposite directions. The air intake is at the bottom and the gas leaves at the top. The combustion reactions occur at the grate that is near the bottom of the gasifier, which are followed by reduction reactions somewhat higher up in the gasifier. In the upper part of the gasifier, heating and pyrolysis of the feedstock occur as a result of heat transfer by forced convection and radiation from the lower zones. The tars and volatiles produced during this process are carried in the gas stream. Ashes are removed from the bottom of the gasifier.

The major advantages of this type of gasifier are its simplicity, high charcoal burn-out and internal heat exchange leading to low gas exit temperatures and high equipment efficiency. The drawback of an updraft gasifier is the high amount of tar content that is produced in the gasifier, which makes the producer gas unsuitable for engine applications.

**2.7.2 Downdraft or Co-current gasifier**

In a downdraft gasifier, the biomass material enters the gasifier through hopper. In this type of gasifier, there is a co-current flow that gives discrete zones of pyrolysis and char gasification. On their way down the acid and tarry pyrolysis products from the fuel pass through a glowing bed of charcoal and therefore are converted into permanent gas i.e. a mixture of hydrogen, carbon dioxide, carbon monoxide and methane. Depending on the temperature of the hot zone and the residence time of the tar vapors, a near complete breakdown of the tars is achieved. However, practically it is highly improbable to achieve a tar-free gas. Also since the levels of organic compounds in condensate are lower for downdraft gasifier and hence it poses less threat to the environment.

The major drawback of downdraft equipment lies in its inability to operate on a number of unprocessed fuels. In particular, fluffy and low-density materials give rise to flow problems and excessive pressure drop, and the solid fuel must be pelletized or briquette before use. Minor drawbacks of the this type of system, as compared to updraft system, are somewhat lower efficiency resulting from the lack of internal heat exchange as well as the lower heating value of the gas.

**2.7.3 Cross-draft gasifier**

Cross-draft gasifiers are an adaptation for the use of charcoal. Charcoal gasification results in very high temperatures (1500 °C and higher) in the oxidation zone which places constraints on the material used for the structure of the gasifier. In cross draft gasifiers the fuel (charcoal) itself provides insulation against these high temperatures. Advantages of the system lie in the very small scale at which it can be operated. Installations below 10 kW (shaft power) can under certain conditions be economically feasible. The reason is the very simple gas-cleaning train (only a cyclone and a hot filter) which can be employed when using this type of gasifier in conjunction with small engines. A disadvantage of cross-draught gasifiers is their minimal tar converting capabilities and the consequent need for high quality (low volatile content) charcoal.

**2.7.4 Fluidized bed gasifier**

The operation, of both up and downdraft gasifiers, is influenced by the morphological, physical and chemical properties of the fuel. Problems commonly encountered are: lack of bunker flow, slagging and extreme pressure drop over the gasifier. As shown in Figure 4, air is blown through abed of solid particles at a sufficient velocity to keep these in a state of suspension. The bed is originally externally heated and the feedstock is introduced as soon as a sufficiently high temperature is reached. The fuel particles are introduced at the bottom of the reactor, very quickly mixed with the bed material and almost instantaneously heated up to the bed temperature. As a result of this treatment the fuel is pyrolyzed very fast, resulting in a component mix with a relatively large amount of gaseous materials. Further gasification and tar-conversion reactions occur in the gas phase. Most systems are equipped with an internal cyclone in order to minimize char blow-out as much as possible. Ash particles are also carried over the top of the reactor and have to be removed from the gas stream if the gas is used in engine applications.

The major advantages of fluidized bed gasifiers come from their feedstock flexibility resulting from easy control of temperature, which can be kept below the melting or fusion point of the ash (rice husks), and their ability to deal with fluffy and fine grained materials (sawdust etc.) without the need of pre-processing. Problems with feeding, instability of the bed and fly-ash sintering in the gas channels can occur with some biomass fuels. Other drawbacks of the fluidized bed gasifier lie in the rather high tar content of the product gas (up to 500 mg/m³ gas), the incomplete carbon burn-out, and poor response to load changes.

**2.7.5 Rotary Kiln Gasifier**

In this type of gasifier, the charge is slowly tumbling which results in limited contact between the charge and the gas phase. Hence, Rotary Kiln gasifier has incomplete gasification unless conditions are favorable for long residence times of the charge in the gasifier.

**2.7.6 Spouted bed Gasifier**

Spouted bed gasifier is a variant of the fluidized bed gasifier. There are multiple spouts present in the gasifier through which coarse material can be introduced in the bed. This kind of gasifier is capable of handling mixed biomass materials of different densities and sizes.

**2.7.7 Entrained flow gasifiers**

They are commonly used for coal because they can be slurry fed in direct gasification mode, which makes solid fuel feeding at high-pressures delightfully inexpensive. There are several commercial designs available for coal but these will not work with more than 10 to 15% biomass in a coal blend. This principal slurry feeding benefit cannot be afforded to biomass because of its high porosity (lower energy density) and moisture holding capacity in a slurry phase. An entrained flow gasifier could be conceived that is pneumatically fed, for example for use with sawdust or other finely divided biomass.

However, the pneumatically fed EFG does not compare to the high-pressure feeding benefits achieved by slurry feeding. ETF’s can operate in slagging & non-slagging modes, referring to either molten ash or dry ash production. Slagging gasification is not practical for biomass due to its lower go/no-go ash fusion limits.

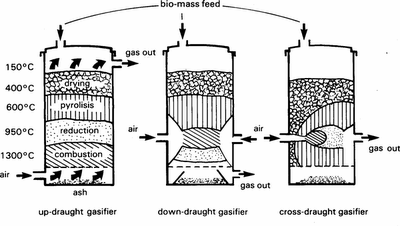


Figure 4: Fixed bed type gasifiers [37]

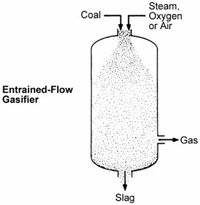
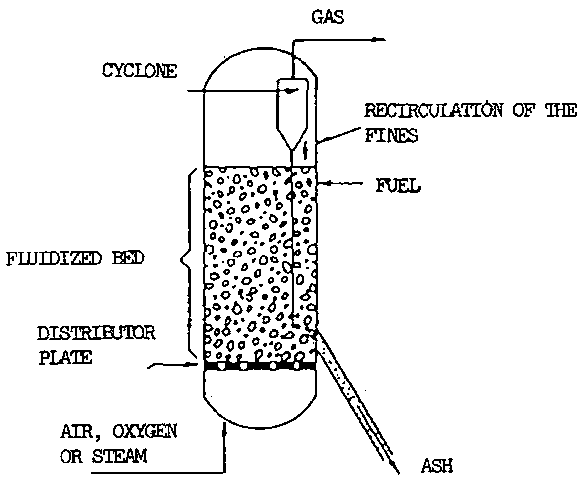


Figure 5: Fluidized and Entrained flow Gasifier [37]

**2.8 CHEMISTRY of Biomass Gasification**

Biomass gasification, a century old technology, is viewed today as an alternative to conventional fuel. In gasification processes, wood, charcoal and other biomass materials are gasified to produce so called producer gas for power or electricity generation. A gasification system basically consists of a gasifier unit, purification system, and energy converters-burner or engine.

Gasification is a thermo-chemical process that converts biomass materials into a gaseous component. The result of gasification is the producer gas, containing carbon monoxide, hydrogen, methane and some other inert gases. Mixed with air, the producer gas can be used in gasoline or a diesel engine with little modifications. The complexity of the gasification process is due the number of reactions taking place, and the considerable number of components in the biomass. The following Thermo-chemical processes that occur during gasification of biomass are:

**2.8.1 Pre Heating**

This involves pre-heating of the fuel and air for better gasification.

**2.8.2 Drying**

Drying is first major process occurring inside the gasifier. It takes place at nearly 50-150 degree C where all the moisture in the wood is converted into steam. The steam helps in reduction further down the system. The rate of drying disaffected by numerous factors such as Temperature, velocity of the feed, moisture content, external surface area and diffusivity.The reaction is suitably represented as:

**Wet biomass (having moisture) +heat → Dry biomass + water vapor**

**2.8.3 Devolatilization/Pyrolysis**

In the devolatilization (pyrolysis) zone, the volatile components which are present in the wood, including various aromatic and tarry compounds, get vaporized and the remaining wood gets converted into char. Typically, pyrolysis occurs at 200-800 degree C and produces char, carbon monoxide, carbon dioxide, water vapor, methane, other higher hydrocarbons, pyroligneous acids and tars. Pyrolysis is affected by various factors such as pyrolysis temperature, rate of heating, physical & chemical characteristics of feed and presence of catalytic compounds. The reaction is shown:

**Biomass + heat → Char(C) + volatiles (CO, CO2, H2O, H2) +Tar (CH4, C6H6, C2H4, C6H5OH etc)**

**2.8.4 Combustion**

The substance of a solid fuel is composed of the elements carbon, hydrogen and oxygen. Nitrogen and sulfur may also exist, but since these are present only in small quantities they will be disregarded in the following discussion. In the types of gasifiers considered here, the solid fuel is heated by combustion of a part of the fuel. The combustion gases are then reduced by being passed through a bed of fuel at high temperature. In complete combustion, carbon dioxide is obtained from the carbon, and water from the hydrogen. Oxygen from the fuel will of course be incorporated in the combustion products thereby decreasing the amount of combustion air needed .Oxidation, or combustion, is described by the following chemical reaction:

**C + O2 → CO2 + heat**

**H2 + 0.5O2 → H2O + heat**

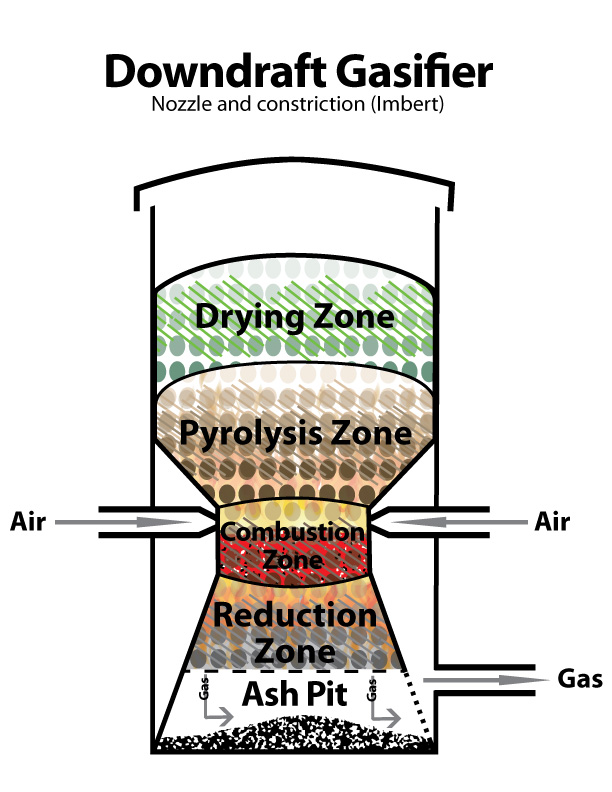
**Tar (heavy hydrocarbons) +O2 → H2O + CO2 + heat**

**2.8.5 Gasification/Reduction**

In the gasification process, primarily the char and other solid/liquid organic compounds gets reduced and oxidized to form various gases which make up the output gas. This is one of the key processes in the process of Biomass gasification and optimization of this process can help in increasing the calorific value of the fuel while at the same time reducing the amount of tar content amount of tar content in the fuel.

In addition to the above processes, various other processes occur in the gasifier like consecutive gas phase reaction involving water shift reaction, steam reforming reaction and other various other ash-catalyzed reactions like

|  |  |
| --- | --- |
| **C + H2O + heat → CO + H2** | **(Primary gasification reaction)** |
| **C + 2H2 → CH4 + heat** | **(Methanation reaction)** |
| **3H2 + CO → CH4 + H2O + heat** | **(Steam reforming)** |
| **H2O + CO → CO2 + H2 + heat** | **(Water gas shift reaction)** |
| **C+ CO2 → 2CO** | **(Bourdard Reaction)** |
| **4H2 + CO2 → CH4 + 2H2O + heat** |  |



**FIGURE 6: downdraft gasifier [37]**

* The above figure shows relative positions of various zones that characterize the different processes occurring while gasification in an Imbert type downdraft gasifier.

**CHAPTER 3**

**LITREATURE REVIEW**

Historically, emphasis has been placed on small-scale gasifier, and numerous designs have been built and tested. Over the past two decades, there has been increasing interest in the use of larger-scale gasifier to provide fuel for advanced power generation concepts such as gas turbines, or for use where strict environmental emission regulations exist. In these cases, the raw product gas must be cleaned and conditioned prior to use. The ability to produce clean energy potentially allows gasification to be used in other situations where combustion is unsuitable including:

* Facilities where stringent emission standards are enforced.
* Locations where public perception of combustors is negative.

**3.1 Liturature review of various authors**

Before proceeding to the present study, following Literature Survey is being carried out:

**Ratnadhariya J. K** [1], shows in his study that the gasification process in the down draft gasifier passes through four stages i.e., drying, pyrolysis, oxidation or combustion & reduction or gasification. For getting optimal operating parameters of down draft gasifier to obtain good quality gas and safe, non –slagging operation it is necessary to study parametric sensitivity of the down draft gasifier.In his paper he also discussed parametric sensitivity of down draft gasifier with the help of three zone KF (Kinetic Free) model. KF model computes gas composition, temperature levels in each zone and performance parameters of the gasifier without involving any reaction kinetics. The drying and pyrolysis zones are clubbed together and form the first zone of the gasifier. The oxidation and reduction

zone make the other two zones of gasifier. Each zone has been modeled through use of Stoichiometry of reaction, mass balance, chemical equilibrium and energy balance. This KF model has been validated with published experimental results and thereafter it is used for the study of sensitivity of gas compositions, temperature profile in each zone and gasifier performance parameters as a function of equivalence ratio, moisture content and C/H ratio. He also found the equivalence ratio in the vicinity of 0.3 and moisture content in the range of 10 to 20%, as the optimal operating parameters to obtain good quality gas and safe, smooth running of gasifier with woody biomass as its feed. Also, this model is capable to identify the suitability of biomass material for pyrolysis / gasification process. His report clearly indicates that biomass material having C/H ratio in the vicinity of 0.719 are the best-feed stock for pyrolysis / gasification.

**Awdhesh kr sharma** [2], presented an Experimental study on 75 kWth, downdraft (biomass) gasifier system to obtain temperature profile, gas composition, calorific value and trends for pressure drop across the porous gasifier bed, cooling–cleaning train and across the system as a whole in both firing as well as non-firing

mode.. He shows in firing mode, the pressure drop across the porous bed, cooling–cleaning train, bed temperature profile, gas composition and gas calorific value are found to be sensitive to the gas flow rate and also the rise in the bed temperature due to chemical reactions strongly influences the pressure drop through the porous gasifier bed. In non-firing mode, the extinguished gasifier bed arrangement gives much higher resistance to flow as compared to a freshly charged gasifier bed. The influence of ash deposition in fired-gasifier bed and tar deposition in sand filters is also examined on the pressure drop through them. He generated an experimental data in his article that is useful for validation of any simulation codes for gasifiers and the pressure drop characteristics may be useful towards the coupling of a gasifier to the gas engine for motive power generation or decentralized electrification applications.

**Jarungthammachote, A. Dutta[4] ,** developed the thermodynamic equilibrium model based on equilibrium constant for predicting the composition of producer gas in a downdraft waste gasifier. To enhance the performance of the model, further modification was made by multiplying the equilibrium constants with coefficients. The modified model was validated with the data reported by different researchers. The results showed that the mole fraction of H2 gradually increases; CO decreases; CH4, which has a very low percentage in the producer gas increases; N2 slightly decreases; and CO2 increases with increasing MC. The reaction temperature, the calorific value, and the second law efficiency, decrease when MC increases.

**J.K. Ratnadhariya a,S.A. Channiwala [5**] proposed a three zone equilibrium and kinetic free model of biomass gasifier. In this three zone: first zone of the model is drying and pyrolysis zone combined together; second zone is oxidation zone; and the third zone is the reduction zone. Each zone has been formulated with: (i) reaction stoichiometry; (ii) constituent balance; and (iii) energy balance along with a few justifying assumptions. In this model he provided an operating range of equivalence ratio and moisture content for the woody biomass materials. Further, through this model he also presented the prediction of the maximum temperature in the oxidation zone of gasifier, which provides useful information for the design of the gasifier and selection of the material for the construction. The main feature of the model lies in the fact that it is capable of handling predictions for all category of biomass materials with a wide operating range of equivalence ratio and moisture content in all of the three principal zones of the gasifier.

**Avdhesh Kr. Sharma [7]**,developed a fluid flow and heat transfer model for the reactive, porous bed of the biomass gasifier to simulate pressure drop, temperature profile in the bed and flow rates. The conservation equations, momentum equation and energy equation are used to describe fluid and heat transport in porous gasifier bed. The model accounted for drag at wall, and the effect of radial as well as axial variation in bed porosity to predict pressure drop in bed. Heat transfer has been modeled using effective thermal conductivity approach. Model predictions are validated against the experiments, while effective thermal conductivity values are tested qualitatively using models available in literature. Parametric analysis has been carried out to investigate the effect of various parameters on bed temperature profile and pressure drop through the gasifier. In his study he recommends that the size of preheating zone may be extended up to pyrolysis zone in order to enhance preheating of input air, while thermal insulation should not be less than 15 cm.

**Kentaro Umeki [8]**, studied a high temperature steam gasification process to generate hydrogen-rich fuel gas from woody biomass. In his study, the performance of the gasification system which employs only high temperature steam exceeding 1200 K as the gasifying agent was evaluated in a 1.2 ton/day scale demonstration plant. He also carried out a numerical analysis to analyze the experimental results. Both the steam temperature and the molar ratio of steam to carbon (S/C ratio) affected the reaction temperature which strongly affects the gasified gas composition. He found the H2 fraction in the produced gas was 35–55 vol.% at the outlet of the gasifier. The highest cold gas efficiency was 60.4%. However, the gross cold gas efficiency was 35%, which considers the heat supplied by high temperature steam. The ideal cold gas efficiency of the whole system with heat recovery processes was 71%.

**M.K. Karmakar , A.B. Datta[10]** ,The objective of his study was to investigate the process of generating hydrogen rich syngas through thermo chemical fluidized bed gasification of biomass. The experiments were performed in a laboratory scale externally heated biomass gasifier. He took Rice husk as a representative biomass and, steam had been used as the fluidizing and gasifying media. A thermodynamic equilibrium model was used to predict the gasification process. The work included the parametric study of process parameters such as reactor temperature and steam biomass ratio which generally influence the percentage of hydrogen content in the product gas. He used Steam here to generate nitrogen free product gas and also to increase the hydrogen concentration in syngas with a medium range heating value of around 12 MJ/Nm3.

**David Brown [12],** addresses the thermo-economic assessment of a mid-scale (20 MWth,wood) wood gasification, gas cleaning and energy conversion process, with particular attention given to electricity generation costs and tar control. Product distributions were estimated with a parametric stoichiometric equilibrium model calibrated using atmospheric air gasification data. He defined a multi-objective optimization problem for a superstructure of alternative energy flow diagrams for each processing step. He also shows the trade-off between total investment costs and the exergy efficiency of electricity production , and analysed to identify operating conditions that minimise tar formation to prevent equipment fouling.

**Yukihiko Okumura [15],** studied the effect of pyrolysis conditions on char reactivity using Raman spectroscopy. This paper reports on the relationship between the properties of biomass char and the gasification rate. First-order kinetic rate constants are determined by fitting the weight loss data using a random pore model. The gasification rate of biomass char increases with the heating rate at pyrolysis. This is due to the coarseness (surface morphology) of biomass char and rough texture, which increases with the heating rate.

**G. Van Oost [17]** , developed an experimental plasma-chemical reactor equipped with a novel hybrid gas–water stabilized torch is available at IPP Prague for the innovative and environmentally friendly plasma treatment of waste streams with a view to their sustainable energetic and chemical valorization and to a reduction of the emission of greenhouse gases. He studied Gasification/pyrolysis of biomass was experimentally using crushed wood as a model substance. He demonstrated homogeneous heating of the reactor volume and proper mixing of plasma with treated material in spite of the low plasma mass flow rate and constricted plasma jet. The economical viability, environmental performance and safety of biofuels/hydrogen produced from syngas resulting from the plasma-thermochemical gasification of a very broad range of second generation biomass feedstock was investigated.

**Kentaro Umeki [18],** proposed a simple expression for the apparent reaction rate of large wood char gasification with steam . Large char samples were gasified under steam atmosphere using a thermo-balance reactor. The apparent reaction rate was expressed as the product of the intrinsic rate and the effective factor.In his study,the effective factor was modified to include the effect of change in char diameter and intrinsic reaction rate during the reaction. Assuming uniform conversion ratio throughout a particle ,he divided the simplified reaction scheme into three stages. In the initial stage, the local conversion ratio increases without particle shrinkage. In the middle stage, the particle shrinks following the shrinking core model without change in the local conversion ratio. In the final stage, the local conversion ratio increases without particle shrinkage. The validity of the modified effective value was confirmed by comparison with experimental results.

**Thilakavathi Mani [21]** presented a model in which Gasification kinetics of wheat straw char withCO2 was investigated using Thermo gravimetric apparatus (TGA).The main objective was to identify the diffusional and surface reaction phenomena that may occur during biomass char gasification experiments withCO2. The effects of temperature (750–900 1C) and particle size (o60–925 mm) on gasification rate of char-CO2 reaction were determined.The 50% conversion (r50) rate showed that the reactivity increases with temperature,and it decreases as the particle size increases. It was found that char gasification within the temperature range studied followed the chemically controlled reaction regime and the influence of pore diffusion was negligible for fine powder particles.

**Giltrap et al. [27]** developed a model for the reduction zone of downdraft biomass gasifier to predict the composition of producer gas under steady state operation. The accuracy of the model is limited by the availability of data on the initial conditions at the top of the reduction zone**. Babu and Sheth [26]** modified the Giltrap’s model by incorporating the variation of char reactivity factor (*CRF*) along the reduction zone of downdraft biomass gasifier.

**Yasuaki Ueki [28],** endorsed the Gasification technology is recognized as one of the possibilities for utilizing biomass effectively. This study focused on woody biomass gasification fundamentals, using a bench-scale packed-bed reactor. In his experiment, pellets of black pine were gasified, using air as the oxidizing agent. Gasification tests were carried out under both updraft and downdraft conditions. Temperature distributions and compositions of syngas inside the gasifier were continuously monitored during gasification experiments at several ports on the wall of the reactor. The syngas at the exit of the gasifier was also sampled to estimate the amount of tar. Lower heating values of the syngas under updraft and downdraft conditions were 4.8 and 3.8 MJ/ m3N, respectively.He shows that it was easier to control the height of the packed bed under the downdraft condition than under the updraft condition. Under the updraft condition, a bridging phenomenon occurred. Tar generation under the downdraft condition was lower than that under the updraft condition. This is because tar passes through a partial combustion zone or higher temperature zone in the downdraft gasifier.

**S. Karellas[29],** shows the use of biomass and waste for decentralized combined heat and power production (CHP) requires highly efficient gasification processes.He developed an allothermal gasifier which produces a hydrogen- rich, high-calorific gas, that can be further used in a microturbine or a fuel cell producing energy.Further he shows, for the operation of such a system, the online analysis of the composition of the product gas is of high importance, since the efficient working of the machines is linked with the gas quality. For this purpose an optical measurement system based on laser spectroscopy has been applied. This system can measure not only the basic components of the product gas (H2, CH4, CO, CO2, H2O), but it also gives information concerning the content of high hydrocarbons, the so-called tars, in the product gas.

**E.D. Gordillo[30]** , presented a two phase biomass char steam gasification kinetic model is developed in a bubbling fluidized bed with nuclear heat as source of energy. This model is capable of predicting the temperature and concentration profiles of gases in the bubble, emulsion gas and solid phases. The robust model calculates the dynamic and steady state profiles, as well as the complex parameters of fluidized bed. Three pilot scale gasifiers were simulated in order to see the effect of the H/D ratio and the bed heating dynamics in the gasification kinetics, these parameters are found to be really important in order to enhance the water-gas shift reaction, and consequently, the hydrogen production.

**Paolo Baggio[31],** presented the energy and the environmental impact analysis of an innovative system based on the pyrolysis of MSW which produces solid (char), liquid (tar) and gas (syngas) fuels used in a combined cycle for electric power generation. The syngas, after filtration and compression, feeds two gas turbines. In turn, the exhaust from the gas turbines, after post-combustion with char and tar, drives a steam turbine power plant. Before being discharged, the flue gas is processed in a selective catalytic reduction (SCR) unit to reduce CO, VOC and NOx content and is filtered to remove particulate matter. This innovative approach to energy recovery from MSW combines high energy efficiency with a low level of polluting emissions. The estimated global efficiency of the plant, referred to the LHV of the MSW, is around 28–30%, a much higher value than ordinarily obtained in traditional waste incineration plants.

**Elisabeth Wetterlund [32]** , shows biomass gasification is a key technology in reaching targets for renewable energy and CO2 emissions reduction.In his study he shows evaluation of policy instruments affecting the profitability of biomass gasification applications integrated in a Swedish district heating (DH) system for the medium-term future (around year 2025). Two polygeneration applications based on gasification technology are considered in this paper: (1) a biorefinery plant co-producing synthetic natural gas (SNG) and district heat; (2) a combined heat and power (CHP) plant using integrated gasification combined cycle technology. Using an optimisation model he identified the levels of policy support, here assumed to be in the form of tradable certificates, required to make biofuel production competitive to biomass based electricity generation under various energy market conditions. It is concluded that the large capital commitment and strong dependency on policy instruments makes it necessary that DH suppliers believe in the long-sightedness of future support policies, in order for investments in large-scale biomass gasification in DH systems .

**Xiuli Zhan [33]** , studied CO2 gasification of petroleum coke using black liquor as a catalyst which was performed in a thermogravimetric analyzer (TGA) under temperatures 1223–1673 K at ambient pressure to evaluate the effect of black liquor loading on petroleum coke gasification. He found that the gasification reactivity of petroleum coke was improved greatly by black liquor. He also found the gasification reactivity was affected by different loading methods in the order: wet grinding > dry grinding > physical impregnation > dry mix. The catalytic activity of black liquor was higher than that of pure alkali metal. The effect of temperature on the gasification reactivity of petroleum coke was changed by black liquor. The reactivity reaches its maximum at 1573 K, clearly demonstrating that black liquor could be an effective catalyst for petroleum coke gasification.

**Liu Hongtao [34]** , studied a two-stage underground coal gasification was to improve the caloric value of the syngas and to extend gas production times. Also a model test using the oxygen-enriched two-stage coal gasification method was carried out. He analyzed composition of the gas produced, the time ratio of the two stages, and the role of the temperature field. The results show that oxygen-enriched two-stage gasification shortens the time of the first stage and prolongs the time of the second stage. The caloric value of the syngas improves with increased oxygen concentration in the first stage. Injection of 80% oxygen-enriched air gave gas with the highest caloric value and also gave the longest production time. The caloric value of the gas obtained from the oxygenenriched two-stage gasification method lies in the range from 5.31 MJ/Nm3 to 10.54 MJ/Nm3.

**3.2 Important findings from literature review**

Followings are the important findings from the literature review:

1. In the equilibrium modeling, Stoichiometry of reaction, mass balance, chemical equilibrium and energy balance are to be performed along with considering the equilibrium constants in order to find the gas composition and gasification temperature.
2. Commonly applied variable in any gasifier are Equivalence ratio and Moisture content of fuel which affects the gasifier performance.
3. With an increase in Moisture content ,the mole fraction of H2 gradually increases; CO decreases; CH4, which has a very low percentage in the producer gas increases; N2 slightly decreases; and CO2 increases,the reaction temperature, the calorific value, and the second law efficiency, decrease.
4. For getting optimal operating parameters of down draft gasifier to obtain good quality gas and safe, non –slagging operation it is necessary to study parametric sensitivity of the down draft gasifier.
5. Equivalence ratio in the vicinity of 0.3 and moisture content in the range of 10 to 20%, as the optimal operating parameters to obtain good quality gas and safe, smooth running of gasifier with woody biomass as its feed.
6. The rise in the bed temperature due to chemical reactions strongly influences the pressure drop through the porous gasifier bed.
7. In firing mode, the pressure drop across the porous bed, cooling–cleaning train, bed temperature profile, gas composition and gas calorific value are found to be sensitive to the gas flow rate.
8. In non-firing mode, the extinguished gasifier bed arrangement gives much higher resistance to flow as compared to a freshly charged gasifier bed.
9. size of preheating zone may be extended up to pyrolysis zone in order to enhance preheating of input air, while thermal insulation should not be less than 15 cm.
10. The steam temperature and the molar ratio of steam to carbon (S/C ratio) affect the reaction temperature which strongly affects the gasified gas composition.
11. The gasification rate of biomass char increases with the heating rate at pyrolysis. This is due to the coarseness (surface morphology) of biomass char and rough texture, which increases with the heating rate.
12. Char gasification within the temperature range studied followed the chemically controlled reaction regime and the influence of pore diffusion was negligible for fine powder particles.
13. The caloric value of the syngas improves with increased oxygen concentration in the first stage. Injection of 80% oxygen-enriched air gives gas with the highest caloric value and also the longest production time.

**3.3 Objective of Present work**

1. Thermodynamic equilibrium modeling of downdraft gasifier dividing it into three different zones viz. drying and pyrolysis zone, oxidation zone and reduction zone for the prediction of the gas composition and temperature in zone.
2. Further, for the simulation part, a 2-D model of downdraft gasifier consistent with main observed phenomenon is proposed ,designed and meshed in GAMBIT. To adapt the model for numerical analysis, the Non-premixed combustion model will be utilized to simulate the process of gasification in the gasifier in FLUENT 6.3.

**Chapter-4**

**THERMODYNAMIC EQULIBRIUM MODELLING OF A BIOMASS GASIFIER**



**4.1 INTRODUCTION**

The gasifier is a device in which gasification process is taking place. This gasification process is a thermochemical conversion of biomass into gaseous fuel (producer gas).

This process in the down draft gasifier passes through four stages i.e., drying, pyrolysis, oxidation or combustion & reduction or gasification. Forgetting optimal operating parameters of down draft gasifier to obtain good quality gas and safe, non –slagging operation, it is necessary to study parametric sensitivity of the down draft gasifier. Thepresent report is an attempt towards the study of parametric sensitivity of down draft gasifier with the help of three zone KF (Kinetic Free) model. KF model computes gas composition, temperature levels in each zone and performance parameters of the gasifier without involving any reaction kinetics. The drying and pyrolysis zones are clubbed together and form the first zone of the gasifier. The oxidation and reduction zone make the other two zones of gasifier. Each zone has been modeled through use of Stoichiometry of reaction, mass balance, chemical equilibrium and energy balance. This KF model has been validated with published experimental results and there after it is used for the study of sensitivity of gas compositions, temperature profile in each zone and gasifier performance parameters as a function of equivalence ratio, moisture content and C/H ratio. This model clearly indicates the equivalence ratio in the vicinity of 0.3 and moisture content in the range of 10 to 20%, as the optimal operating parameters to obtain good quality gas and safe, smooth running of gasifier with woody biomass as its feed. Also, this model is capable to identify the suitability of biomass material for pyrolysis/ gasification process. It clearly indicates that biomass material having C/H ratio in the vicinity of 0.719 are the best-feed stock for pyrolysis / gasification.

**4.2 PHYSICAL DESCRIPTION AND FORMULATION OF MODEL**

Fig 1 gives overall view of the physical model of downdraft gasifier along with possible reactions in the different zones i.e., drying & pyrolysis, oxidation and reduction. Drying and pyrolysis zones are clubbed together. Product composition and temperature in this zone is computed assuming equilibrium of water gas, methanation and water gas shift reaction along with condition of mass and energy

balance.

Dry wood+Moisture

CH1.451O0.697 +H2O

**Drying and pyrolysis zone reactions**

C+H2O=CO+H2

C+2H2=CH4

CO+H2O=CO2+H2

hp1

Char (C)

Cop +CO2p +H2p +H2Op +CH4p

**Figure 7: Drying and Pyrolysis Zone**

These products enter the oxidation zone where incoming air reacts and complete oxidation of hydrogen to H2O and partial oxidation of char and methane takes place. The char oxidation yields CO and CO2, which are assumed to follow Evans and Emmons relationship [4]. The extent of methane oxidation is assumed to be 60% on molar basis, this proportion being arrived at after several trials towards comparability of model and experimental results. Channiwala [5] in his work assumed this methane carry over as 50%.

(CHAR +GASES +AIR)P

**Oxidation zone reactions**

C+O2=CO2

C+(1/2)O2=CO

CO+(1/2)O2=CO2

H2+(1/2)O2=H2O

XCH4+XO2=(X/2)CH4+(X/2)CO2+XH2O

h1OXD

Char (C)

CoOXD +CO2OXD +H2OOXD +CH4OXD+N2OXD

**Figure:8 Oxidation Zone**

The products from oxidation zone enter reduction zone. The balance 40% methane is assumed to be carried forward through this zone while char carry over is assumed to be 3% on molar basis based on the work of Channiwala [5]. The other gas constituents in reduction zone are assumed to be at shift equilibrium. The product distribution and temperature level in this zone is obtained using mass and energy balance equations along with the condition of shift equilibrium.

(Char+Gases)oxd

**Reduction zone reactions**

C+H2O=CO+H2

C+CO2=2CO

CO+H2O=CO2+H2

hR1

Char (CR)

RAW GAS

COR +CO2R+H2R +H2OR +CH4R+N2R

COR +CO2R +H2R+H2OR+CH4R+N2R

**Figure 9: Reduction Zone**

**4.3 Methodology for gas composition and temperature in each zone**

**4.3.1 Drying and pyrolysis Zone**

To develop the model A generalized form of equation is used of gasification process. For the present study,**Sababul Wood (CH1.451O0.697 ,HHV=19.777 MJ/kg)** is being used as a biomass fuel.

**CHxOy + wH2O → Char+N1 CO + N2 CO2 +N3 H2  + N4 H2O + N5 CH4**

**4.3.1.1 Mass balance Equations**

To find the five unknown species of the producer gas, five equations were required. Those equations were generated using mass balance and equilibrium constant relationships. Considering the global gasification reaction, the first three equations were formulated by balancing each chemical element as shown;

Carbon balance:

**N1+N2+N5-0.237=0**

Hydrogen balance:

**2N3+2N4+4N5-x-2w=0**

Oxygen balance:

**N1+2N2+N4-w-y=0**

Chemical equilibrium is usually explained by using equilibrium constant. The remaining two equations were obtained from the equilibrium constant of the reactions occurring in the gasification zone as shown below:

Water-gas reaction: C + H2O = CO + H2,

Methane reaction: C + 2H2 = CH4.

Using relations involving equilibrium constants K1 and K2 and species in these reactions we get 2 more equations as:

**N1\*N4\*K1-N2\*N3=0** (from Water gas shift reaction)

**N5\*(N1+N2+N3+N4+N5)- K2\*N32 =0** ( from Methanation reaction)

Following equations were used for the equilibrium state of ideal gas mixture because of the requirements of K1 and K2 values:

**ln(K) = - (Δ G0T)/(R\*T)**

**Δ G= ∑ νi Δg0f, T, i**

Where R is the universal gas constant, 8.314 kJ/(kmol - K),Δ G0T is the standard Gibbs function of reaction, and Δg0f,T,I represents the standard Gibbs function of formation at given temperature T of the gas species i which can be expressed by the empirical equation :

**(Δg0f,T )=(h0f)- a T lnT- b T2 - (c/2)T3 – (d/3) T4 + (e/2T)+ f + g T**

The values of coefficients a–g and the enthalpy of formation of the gases are presented in **APPENDIX A**

For calculating K1 and K2, the temperature in the gasification or reduction zone must be known. In this study, it was determined using energy balance method.

**4.3.1.2 Energy Balance Equations**

The temperature of the gasification zone needs to be calculated in order to calculate the equilibrium constants. For this reason, either energy or enthalpy balance was performed for the gasification process which was usually assumed to be an adiabatic process. When the temperature in gasification zone is T and the temperature at inlet state is assumed to be 298K (25 degree C), the enthalpy balance for this process can be written as

**∑ h0f,j (j=reactant specie) = ∑( h0f,I + Δh0T,i)(i=product specie)**

Where h0f is the enthalpy of formation in kJ/kmol and its value is zero for all chemical elements at reference state (298 K, 1 atm), and Δh0T represents the enthalpy difference between any given state and at reference state. It can be approximated by:

**ΔhT =∫Cp dt**

Where Cp is specific heat at constant pressure in kJ/kmol-K and is a function of temperature. It can be defined by the empirical equation below:

**Cp = a1 T + b1 T2 + c1 T3 +d1 T4 + K**

Where K is a constant obtained from the integration and a1, b1, c1and d1are the specific gas species coefficients, which are shown in **APPENDIX A.**

Hence using above equations we can find the required gasification Temperature.

**4.3.2 Oxidation Zone**

The products coming out of the drying and pyrolysis zone will now enter to the Oxidation zone. The Char along with the product gases of drying and pyrolysis Zone will now react with air and complete oxidation of hydrogen to H2O and partial oxidation of char and methane takes place. The char oxidation yields CO and CO2, which are assumed to follow Evans and Emmons relationship [4] .They found while studying combustion of wood charcoal observed that when combustion actually proceeds in an oxygen deficient environment, the CO/CO2 distribution is related to the temperature as:

**Nco/ Nco2= 4.3 \* e-3390 / Toxd**

The extent of methane oxidation is assumed to be 60% on molar basis, this proportion being arrived at after several trials towards comparability of model and experimental results.

Now general equation for Oxidation zone:

**Char+N1 CO + N2 CO2 +N3 H2  + N4 H2O + N5 CH4+m\*(O2+3.76\*N2) →Charoxd+N1oxdCO+N2oxdCO2+N3oxdH2O+N4oxdCH4+N5oxdN2**

**4.3.2.1 Mass Balance Equation**

For Finding out the gas constituents after the oxidation zone, following mass balance will be required:

Carbon balance:

**Charoxd+N1oxd+N2oxd+N4oxd-(Char+N1+N2+N5)=0**

Hydrogen balance:

**2\*N3oxd+4\*N4oxd-(2\*N3+2\*N4+4\*N5)=0**

Oxygen balance:

**N1oxd+2\*N2oxd+N3oxd-(N1+2\*N2+N4+2\*m)=0**

Nitrogen balance:

**N5oxd-(2\*3.76\*m)=0**

Evans and Emmons relationship:

**N1oxd/ N2oxd= 4.3 \* e-3390 / Toxd**

**4.3.2.2 Energy Balance Equations**

Now Temperature of the Oxidation zone can be calculated through energy balance as we have done earlier.

**∑ h0f,j (j=reactant specie) = ∑( h0f,I + Δh0T,i)(i=product specie)**

Where h0f is the enthalpy of formation in kJ/kmol and its value is zero for all chemical elements at reference state (298 K, 1 atm), and Δh0T represents the enthalpy difference between any given state and at reference state. It can be approximated by:

**ΔhT =∫Cp dt**

Where Cp is specific heat at constant pressure in kJ/kmol-K and is a function of temperature. It can be defined by the empirical equation below:

**Cp = a1 T + b1 T2 + c1 T3 +d1 T4 + K**

Where K is a constant obtained from the integration and a1, b1, c1and d1are the specific gas species coefficients, which are shown in **APPENDIX A.**

Hence using above equations we can find the required Oxidation Temperature.

**4.3.3 Reduction Zone**

The products from oxidation zone enter reduction zone. The balance 40% methane is assumed to be carried forward through this zone while char carry over is assumed to be 3% on molar basis based on the work of Channiwala [5]. The other gas constituents in reduction zone are assumed to be at shift equilibrium. The product distribution and temperature level in this zone is obtained using mass and energy balance equations along with the condition of shift equilibrium.

Now General equation for Reduction Zone:

**Charoxd+N1oxdCO+N2oxdCO2+N3oxdH2O+N4oxdCH4+N5oxdN2→Charred+N1redCO+N2redCO2+N3redH2+N4redH2O+N5redCH4+N6redN2**

**4.3.2.1 Mass Balance Equation**

For Finding out the gas constituents after the Reduction Zone, following mass balance will be required:

Carbon balance:

**Charred+N1red+N2red+N5red-(Charoxd+N1oxd+N2oxd+N4oxd)=0**

Hydrogen Balance:

**2\*N3red+2\*N4red+N5red-(2\*N3oxd+4\*N4oxd)=0**

Oxygen Balance:

**N1red+2\*N2red+N4red-(N1oxd+2\*N2oxd+N3oxd)=0**

Now as we have done in Drying and Pyrolysis Zone ,Using relations involving equilibrium constant K1 and species in the water-gas shift reaction we get one more equation as:

**N1red\*N4red\*K1-N2red\*N3red=0** (from Water gas shift reaction)

Following equation will be used for the equilibrium state of ideal gas mixture because of the requirements of K1 values:

**ln(K) = - (Δ G0T)/(R\*T)**

**Δ G= ∑ νi Δg0f, T, i**

Where R is the universal gas constant, 8.314 kJ/(kmol - K),Δ G0T is the standard Gibbs function of reaction, and Δg0f,T,I represents the standard Gibbs function of formation at given temperature T of the gas species i which can be expressed by the empirical equation :

**(Δg0f,T )=(h0f)- a T lnT- b T2 - (c/2)T3 – (d/3) T4 + (e/2T)+ f + g T**

The values of coefficients a–g and the enthalpy of formation of the gases are presented in **APPENDIX A**

For calculating K1 and K2, the temperature in the gasification or reduction zone must be known. In this study, it was determined using energy balance method.

**4.3.1.2 Energy Balance Equations**

The temperature of the gasification zone needs to be calculated in order to calculate the equilibrium constants. For this reason, either energy or enthalpy balance was performed for the gasification process which was usually assumed to be an adiabatic process. When the temperature in gasification zone is T and the temperature at inlet state is assumed to be 298K (25 degree C), the enthalpy balance for this process can be written as

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Where h0f is the enthalpy of formation in kJ/kmol and its value is zero for all chemical elements at reference state (298 K, 1 atm), and Δh0T represents the enthalpy difference between any given state and at reference state. It can be approximated by:

**ΔhT =∫Cp dt**

Where Cp is specific heat at constant pressure in kJ/kmol-K and is a function of temperature. It can be defined by the empirical equation below:

**Cp = a1 T + b1 T2 + c1 T3 +d1 T4 + K**

Where K is a constant obtained from the integration and a1, b1, c1and d1are the specific gas species coefficients, which are shown in **APPENDIX A.**

Hence using above equations we can find the required Reduction Temperature.

**4.4 Results and Calculations**

The validation of three-zone KF model has been carried out through comparison of final gas composition with published literature. In all cases char composition is kept same due to unavailability of this data in literature. The data of wood and char compositions are taken from the Channiwala [5]. The heat loss in all calculation is assumed to be 10% of product of ER & HHV of the material. Table 1 shows the comparison of model prediction with published experimental results. Also Table 2 shows the zone wise prediction of Temperature level. It can be seen from comparisons of results presented in Table 1 & 2 that the model predictions are in good agreements with published experimental results. The predictions of CO, CO2, H2, N2 & the hydrocarbon in the form of CH4 are in good agreement with the published experimental results as is reflected from their error levels. The better agreement even for CH4 prediction certainly justifies the assumption of 60% methane oxidation and 40% methane carry over along with 3% char carry over in reduction zone. Predictions of Pyrolysis zone temperature compares well with experimental results while over prediction of oxidation and reduction zone temperatures may be due to use of Evans and Emmons relationship. The model thus stands validated over the wide range of biomass material and operating conditions.

Below given tables will help in comparing the present study and the experimental results.

TABLE 4

|  |  |  |
| --- | --- | --- |
| ER = 0.329 | MC = 10% | HHV = 19.777 MJ/Kg |

Material information

TABLE 5

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | ER | CO | CO2 | H2 | CH4 | N2 |
| EXP | 0.329 | 21.50 | 11.00 | 19.00 | 1.40 | 47.10 |
| MODEL | 0.329 | 19.01 | 11.31 | 16.46 | 2.078 | 41.3 |

Gas composition comparison with experimental results

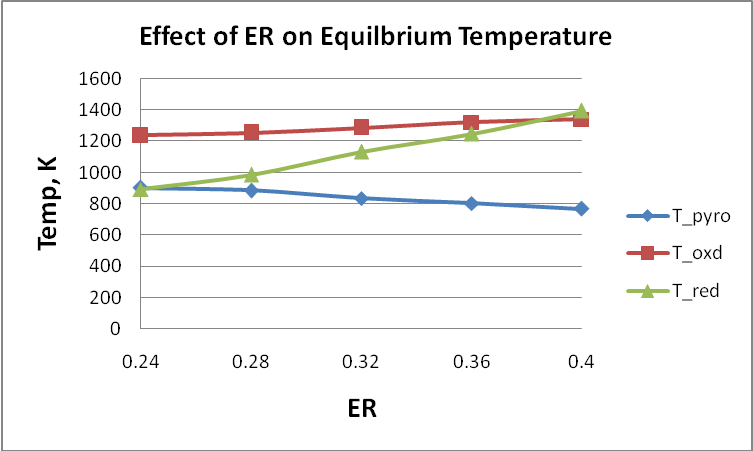
TABLE 6

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ER | MOISTURE CONTENT | TEMPD,P | TEMPOXD | TEMPRED |
| 0.329(EXP) | 10.9 | 888 | 1351 | 1112 |
| 0.329(MODEL) | 10.9 | 751.8 | 1285 | 1160 |

Zone wise temperature comparison with experimental results

**4.4.1 Effect of equivalence ratio on Equilibrium Temperature**

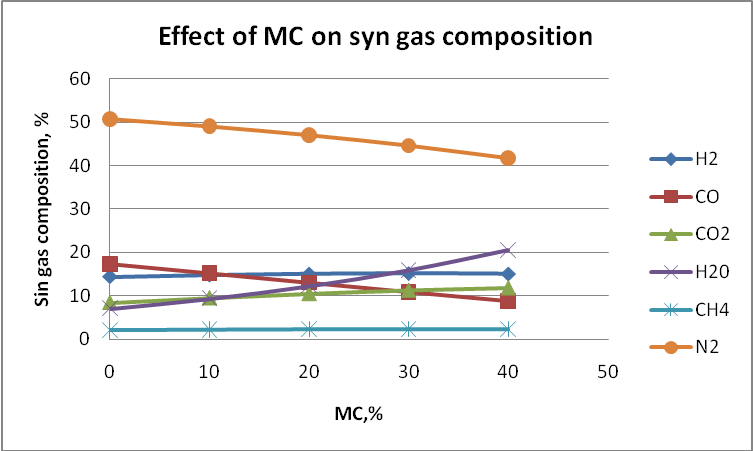
Fig. shown below shows the influence of equivalence ratio on the temperature at each zone. Temperature of pyrolysis zone is remaining constant with increasing equivalence ratio while temperature of oxidation and reduction zones are increasing with increasing equivalence ratio. The rate of increase of temperature as a function of equivalence ratio is higher in reduction zone as compared to oxidation zone, because the products of the oxidation zone enters at a high temperature in reduction zone plus the amount of char needed for endothermic reduction reactions is reduced, because at higher equivalence ratio most of the char is utilized in oxidation zone .



**Plot 1: Effect of ER on Equilibrium temperature**

**4.4.2 Effect of moisture content on Gas composition**

Fig represents the variation in composition in reduction zone with moisture content for a constant equivalence ratio as 0.3 and subabul wood as biomass material. The decreasing N2 concentration is essentially due to increased availability of the moles of moisture. Higher moisture level also seem to reduce CO concentration level and increase CO2 and H2 level due to equilibrium of water gas shift reaction. The variation of CH4 concentration are quite interesting, it has a direct bearing with the pyrolysis zone results.



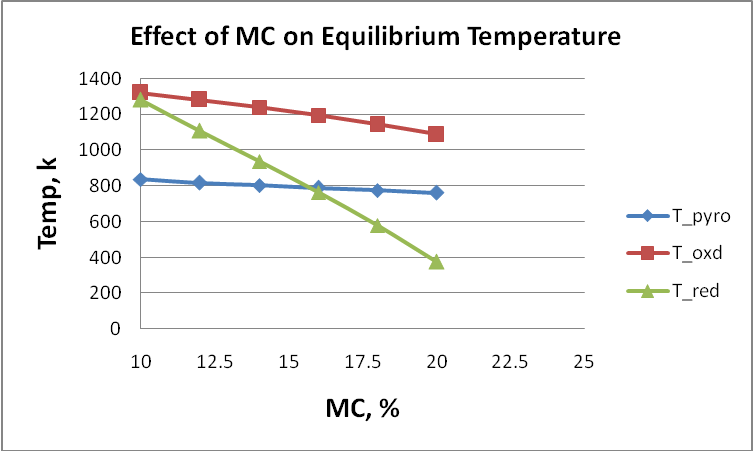
**Plot 2: Effect of MC on syn gas composition**

**4.4.3 Effect of MC on Equilibrium temperature**

Fig. represents the influence of moisture content on equilibrium temperatures of pyrolysis, oxidation and reduction zones. Very obviously the temperatures at each zone decreases with increasing moisture content because higher moisture content consumes more amount of heat energy as a latent heat and thereby reduces the

temperature levels.

**Plot 3: Effect of MC on Equilibrium Temperature**



**4.5 conclusions**

Based on the results the following conclusions may be derived.

(1) The comparison of KF model predications with published experimental results and the illustrated closeness between the two proves the quantitative and qualitative validity of the KF model for most parameters of interest. This means that the present model may be accepted for performance prediction of downdraft

gasifier.

(2) Dividing the model in three different zone facilitates in examining the parametric sensitivity in different zones,which is quite useful in predicting the design parameters.

(3) Inclusion of independent oxidation zone in the model facilitates the predictions of maximum temperature in the gasifier and thereby provides important information needed for design and selections of materials of constructions.

(4) The model predictions to parametric sensitivity study such as the influence of equivalence ratio; moisture content provide extremely useful information regarding the effect of these parameters on the gas quality and temperature levels in different zones of downdraft gasifier. This results suggested the equivalence ratio in the vicinity of 0.3 and moisture content in the range of 10 to 20% should be the operating parameters to obtain good quality of gas & safe, non slagging operations of gasifier with the woody biomass as its feed.

**CHAPTER 5**

**METHODOLOGY FOR CFD MODELLING**



In this chapter, the main methodology used for CFD modeling of a downdraft gasifier is discussed. FLUENT 6.3 has been chosen to carry out the simulation for the numerical simulations. This software has the capability on predicting the fluid flow, heat and mass transfer, chemical reaction, and related phenomena. This software help engineers with detailed product development, design optimization, trouble shooting, scale-up and retrofitting that can help in reduces engineering cost, while improving the final design of products in many applications, and one of them is combustion system design.

**5.1 Theoretical considerations on CFD**

Computational fluid dynamics or CFD is the analysis of of system involving fluid flow,heat transfer and associated phenomenon such as chemical reaction by means of computer based simulations.The CFD codes are arranged by the numerical algorithm accordingly, so that the fluid flow problem can be tackled. There are three main elements of CFD codes in the CFD packages which consist of *pre-processor*, *solver* and *post-processor*.

* **Pre-processor**

The pre-processor contains all the fluid flow inputs for a flow problem. It can be seen as a user-friendly interface and a conversion of all the input into the solver in CFD program. In this stage, quite a lot of activities are carried out before the problem is being solved. These stages are listed as below:

**1. Definition of the geometry**

* The region of interest which is the computational domain.

**2. Grid generation**

* The subdivision of the domain into a number of smaller and non overlapping domains. The grid mesh of cells is carried out for the geometry.

**3. Selection of the physical and chemical properties**

* The geometry to be modelled.

**4. Definition of the fluid properties**

**5. Specifications of correct boundary conditions**

* This is done at model’s cells.

The solution of the flow problem such as temperature, velocity, pressure etc. is defined at the nodes insides each cell. The accuracy of the CFD solution governed by the number of cells in the grid and is dependent on the fineness of the grid.

* **Solver**

In the numerical solution technique, there are three different streams that form the basis of the solver. There are *finite differences*, *finite element* and *finite volume methods*. The differences between them are the way in which the flow variables are approximated and the discretization processes are done.

**1. Finite difference element, FDM**

Describes the unknown flow variables of the flow problem by means of point samples at node points of a grid coordinate. By FDM, the Taylor’s expansion is usually used to generate finite differences approximation.

**2. Finite element method, FEM**

Use the simple piecewise functions valid on elements to describe the local variations of unknown flow variables. Governing equation is precisely satisfied by the exact solution of flow variables. In FEM, residuals are used to measure the errors.

**3. Finite volume method, FVM**

It was originally developed as a special finite difference formulation. The main computational commercial CFD codes packages using the FVM approaches involves PHOENICS, FLUENT, FLOW 3D and STAR-CD.

Basically, the numerical algorithm in these CFD commercial packages involved the formal integration of the governing equation over all the finite control volume, the discretization process involves the substitution of variety FDM types to approximate the integration equation of the flow problem and the solution is obtained by iterative method.

Discretization in the solver involves the approaches to solve the numerical integration of the flow problem. Two different approaches have been used and once at a time:

**1. Explicit approach**

Usually, this is the most approach that makes sense. It is relatively simple to set up and program. The limitation is that for a given Δ*t* and Δ*x,* must be less than some limit imposed by stability constraints. In some cases,Δ*t* must be very small to maintain the stability and consequently long running time required for the calculation over a given time interval, t.

**2. Implicit approach**

For this approach, the stability can be maintained over a large value of Δ*t* and fewer time steps are required for making calculations thus resulting in less computing time. Adversely, it is complicated to set up and program. The computer time per time step is much larger than the explicit approach due to the matrix manipulation which is required for each time step. This approach is very accurate to follow the exact transients i.e. the time variations of the independent variables.

* **Post-processor**

A FLUENT package provides the data visualization tools to visualize the flow problem. This includes – vectors plots, domain geometry and grid display, line and shaded counter plots, particle tracking etc. Recent facilities aided with animation for dynamic result display and also have data export facilities for further manipulation external to the code.

* **Problem solving**

In computational fluid dynamics, using the FLUENT codes provides to solve the problem numerically. The fundamental involves determining the convergence, whether the solution is consistent and stable for all range of flow variables.

* *Convergence* – is a property of a numerical method to produce a solution that approaches the exact solution of which the grid spacing, control volume size is reduced to a specific value or to zero value
* *Consistent* – to produce the system of algebraic equations which can be equivalent to the original governing equation
* *Stability* – associates with the damping of errors as a numerical method proceeds. If a technique chosen is not stable, even the round-off error in the initial data can leads to wild oscillations or divergence.
  1. **Physical Characteristics of the Problem and Assumptions Made**

The physical characteristics of the problem are as follow:

* Two-dimensional
* Buoyancy force and gravity considered
* Varying fluid properties
* Impermeable walls
* Radition is considered

The following are the general assumptions made in this study:

1. The flow is steady.
2. No-slip condition (zero velocity) is imposed on wall surfaces.
3. Chemical reaction is faster than the time scale of turbulence eddies.
4. Low Mach number for the combustion approximation.
5. Single-phase gaseous flow of ideal gas.
6. Neglect the electromagnetic radiation and particle radiation interaction.
   1. **TURBULENCE MODELS**

Turbulence modeling is a key issue in most CFD simulations. Virtually all engineering applications are turbulent and hence require a turbulence model. Various classes of turbulence models are as follows:

1. **RANS-based models** 
   * Linear eddy-viscosity models
   * Algebraic models
   * Non-linear eddy viscosity models and algebraic stress models
   * Reynolds stress transport models
2. **Large eddy simulations**
3. **Detached eddy simulations and other hybrid models**
4. **Direct numerical simulations**

The K-epsilon model which is employed in this study is one of the most common turbulence models. It is a two equation model that means, it includes two extra transport equations to represent the turbulent properties of the flow. This allows a two equation model to account for history effects like convection and diffusion of turbulent energy. The first transported variable is turbulent kinetic energy, . The second transported variable in this case is the turbulent dissipation,. It is the variable that determines the scale of the turbulence, whereas the first variable, , determines the energy in the turbulence.



There are two major formulations of K-epsilon models. That of Launder and Sharma is typically called the "Standard" K-epsilon Model. The original impetus for the K-epsilon model was to improve the mixing-length model, as well as to find an alternative to algebraically prescribing turbulent length scales in moderate to high complexity flows.

The various governing equations of standard K-epsilon model are as follows,

For turbulent kinetic energy



For dissipation



For modeling viscosity



For modeling of



Where is the modulus of the mean rate-of-strain tensor, defined as :



For effect of buoyancy



Where Prt is the turbulent Prandtl number for energy and gi is the component of the gravitational vector in the ith direction. For the standard and realizable - models, the default value of Prt is 0.85.

The coefficient of thermal expansion, , is defined as



## Model constants



* 1. **COMBUSTION MODEL**

The biomass gasification simulation involves modeling a continuous gas phase flow field and its interaction with a discrete phase of biomass particles. The biomass particles, traveling through the gas, will undergo devolatilization and char combustion, creating a source of fuel for reaction in the gas phase. The reaction can be modeled using either the species transport model or the non-premixed combustion model. Here we will model a downdraft gasifier furnace using the non-premixed combustion model for the reaction chemistry. The non-premixed combustion model uses a modeling approach that solves transport equations for one or two conserved scalars, the mixture fractions. Multiple chemical species, including radicals and intermediate species, may be included in the problem definition. Their concentrations will be derived from the predicted mixture fraction distribution. Property data for the species are accessed through a chemical database and turbulence chemistry interaction is modeled using a β-function for the PDF.

Combustion is simplified to a mixing problem, and the difficulties associated with closing non-linear mean reaction rates are avoided. Once mixed, the chemistry can be modeled as being in chemical equilibrium with the Equilibrium model, being near chemical equilibrium with the Steady Laminar Flamelet model or significantly departing from chemical equilibrium with the Unsteady Laminar Flamelet model.

*Restrictions and Special Cases for Using the Non-Premixed Model (Restrictions on the Mixture Fraction Approach)*

The unique dependence of Øi (species mass fractions, density, or temperature) on mixture fraction requires that the reacting system meet the following conditions:

* The chemical system must be of the diffusion type with discrete fuel and oxidizer inlets (spray combustion and pulverized fuel flames may also fall into this category) and the flow must be turbulent.
* The Lewis number must be unity. (This implies that the diffusion coefficients for all species and enthalpy are equal, a good approximation in turbulent flow).
* When a single mixture fraction is used, the following conditions must be met:
  + Only one type of fuel is involved. The fuel may be made up of a burnt mixture of reacting species (e.g., 90% CH4 and 10% CO) and you may include multiple fuel inlets. The multiple fuel inlets must have the same composition; however, two or more fuel inlets with different fuel composition are not allowed (e.g., one inlet of CH4 and one inlet of CO). Similarly, in spray combustion systems or in systems involving reacting particles, only one off-gas is permitted.
  + Only one type of oxidizer is involved. The oxidizer may consist of a mixture of species (e.g., 21% O2 and 79% N2) and you may have multiple oxidizer inlets. The multiple oxidizer inlets must, however, have the same composition. Two or more oxidizer inlets with different composition are not allowed (e.g., one inlet of air and a second inlet of pure oxygen).

Various governing equations of this model are:

The basis of the non-premixed modeling approach is that under a certain set of simplifying assumptions, the instantaneous thermochemical state of the fluid is related to a conserved scalar quantity known as the mixture fraction ,f. The mixture fraction can be written in terms of the atomic mass fraction as



**ffuel+fox=1**

Where Zi is the elemental mass fraction for some element,. The subscript ox denotes the value at the oxidizer stream inlet and the subscript fuel denotes the value at the fuel stream inlet. The mixture fraction is thus the elemental mass fraction that originated from the fuel stream. Note that this mass fraction includes all elements from the fuel stream, including inert species such as N2 and any oxidizing species mixed with the fuel, such as O2.



Transport Equations for the Mixture Fraction

The mean (time-averaged) mixture fraction equation is



Conservation equation for the mean mixture fraction variance,(f’bar)2



Then the mixture fraction for the system is related to equivalence ratio, Ө as

**f= Ø/ (Ø+r).**

When the non-adiabatic non-premixed combustion model is enabled, **FLUENT** solves the total enthalpy form of the energy equation:



The total enthalpy, H is defined as



Where Hj is enthalpy of species j and Yj is mass fraction and H0 is the enthalpy of specie j at reference temperature Tref.



The Probability Density Function, written as p(f), can be thought of as the fraction of time that the fluid spends in the vicinity of the state f. Figure 10 plots the time trace of mixture fraction at a point in the flow (right-hand side) and the probability density function of f (left-hand side). The fluctuating value of f, plotted on the right side of the figure, spends some fraction of time in the range denoted as Δf. p(f), plotted on the left side of the figure, takes on values such that the area under its curve in the band denoted, Δf, is equal to the fraction of time that f spends in this range. Written mathematically

**Δf. p(f)=limitT→∞ (1/T).∑Ti**

Where T is the time scale and Ti is the amount of time that f spends in the f band. The shape of the function p(f) depends on the nature of the turbulent fluctuations in Δf. In practice, p(f) is unknown and is modeled as a mathematical function that approximates the actual PDF shapes that have been observed experimentally.

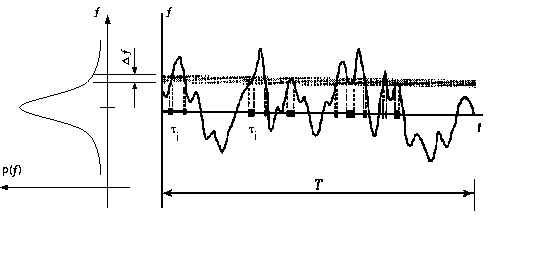


Figure 10: PDF function

The shape of the assumed PDF, p(f), is described in FLUENT by one of two mathematical functions:

* The double-delta function (two-mixture-fraction cases only)
* The beta-function (single- and two-mixture-fraction cases)

The double-delta function is the most easily computed, while the beta-function most closely represents experimentally observed PDFs. The shape produced by this function depends solely on the mean mixture fraction, fbar, and its variance, f’2.Here for modeling the Beta function was employed.

* 1. **MODEL SETTING**
     1. **Numerical Procedure**

The procedure for performing the simulation in FLUENT is outlined below.

1. Create and mesh the geometry model using GAMBIT
2. Import geometry into FLUENT
3. Define the solver model
4. Define the turbulence model
5. Define the species model
6. Define the materials and the chemical reactions
7. Define the boundary conditions
8. Initialize the calculations
9. Iterate/calculate until convergence is achieved.
10. Post-process the results for the first order and second order upwind consideration.

**5.5.2 Dimensions and boundary conditions**

The geometry of the gasifier used in the simulation is shown in Figure below. The downdraft gasifier is mainly divided into four regions: a fuel hopper at the top, followed by a subsequent section where pyrolysis occurs and then the combustion region which has 2 injectors attached to it and finally the outlet pipe from where the syn gas or producer gas is ejected. The gasifier has two air injectors that are positioned symmetrically. The length of each nozzle is taken to be 100 mm and diameter of each nozzle is 25 mm. The Dimensions of gasifier as shown in next figure are in cm. It is a small scale gasifier operating at pressure of 1 atmosphere.

25cm

160cm

25mm

23.7cm

17mm

Figure 11: Dimensioned schematic of downdraft gasifier

FLUENT has a wide range of boundary conditions that permit flow to enter and exit the solution domain. FLUENT provides 10 types of boundary cell types for the specification of flow inlets and exits: velocity inlet, pressure inlet, mass flow inlet, pressure outlet, pressure far-field, outflow, inlet vent, intake fan, outlet vent, and exhaust fan.

The inlet and exit boundary condition options in FLUENT that were used in this 2-dimensional model are as follows:

* *Velocity inlet* boundary conditions are used to define the velocity and scalar properties of the flow at inlet boundaries.
* *Pressure inlet* boundary conditions are used to define the total pressure and other scalar quantities at flow inlets.
* *Mass flow* inlet boundary conditions are used in compressible flows to prescribe a mass flow rate at an inlet. It is not necessary to use mass flow inlets in incompressible flows because when density is constant, velocity inlet boundary conditions will fix the mass flow.
* *Pressure outlet* boundary conditions are used to define the static pressure at flow outlets (and also other scalar variables, in case of backflow). The use of a pressure outlet boundary condition instead of an outflow condition often results in a better rate of convergence when backflow occurs during iteration.
* Walls were specified as stationary walls with zero slip condition and either with zero flux condition or constant temperature type.

The schematic diagram with boundary conditions that have been used in the model are illustrated in figure below.

**FUEL INLET**

**TEMPERATURE: 400K**

**MASS FLOW RATE: 0.0041 Kg/s**

**TURBULENT INTENSITY: 5%**

**C: 51.034% N: 3.012%**

**H: 6.776% O: 39.178%**

**AIR INLET (2 no’s)**

**TEMPERATURE: 600K**

**MASS FLOW**

**RATE: 0.0070Kg/s**

**TURBULENT INTENSITY: 5%**

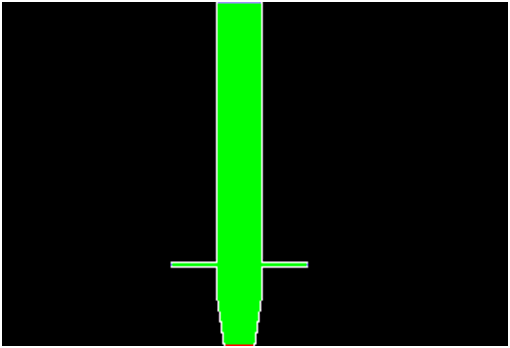
**O: 21%**

**N: 79%**

**GAS OUTLET**

**BACKFLOW TEMPERATURE: 800K**

**BACKFLOW TURBULENT INTENSITY: 5%**



**Figure 12: schematic showing various boundary conditions used in gasifier model.**

**CHAPTER 6**

**OBSERVATIONS AND CALCULATIONS**



**6.1 INTRODUCTION**

The objective of this study is to model the Biomass gasification process which is considered to be a very complicated process. There are many parameters that affect the efficiency of producer gas production in Biomass gasifier, such as fuel type, Moisture content in the fuel, equivalence ratio etc. **Awadhesh Kr. Sharma [7],** presenteda CFD model on fluid flow and heat transfer model for the reactive, porous bed of the biomass gasifier to simulate pressure drop, temperature profile in the bed and flow rates. The conservation equations, momentum equation and energy equation were used to describe fluid and heat transport in porous gasifier bed. The model also accounted for drag at wall, and the effect of radial as well as axial variation in bed porosity to predict pressure drop in bed. Heat transfer has been modeled using effective thermal conductivity approach. He validated his model predictions against the experiments, while effective thermal conductivity values are tested qualitatively using models available in literature. Parametric analysis has been carried out to investigate the effect of various parameters on bed temperature profile and pressure drop through the gasifier. The temperature profile was found to be very sensitive to gas flow rate, and heat generation in oxidation zone, while high bed temperature, gas flow rate and the reduction in feedstock particle size are found to cause a marked increase in pressure drop through the gasifier.

This study of gasification/thermal flow interactions and investigate the effects of these different input parameters on the performance of down draft biomass gasifier by modeling the gasification process and employing the Computational Fluid Dynamics (CFD) technology would contribute to the industry resolving concerns and improve gasifier efficiency and reliability. The specific goals are:

1. Incorporate the gasification models into a commercial CFD code
2. Simulate a Down draft biomass gasifier
3. Investigate the effects of equivalence ratio over the composition of the producer gas and the calorific value.

Investigation of down draft biomass gasification processes simulation has-been carried out with the help of FLUENT, a CFD tool to simulate. The following different operating conditions and parameters on which the study is focused:

1. Gas outlet temperature
2. Maximum reaction temperature
3. Species mass fraction at the reactor out
4. Calorific value of the gas produced.

The operating conditions and the model parameters used in the simulations for various cases are summarized below. The simulation results on the gas temperature, carbon fuel conversion, and mole fractions of species at the gasifier outlet are discussed in details in the following article. But before this the analysis of result of downdraft gasifier operating at equivalence ratio of 0.4 are discussed in detail.

**6.2 MODEL DESCRIPTION**

The downdraft gasifier operates by heating the biomass fuel (which is composed of municipal waste matter) using burner/torches that are connected at both side of cylinder. The biomass pellets are heated in the reactor using air as the gasifying medium to produce a syngas which contains varying amount of H2, CO, CH4, CO2 and N2. The outer wall also are being applied a heat until the wood breaks, decomposes and gives off gas which can be used as a fuel which is can be used in gas turbine. The following figure shows the geometry of downdraft gasifier model which has been designed and then meshed in GAMBIT and subsequently imported in FLUENT.

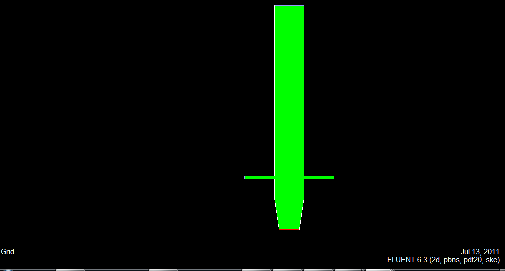


Figure 13: Meshed model of gasifier generated in GAMBIT

**5.3 CONTOURS of DOWNDRAFT GASIFIER**

In order to get the solution convergent the first order discretization scheme was employed in FLUENT and the solution converged in 234 iterations. The second order discretization scheme was however not used because of the large number of sinusoidal fluctuations seen in the second order discretization scheme even after modifying the relaxation factors. The relaxation factors used in FLUENT code can be found in **APPENDIX-B**.

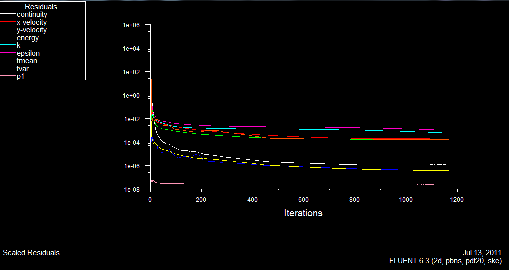


Figure 14: Convergence of iterations in fluent

**5.3.1 Static pressure and Temperature contours**

The static pressure and temperature contours obtained after successful iteration are shown.



Figure 15: Static pressure contour

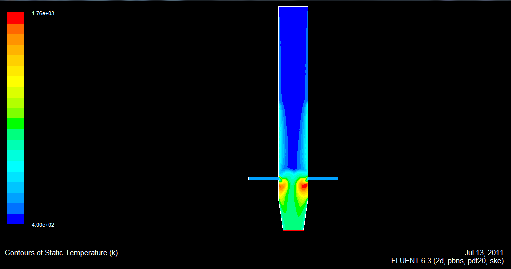
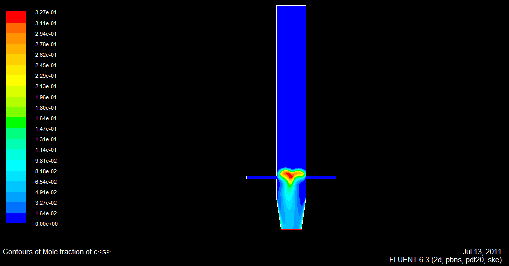


Figure 16: Static Temperature Contours

**5.3.2 Species mole fractions Contours**



**Figure 17: Mole fraction of N2**



**Figure 18: Mole fraction of solid char**

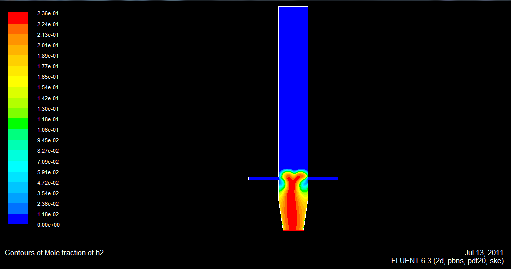


Figure 19: Mole fraction of hydrogen

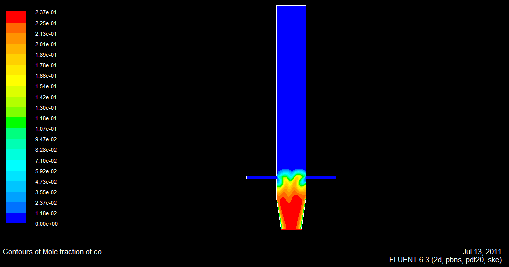


Figure 20: Mole fraction of carbon monoxide

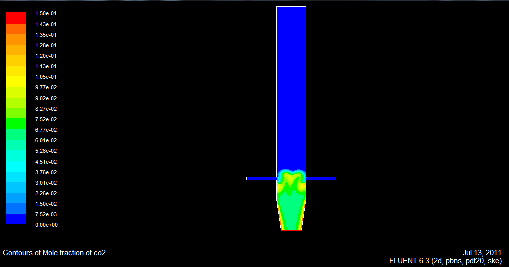


Figure 21: Mole fraction of carbon dioxide

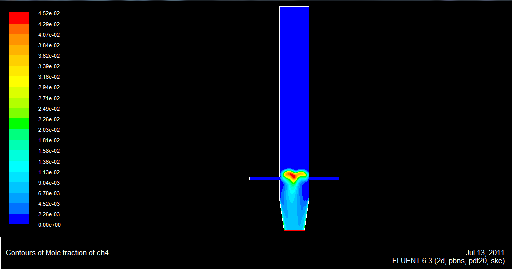


Figure 22: Mole fraction of methane

* 1. **CALCULATIONS**

The equivalence ratio, ER is defined as

**Ø = (actual fuel-air ratio) / (stoichiometric fuel-air ratio)**

The following article now sees the effect of changing the ER from 0.2 to 0.4.

**TABLE 7: CALCULATION OF CALORIFIC VALUE OF GAS**

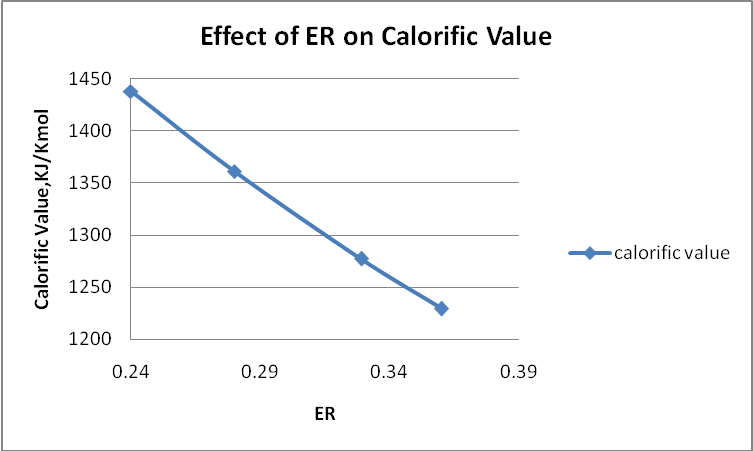
|  |  |  |  |
| --- | --- | --- | --- |
| **Components** | **Percentage Composition** | **Calorific value of individual component** | **Calorific value contribution to overall mol. wt** |
| **ER=0.329** |  |  |  |
| **CO** | 19.01 | 12.71 | 241.6171 |
| **H2** | 16.46 | 12.78 | 210.3588 |
| **CH4** | 2.079 | 39.76 | 82.66 |
| **CO2** | 11.31 | 0 | 0 |
| **N2** | 41.29 | 0 | 0 |
| **Gross CV** |  |  | **534.6359** |

Grass calorific value = 534.6359/100 = 5.346 Mj/m3 = 1277.35 kcal/ m3

Following the above procedure the calorific value for all the four cases is calculated and the values are tabulated as below:

**Table 8: Calorific value v/s ER.**

|  |  |
| --- | --- |
| **ER** | **Calorific value(kcal/m3)** |
| 0.24 | 1437.93 |
| 0.28 | 1361.198 |
| 0.329 | 1277.35 |
| 0.36 | 1229.45 |



**plot 6: effect of ER on calorific value of syn gas**

**6.5 SEcond law efficiency**

Exergy analysis is a very important tool for the evaluation of the performance of a gasifier. In real processes, exergy is not conserved because of irreversibilities. Exergy efficiency or second law efficiency is defined as

**Eff=(Eprod/Efeed)**

where Eprod and Efeed are exergies of producer gas and feedstock, respectively. In this case, kinetic exergy and potential exergy are also negligible, thus the exergy can be divided into two major components shown below

**E=€ch+€ph**

where Ech and Eph are chemical exergy and physical exergy, respectively. The dead state used in the following calculation is defined at Po at1 atm, To at 298 K. Kotas [35] suggested that the specific chemical exergy of ideal mixture gas, in kJ/kmol, can be calculated by

**Ech,M=∑xi\*€ch,i+∑xi\*ln(xi)**

where xi is mole fraction of ith component and €ch,iis standard chemical exergy of ith component, in kJ/kmol and they are presented in Table given below.

**Table 9: Standard Chemical exergy of producer gas,₡ch,i, KJ/Kmol**

|  |  |
| --- | --- |
| **H2** | **238490** |
| **CO** | **275430** |
| **CO2** | **20140** |
| **H20** | **11710** |
| **CH4** | **836510** |
| **N2** | **720** |

The physical exergy of each gas species can be calculated by

**Eph,M=(h-h0)-T0\*(s-s0)**

where h and s are enthalpy and entropy at any pressure (P), temperature (T), ho and so are enthalpy and entropy at Po,To.

For the solid fuel,Exergy can be calculated as,in kj/kg

**€solid=₡dry\*(LHV+mw\*hfg)**

Where,

**₡dry=(1.0438+0.1882(H/C)-0.2509(1+0.7256(H/C))+0.0383(N/C))**

**(1-0.3035(O/C))**

Where, mw is the mass fraction of moisture in fuel, and hfg is enthalpy of vaporization in kj/kg.Values of C,H,O and N are taken from the ultimate analysis of sababul wood carried out by V. Kirubakaran, [9].

Following table depicts the Second law efficiency for the given values of ER nad MC.

|  |  |  |
| --- | --- | --- |
| ER | MC | Second law efficiency |
| 0.329 | 10.9 | 81.266 |

In the next chapter the discussion of contours obtained from CFD modeling as well effect of equivalence ratio on various operating conditions of gasifier are undertaken.

**CHAPTER -7**

**DISCUSSIONS & RESULTS**



Investigation of down draft biomass gasifier has been carried out with help of FLUENT, a CFD tool to simulate the effect of equivalence ratio on the product gas composition. The product gas composition is studied with variation in equivalence ratios. It is assumed that the syngas hence produced is exhausted from gas outlet of gasifier at a certain pressure which is assumed to be atmospheric. The following paragraphs explain the observed contours and plots of previous chapter.The following inferences can be drawn:

1. From the static pressure contour one can see that the pressure first increases along height of reactor and reaches a maximum value near nozzles where combustion occurs and then the pressure decreases along height of reactor till that at the gas outlet static pressure is zero indicating syn gas exits at atmospheric pressure.
2. From the static temperature contour and plot along the height of reactor we can observe following points:

* There is a formation of different zones along the height of the reactor with reference to the temperature at that particular zone.
* The temperature near fuel hopper is about 450K which increases to 850K as fuels moves down the reactor. This is due to the fact that pyrolysis has started to occur.
* The maximum temperature is obtained near the air nozzles because there due to combustion process large amount of heat is generated which raises temperature to 1760K.After this the temperature drops to range of 800-950K indicating the reduction reactions that occur.
* The gas which exits from syn gas outlet is about range of 955K

1. Also it can be inferred from plot of equivalence ratio and gas outlet and reaction temperature that as the equivalence ratio decreases from 0.4 to 0.2 the gas outlet temperature and the maximum reaction temperature increases which emphasizes that below ER 0.2 combustion phenomenon is more dominant than pyrolysis and below ER 0.4 pyrolysis is dominant.
2. From the contours and plots of species mole fractions of syn gas following points are worth mentioning:

* From plots of species at gas outlets we can infer that either the gas specie is increasing purely or decreasing.
* The nitrogen has the maximum concentration in syn gas composition and its value decreases as ER is increased and Methane has the lowest concentration and its value also decreases as ER is increased.
* All the species namely CO, CO2, CH4 and H2 are formed above nozzles because of pyrolysis of preheated biomass. With these volatiles the Char (solid carbon is also produced and it is seen that as ER is increased the percentage of Solid char is decreased. The reaction is shown as

**Biomass → C (Char) + tar + (CO + CO2 + H2 + CH4 + H2O)**

* Secondly the char would have reacted with oxygen present in preheated air passed through air inlet nozzle to obtain carbon dioxide and other subsidiary reactions as sequenced below:-

**C + O 2 → CO2 + heat**

**C + CO2 → 2CO**

**C + 2H2 → CH4 + heat**

**3H2 + CO → CH4 + H2O + heat**

**H2O + CO → CO2 + H2 + heat  
 4H2 + CO2 → CH4 + 2H2O + heat**

* From the contour of carbon monoxide we can see that CO starts forming after the air enters the gasifier and keeps on forming till the outlet surface. The red region indicates the maximum concentration of formation of CO gas in that region. As can be seen that the region where there is Carbon dioxide further reacts with carbon in biomass fuel to form carbon monoxide The reaction for its formation is:-

**C + CO 2 → 2 CO**

**C + H2O + heat → CO + H2**

* The contour of carbon dioxide depicts that the maximum concentration of CO2 formation takes place a little after the fuel inlet and goes on forming till the outlet surface. These CO2 forming regions show the complete combustion of the biomass. The other source of Carbon dioxide formation is water gas shift reaction. This is reversible reaction occurring in gasifier.

**H2O + CO → CO2 + H2 + heat**

* The hydrogen mole fraction contour indicates that hydrogen formation starts at the same point where carbon dioxide were forming and this can be justified on the basis of reaction:-

**H2O + CO → CO2 + H2 + heat**

* + - Secondly in the region just adjacent to the air inlet nozzle the hydrogen reacts with oxygen and gets converted into steam, hence its low concentration.

**H2+ ½ O2→ H2O+heat**

1. From plots of ER vs. the mole fractions of producer gas species one can see very less variations in mole fractions of each gas species .The noticeable observation is from the ER vs. calorific value of gas which leads us to the fact that at ER=0.35 the calorific value and the gasification efficiency are maximum and hence is the best ER for gasification.

**CHAPTER-8**

**CONCLUSIONS & RECOMMENDATIONS FOR FUTURE WORK**



1. The analysis of Biomass Gasification in CFD software yields syngas that is a mixture of Carbon Monoxide(20.60%), Hydrogen(21.21%), carbon dioxide(7.65%) and traces of methane(0.8436%) and other compounds at a temperature of about 700 degree Celsius.
2. In the dissertation, some of the results obtained from this simulation is not very accurate. This is because of several factors such as model’s parameters, geometry, meshing, grid and discretization that play an important role in the result accuracy. As for model’s geometry, 2-dimensional model is used because of easy iterations and time consuming. Thus, first-order discretization leads to convergent result.
3. After carrying out process simulation of Biomass Gasification it has been concluded that the biomass gasification can be viewed upon as a clean alternative to fossil fuels and this product gas can be directly used in internal gas combustion engines or in conjunction with other systems such as in CHP plants.

The current project enabled the basic understanding and formulation of 2d models for study of the gasification using CFD code. However more detailed models are required for extending these models to achieve results which can be applied into practical situations.

The following list of possibilities is present for future work on this subject:

* Study of tar and tar modeling in a gasifier
* Construction of steady state models for pyrolysis and gasification zones.
* Comprehensive modeling of a gasifier in which the various models developed can be combined to obtain realistic results.
* Formulation of a design procedure for construction of a biomass gasifier and pyrolyzer on the basis of the above models.
* Formulation of simulation and design procedure for modeling various pollutants associated with gasification so that in future the gasifier can be modelled based on simulation and evaluated and so can be used for reference when any gasifier is to be built in any local community.



NOMENCLATURE USED



CP  Molar specific heat at constant pressure (kJ/kmol-K)

CV Calorific value of fuel (kcal/m3 or Mj/m3)

ER Equivalence Ratio

G Gibbs energy (kJ/kg)

H Enthalpy (kJ/kg)

HHV Higher heating value of fuel (Mj/kg)

LHV Lower heating value of fuel (Mj/kg)

MC Moisture content percentage

n No. of moles

s Entropy( Kj/kg-K)

R Universal gas constant

T Temperature (K)

GREEK SYMBOLS

ή Efficiency

µ Viscosity

Ø Equivalence Ratio

Δ Change in

Σ Sum of

**₡ Exergy**

**APPENDICES**

**APPENDIX-A**

**TABLE 10: The value of h0f (kJ/mol) and coefficients of the empirical equation for Δg0f,T (kJ/mol)**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| COMPOUND | h0f | a\*10-3 | b\*10-6 | c\*10-9 | d\*10-12 | e\*102 | f\*10-1 | g\*10-2 |
| CO | -110.5 | 5.619 | -11.90 | 6.383 | 1.846 | -4.891 | 8.684 | -6.131 |
| CO2 | -393.5 | -19.49 | 31.22 | -24.48 | 6.946 | -4.891 | 52.70 | -12.07 |
| H2O | -241.8 | -8.95 | -3.672 | 5.209 | -1.478 | 0 | 28.68 | -1.722 |
| CH4 | -74.8 | -46.2 | 11.30 | 13.19 | -6.647 | -4.891 | 141.1 | -22.34 |

**TABLE 11: COEFFICIENT OF SPECIFIC HEAT FOR EMPERICAL EQUATION**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| GAS SPECIES | a1 | b1 | c1 | d1 | Temperature range |
| H2 | 29.11 | -0.1916 | 0.4003 | -0.8704 | 273-1800 |
| CO | 28.16 | 0.1675 | 0.5372 | -2.222 | 273-1800 |
| CO2 | 22.26 | 5.981 | -3.501 | -7.469 | 273-1800 |
| H2O | 32.24 | 0.1923 | 1.055 | -3.595 | 273-1800 |
| CH4 | 19.89 | 5.204 | 1.269 | -11.01 | 273-1800 |
| N2 | 28.90 | -0.1571 | 0.8081 | -2.873 | 273-1800 |

**APPENDIX-B**

**Methodology for EES calculation:**

**Drying / Pyrolysis Zone:**

R=8.314

T=800

ER=0.329

MC%=10.9

MC=(MC%)/100

A1g=5.619\*10^(-3)

A2g=-19.49\*10^(-3)

A3g=-8.950\*10^(-3)

A4g=-46.2\*10^(-3)

B1g=-11.90\*10^(-6)

B2g=31.22\*10^(-6)

B3g=-3.672\*10^(-6)

B4g=11.30\*10^(-6)

C1g=6.383\*10^(-9)

C2g=-24.48\*10^(-9)

C3g=5.209\*10^(-9)

C4g=13.19\*10^(-9)

D1g=-1.846\*10^(-12)

D2g=6.946\*10^(-12)

D3g=-1.478\*10^(-12)

D4g=-6.647\*10^(-12)

E1g=-4.891\*10^(2)

E2g=-4.891\*10^(2)

E3g=0

E4g=-4.891\*10^(2)

F1g=0.8684

F2g=5.270

F3g=2.868

F4g=14.11

G1g=-6.131\*10^(-2)

G2g=-12.07\*10^(-2)

G3g=-1.722\*10^(-2)

G4g=-22.34\*10^(-2)

H\_co=-110525

H\_co2=-393509

H\_h2o=-241818

H\_ch4=-74820

H41=-285830

h\_fg=2258.02

(DELTAG\_2)=((H\_ch4)-(A4g\*T\*ln(T))-(B4g\*T^(2))-(0.5\*C4g\*T^(3))-(0.333\*D4g\*T^(4))+(0.5\*E4g)/T+F4g+(G4g\*T))

(DELTAG\_1)=-(DELTAG\_CO2)+(DELTAG\_CO)+(DELTAG\_H2O)

(DELTAG\_CO2)=(H\_co2-A2g\*T\*ln(T)-(B2g)\*T^(2)-(0.5\*C2g\*T^(3))-(0.333\*D2g\*T^(4))+(0.5\*E2g)/T+(F2g)+G2g\*T)

(DELTAG\_CO)=(H\_co-A1g\*T\*ln(T)-(B1g)\*T^(2)-(0.5\*C1g\*T^(3))-(0.333\*D1g\*T^(4))+(0.5\*E1g)/T+(F1g)+G1g\*T)

(DELTAG\_H2O)=(H\_h2o-A3g\*T\*ln(T)-(B3g)\*T^(2)-(0.5\*C3g\*T^(3))-(0.333\*D3g\*T^(4))+(0.5\*E3g)/T+(F3g)+G3g\*T)

ln(K\_1)\*1000=-(DELTAG\_1)/(R\*T)

ln(K\_2)\*1000=-(DELTAG\_2)/(R\*T)

N1%=(N1/(N\_T))\*100

N2%=(N2/(N\_T))\*100

N3%=(N3/(N\_T))\*100

N4%=(N4/(N\_T))\*100

N5%=(N5/(N\_T))\*100

N\_T=(N1+N2+N3+N4+N5)

alpha=1.451

beta=0.697

w=0.15

mw=12+alpha+16\*beta

alpha+2\*w=2\*alpha\_s

beta+w+2\*m\_s=2+alpha\_s

ER=(m/m\_s)

(N1)+(N2)+(N5)+0.237-1=0

(2\*N3)+(2\*N4)+(4\*N5)-(alpha)-(2\*w)=0

(N1)+(2\*N2)+(N4)-(w)-(beta)=0

(N1)\*(N4)\*(K\_1)-((N3)\*(N2))=0

(K\_2)\*((N3)^2)-(N5\*(N\_T))=0

A\_h2=29.11

A\_co=28.16

A\_co2=22.26

A\_h2o=32.24

A\_ch4=19.89

A\_n2=28.90

B\_h2=-0.1916\*10^(-2)

B\_co=0.1675\*10^(-2)

B\_co2=5.981\*10^(-2)

B\_h2o=0.1923\*10^(-2)

B\_ch4=5.204\*10^(-2)

B\_n2=-0.1571\*10^(-2)

C\_h2=0.4003\*10^(-5)

C\_co=0.5372\*10^(-5)

C\_co2=-3.501\*10^(-5)

C\_h2o=1.055\*10^(-5)

C\_ch4=1.269\*10^(-5)

C\_n2=0.8081\*10^(-5)

D\_h2=-0.8704\*10^(-9)

D\_co=-2.222\*10^(-9)

D\_co2=-7.469\*10^(-9)

D\_h2o=-3.595\*10^(-9)

D\_ch4=-11.01\*10^(-9)

D\_n2=-2.873\*10^(-9)

(T\_0)=298

H0-w\*H41-h\_loss=(N1\*H\_co)+(N2\*H\_co2)+(N4\*H\_h2o)+(N5\*H\_ch4)+(N1\*A\_co+N2\*A\_co2+N3\*A\_h2+N4\*A\_h2o+N5\*A\_ch4)\*(T\_1)+(N1\*B\_co+N2\*B\_co2+N3\*B\_h2+N4\*B\_h2o+N5\*B\_ch4)\*(T\_1)^(2)+(N1\*C\_co+N2\*C\_co2+N3\*C\_h2+N4\*C\_h2o+N5\*C\_ch4)\*(T\_1)^(3)+(N1\*D\_co+N2\*D\_co2+N3\*D\_h2+N4\*D\_h2o+N5\*D\_ch4)\*(T\_1)^(4)-K

K=(N1\*A\_co+N2\*A\_co2+N3\*A\_h2+N4\*A\_h2o+N5\*A\_ch4)\*(T\_0)+(N1\*B\_co+N2\*B\_co2+N3\*B\_h2+N4\*B\_h2o+N5\*B\_ch4)\*(T\_0)^(2)+(N1\*C\_co+N2\*C\_co2+N3\*C\_h2+N4\*C\_h2o+N5\*C\_ch4)\*(T\_0)^(3)+(N1\*D\_co+N2\*D\_co2+N3\*D\_h2+N4\*D\_h2o+N5\*D\_ch4)\*(T\_0)^(4)

ERROR=((T-T\_1)/T)\*100

HHV=486573.5

m\_h=(alpha\*1)/(12\*1+alpha\*1+beta\*16)

LHV=HHV-h\_fg\*18\*(9\*m\_h+MC)

H0=(LHV)+H\_co2+(alpha\_s)\*h\_h2o

h\_loss=(10/100)\*(ER\*HHV)

**Oxidation Zone:**

"Oxidation Zone Calculation"

N\_char%=(N\_char/(N\_T))\*100 {no of moles of char in oxidation zone}

N1\_oxd%=(N1\_oxd/(N\_T))\*100 {no. of moles CO in oxidation zone}

N2\_oxd%=(N2\_oxd/(N\_T))\*100 {no. of moles of CO2 in oxidation zone}

N3\_oxd%=(N3\_oxd/(N\_T))\*100 {no. of moles of H2O in oxidation zone}

N4\_oxd%=(N4\_oxd/(N\_T))\*100 {No. of moles of CH4 in Oxidation zone}

N5\_oxd%=(N5\_oxd/(N\_T))\*100 {No. of moles of N2 in Oxidation Zone}

N\_T=(N\_char+N1\_oxd+N2\_oxd+N3\_oxd+N4\_oxd+N5\_oxd)

N1=0.4601

N2=0.145

N3=0.4629

N4=0.1468

N5=0.1579

N4\_oxd=0.4\*N5

ER\_oxd=0.329

ER\_oxd=(m\_oxd)/(m\_oxd\_s)

MC%=10.9

MC=(MC%)/100

T\_1=1200

N\_char+N1\_oxd+N2\_oxd+N4\_oxd-(0.237+N1+N2+N5)=0

2\*N3\_oxd+4\*N4\_oxd-(2\*N3+2\*N4+4\*N5)=0

N1\_oxd+2\*N2\_oxd+N3\_oxd-2\*m\_oxd-(N1+2\*N2+N4)=0

2\*N5\_oxd-2\*3.76\*m\_oxd=0

(1/4.3)\*((N1\_oxd)/(N2\_oxd))=exp(-3390/T\_1)

"stoichiometric balance after complete combustion"

n\_co2\_s=0.237+N1+N2+N5

2\*n\_h2o\_s=2\*N3+2\*N4+4\*N5

2\*m\_oxd\_s+N1+2\*N2+N4=2+n\_h2o\_s

"energy balance to find out oxidation Temperature"

alpha=1.451

beta=0.697

MC=(18\*w)/(18\*w+mw)

mw=12+alpha\*1+beta\*16

H\_co=-110525

H\_co2=-393509

H\_h2o=-241818

H\_ch4=-74820

H41=-285830

h\_fg=2258.02

A\_co=28.16

A\_co2=22.26

A\_h2o=32.24

A\_ch4=19.89

A\_n2=28.90

B\_co=0.1675\*10^(-2)

B\_co2=5.981\*10^(-2)

B\_h2o=0.1923\*10^(-2)

B\_ch4=5.204\*10^(-2)

B\_n2=-0.1571\*10^(-2)

C\_co=0.5372\*10^(-5)

C\_co2=-3.501\*10^(-5)

C\_h2o=1.055\*10^(-5)

C\_ch4=1.269\*10^(-5)

C\_n2=0.8081\*10^(-5)

D\_co=-2.222\*10^(-9)

D\_co2=-7.469\*10^(-9)

D\_h2o=-3.595\*10^(-9)

D\_ch4=-11.01\*10^(-9)

D\_n2=-2.873\*10^(-9)

(T\_0)=298

sigma\_h\_f=(N1\_oxd\*H\_co)+(N2\_oxd\*H\_co2)+(N3\_oxd\*H\_h2o)+(N4\_oxd\*H\_ch4)

sigma\_1=(N1\_oxd\*A\_co+N2\_oxd\*A\_co2+N3\_oxd\*A\_h2o+N4\_oxd\*A\_ch4+N5\_oxd\*A\_n2)

sigma\_2=(N1\_oxd\*B\_co+N2\_oxd\*B\_co2+N3\_oxd\*B\_h2o+N4\_oxd\*B\_ch4+N5\_oxd\*B\_n2)

sigma\_3=(N1\_oxd\*C\_co+N2\_oxd\*C\_co2+N3\_oxd\*C\_h2o+N4\_oxd\*C\_ch4+N5\_oxd\*C\_n2)

sigma\_4=(N1\_oxd\*D\_co+N2\_oxd\*D\_co2+N3\_oxd\*D\_h2o+N4\_oxd\*D\_ch4+N5\_oxd\*D\_n2)

H0+w\*H41+h\_loss=((sigma\_h\_f)+(sigma\_1)\*(T\_oxd)+((sigma\_2)\*(T\_oxd)^(2))+((sigma\_3)\*(T\_oxd)^(3))-((sigma\_4)\*(T\_oxd)^(4)))-K

K=(sigma\_1)\*(T\_0)+(sigma\_2)\*(T\_0)^(2)+(sigma\_3)\*(T\_0)^(3)+(sigma\_4)\*(T\_0)^(4)

ERROR=((T\_1-T\_oxd)/(T\_1))\*100

HHV=486573.5

m\_h=(alpha\*1)/(12\*1+alpha\*1+beta\*16)

LHV=HHV-h\_fg\*18\*(9\*m\_h+MC)

H0=(LHV)+(n\_co2\_s)\*H\_co2+(n\_h2o\_s)\*H\_h2o

h\_loss=(10/100)\*(ER\_oxd\*HHV)

**Reduction Zone:**

R=8.314

ASH=0

MC%=10.9

MC=(MC%)/100

T=1000

ER\_r=0.329

A1g=5.619\*10^(-3)

A2g=-19.49\*10^(-3)

A3g=-8.950\*10^(-3)

B1g=-11.90\*10^(-6)

B2g=31.22\*10^(-6)

B3g=-3.672\*10^(-6)

C1g=6.383\*10^(-9)

C2g=-24.48\*10^(-9)

C3g=5.209\*10^(-9)

D1g=-1.846\*10^(-12)

D2g=6.946\*10^(-12)

D3g=-1.478\*10^(-12)

E1g=-4.891\*10^(2)

E2g=-4.891\*10^(2)

E3g=0

F1g=0.8684

F2g=5.270

F3g=2.868

"

G1g=-6.131\*10^(-2)

G2g=-12.07\*10^(-2)

G3g=-1.722\*10^(-2)

(DELTAG\_1)=-(DELTAG\_CO2)+(DELTAG\_CO)+(DELTAG\_H2O)

(DELTAG\_CO2)=(H\_co2-A2g\*T\*ln(T)-(B2g)\*T^(2)-(0.5\*C2g\*T^(3))-(0.333\*D2g\*T^(4))+(0.5\*E2g)/T+(F2g)+G2g\*T)

(DELTAG\_CO)=(H\_co-A1g\*T\*ln(T)-(B1g)\*T^(2)-(0.5\*C1g\*T^(3))-(0.333\*D1g\*T^(4))+(0.5\*E1g)/T+(F1g)+G1g\*T)

(DELTAG\_H2O)=(H\_h2o-A3g\*T\*ln(T)-(B3g)\*T^(2)-(0.5\*C3g\*T^(3))-(0.333\*D3g\*T^(4))+(0.5\*E3g)/T+(F3g)+G3g\*T)

ln(K\_1)\*1000=-(DELTAG\_1)/(R\*T)

N\_char\_oxd=0.511

N1\_oxd=0.08653

N2\_oxd=0.3393

N3\_oxd=0.7992

N4\_oxd=0.06316

N5\_oxd=1.255

N\_T=(N1\_r+N2\_r+N3\_r+N4\_r+N5\_r+N6\_r)

N1\_r%=(N1\_r/(N\_T))\*100

N2\_r%=(N2\_r/(N\_T))\*100

N3\_r%=(N3\_r/(N\_T))\*100

N4\_r%=(N4\_r/(N\_T))\*100

N5\_r%=(N5\_r/(N\_T))\*100

N6\_r%=(N6\_r/(N\_T))\*100

N\_char\_r=(3/100)\*N\_char\_oxd

N5\_r=N4\_oxd

N6\_r=3.76\*m

alpha=1.451

beta=0.697

mw=12+(alpha)+(16\*beta)

MC=(18\*w)/(18\*w+mw)

alpha+(2\*w)=(2\*A\_1s)

beta+w+(2\*m\_s)=2+(A\_1s)

ER\_r=(m/m\_s)

N\_char\_r+N1\_r+N2\_r+N5\_r-(N\_char\_oxd+N1\_oxd+N2\_oxd+N4\_oxd)=0

N3\_r+N4\_r-N3\_oxd=0

N1\_r+2\*N2\_r+N4\_r-(N1\_oxd+2\*N2\_oxd+N3\_oxd)=0

(N1\_r)\*(N4\_r)\*(K\_1)-(N2\_r)\*(N3\_r)=0

H\_co=-110525

H\_co2=-393509

H\_h2o=-241818

H\_ch4=-74820

H41=-285830

h\_fg=2258.02

"energy balance to get reduction zone temperature"

A\_3=29.11

A\_1=28.16

A\_2=22.26

A\_4=32.24

A\_5=19.89

A\_6=28.90

B\_3=-0.1916\*10^(-2)

B\_1=0.1675\*10^(-2)

B\_2=5.981\*10^(-2)

B\_4=0.1923\*10^(-2)

B\_5=5.204\*10^(-2)

B\_6=-0.1571\*10^(-2)

C\_3=0.4003\*10^(-5)

C\_1=0.5372\*10^(-5)

C\_2=-3.501\*10^(-5)

C\_4=1.055\*10^(-5)

C\_5=1.269\*10^(-5)

C\_6=0.8081\*10^(-5)

D\_3=-0.8704\*10^(-9)

D\_1=-2.222\*10^(-9)

D\_2=-7.469\*10^(-9)

D\_4=-3.595\*10^(-9)

D\_5=-11.01\*10^(-9)

D\_6=-2.873\*10^(-9)

(T\_0)=298

sigma\_h\_f=((N1\_r)\*H\_co)+((N2\_r)\*H\_co2)+((N4\_r)\*H\_h2o)+((N5\_r)\*H\_ch4)

sigma\_1=((N1\_r)\*A\_1+(N2\_r)\*A\_2+(N3\_r)\*A\_3+(N4\_r)\*A\_4+(N5\_r)\*A\_5+(N6\_r)\*A\_6)

sigma\_2=((N1\_r)\*B\_1+(N2\_r)\*B\_2+(N3\_r)\*B\_3+(N4\_r)\*B\_4+(N5\_r)\*B\_5+(N6\_r)\*B\_6)

sigma\_3=((N1\_r)\*C\_1+(N2\_r)\*C\_2+(N3\_r)\*C\_3+(N4\_r)\*C\_4+(N5\_r)\*C\_5+(N6\_r)\*C\_6)

sigma\_4=((N1\_r)\*D\_1+(N2\_r)\*D\_2+(N3\_r)\*D\_3+(N4\_r)\*D\_4+(N5\_r)\*D\_5+(N6\_r)\*D\_6)

H0+w\*H41+h\_loss=((sigma\_h\_f)+(sigma\_1)\*(T\_R)+(sigma\_2)\*(T\_R)^(2)+(sigma\_3)\*(T\_R)^(3)+(sigma\_4)\*(T\_R)^(4))-K

K=(sigma\_1)\*(T\_0)+(sigma\_2)\*(T\_0)^(2)+(sigma\_3)\*(T\_0)^(3)+(sigma\_4)\*(T\_0)^(4)

ERROR=((T-T\_R)/T)\*100

HHV=486573.5

m\_h=(alpha\*1)/(12\*1+alpha\*1+beta\*16)

LHV=HHV-h\_fg\*18\*(9\*m\_h+MC)

H0=(LHV)+H\_co2+(A\_1s)\*H\_h2o

h\_loss=(10/100)\*(ER\_r\*HHV)

**APPENDIX-C**

**DOWNDRAFT GASIFIER MODEL FLUENT CODE:**

FLUENT

Version: 2d, pbns, pdf20, ske (2d, pressure-based, 20 species pdf, standard k-epsilon)

Release: 6.3.26

Title:

Models

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Model Settings

-------------------------------------------------------------------------------------------------------------------------------

Space 2D

Time Steady

Viscous Standard k-epsilon turbulence model

Wall Treatment Standard Wall Functions

Heat Transfer Enabled

Solidification and Melting Disabled

Radiation P1 Model

Species Transport PDF ((c h o n n2 o2 empirical-fuel c<s> h2 co h2o co2 ch4 oh c2h2 ch3 ho2 c2n2 c4h2 c2h4) species)

Coupled Dispersed Phase Disabled

Pollutants Disabled

Pollutants Disabled

Soot Disabled

Boundary Conditions

-------------------

Zones

name id type

---------------------------------------

fluid 2 fluid

tier\_wall 3 wall

wall\_4 4 wall

wall\_3 5 wall

wall\_2 6 wall

wall\_1 7 wall

air\_inlet 8 mass-flow-inlet

gas\_outlet 9 pressure-outlet

fuel\_inlet 10 mass-flow-inlet

default-interior 12 interior

Boundary Conditions

fluid

Condition Value

---------------------------------------------------------------------

Material Name pdf-mixture

Specify source terms? no

Source Terms ()

Specify fixed values? no

Fixed Values ()

Motion Type 0

X-Velocity Of Zone (m/s) 0

Y-Velocity Of Zone (m/s) 0

Rotation speed (rad/s) 0

X-Origin of Rotation-Axis (mm) 0

Y-Origin of Rotation-Axis (mm) 0

Deactivated Thread no

Laminar zone? no

Set Turbulent Viscosity to zero within laminar zone? yes

Porous zone? no

X-Component of Direction-1 Vector 1

Y-Component of Direction-1 Vector 0

Relative Velocity Resistance Formulation? yes

Direction-1 Viscous Resistance (1/m2) 0

Direction-2 Viscous Resistance (1/m2) 0

Choose alternative formulation for inertial resistance? no

Direction-1 Inertial Resistance (1/m) 0

Direction-2 Inertial Resistance (1/m) 0

C0 Coefficient for Power-Law 0

C1 Coefficient for Power-Law 0

Porosity 1

Solid Material Name aluminum

tier\_wall

Condition Value

---------------------------------------------------------------

Wall Thickness (mm) 0

Heat Generation Rate (w/m3) 0

Material Name aluminum

Thermal BC Type 0

Temperature (k) 600

Heat Flux (w/m2) 0

Convective Heat Transfer Coefficient (w/m2-k) 0

Free Stream Temperature (k) 300

Wall Motion 0

Shear Boundary Condition 0

Define wall motion relative to adjacent cell zone? yes

Apply a rotational velocity to this wall? no

Velocity Magnitude (m/s) 0

X-Component of Wall Translation 1

Y-Component of Wall Translation 0

Define wall velocity components? no

X-Component of Wall Translation (m/s) 0

Y-Component of Wall Translation (m/s) 0

Internal Emissivity 0.60000002

External Emissivity 1

External Radiation Temperature (k) 300

Wall Roughness Height (mm) 0

Wall Roughness Constant 0.5

Rotation Speed (rad/s) 0

X-Position of Rotation-Axis Origin (mm) 0

Y-Position of Rotation-Axis Origin (mm) 0

X-component of shear stress (pascal) 0

Y-component of shear stress (pascal) 0

Surface tension gradient (n/m-k) 0

Specularity Coefficient 0

wall\_4

Condition Value

---------------------------------------------------------------

Wall Thickness (mm) 0

Heat Generation Rate (w/m3) 0

Material Name aluminum

Thermal BC Type 0

Temperature (k) 700

Heat Flux (w/m2) 0

Convective Heat Transfer Coefficient (w/m2-k) 0

Free Stream Temperature (k) 300

Wall Motion 0

Shear Boundary Condition 0

Define wall motion relative to adjacent cell zone? yes

Apply a rotational velocity to this wall? no

Velocity Magnitude (m/s) 0

X-Component of Wall Translation 1

Y-Component of Wall Translation 0

Define wall velocity components? no

X-Component of Wall Translation (m/s) 0

Y-Component of Wall Translation (m/s) 0

Internal Emissivity 0.60000002

External Emissivity 1

External Radiation Temperature (k) 300

Wall Roughness Height (mm) 0

Wall Roughness Constant 0.5

Rotation Speed (rad/s) 0

X-Position of Rotation-Axis Origin (mm) 0

Y-Position of Rotation-Axis Origin (mm) 0

X-component of shear stress (pascal) 0

Y-component of shear stress (pascal) 0

Surface tension gradient (n/m-k) 0

Specularity Coefficient 0

wall\_3

Condition Value

---------------------------------------------------------------

Wall Thickness (mm) 0

Heat Generation Rate (w/m3) 0

Material Name aluminum

Thermal BC Type 0

Temperature (k) 1200

Heat Flux (w/m2) 0

Convective Heat Transfer Coefficient (w/m2-k) 0

Free Stream Temperature (k) 300

Wall Motion 0

Shear Boundary Condition 0

Define wall motion relative to adjacent cell zone? yes

Apply a rotational velocity to this wall? no

Velocity Magnitude (m/s) 0

X-Component of Wall Translation 1

Y-Component of Wall Translation 0

Define wall velocity components? no

X-Component of Wall Translation (m/s) 0

Y-Component of Wall Translation (m/s) 0

Internal Emissivity 0.60000002

External Emissivity 1

External Radiation Temperature (k) 300

Wall Roughness Height (mm) 0

Wall Roughness Constant 0.5

Rotation Speed (rad/s) 0

X-Position of Rotation-Axis Origin (mm) 0

Y-Position of Rotation-Axis Origin (mm) 0

X-component of shear stress (pascal) 0

Y-component of shear stress (pascal) 0

Surface tension gradient (n/m-k) 0

Specularity Coefficient 0

wall\_2

Condition Value

---------------------------------------------------------------

Wall Thickness (mm) 0

Heat Generation Rate (w/m3) 0

Material Name aluminum

Thermal BC Type 0

Temperature (k) 900

Heat Flux (w/m2) 0

Convective Heat Transfer Coefficient (w/m2-k) 0

Free Stream Temperature (k) 300

Wall Motion 0

Shear Boundary Condition 0

Define wall motion relative to adjacent cell zone? yes

Apply a rotational velocity to this wall? no

Velocity Magnitude (m/s) 0

X-Component of Wall Translation 1

Y-Component of Wall Translation 0

Define wall velocity components? no

X-Component of Wall Translation (m/s) 0

Y-Component of Wall Translation (m/s) 0

Internal Emissivity 0.60000002

External Emissivity 1

External Radiation Temperature (k) 300

Wall Roughness Height (mm) 0

Wall Roughness Constant 0.5

Rotation Speed (rad/s) 0

X-Position of Rotation-Axis Origin (mm) 0

Y-Position of Rotation-Axis Origin (mm) 0

X-component of shear stress (pascal) 0

Y-component of shear stress (pascal) 0

Surface tension gradient (n/m-k) 0

Specularity Coefficient 0

wall\_1

Condition Value

---------------------------------------------------------------

Wall Thickness (mm) 0

Heat Generation Rate (w/m3) 0

Material Name aluminum

Thermal BC Type 0

Temperature (k) 500

Heat Flux (w/m2) 0

Convective Heat Transfer Coefficient (w/m2-k) 0

Free Stream Temperature (k) 300

Wall Motion 0

Shear Boundary Condition 0

Define wall motion relative to adjacent cell zone? yes

Apply a rotational velocity to this wall? no

Velocity Magnitude (m/s) 0

X-Component of Wall Translation 1

Y-Component of Wall Translation 0

Define wall velocity components? no

X-Component of Wall Translation (m/s) 0

Y-Component of Wall Translation (m/s) 0

Internal Emissivity 0.60000002

External Emissivity 1

External Radiation Temperature (k) 300

Wall Roughness Height (mm) 0

Wall Roughness Constant 0.5

Rotation Speed (rad/s) 0

X-Position of Rotation-Axis Origin (mm) 0

Y-Position of Rotation-Axis Origin (mm) 0

X-component of shear stress (pascal) 0

Y-component of shear stress (pascal) 0

Surface tension gradient (n/m-k) 0

Specularity Coefficient 0

air\_inlet

Condition Value

---------------------------------------------------------

Mass Flow Specification Method 0

Mass Flow-Rate (kg/s) 0.0070000002

Mass Flux (kg/m2-s) 1

Average Mass Flux (kg/m2-s) 1

Upstream Torque Integral (n-m) 1

Upstream Total Enthalpy Integral (w/m2) 1

Total Temperature (k) 600

Supersonic/Initial Gauge Pressure (pascal) 0

Direction Specification Method 1

Reference Frame 0

X-Component of Flow Direction 1

Y-Component of Flow Direction 0

X-Component of Axis Direction 1

Y-Component of Axis Direction 0

Z-Component of Axis Direction 0

X-Coordinate of Axis Origin (mm) 0

Y-Coordinate of Axis Origin (mm) 0

Z-Coordinate of Axis Origin (mm) 0

Turbulent Specification Method 3

Turbulent Kinetic Energy (m2/s2) 1

Turbulent Dissipation Rate (m2/s3) 1

Turbulent Intensity (%) 0.099999994

Turbulent Length Scale (mm) 1

Hydraulic Diameter (mm) 0.0025000002

Turbulent Viscosity Ratio 10

External Black Body Temperature Method 0

Black Body Temperature (k) 300

Internal Emissivity 0.60000002

Mean Mixture Fraction 0

Mixture Fraction Variance 0

is zone used in mixing-plane model? no

gas\_outlet

Condition Value

---------------------------------------------------------

Gauge Pressure (pascal) 0

Backflow Total Temperature (k) 800

Backflow Direction Specification Method 1

X-Component of Flow Direction 1

Y-Component of Flow Direction 0

X-Component of Axis Direction 1

Y-Component of Axis Direction 0

Z-Component of Axis Direction 0

X-Coordinate of Axis Origin (mm) 0

Y-Coordinate of Axis Origin (mm) 0

Z-Coordinate of Axis Origin (mm) 0

Turbulent Specification Method 3

Backflow Turbulent Kinetic Energy (m2/s2) 1

Backflow Turbulent Dissipation Rate (m2/s3) 1

Backflow Turbulent Intensity (%) 0.099999994

Backflow Turbulent Length Scale (mm) 1

Backflow Hydraulic Diameter (mm) 0.017000001

Backflow Turbulent Viscosity Ratio 10

External Black Body Temperature Method 0

Black Body Temperature (k) 300

Internal Emissivity 0.60000002

Mean Mixture Fraction 0

Mixture Fraction Variance 0

is zone used in mixing-plane model? no

Specify targeted mass flow rate no

Targeted mass flow (kg/s) 1

fuel\_inlet

Condition Value

--------------------------------------------------------

Mass Flow Specification Method 0

Mass Flow-Rate (kg/s) 0.0041

Mass Flux (kg/m2-s) 1

Average Mass Flux (kg/m2-s) 1

Upstream Torque Integral (n-m) 1

Upstream Total Enthalpy Integral (w/m2) 1

Total Temperature (k) 400

Supersonic/Initial Gauge Pressure (pascal) 0

Direction Specification Method 1

Reference Frame 0

X-Component of Flow Direction 1

Y-Component of Flow Direction 0

X-Component of Axis Direction 1

Y-Component of Axis Direction 0

Z-Component of Axis Direction 0

X-Coordinate of Axis Origin (mm) 0

Y-Coordinate of Axis Origin (mm) 0

Z-Coordinate of Axis Origin (mm) 0

Turbulent Specification Method 3

Turbulent Kinetic Energy (m2/s2) 1

Turbulent Dissipation Rate (m2/s3) 1

Turbulent Intensity (%) 0.099999994

Turbulent Length Scale (mm) 1

Hydraulic Diameter (mm) 0.025

Turbulent Viscosity Ratio 10

External Black Body Temperature Method 0

Black Body Temperature (k) 300

Internal Emissivity 0.60000002

Mean Mixture Fraction 1

Mixture Fraction Variance 0

is zone used in mixing-plane model? no

default-interior

Condition Value

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Solver Controls

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Equations

Equation Solved

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Flow yes

Turbulence yes

Energy yes

P1 yes

Pdf yes

Numerics

Numeric Enabled

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Absolute Velocity Formulation yes

Relaxation

Variable Relaxation Factor

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Pressure 0.5

Density 0.80000001

Body Forces 1

Momentum 0.30000001

Turbulent Kinetic Energy 0.69999999

Turbulent Dissipation Rate 0.69999999

Turbulent Viscosity 1

Energy 1

Temperature 1

P1 0.80000001

Mean Mixture Fraction 1

Mixture Fraction Variance 0.89999998

Linear Solver

Solver Termination Residual Reduction

Variable Type Criterion Tolerance

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Pressure V-Cycle 0.1

X-Momentum Flexible 0.1 0.7

Y-Momentum Flexible 0.1 0.7

Turbulent Kinetic Energy Flexible 0.1 0.7

Turbulent Dissipation Rate Flexible 0.1 0.7

Energy Flexible 0.1 0.7

P1 Flexible 0.1 0.7

Mean Mixture Fraction Flexible 0.1 0.7

Mixture Fraction Variance Flexible 0.1 0.7

Pressure-Velocity Coupling

Parameter Value

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Type SIMPLE

Discretization Scheme

Variable Scheme

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Pressure PRESTO!

Momentum Second Order Upwind

Turbulent Kinetic Energy Second Order Upwind

Turbulent Dissipation Rate Second Order Upwind

Energy Second Order Upwind

Mean Mixture Fraction Second Order Upwind

Mixture Fraction Variance First Order Upwind

Solution Limits

Quantity Limit

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Minimum Absolute Pressure 1

Maximum Absolute Pressure 4.9999999e+10

Minimum Temperature 1

Maximum Temperature 2500

Minimum Turb. Kinetic Energy 9.9999998e-15

Minimum Turb. Dissipation Rate 9.9999997e-21

Maximum Turb. Viscosity Ratio 10000000

Material Properties

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Material: pdf-mixture (mixture)

Property Units Method Value(s)

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Mixture Species names (c h o n n2 o2 empirical-fuel c<s> h2 co h2o co2 ch4 oh c2h2 ch3 ho2 c2n2 c4h2 c2h4)

Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k mixing-law #f

Thermal Conductivity w/m-k constant 0.045400001

Viscosity kg/m-s constant 1.72e-05

Absorption Coefficient 1/m wsggm-domain-based #f

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (c2h4 . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: -255.32065 8.2870323 -0.010043079 8.2544018e-06 -2.8860316e-09) (1000-5000: 1045.7232 3.4038836 -0.0013094842 2.3249173e-07 -1.5609446e-11)

Molecular Weight kg/kgmol constant 28.05376

Standard State Enthalpy j/kgmol constant 52463938

Standard State Entropy j/kgmol-k constant 219170.06

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: c2h4 (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: -255.32065 8.2870323 -0.010043079 8.2544018e-06 -2.8860316e-09) (1000-5000: 1045.7232 3.4038836 -0.0013094842 2.3249173e-07 -1.5609446e-11)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 28.05376

Standard State Enthalpy j/kgmol constant 52463938

Standard State Entropy j/kgmol-k constant 219170.06

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (c4h2 . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 665.21373 3.2902012 -0.0016386027 -1.1020194e-06 1.0093847e-09) (1000-5000: 1500.0074 1.0043753 -0.00032367009 4.5754939e-08 -2.3013271e-12)

Molecular Weight kg/kgmol constant 50.05988

Standard State Enthalpy j/kgmol constant 4.6741459e+08

Standard State Entropy j/kgmol-k constant 250152.98

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: c4h2 (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 665.21373 3.2902012 -0.0016386027 -1.1020194e-06 1.0093847e-09) (1000-5000: 1500.0074 1.0043753 -0.00032367009 4.5754939e-08 -2.3013271e-12)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 50.05988

Standard State Enthalpy j/kgmol constant 4.6741459e+08

Standard State Entropy j/kgmol-k constant 250152.98

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (c2n2 . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 681.54519 1.9050164 -0.0021443022 1.4687671e-06 -4.440258e-10) (1000-5000: 1046.2553 0.63668596 -0.00026111898 4.855141e-08 -3.3731163e-12)

Molecular Weight kg/kgmol constant 52.0354

Standard State Enthalpy j/kgmol constant 3.0911739e+08

Standard State Entropy j/kgmol-k constant 241531.82

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: c2n2 (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 681.54519 1.9050164 -0.0021443022 1.4687671e-06 -4.440258e-10) (1000-5000: 1046.2553 0.63668596 -0.00026111898 4.855141e-08 -3.3731163e-12)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 52.0354

Standard State Enthalpy j/kgmol constant 3.0911739e+08

Standard State Entropy j/kgmol-k constant 241531.82

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (ho2 . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 750.64746 1.2586592 -0.0009549455 5.9301684e-07 -2.037611e-10) (1000-5000: 1025.7778 0.53686973 -0.00013371124 1.5396699e-08 -7.1568424e-13)

Molecular Weight kg/kgmol constant 33.00674

Standard State Enthalpy j/kgmol constant 10455847

Standard State Entropy j/kgmol-k constant 228992.05

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: ho2 (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 750.64746 1.2586592 -0.0009549455 5.9301684e-07 -2.037611e-10) (1000-5000: 1025.7778 0.53686973 -0.00013371124 1.5396699e-08 -7.1568424e-13)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 33.00674

Standard State Enthalpy j/kgmol constant 10455847

Standard State Entropy j/kgmol-k constant 228992.05

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (ch3 . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1344.0481 6.1516893 -0.0092917111 8.9688045e-06 -3.2433514e-09) (1000-5000: 1572.7762 3.3943341 -0.0012333933 2.0932153e-07 -1.3560577e-11)

Molecular Weight kg/kgmol constant 15.03482

Standard State Enthalpy j/kgmol constant 1.4569786e+08

Standard State Entropy j/kgmol-k constant 194048.5

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: ch3 (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1344.0481 6.1516893 -0.0092917111 8.9688045e-06 -3.2433514e-09) (1000-5000: 1572.7762 3.3943341 -0.0012333933 2.0932153e-07 -1.3560577e-11)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 15.03482

Standard State Enthalpy j/kgmol constant 1.4569786e+08

Standard State Entropy j/kgmol-k constant 194048.5

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (c2h2 . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 642.96475 4.850569 -0.0051611824 2.8990773e-06 -6.1077248e-10) (1000-5000: 1416.7365 1.7166611 -0.00061079483 1.049397e-07 -6.8867404e-12)

Molecular Weight kg/kgmol constant 26.03788

Standard State Enthalpy j/kgmol constant 2.2676688e+08

Standard State Entropy j/kgmol-k constant 200915.22

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: c2h2 (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 642.96475 4.850569 -0.0051611824 2.8990773e-06 -6.1077248e-10) (1000-5000: 1416.7365 1.7166611 -0.00061079483 1.049397e-07 -6.8867404e-12)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 26.03788

Standard State Enthalpy j/kgmol constant 2.2676688e+08

Standard State Entropy j/kgmol-k constant 200915.22

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (oh . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1778.142 0.09048502 -0.00081942281 1.1670261e-06 -4.1218601e-10) (1000-5000: 1409.2737 0.49569933 -0.00011130917 1.0631324e-08 -2.5060852e-13)

Molecular Weight kg/kgmol constant 17.00734

Standard State Enthalpy j/kgmol constant 38985683

Standard State Entropy j/kgmol-k constant 183602.61

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: oh (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1778.142 0.09048502 -0.00081942281 1.1670261e-06 -4.1218601e-10) (1000-5000: 1409.2737 0.49569933 -0.00011130917 1.0631324e-08 -2.5060852e-13)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 17.00734

Standard State Enthalpy j/kgmol constant 38985683

Standard State Entropy j/kgmol-k constant 183602.61

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (ch4 . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 403.5915 9.0574851 -0.014425329 1.5805453e-05 -6.3431579e-09) (1000-5000: 872.48132 5.3055622 -0.0020083285 3.5167054e-07 -2.3339494e-11)

Molecular Weight kg/kgmol constant 16.04276

Standard State Enthalpy j/kgmol constant -74892973

Standard State Entropy j/kgmol-k constant 186057.77

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: ch4 (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 403.5915 9.0574851 -0.014425329 1.5805453e-05 -6.3431579e-09) (1000-5000: 872.48132 5.3055622 -0.0020083285 3.5167054e-07 -2.3339494e-11)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 16.04276

Standard State Enthalpy j/kgmol constant -74892973

Standard State Entropy j/kgmol-k constant 186057.77

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (co2 . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 429.93022 1.8744798 -0.0019664917 1.2972557e-06 -3.9999695e-10) (1000-5000: 841.37933 0.59324115 -0.00024151756 4.5227419e-08 -3.153141e-12)

Molecular Weight kg/kgmol constant 44.0098

Standard State Enthalpy j/kgmol constant -3.9354283e+08

Standard State Entropy j/kgmol-k constant 213734.59

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: co2 (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 429.93022 1.8744798 -0.0019664917 1.2972557e-06 -3.9999695e-10) (1000-5000: 841.37933 0.59324115 -0.00024151756 4.5227419e-08 -3.153141e-12)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 44.0098

Standard State Enthalpy j/kgmol constant -3.9354283e+08

Standard State Entropy j/kgmol-k constant 213734.59

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (h2o . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1563.0818 1.6037598 -0.0029327939 3.2161116e-06 -1.1568305e-09) (1000-5000: 1233.2377 1.4105281 -0.00040291547 5.5427906e-08 -2.949834e-12)

Molecular Weight kg/kgmol constant 18.01528

Standard State Enthalpy j/kgmol constant -2.4184276e+08

Standard State Entropy j/kgmol-k constant 188713.27

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: h2o (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1563.0818 1.6037598 -0.0029327939 3.2161116e-06 -1.1568305e-09) (1000-5000: 1233.2377 1.4105281 -0.00040291547 5.5427906e-08 -2.949834e-12)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 18.01528

Standard State Enthalpy j/kgmol constant -2.4184276e+08

Standard State Entropy j/kgmol-k constant 188713.27

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (co . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 968.39484 0.44879012 -0.0011522231 1.656891e-06 -7.3464085e-10) (1000-5000: 897.9353 0.4282339 -0.0001671401 3.0234596e-08 -2.0513808e-12)

Molecular Weight kg/kgmol constant 28.0104

Standard State Enthalpy j/kgmol constant -1.1053974e+08

Standard State Entropy j/kgmol-k constant 197546.27

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: co (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 968.39484 0.44879012 -0.0011522231 1.656891e-06 -7.3464085e-10) (1000-5000: 897.9353 0.4282339 -0.0001671401 3.0234596e-08 -2.0513808e-12)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 28.0104

Standard State Enthalpy j/kgmol constant -1.1053974e+08

Standard State Entropy j/kgmol-k constant 197546.27

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (h2 . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 13602.855 3.4024177 -0.0033585231 -3.9080689e-07 1.7053957e-09) (1000-5000: 12337.891 2.8873611 -0.00023236285 -3.8074924e-08 6.5279369e-12)

Molecular Weight kg/kgmol constant 2.01588

Standard State Enthalpy j/kgmol constant 2448.5948

Standard State Entropy j/kgmol-k constant 130593.59

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: h2 (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 13602.855 3.4024177 -0.0033585231 -3.9080689e-07 1.7053957e-09) (1000-5000: 12337.891 2.8873611 -0.00023236285 -3.8074924e-08 6.5279369e-12)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 2.01588

Standard State Enthalpy j/kgmol constant 2448.5948

Standard State Entropy j/kgmol-k constant 130593.59

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (c<s> . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 constant 2000

Cp (Specific Heat) j/kg-k polynomial (273-1000: -464.18404 4.9712284 -0.0038992607 1.4829568e-06 -2.8855917e-10) (1000-5000: 1031.5336 1.1505684 -0.0004629064 8.9358187e-08 -6.3721819e-12)

Molecular Weight kg/kgmol constant 12.011

Standard State Enthalpy j/kgmol constant 1174.647

Standard State Entropy j/kgmol-k constant 5735.9101

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: c<s> (fluid)

Property Units Method Value(s)

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Density kg/m3 constant 2000

Cp (Specific Heat) j/kg-k polynomial (273-1000: -464.18404 4.9712284 -0.0038992607 1.4829568e-06 -2.8855917e-10) (1000-5000: 1031.5336 1.1505684 -0.0004629064 8.9358187e-08 -6.3721819e-12)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 12.011

Standard State Enthalpy j/kgmol constant 1174.647

Standard State Entropy j/kgmol-k constant 5735.9101

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (empirical-fuel . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k constant 1200

Molecular Weight kg/kgmol constant 28

Standard State Enthalpy j/kgmol constant 0

Standard State Entropy j/kgmol-k constant 0

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: empirical-fuel (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k constant 1200

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 28

Standard State Enthalpy j/kgmol constant 0

Standard State Entropy j/kgmol-k constant 0

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (o2 . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 834.82638 0.29295803 -0.0001495637 3.4138851e-07 -2.2783585e-10) (1000-5000: 960.7523 0.15941258 -3.2708853e-05 4.6127636e-09 -2.9528327e-13)

Molecular Weight kg/kgmol constant 31.9988

Standard State Enthalpy j/kgmol constant -847.64045

Standard State Entropy j/kgmol-k constant 205041.62

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: o2 (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 834.82638 0.29295803 -0.0001495637 3.4138851e-07 -2.2783585e-10) (1000-5000: 960.7523 0.15941258 -3.2708853e-05 4.6127636e-09 -2.9528327e-13)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 31.9988

Standard State Enthalpy j/kgmol constant -847.64045

Standard State Entropy j/kgmol-k constant 205041.62

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (n2 . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 979.04296 0.41796388 -0.001176279 1.6743942e-06 -7.2562943e-10) (1000-5000: 868.62287 0.44162954 -0.00016872292 2.9967875e-08 -2.0043856e-12)

Molecular Weight kg/kgmol constant 28.0134

Standard State Enthalpy j/kgmol constant 1429.881

Standard State Entropy j/kgmol-k constant 191509.42

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: n2 (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 979.04296 0.41796388 -0.001176279 1.6743942e-06 -7.2562943e-10) (1000-5000: 868.62287 0.44162954 -0.00016872292 2.9967875e-08 -2.0043856e-12)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 28.0134

Standard State Enthalpy j/kgmol constant 1429.881

Standard State Entropy j/kgmol-k constant 191509.42

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (n . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1485.8163 -0.012940529 3.2176116e-05 -3.3523766e-08 1.2464974e-11) (1000-5000: 1454.4726 0.063286132 -4.4314043e-05 1.1157564e-08 -6.0902132e-13)

Molecular Weight kg/kgmol constant 14.0067

Standard State Enthalpy j/kgmol constant 4.7262532e+08

Standard State Entropy j/kgmol-k constant 153187.62

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: n (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1485.8163 -0.012940529 3.2176116e-05 -3.3523766e-08 1.2464974e-11) (1000-5000: 1454.4726 0.063286132 -4.4314043e-05 1.1157564e-08 -6.0902132e-13)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 14.0067

Standard State Enthalpy j/kgmol constant 4.7262532e+08

Standard State Entropy j/kgmol-k constant 153187.62

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (o . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1531.1577 -0.851299 0.0012581269 -8.3294264e-07 2.0218614e-10) (1000-5000: 1321.021 -0.014317108 -1.6124204e-06 2.3650336e-09 -2.2699264e-13)

Molecular Weight kg/kgmol constant 15.9994

Standard State Enthalpy j/kgmol constant 2.49195e+08

Standard State Entropy j/kgmol-k constant 160943.58

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: o (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1531.1577 -0.851299 0.0012581269 -8.3294264e-07 2.0218614e-10) (1000-5000: 1321.021 -0.014317108 -1.6124204e-06 2.3650336e-09 -2.2699264e-13)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 15.9994

Standard State Enthalpy j/kgmol constant 2.49195e+08

Standard State Entropy j/kgmol-k constant 160943.58

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (h . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 20622.11 0 0 0 0) (1000-5000: 20622.11 0 0 0 0)

Molecular Weight kg/kgmol constant 1.00794

Standard State Enthalpy j/kgmol constant 2.1797701e+08

Standard State Entropy j/kgmol-k constant 114603.82

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: h (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 20622.11 0 0 0 0) (1000-5000: 20622.11 0 0 0 0)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 1.00794

Standard State Enthalpy j/kgmol constant 2.1797701e+08

Standard State Entropy j/kgmol-k constant 114603.82

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: (c . pdf-mixture) (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1729.5876 0.055971935 -0.0001867419 2.1048751e-07 -7.6605439e-11) (1000-5000: 1801.2352 -0.12370659 6.2902963e-05 -7.9601502e-09 2.291856e-13)

Molecular Weight kg/kgmol constant 12.011

Standard State Enthalpy j/kgmol constant 7.1674177e+08

Standard State Entropy j/kgmol-k constant 158005.45

Reference Temperature k constant 298.15

Speed of Sound m/s none #f

Material: c (fluid)

Property Units Method Value(s)

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Density kg/m3 pdf #f

Cp (Specific Heat) j/kg-k polynomial (300-1000: 1729.5876 0.055971935 -0.0001867419 2.1048751e-07 -7.6605439e-11) (1000-5000: 1801.2352 -0.12370659 6.2902963e-05 -7.9601502e-09 2.291856e-13)

Thermal Conductivity w/m-k constant 0.0454

Viscosity kg/m-s constant 1.72e-05

Molecular Weight kg/kgmol constant 12.011

Standard State Enthalpy j/kgmol constant 7.1674177e+08

Standard State Entropy j/kgmol-k constant 158005.45

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: air (fluid)

Property Units Method Value(s)

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Density kg/m3 constant 1.225

Cp (Specific Heat) j/kg-k constant 1006.43

Thermal Conductivity w/m-k constant 0.0242

Viscosity kg/m-s constant 1.7894e-05

Molecular Weight kg/kgmol constant 28.966

Standard State Enthalpy j/kgmol constant 0

Standard State Entropy j/kgmol-k constant 0

Reference Temperature k constant 298.15

Absorption Coefficient 1/m constant 0

Scattering Coefficient 1/m constant 0

Scattering Phase Function isotropic #f

Thermal Expansion Coefficient 1/k constant 0

Speed of Sound m/s none #f

Material: aluminum (solid)

Property Units Method Value(s)

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Density kg/m3 constant 2719

Cp (Specific Heat) j/kg-k constant 871

Thermal Conductivity w/m-k constant 202.4

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