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Investigating Downdraft Gasification of Biomass

A thesis presented in partial fulfilment of the requirements for the degree of

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in
Physics

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Abstract

Gasification of biomass is a potential source of renewable energy. Downdraft gasifiers are comparatively cheap and can produce gases with low tar content. We constructed a simple, phenomenological model of downdraft gasification which we compared to both previously published data and our own experimental results. The steady-state gas compositions predicted by the model were quite close to those found experimentally, although the model tended to over-predict the amount of methane in the dry product gas. The steady-state gas composition predicted depended upon the conditions assumed at the top of the gasifier.

The experimental part of this investigation looked at the effect of the air flow rate into the gasifier and the length of the gasifier bed. However, the uncertainties in the experimental measurements were too large to determine whether the experimental results followed the same trends as predicted by the model.

The gasifier was run successfully using both 18.7% moisture content pine chips and 12.3% moisture content walnut shells (weight percentage, dry basis) as fuel. Both fuel types produced dry exit gases of similar compositions.

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1. Introduction

Energy production is an area of extremely high interest internationally. The global demand for energy is increasing and is expected to continue increasing for the foreseeable future. However, a high proportion of the current energy usage comes from burning fossil fuels – of which there is only a finite supply. In addition, the burning of fossil fuels releases CO_2 into the atmosphere which is believed to contribute to changes in global climate patterns via the “Greenhouse Effect”. Thus, there is a need to research alternatives to fossil fuels as well as finding methods to increase the efficiency of fossil fuel use.

Gasification is a method for converting solid fuels into gaseous fuels. The producer gas from a gasifier can be burned directly as a fuel, used to power a gas turbine or internal combustion engine or processed further to produce various organic chemicals. Commercial gasification of coal is well-established.

Biomass has several advantages over coal. Sustainably managed biomass is a renewable energy resource. Burning plant-derived biomass does release CO_2 into the atmosphere, however the amount released will be no more than the total CO_2 absorbed by the plant over the course of its lifetime. So as long as the biomass is replanted at the same rate as it is harvested, then the net CO_2 released into the atmosphere is zero. Biomass also has a lower sulfur content than coal so sulfur dioxide production is less significant. In addition, some industries produce large quantities of biomass as a by-product. However, biomass tends to have a low energy density and therefore it is uneconomic to transport it large distances. This means that any processing should occur as close to the point of production as possible.

Downdraft gasification is a comparatively cheap method of gasification that can produce gases with a low tar content. In this thesis we started developing a model of downdraft gasification that accounted for the chemical and physical processes occurring and that could describe a range of downdraft gasifiers under different operating conditions. A series of experiments operating a downdraft gasifier using different bed lengths, fuel types and air flows were performed to provide data to compare with the

model. The model predictions were also compared to published experimental results from other downdraft gasifiers.

1.1 The World Energy Situation

A large proportion of the world's energy demands are supplied by burning fossil fuels. The world demand for energy is increasing, but there is also interest in reducing the amount of fossil fuels consumed and making greater use of renewable energy sources. This is due to both the finite supply of fossil fuels and concerns about the environmental effects of fossil fuel burning.

Burning fossil fuels releases carbon dioxide into the atmosphere which is believed to contribute to global climate changes via the "Greenhouse effect". Also released (although in smaller quantities) are sulfur and nitrogen oxides which can cause acid rain in addition to contributing to the Greenhouse effect.

In order to reduce the possible negative effects of Greenhouse gases accumulating in the atmosphere there have been international agreements made to reduce the level of Greenhouse gases released. The Kyoto Protocol to the United Nations Framework Convention on Climate Change states that Governments should adopt policies to reduce CO₂ emissions with the target of reducing average emissions for the period 2008-2012 to 5% below 1990 levels. New Zealand is a signatory to this agreement.

There are many potential sources of renewable energy for example: solar, wind, hydro, biomass and geothermal power. These energy sources can only be practically exploited in certain locations and in the case of solar and wind power do not produce energy continuously. Attempts to reduce the amount of fossil fuels consumed are likely to involve using many different forms of renewable energy generation as well as increasing the efficiency of energy usage.

Nuclear energy is also an energy source that does not emit CO₂ into the atmosphere. However, nuclear power generation does create radioactive waste that is difficult to

dispose of safely. There have been several disasters involving nuclear power plants that have reduced the popularity of nuclear power. New Zealand, in particular, has a strong "anti-nuclear" policy.

New Zealand Energy Usage

New Zealand's "end-use" energy consumption (i.e. not including energy consumed in energy transformation and transmission) for the 2001 was 459.2 PJ (Ministry of Economic Development, 2002). This was an increase of approximately 0.15% above the previous year. The Figure 1.1 shows the percentage of New Zealand's energy demands met by fuel type for 2001 (Ministry of Economic Development, 2002):

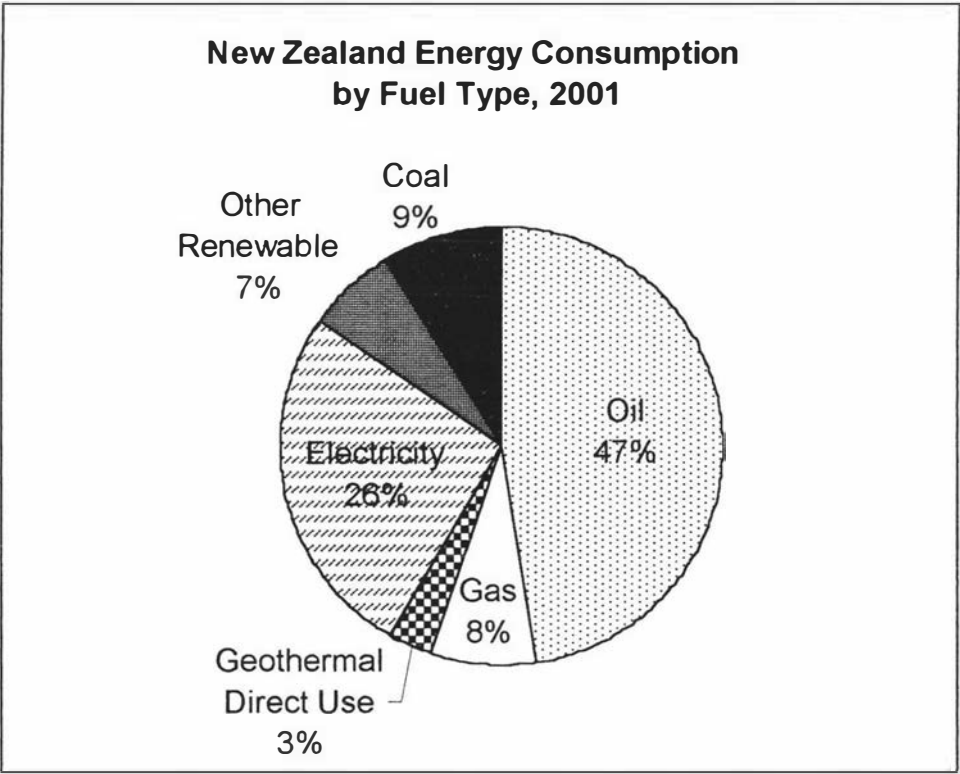


Figure 1.1: New Zealand energy consumption by fuel type for the calendar year 2001 (Ministry of Economic Development, 2002).

The majority of New Zealand's energy demands are met by fossil fuels, particularly oil and oil products (most of which must be imported). Figure 1.2 shows the CO₂ emissions by sector for the 2001 calendar year.

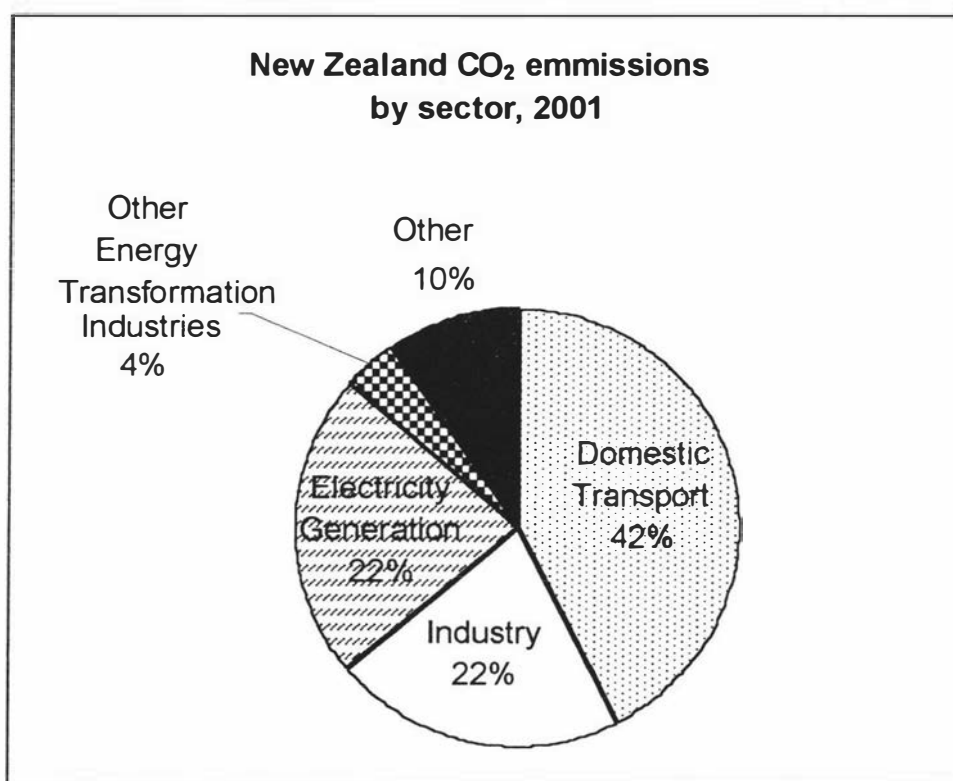


Figure 1.2: New Zealand CO₂ emissions by sector for the calendar year 2001 (Ministry of Economic Development, 2002).

Transport is the single largest contributor to CO₂ emissions. While renewable biofuels suitable for running transport vehicles can be derived from biomass using gasification followed by other refinement techniques, we shall mainly concentrate on electricity generation which is the second largest contributor to New Zealand CO₂ emissions.

Figure 1.3 shows electricity generation by fuel type for the year ended March 2002 (Ministry of Economic Development, 2002). (Note that the output from any co-generation is included in the total energy generated.)

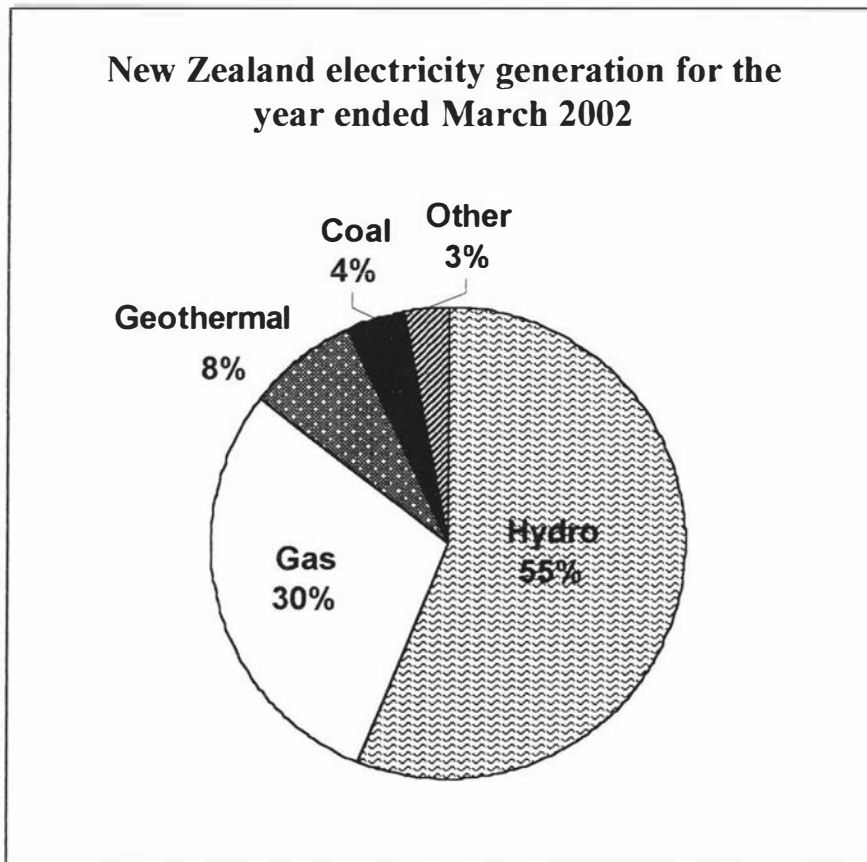


Figure 1.3: New Zealand electricity generation for the year ended March 2002
(Ministry of Economic Development, 2002).

By international standards, New Zealand currently has a high proportion of electricity produced using renewable energy sources. However, the existing hydro-generators have a finite generating capacity which is weather dependent. New generation capacity tends to come from non-renewable sources such as natural gas. New Zealand has an open electricity generation market, which means that any new electricity generators must be able to compete financially with the existing generators. The Government may introduce financial incentives, such as a carbon tax, to encourage the development of new renewable energy sources.

1.2 Gasification

Gasification is a process for turning a solid fuel into a fuel gas. Gasification can occur via thermochemical or biological processes. In this thesis we shall concentrate on thermochemical gasification.

The basic gasification reaction is: $\text{Solid} + \text{Air} + \text{Heat} \rightarrow \text{CO} + \text{H}_2 + \text{other products}$.
The $\text{CO} + \text{H}_2$ can then be used as a fuel.

The gasification process can be broken down into three stages - pyrolysis (devolatilisation), combustion and reduction. Pyrolysis is the thermal decomposition of the fuel that releases the volatile hydrocarbons and leaves solid char. The volatile hydrocarbons released can be broken into lighter molecules ("cracked") if the temperature is greater than 600°C . This is desirable as heavy molecules tend to condense at higher temperatures than lighter molecules and this can cause problems for downstream processes. The high boiling point molecules in the product gas are commonly referred to as "tars".

The combustion stage occurs when carbon in the char and/or the volatile hydrocarbons from pyrolysis react with oxygen entering the gasifier to produce carbon dioxide plus heat. In some gasifiers the pyrolysis and combustion stages can occur simultaneously.

Finally reduction occurs when the carbon dioxide absorbs heat and reacts with the char to produce carbon monoxide fuel gas. If water is present then hydrogen gas can form (which also makes a good fuel).



As these reactions are both endothermic they will act as a moderating influence on the upper temperature of the gasifier.

The product gases can then be used as fuel. The exact production of a gasifier depends on many factors including gasifier design and feed material used. Typically the product gas will contain between 14-40% CO and 6-42% H₂ that can be used as fuel (Redshaw and Dawber, 1996).

There are several different gasifier designs – each with its own advantages and disadvantages. Three major gasifier designs are discussed below:

Downdraft

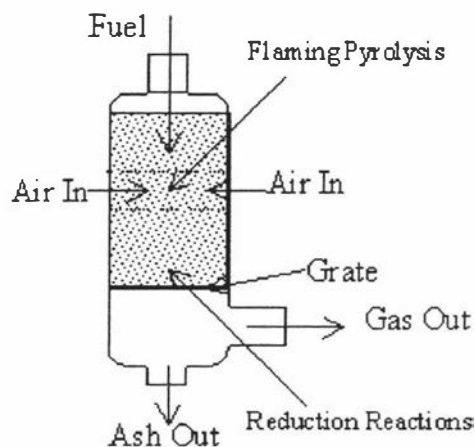


Figure 1.4: Schematic of a typical downdraft gasifier.

In a downdraft gasifier the feedstock is fed into a fixed bed and air (or oxygen) is fed into the middle of the bed which becomes the combustion zone. The heat from the combustion pyrolyses the fuel around the combustion zone. The pyrolysis products are drawn through the combustion zone where the temperature is high enough to thermally crack and oxidise any tars that have been produced. In practice the level of tars that will be in the product gas is a function of temperature. The resulting carbon dioxide is reduced to carbon monoxide in the lower part of the gasifier bed.

The advantage of downdraft gasifiers is that all the pyrolysis gases must pass through the combustion zone before exiting the gasifier. This makes it possible in theory to produce essentially tar free gas. However, the need to ensure that there is sufficient oxygen available throughout the entire cross-section of the combustion zone does

constrain the physical dimensions of a downdraft gasifier. Sime (1998) found that the throughput of a downdraft gasifier could be increased by operating at high pressure. This could allow the energy output of a downdraft gasifier to be increased without increasing the physical dimensions.

Updraft

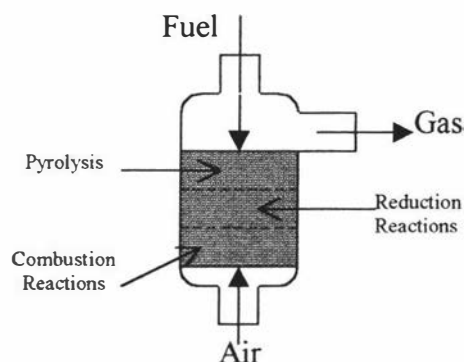


Figure 1.5: Schematic of a typical updraft gasifier.

In the updraft gasifier, oxidation of char occurs at the bottom of the gasifier. The heat from this exothermic reaction drives the other processes in the gasifier. In the area above the oxidation region the high temperature favours the reduction of the rising CO_2 and H_2O . Finally, at the top of the gasifier the heat from the rising product gas pyrolyses the incoming fuel. The disadvantage of this design is that the pyrolysis products are mixed with the outgoing fuel gas. Thus the product gas will have a high oil and tar content and will require extra cleaning before it can be used.

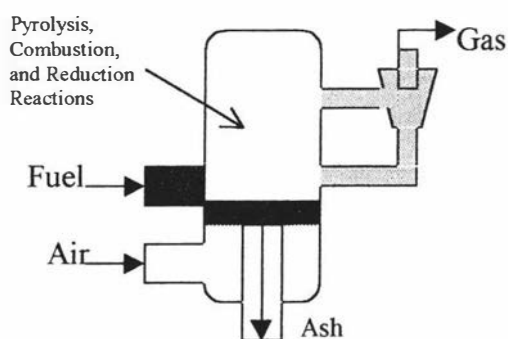


Figure 1.6: Schematic of a typical fluidised bed gasifier.

A fluidised bed gasifier has a bed of fine, inert particulate material. The bed material is "fluidised" by blowing air at a sufficiently high velocity through the bed so that the bed particles move about in a turbulent manner similar to a boiling liquid. The fuel is fed into the bed and must be of sufficiently small particle size. The rate of heat transfer from the bed is relatively high due to the turbulent movement of the particles.

Fluidised bed gasifiers can be used at relatively low temperatures reducing the amount of sulfur and nitrogen oxides that are released from the fuel. A large proportion of the sulfur dioxide can be captured by placing limestone or dolomite within the bed. However, the gas produced will still have a high tar content. The composition of the output gas depends upon its residence time within the gasifier.

1.3 Review of Related Research

There is a large body of literature on gasification. This section is intended to be a representative review of recent work in the field, rather than a comprehensive review.

(A) Electricity Production Using Gasification

The product gas from a gasifier can be used to run a gas turbine and produce electricity. Increased efficiency can be gained if the waste heat from the gas cycle is used to

produce steam to run a secondary steam turbine. This arrangement is called an Integrated Gasification Combined Cycle (IGCC) plant.

Several IGCC plants have been built using coal as a fuel, particularly in the United States as part of the Department of Energy's "Clean Coal Technology Program". The gasifier is usually a fluidised bed or entrained flow design as these can produce a larger throughput reducing the cost of electricity production on a per kilowatt-hour basis. Joshi and Lee (1996) reviewed IGCC technology.

A variation of the IGCC was built in Morwell, Australia to run on low-rank brown coals (Anderson et al., 1998). This design, called Integrated Drying and Gasification Combined Cycle (IGDCC), used the heat of the exit gas to dry the incoming fuel.

(B) Gasification of Biomass

Many industries produce biomass by-products. Gasification and electricity generation is one possible use for these products. As gasification is only one possible use of these by-products (heat generation is usually also an alternative) a good understanding of the potential value of the product gas is necessary in order to determine whether gasification represents the optimal use of these by-products.

The Technical Research Centre of Finland (VTT) has been investigating the use of peat and wood wastes in IGCC. The experimental research over the period 1988-92 was reviewed by Kurkela et al. (1993).

Air-blown downdraft gasification of hazel nut shells has been investigated in a pilot scale downdraft gasifier (Midilli et al., 2001; Dogru et al., 2002). The maximum gross calorific value of the gas produced was 5.15 MJ/Nm^3 .

Chee (1987), Senelwa (1997) and Sime (1998) all studied air-blown downdraft gasification of biomass. Chee used a downdraft gasifier that was open to the atmosphere at the top with a rotating grate and a fan at the bottom of the gasifier to draw the gas through the bed. There was a secondary air supply through tuyeres in the centre of the bed. The effect of different fuel types, fuel moisture contents, grate rotation and

fan speeds were examined. However, the results were often quoted in terms that were specific to the apparatus used (e.g. "fan speed 1").

Senelwa (1997) investigated the potential of short rotation forestry as a source of energy in Kenya. As part of this study several different wood species were gasified in a downdraft gasifier. This gasifier had a port that was open to the atmosphere and relied on a pump in the exit line to draw air into the gasifier.

Sime (1998) used a downdraft gasifier that operated using a positive pressure difference. Air was pumped into the gasifier through an inlet port that distributed the air around the circumference of the gasifier bed. With the exception of the inlet and exit lines the gasifier was sealed from the atmosphere. Sime conducted experiments with the gasifier pressurised at pressures up to 800 kPa. The following observations were made from the experiments performed using pine chips in air pressures of 100-800 kPa:

- The throughput (input flowrate) of the downdraft gasifier increased with increasing pressure.
- The output gas contained (as a percentage of the dry volume) 9.2% H₂, 20.1% CO and 2.4% CH₄ and had a dry higher heating value¹ (HHV) of 104 kJ.mol⁻¹. The HHV did not change significantly with pressure.
- The exit temperature increased with increasing pressure.

The downdraft gasifier used by Sime was also used (with some minor modifications) to collect the experimental results in Chapter 4 of this thesis.

(C) Modelling Gasification

Desrosiers (1981) calculated the effect of varying the temperature, pressure, feed moisture content and fuel/oxidant ratio on gasifier performance assuming the gases reach chemical equilibrium. In practice, the gas produced by a gasifier may not have reached chemical equilibrium. How close the product gas is to the equilibrium composition depends upon factors such as gas residence time and particle size.

¹ The higher heating value of a gas is the heat of combustion assuming that water is produced in the liquid rather than gaseous phase.

As fluidised bed gasifiers are commonly used in large-scale gasification operations there has been some interest in modelling fluidised bed gasification. Modelling of fluidised bed coal gasification was reviewed by Gururajan et al. (1992). Ergüdenler et al. (1997, a-c) published a series of paper in which a model of a fluidised bed straw gasifier was developed then compared to the experimental results produced by a real gasifier.

Yoon et al. (1978) simulated an updraft coal gasifier under steady-state operation.

Wang and Kinoshita (1993) created a kinetic model of biomass gasification and estimated the kinetic parameters of the chemical reactions by finding the best agreement between the model predictions and earlier experimental measurements (Wang and Kinoshita, 1992). The model treated the gases as remaining in a well-mixed reaction zone for a given residence time. Therefore their model was physically similar to a fluidised-bed gasifier, but different from a fixed-bed gasifier where the gases travel vertically through the bed with time.

Other work has concentrated on modelling the reactivity of individual char particles (Lee et. al., 1984; Kyotani et. al., 1993; Bhatia, 1998).

1.4 Thesis Organisation

This thesis is divided into six chapters plus three appendices containing supplementary material.

Chapter 1 discusses the general principles of gasification and the potential uses of biomass gasification. A literature review of other research in this area is also included.

Chapter 2 details the downdraft gasifier used in the experimental part of this project. The experimental methods used to collect data and calibrate instruments are also discussed.

Chapter 3 describes the development of the mathematical models. The model predictions are then compared to previously published experimental data.

Chapter 4 contains the experimental data collected operating a downdraft gasifier using different bed lengths, fuels and air flow rates.

In Chapter 5 the experimental data from Chapter 4 is analysed and compared with the model predictions from Chapter 3.

Chapter 6 contains a discussion and the overall conclusions of this work.

The three appendices contain calculations of the "real gas" correction to the ideal gas law assumed in the model, the formulae used to calculate the equilibrium constants of the chemical reactions at different temperatures, and MATLAB scripts implementing the models developed in Chapter 3.

2. Experimental Apparatus

The downdraft gasifier used for our experimental measurements was originally designed and built by Richard Sime (1998). As we were not planning to run the gasifier at high pressures some minor modifications were made; the fuel feed port at the top of the gasifier and the gas exit pipe were widened. The major modification was the addition of a burner unit for automating the start-up process. This is discussed in further detail in Section 2.1 below.

Figure 2.1 shows a schematic diagram of the downdraft gasifier used:

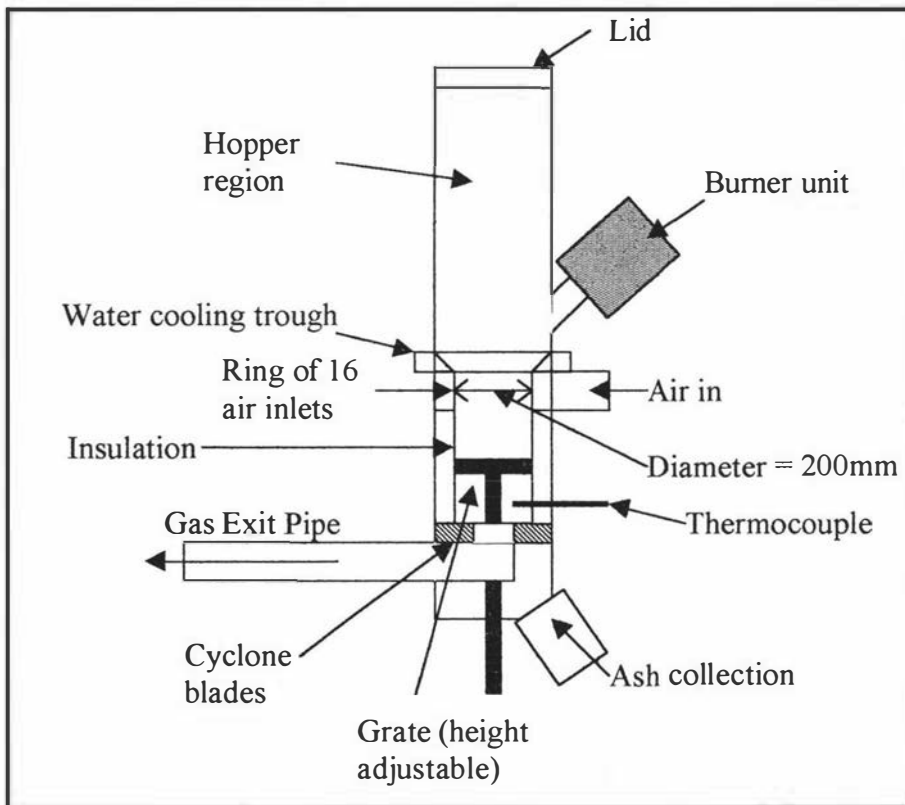


Figure 2.1: Downdraft gasifier configuration

2.1 Gasifier Ignition System

The biggest alteration to the gasifier was the addition of an ignition system. Sime (1998) ignited the gasifier by inserting an oxygen/propane torch into a small opening in the side of the gasifier. However, this did not always produce ignition across the entire cross-section of the bed, particularly when fuels with high moisture content were used.

The new ignition system involved mounting a Nu-Way NG2 burner unit on the side of the gasifier. The Nu-Way burner ran on LPG and had built-in safety features¹ to reduce the risk of explosive concentrations of LPG and air accumulating. The burner unit was mounted at an angle on the side of the gasifier so that the pilot flame would pass through the centre of the ring of air inlets.

The burner unit needed protection from the tars and smoke produced within the gasifier during operation. In a commercial gasifier this could have been achieved by having a sliding plate physically isolate the burner unit from the gasification chamber once ignition had been achieved. However, for safety reasons, a sensor system would have been required to prevent the burner unit from starting up while the plate was closed. This was considered too expensive for our purposes.

The burner unit was altered so that it could also operate as a fan in addition to its normal burner mode. The initial plan was to run the burner unit as a fan once ignition had occurred. The air from the fan would keep smoke from travelling back through the burner unit and would double as the air supply for the gasifier.

A test run of this system was performed using pine chips. The outside of the gasifier was continuously water-cooled to prevent the burner unit from over-heating (the burner unit was attached to the gasifier above the original combustion zone where there was less insulation). Smoke soon emerged from the exhaust pipe indicating that ignition occurred. However, the product gas remained smoky throughout the entire run, indicating that the pyrolysis products were not being cracked (when the gasifier is

¹ A 30 s fan cycle prior to attempting ignition and an automatic shut down if flame failure was detected.

running successfully the product gas should be almost colourless). The most likely reason for this was that the asymmetry of the air supply meant that the bed was hotter on the side close to the burner unit where combustion was occurring vigorously and cooler at the opposite wall. This left a pathway through which pyrolysis products could travel without reaching temperatures high enough to cause cracking. When the interior of the gasifier was inspected after the run a small amount of char remained on the grate on the side opposite the burner unit.

In the following trial we connected a vacuum cleaner (set to blow) to the original air inlet to be run in conjunction with the burner fan. The original air inlet distributed the air through a ring of sixteen holes evenly spaced around the inner circumference of the gasifier so that there was sufficient oxygen to support combustion across the entire cross-section of the bed. The bed was ignited using the burner unit as before. Once ignition had been achieved the burner unit was switched to fan only mode and the vacuum cleaner started. The speed of the burner fan was controlled using a Variac variable transformer connected to the power supply of the burner unit. However, twenty minutes into the run smoke began to blow back through the burner unit. This could not be reliably prevented by adjusting the fan speed and/or cutting off the air from the vacuum cleaner so we had to physically remove the burner to prevent damage from tars condensing inside the unit.

Future runs were started using the burner unit to ignite the bed. However, once ignition had been established the burner unit was removed from the gasifier, the burner port sealed and a vacuum cleaner (set to blow) connected to the original air inlet. A Variac variable transformer attached to the power supply of the vacuum cleaner was used to vary the flow rate of air into the gasifier. This method led to successful gasification runs the results of which are discussed in Chapter 4.

The pine chips used in the main gasifier runs had been in storage for several years. An attempt was made to gasify pine chips that had been cut within a couple of weeks of the run. The burner unit could initially ignite the fuel but combustion could not be sustained without the burner. The moisture content of the fuel was over 130% by weight (dry basis). After a couple of attempts the fuel was inspected. Some of the fuel had charred

but there was a significant amount of fuel that appeared unchanged. A sample of the remaining fuel containing a mixture of charred and uncharred pieces was measured to have a moisture content of 110% by weight (dry basis). Running the burner may have dried the fuel a little but it was still insufficiently dry to gasify.

A second attempt was made with the gasifier filled with 18.7% moisture content pine chips to above the level of the air inlets and the rest of the gasifier filled with the wet pine chips so that the gasification reactions could get well established on the drier chips before the wet fuel moved into the combustion region. This run started well with some CO production noticed in the early phases, but gas production died off part-way through the run. Inspection of the hopper afterwards showed that there was still a large amount of unburnt fuel remaining. The most likely explanation was that gas production stopped when the gasifier started having to burn the wet fuel.

2.2 Transducers and Calibration

Conditions inside the gasifier are very hot and dirty making it unsuitable for many types of transducers. Electronic transducers capable of withstanding these conditions were expensive. Therefore we decided to limit the measurements taken to those that could be taken using readily available transducers.

(A) Temperature

The exit gas temperature was measured using an N-type thermocouple inserted into the exit gas stream. The thermocouple was connected to a miniPOD data logger that recorded the thermocouple voltage every 2 seconds. The reference temperature used was ambient temperature rather than 0°C. This meant that the results could be affected by variations in the ambient temperature from day to day but with exit temperatures in excess of 900 K variations of the order of a few degrees would not introduce significant errors.

Figure 2.2 shows the thermocouple voltage measured compared with the temperature of an electric furnace. The equation of the line of least squares shown was used to calculate the exit gas temperature from the thermocouple voltage for temperatures greater than 300°C.

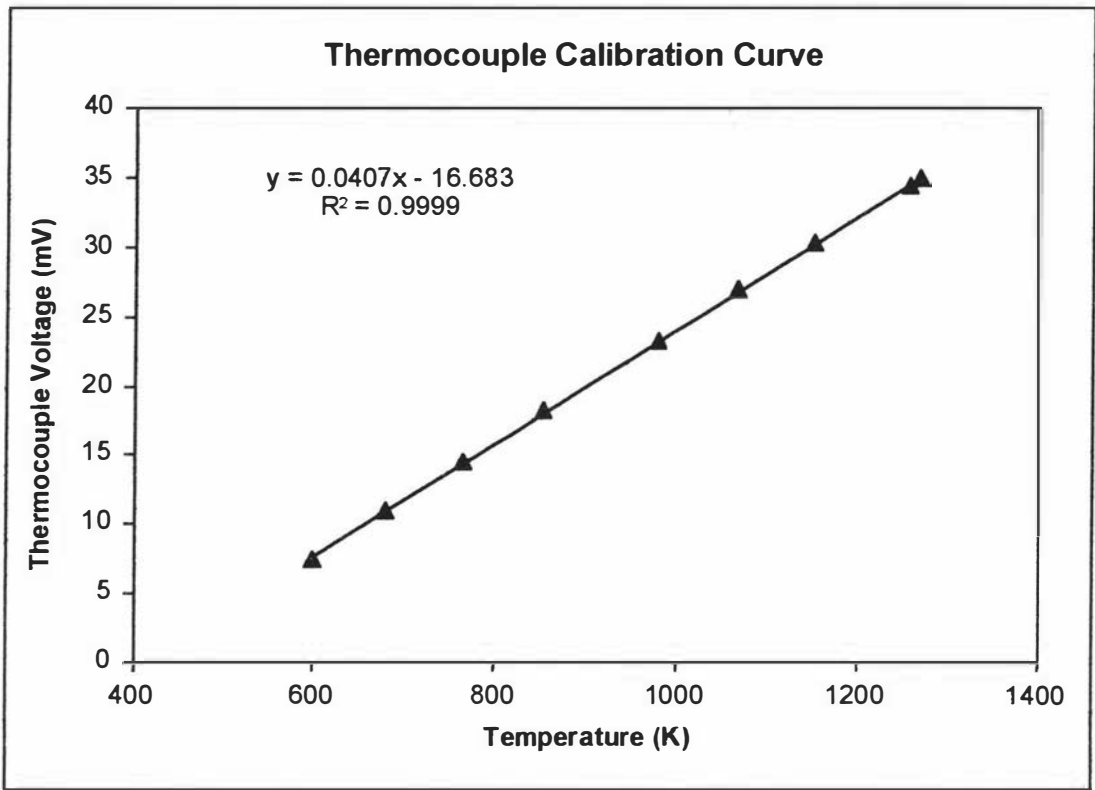


Figure 2.2: Calibration of N-type thermocouple used in experiments.

(B) Inlet Air Flow Rate

The gasifier air supply was pumped into the air inlet by a vacuum cleaner set to blow. The air flow rate was controlled by attaching a Variac variable transformer to the vacuum cleaner power supply. The volume flow rate of air from the vacuum cleaner at different Variac settings was found by measuring the time taken to inflate a long (>20 m) plastic tube of known volume. The results are plotted in Figure 2.3.

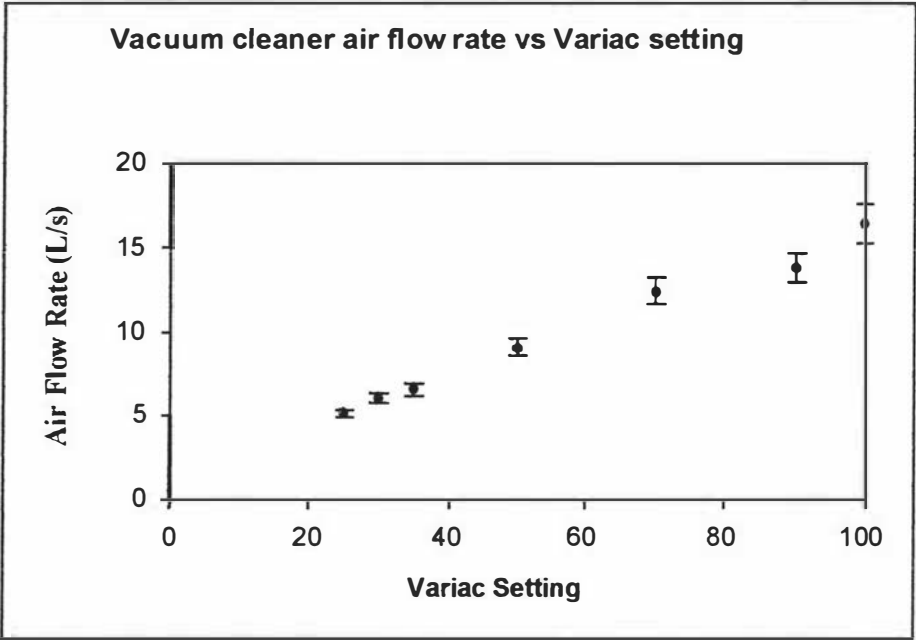


Figure 2.3: Volume flow rate of air out of vacuum cleaner vs the setting of the Variac variable transformer attached to the vacuum cleaner power supply.

So the volume flow rate of air out of the vacuum cleaner for a given Variac setting was known when the vacuum cleaner was working against atmospheric pressure. However, when connected to an operating gasifier the vacuum cleaner works against a back pressure from the gases inside the gasifier. The actual volume output of the vacuum cleaner can be determined by measuring the air speed at the vacuum cleaner air inlet. We used a Testovent 4000 rotating-fan digital anemometer to measure the air speed at the vacuum cleaner inlet at the Variac settings for which the volume flow rates had been calculated. Figure 2.4 below shows the relationship between the air speed at the vacuum cleaner air inlet plotted against the output volume flow rate of the vacuum cleaner.

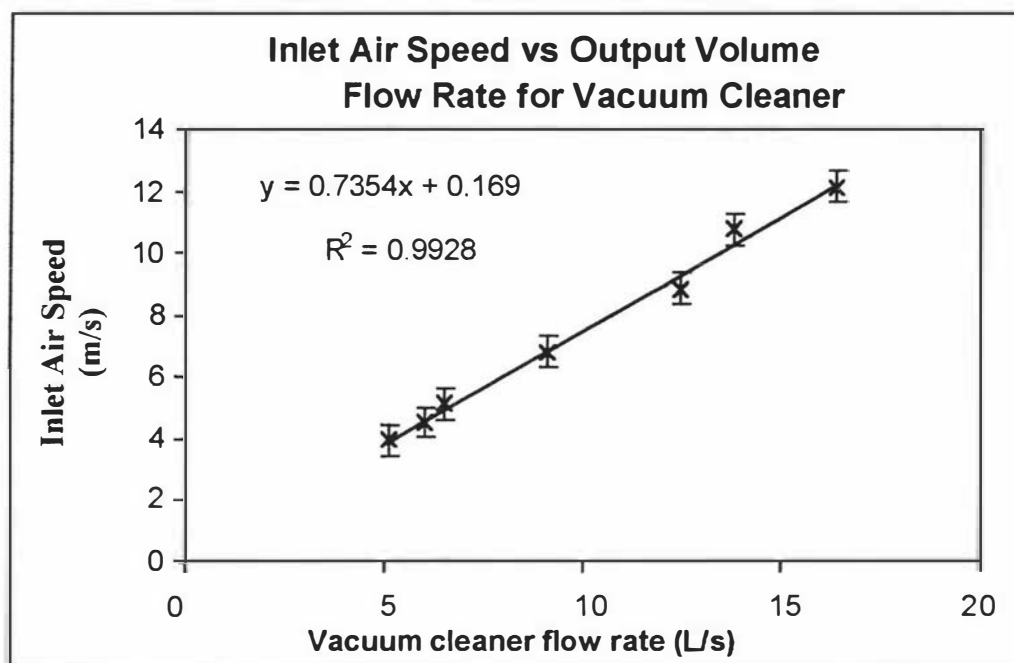


Figure 2.4: Air speed at vacuum cleaner inlet vs. the volume flow rate output of the vacuum cleaner.

Unfortunately the anemometer was not available for every gasifier run, so we took a series of readings of the vacuum cleaner inlet air speed as the Variac setting was varied with the vacuum cleaner connected to an operating gasifier. The relationship between vacuum cleaner inlet air speed and output flow rate from Fig. 2.4 was then used to calculate the output flow rate produced by the vacuum cleaner when working against the back pressure from the gasifier. Figure 2.5 shows the volume flow rates produced by the vacuum cleaner connected to an operating gasifier for given Variac settings compared to the volume flow rates produced when the vacuum cleaner is only working against atmospheric pressure.

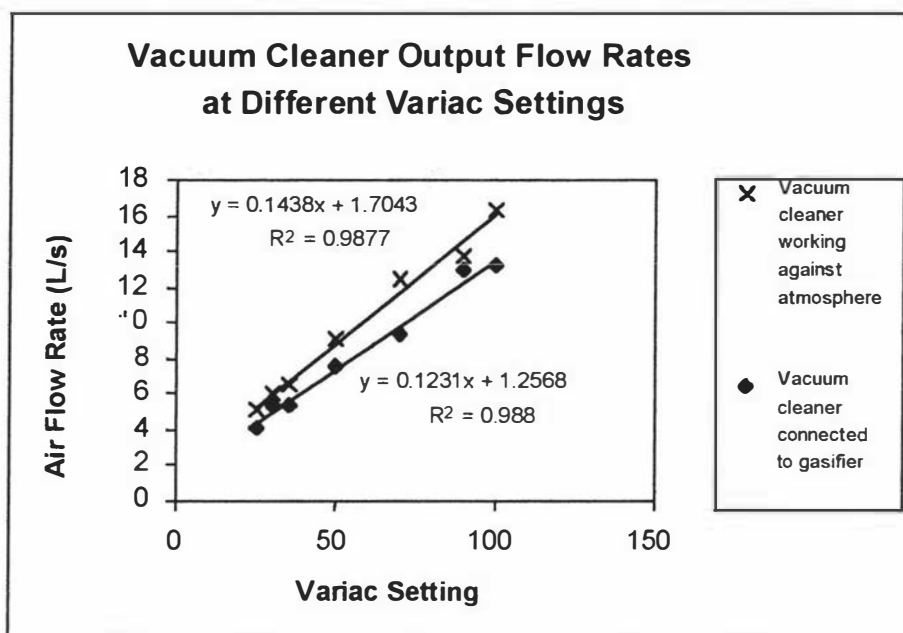


Figure 2.5: Air flow rate produced by vacuum cleaner at different Variac settings when operating against atmospheric pressure and when connected to an operating gasifier. Volume flow rates are assumed to be at standard temperature and pressure.

The output flow rate of the vacuum cleaner was noticeably reduced when it was working against back pressure from an operating gasifier. In later experiments we assumed that the output flow rate of the vacuum cleaner at a given Variac setting was the same as that found in Figure 2.5 for the vacuum cleaner connected to an operating gasifier. The back pressure produced within the gasifier will vary between runs and within a single run, but we assumed that the effect of such variations on the vacuum cleaner output was less than the effect of the vacuum cleaner being connected to an operating gasifier compared to working against atmospheric pressure only. So the difference between the two plots in Figure 2.5 formed an upper bound on the uncertainty in the volume flow rate produced by the vacuum cleaner.

(C) Exit Gas Flow Rate

The gas exited the gasifier at about 700°C and sometimes contained tars and entrained particles. Therefore it was decided to use a simple Venturi meter to measure the exit gas flow rate rather than risk damaging sensitive electronic equipment.

A Venturi meter is a device for measuring the rate of fluid flow within a pipe by measuring the pressure difference between the regions of different cross-sectional area within the pipe. The work done moving a volume V of gas between two points equals the difference in the total mechanical energy of the gas at the two points. If both points are at the same height this gives:

$$(2.1) \quad \Delta PV = \frac{1}{2}m_2v_2^2 - \frac{1}{2}m_1v_1^2$$

where ΔP is the pressure difference between the two points,
 m_i is the mass of gas in volume V at point i , and
 v_i is the velocity of the gas at point i .

Dividing by V gives:

$$(2.2) \quad \Delta P = \frac{1}{2}\rho_2v_2^2 - \frac{1}{2}\rho_1v_1^2$$

where ρ_i is the mass density of the gas at position i .

The gas velocity, v , is related to the volume flow rate, U , by the following relationship:

$$(2.3) \quad U = vA$$

where A is the cross-sectional area of the pipe.

In order to keep the total mass flow constant we must have:

$$(2.4) \quad \rho_1U_1 = \rho_2U_2$$

Therefore Equation 2.2 can be rewritten as:

$$(2.5) \quad \Delta P = \frac{1}{2} \left((\rho_1 + \Delta\rho) \left(\frac{U_1\rho_1}{(\rho_1 + \Delta\rho)A_2} \right)^2 - \rho_1 \frac{U_1^2}{A_1^2} \right)$$

Rearranging gives:

$$(2.5) \quad \Delta P = \frac{1}{2} \rho_1 U_1^2 \left(\frac{\rho_1}{(\rho_1 + \Delta \rho)} \cdot \frac{1}{A_2^2} - \frac{1}{A_1^2} \right)$$

Therefore the pressure difference between a point in the unstricted part of the pipe and a point within the constricted region depends upon the square of the volume flow rate of the gas.

A 40 mm diameter constriction was placed in the ~60 mm diameter exit pipe. The pressure difference between the constricted and unstricted regions was measured using a water manometer with one arm that could be set at an angle.

From Equation 2.5 the pressure difference measured depends upon the density of the gas in addition to the volume flow rate. The density of the gas depends upon its composition and is inversely proportional to temperature. Therefore pressure difference across the constriction should be proportional to V^2/T if the gas composition is kept constant.

The relationship between the volume flow rate and the pressure drop across the constriction was tested using the digital anemometer to measure the air speed and temperature of a hairdryer with different heat and fan speed settings while the pressure drop across the constriction was measured with the water manometer. The volume flow rate was calculated by multiplying the measured air velocity by the unstricted cross-sectional area of the pipe.

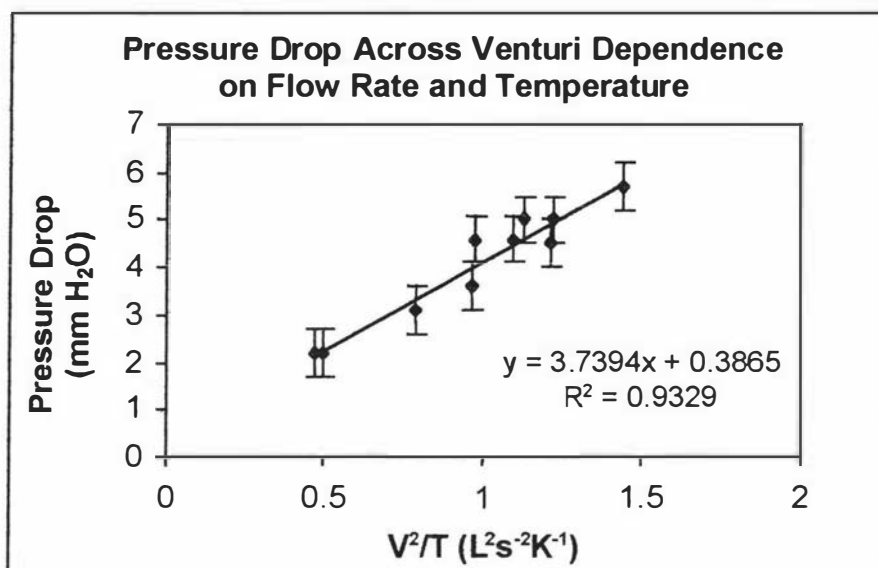


Figure 2.6: Pressure drop across the Venturi constriction plotted as a function of volume flow rate and temperature. The line of least squares is shown.

Figure 2.6 shows that the pressure drop across the Venturi constriction is a linear function of V^2/T . The data points had temperatures ranging from 300 to 375 K and volume flow rates ranging from 12.6 to 22.7 L/s. The exit gas temperatures of an operating gasifier are significantly higher than those used in this calibration, but we assumed that the relationship found in Figure 2.6 holds. Air was used in the calibration runs but the gas produced by an operating gasifier will vary in its composition. However, the density of a typical producer gas is close to that of air at the same temperature.

(D) Pressure Gradient across bed

The pressure gradient across the bed was measured using a water manometer with one side connected to the gasifier above the air inlets and one end connected to the gasifier beneath the grate level. It was assumed that there was negligible pressure drop in the gasifier bed above the air inlets or in the region below the grate.

The burner unit was operated in fan mode to provide the air flow through the bed. A Variac variable transformer was attached to the power supply of the burner unit. The volume flow rate of the fan was adjusted using the Variac to alter the power supplied to

the unit. The volume flow rate of the fan at a given power setting had been measured using the same method used to calculate the air flow rate of the vacuum cleaner in Section 2.2(C) above. The volume flow rate was converted to a superficial gas velocity by dividing it by the cross-sectional area of the gasifier.

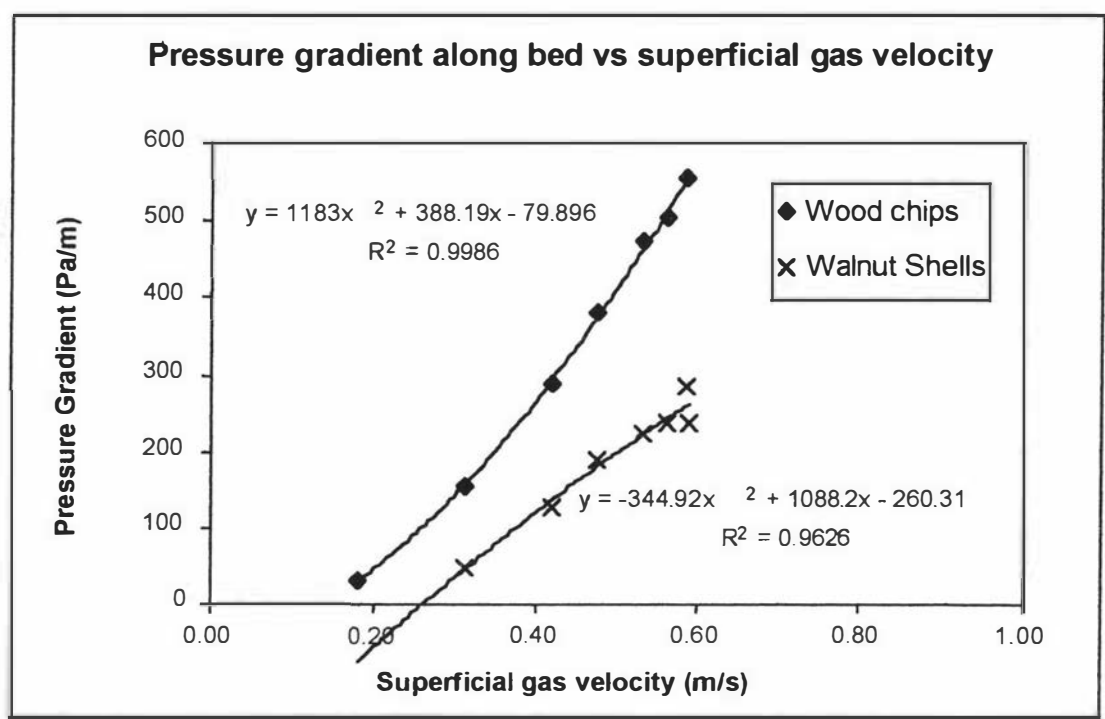


Figure 2.7: Pressure gradient (going up the bed) as a function of superficial gas velocity for gasifier beds of wood chips and walnut shells. A quadratic fit is shown.

Figure 2.7 shows the pressure gradient measured up the gasifier bed as a function of superficial gas velocity for a bed of wood chips and one of walnut shells. The quadratic equations found by the method of least squares were used to provide the relationship between dP/dz and v for the model in Chapter 3. In practice, the gasifier bed composition will be non-uniform with fresh fuel in the hopper region and char particles of decreasing size beneath the combustion zone.

(E) Fuel Moisture Content

The moisture content of the fuel was measured by heating the fuel at above 100°C and measuring the change in mass. The sample was repeatedly heated and reweighed until

consecutive measurements varied by less than 0.1%. The moisture content of the wood chips was 18.7% and the moisture content of the walnut shells was 12.3%.

(F) CO detector

A portable carbon monoxide (CO) detector was used around the gasifier to ensure that toxic levels of CO did not accumulate. Detecting high level of ambient CO was a sign that the gasifier exhaust should be ignited. If the exhaust could not be ignited in a reasonable time period then the gasifier was shut down.

2.3 Gas Collection and Analysis

(A) Gas Sampling

Gas samples were taken from the exit pipe, run through a copper cooling coil immersed in cold water then collected using a 60 mL syringe with stop-cock attachment. The aim of the copper coils was to cool the gas so that the syringes would not be damaged and to condense out any tars and water vapour (which the gas chromatograph was unable to separate).

(B) Gas Chromatograph

The gas samples were analysed using a Shimadzu GC-8A gas chromatograph with a thermal conductivity detector (TCD) using helium as a carrier gas. The column was a silica gel packed column capable of separating H_2 , CO, CH_4 , and CO_2 but could not separate O_2 from N_2 . Some earlier samples were analysed using an Alltech CTRI column that could separate N_2 from O_2 but could not detect H_2 .

To find out how long a sample could be kept in the syringe some samples were analysed at different time intervals to see how the composition changed with time. H_2 was the smallest of the molecules in the mixture and therefore the most likely to leak out. Ideally samples would be analysed either "inline" or immediately after collection. However, the times that the gasifier and gas chromatograph could be used meant that there was usually a 24-hour delay between collection and analysis of samples.

We expected that the rate of H₂ loss from the syringe would be proportional to the amount of H₂ within the syringe. This would give an exponential decay in the H₂ concentration over time. Because several different samples were used, the H₂ concentrations were normalised relative to the H₂ concentration detected on Day 1 (the time of the sample collection was Day 0).

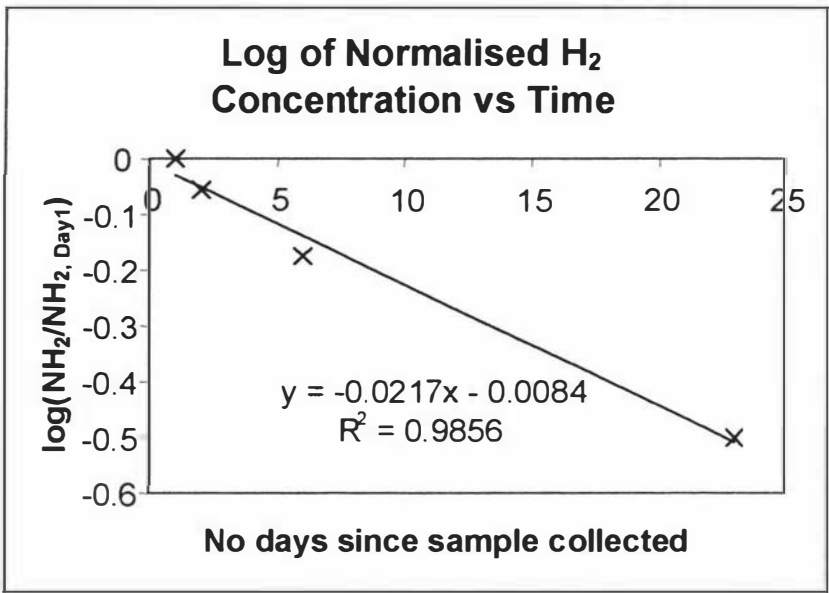


Figure 2.8: Log of the H₂ remaining in sample (relative to concentration 1 day after collection) vs time.

Figure 2.8 shows the log of the normalised H₂ concentrations plotted against time. The data lies approximately on a straight line. The intercept of the line is equal to the log of the ratio of the hydrogen concentration on Day 0 to the hydrogen concentration on Day 1. If the H₂ concentration on Day 1 were exactly the same as Day 0 then the ratio of the H₂ concentrations would be one and taking the log would give zero. The y-intercept of the best-fit line was -0.01 ± 0.02 . As zero is included within this range we can assume that there was only a small amount of H₂ lost during the 24-hour period between collection and analysis.

3. Steady State and Time Dependent Models

Most published models of downdraft gasification have been empirical descriptions of the performance of a specific gasifier (e.g. Chee 1987). Our aim was to develop a model that could be used to predict the performance of any downdraft gasifier, given certain operating parameters, based on the physical and chemical processes occurring. However, the values of some of the parameters introduced were set using data from previously published experiments.

Wang and Kinoshita (1993) modelled the kinetics of the reactions occurring in the reduction zone of a gasifier assuming a given gas residence time and temperature. They considered the following set of reactions and determined values for the kinetic parameters that gave the best agreement with earlier experimental results (Wang and Kinoshita, 1992).

Reaction 1: $C + CO_2 \leftrightarrow 2CO$

Reaction 2: $C + H_2O \leftrightarrow CO + H_2$

Reaction 3: $C + 2H_2 \leftrightarrow CH_4$

Reaction 4: $CH_4 + H_2O \leftrightarrow CO + 3H_2$

Wang and Kinoshita (1993) also considered the water-gas shift reaction ($CO + H_2O \leftrightarrow CO_2 + H_2$) but found that it had little effect on the final result.

Their model was physically similar to a well-mixed fluidised bed. However in a downdraft gasifier the gas travels down the bed as it reacts, so there is one-dimensional variation in the gas temperature and composition.

We used the reaction kinetics parameters found by Wang and Kinoshita to build models of the gas composition and temperature within a downdraft gasifier.

3.1 1-Dimensional Steady-State Model

Several simplifying assumptions were made to develop the first model. The gasifier was assumed to have no variation in the radial direction and to be in a steady state with respect to time. Heat transfer between the gaseous and solid phases was also neglected.

The pyrolysis and cracking reactions introduce a large number of intermediate chemical species and reactions that could be present. Rather than try to account for all of these reactions we restricted our model to the region of the gasifier beneath the pyrolysis and combustion zones and considered only Reactions 1 to 4 listed above. The pyrolysis, combustion and cracking reactions were treated as a source of initial CO, CO₂, CH₄ and H₂O.

We assumed that there was always a plentiful supply of carbon from the fuel, so the chemical species that needed to be tracked were CO₂, CO, CH₄, H₂O and H₂. N₂ from the inlet air was also tracked. Although N₂ does not participate in any of the reactions considered, it does "dilute" the final product gas.

(A) Reaction Rates

According to Graboski (1981) at typical gasifier temperatures the reaction rates within the gasifier will be limited by pore diffusion rather than the surface reaction kinetics. However, the relative rates of the different chemical reactions are important in determining the relative amounts of each chemical species in the product gas. We therefore determined the reaction rates using reaction kinetics and assumed that pore diffusion would affect the rates of all reactions equally. The reaction rate equations included a constant pre-multiplier that could be altered to account for differences in char reactivity, pore diffusion and other factors.

The reaction rates were all considered to have an Arrhenius-type temperature dependence and to be proportional to the difference between the actual reactant/product ratio and the corresponding equilibrium ratio. Thus we obtained:

$$(3.1) \quad r_1 = A_1 \exp\left(\frac{-E_1}{RT}\right) \left(P_{CO_2} - \frac{P_{CO}^2}{K_1} \right)$$

$$(3.2) \quad r_2 = A_2 \exp\left(\frac{-E_2}{RT}\right) \left(P_{H_2O} - \frac{P_{CO} P_{H_2}}{K_2} \right)$$

$$(3.3) \quad r_3 = A_3 \exp\left(\frac{-E_3}{RT}\right) \left(P_{H_2}^2 - \frac{P_{CH_4}}{K_3} \right)$$

$$(3.4) \quad r_4 = A_4 \exp\left(\frac{-E_4}{RT}\right) \left(P_{CH_4} P_{H_2O} - \frac{P_{CO} P_{H_2}^3}{K_4} \right)$$

where r_i is the rate of reaction i in $\text{mol.m}^{-3}.\text{s}^{-1}$

A_i is the frequency factor for reaction i ,

E_i is the activation energy of reaction i in J.mol^{-1} ,

R is the gas constant in $\text{J.mol}^{-1}.\text{K}^{-1}$,

T is the temperature in K,

P_x is the partial pressure of gaseous species x , and

K_i is the equilibrium constant of reaction i .

The values for the activation energies for these reactions were taken from Wang and Kinoshita (1993). However, we had incorporated several factors into our constant pre-multipliers, such as char particle size and number of active carbon sites, that were considered separately by Wang and Kinoshita. So to calculate our frequency factors we multiplied the values found by Wang and Kinoshita by a "Char Reactivity Factor" (C_{RF}), that represents the relative reactivity of different char types. That is, we used $A_i = A'_i \cdot C_{RF}$ where A'_i is the value found by Wang and Kinoshita.

The equilibrium constants K_i were temperature dependent and were calculated from tabulated values of $\log_{10}K$ (Barin, 1993). These calculations are included in Appendix B.

(B) Mass and Energy Balances

We assumed a cylindrical gasifier bed of uniform cross-sectional area A with negligible radial variation in the properties of both the bed and the gas. The axial distance was z . The gases were assumed to behave ideally. We then considered thin cross-sections of thickness Δz . For each chemical species in the gas, the change in the molar flow rate across Δz must equal the net rate of creation of species by chemical reactions within the volume. Therefore for small Δz we obtained:

$$(3.5) \quad n_x(z)Av(z) = n_x(z + \Delta z)Av(z + \Delta z) + R_x A \Delta z$$

where n_x is the molar density of species x in mol.m^{-3} ,
 v is the superficial gas velocity in m.s^{-1} , and
 R_x is the net rate of formation of species x by chemical reactions in
 $\text{mol.m}^{-3}.\text{s}^{-1}$.

Equation 3.5 can be used to generate expressions for the molar concentrations of each of the six gaseous species considered (CO_2 , CO , H_2O , H_2 , CH_4 , N_2). Similarly the total molar density of all gases, n , can be expressed as the sum of the molar densities of each of the six component gases. Table 3.1 gives the net rates of formation of each gas species in terms of the reaction rates of Reactions 1- 4.

Species	$R_x (\text{mol.m}^3.\text{s}^{-1})$
N_2	0
CO_2	$-r_1$
CO	$2r_1 + r_2 + r_4$
CH_4	$r_3 - r_4$
H_2O	$-r_2 - r_4$
H_2	$r_2 - 2r_3 + 3r_4$
Total number of gas molecules	$r_1 + r_2 - r_3 + 2r_4$

Table 3.1: Net rate of production of the different gaseous species by chemical reactions in terms of the rates of Reactions 1 - 4.

Rearranging Equation 3.5 and taking the limit as $\Delta z \rightarrow 0$ gave:

$$(3.6) \quad \frac{d(n_x v)}{dz} = R_x$$

or

$$(3.7) \quad \frac{dn_x}{dz} = \frac{1}{v} \left(R_x - n_x \frac{dv}{dz} \right)$$

Similarly, for steady-state operation, any change in the energy flow rate over distance Δz must be equal to the rate of energy released by reactions within the volume minus the rate of work done by the gas. This neglects changes in the kinetic and gravitational

potential energy of the gas which were relatively insignificant. The thermal energy of N moles of gas species x is Nc_xT where c_x is the molar heat capacity of the gas in $\text{J.K}^{-1}.\text{mol}^{-1}$. For a chemical reaction the change in enthalpy ΔH in J.mol^{-1} represents the change in the internal chemical energy of the system due to the reaction. Thus the rate of energy released due to chemical reactions is $-\sum_i r_i \Delta H_i$ where i ranges over all the reactions being considered.

The change in enthalpy and molar heat capacities at standard pressure and temperature from Aylward and Findlay (1974) were used. The temperature dependence of these values was neglected.

Thus from the energy balance we obtained the following relation:

$$(3.8) \quad v_{z+\Delta z} A \left(\sum_x n_x c_x T \right)_{z+\Delta z} - v_z A \left(\sum_x n_x c_x T \right)_z = - \sum_i r_i \Delta H_i A \Delta z - \Delta(PAv)$$

where P is the total pressure in Pa,

the subscript x ranges over all chemical species and

the subscript i ranges over all chemical reactions under consideration.

Dividing by $A\Delta z$ and taking the limit as $\Delta z \rightarrow 0$ gave:

$$(3.9) \quad \frac{d(v \sum_x n_x c_x T)}{dz} = - \sum_i r_i \Delta H_i - \frac{d(Pv)}{dz}$$

Rearranging we obtained:

$$(3.10) \quad \frac{dT}{dz} = \frac{1}{v \sum_x n_x c_x} \left(- \sum_i r_i \Delta H_i - v \frac{dP}{dz} - P \frac{dv}{dz} - \sum_x R_x c_x T \right)$$

Equations 3.7 and 3.10 gave a total of seven differential equations when all six gaseous species were considered. However, the state of the gasifier at any given point is described by the concentration of each gas species, the temperature, the superficial gas

velocity and the total pressure. So to complete our system of differential equations we still needed expressions for dP/dz and dv/dz .

The pressure gradient, dP/dz , is known to depend upon the superficial gas velocity. The following empirical formula relates the pressure gradient of a fluid flowing through a bed of solid particles to the physical properties of the bed and the fluid (Rhodes, 1998):

$$(3.11) \quad -\frac{dP}{dz} = \frac{150\mu(1-\varepsilon)^2}{D_p^2 \varepsilon^3} v + \frac{1.75\rho(1-\varepsilon)}{D_p \varepsilon^3} v^2$$

where μ is the fluid viscosity,

ε is the void fraction of the bed,

D_p is the average particle diameter in the bed and

ρ is the mass density of the fluid.

However, we found coefficients for v and v^2 empirically in Chapter 2 by measuring the pressure drop across a bed of pine chips of fixed length at room temperature over a range of different air speeds. We used these coefficients in our expression for dP/dz throughout the gasifier, although the bed of an operating downdraft gasifier will vary in composition from fresh fuel at the top to smaller char particles just above the grate.

To get an expression for dv/dz we took the ideal gas law:

$$(3.12) \quad P = nRT$$

where n is the molar concentration of all gaseous species (in mol.m^{-3}),

P is the total pressure (in Pa),

R is the gas constant in ($\text{J.mol}^{-1}.\text{K}^{-1}$), and

T is the absolute temperature (in K).

The ideal gas law is an approximation where it is assumed that the gas molecules are sufficiently far apart that the size of the molecules can be neglected and that the intermolecular forces are insignificant. This approximation works well for gases at high temperature and low pressure, but less well for gases that are near condensation.

Appendix A contains calculations of the correction terms to the ideal gas equation for the gases considered in the model at typical gasification temperatures and pressures. In all cases the correction term made less than 1% difference.

Differentiating Equation 3.12 with respect to z gave:

$$(3.13) \quad \frac{dP}{dz} = \frac{dn}{dz}RT + nR \frac{dT}{dz}$$

An expression for dn/dz was found by summing the expressions for dn_x/dz from Equation 3.7 for each gaseous species x . This gave us expressions for dn/dz and dT/dz that depended upon dv/dz . We substituted Equations 3.7 and 3.10 into 3.13 and rearranged to get:

$$(3.14) \quad \frac{dv}{dz} = \frac{1}{\sum_x n_x c_x + nR} \left(\frac{\sum_x n_x c_x \sum_x R_x}{n} - \frac{\sum_i r_i \Delta H_i}{T} - \frac{dP}{dz} \left(\frac{v}{T} + \frac{v \sum_x n_x c_x}{P} \right) - \sum_x R_x c_x \right)$$

This gave us a set of nine coupled first-order ordinary differential equations in the system variables n_x (where x ranges over the six different gas species considered), P , v and T , that can be solved using commercially-available computer software. We used the ODE45 function in MATLAB. Appendix C contains the MATLAB scripts used to run this model.

(C) Model Sensitivity to Initial Conditions

The computer model required initial values for the temperature, pressure, superficial gas velocity and gas composition within the gasifier. To find out the degree to which the initial values selected affected the results we ran a series of simulations varying one factor at a time. Table 3.2 below shows the base values used for the parameters when they were not being varied.

	Value
Temperature	1200 K
Pressure	101 300 Pa
Velocity	1 m.s ⁻¹
Gas composition (Mol %)	
CO ₂	10 %
CO	10 %
CH ₄	10 %
H ₂ O	10 %
H ₂	0 %
N ₂	The remainder
C_{RF}	500

Table 3.2: Initial values used in simulations to test the model sensitivity.

Varying Initial Temperature

The temperature at the top of the reduction zone depends upon factors such as the moisture content of the fuel and the air flow rate. Therefore the initial temperature is likely to vary for different fuel types.

The effects of different initial temperatures on the temperature profile and the higher heating value (HHV) of the dry product gas were plotted in Figures 3.1(A) and (B) respectively.

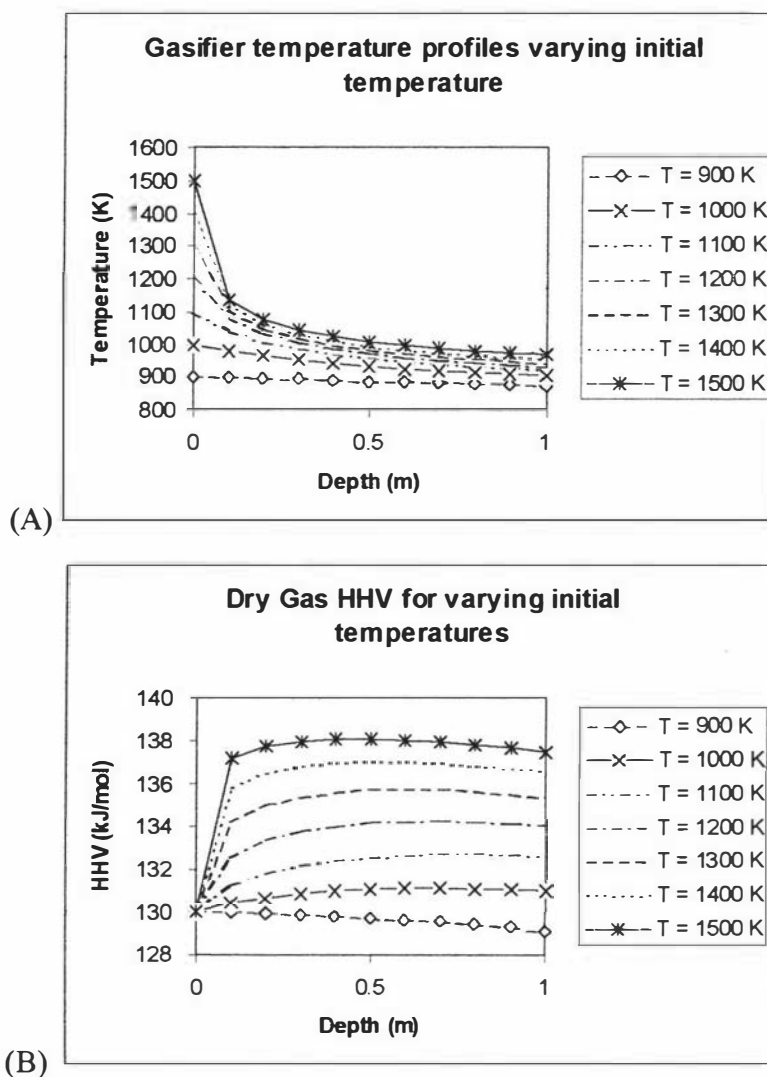


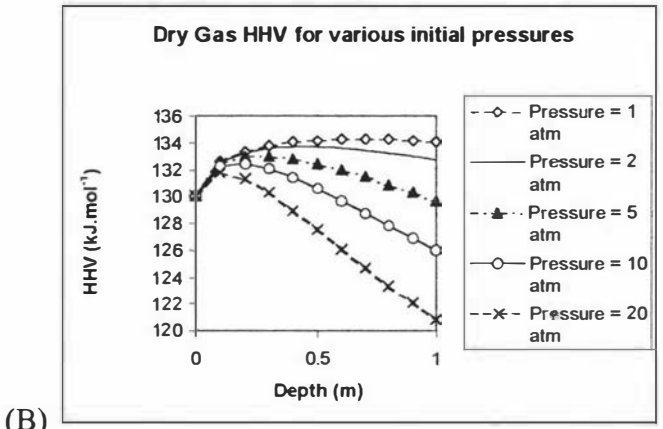
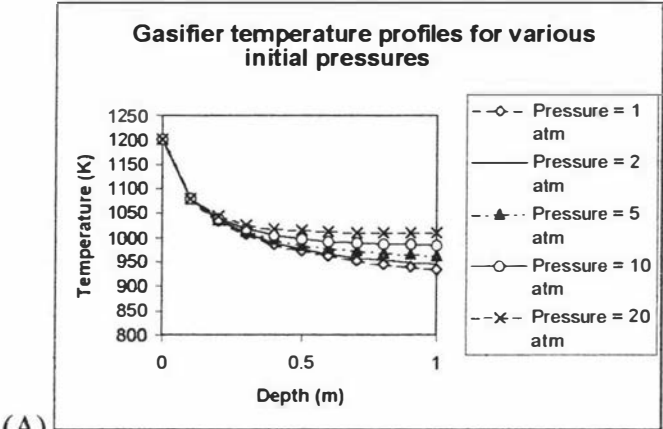
Figure 3.1: The effects of changing the temperature at the top of the reduction zone on (A) the temperature profile within the gasifier, and (B) the HHV of the dry gas.

Figure 3.1 (A) shows the steady state temperature profiles of the gasifier bed for different initial temperatures. There was a trend for the temperature to approach a stable temperature of approximately 900 K provided that the initial temperature was greater than 900 K.

The dry gas higher heating value (Figure 3.1(B)) tended to rapidly approach a maximum value then slowly deteriorate. Higher initial temperatures result in higher HHVs as the high temperature promotes the endothermic reduction reactions that produce CO and H₂. The overall variation in the gas heating values produced using initial temperatures ranging from 900 - 1500 K was about 8%.

Varying Initial Pressure

Sime (1998) proposed that the throughput of downdraft gasifiers could be improved by operating at high pressures. Figures 3.2 (A)-(C) show the effects of increasing the initial pressure on the gasifier temperature profile, dry gas HHV and molar flux of dry gas respectively. It has been assumed that the increase in pressure has not changed the values of any of the other parameters.



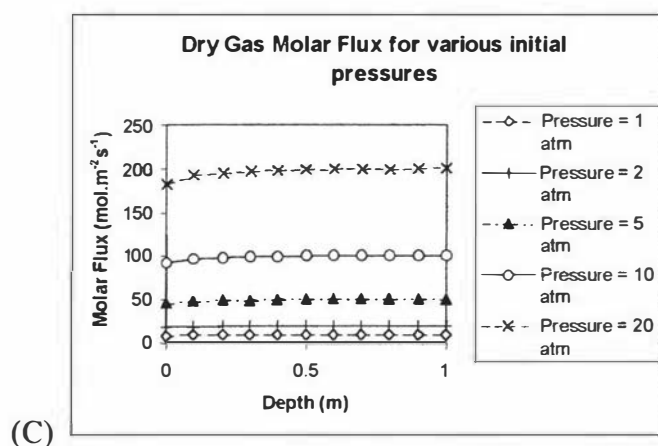


Figure 3.2: The effects of changing the initial pressure on (A) the gasifier temperature profile, (B) the dry gas HHV and (C) the molar flux of dry gas predicted.

An increase in pressure is expected to shift the equilibrium point of a reaction towards the direction that produces the smallest number of gaseous molecules. This means that the (forward) rates of Reactions 1, 2 and 4 would be expected to decrease with increasing pressure while the (forward) rate of Reaction 3 would increase. This was seen in the model predictions as a drop in the HHV of the dry gas produced at higher pressures due to a decrease in the rate of production of CO and H₂, and also by the fact that at high pressure the temperature levels off at a higher value as chemical equilibrium is achieved earlier.

However, the higher pressure did lead to a higher molar flux of dry gas out of the gasifier (Figure 3.2(C)). This increased rate of production meant that the rate of chemical energy exiting the gasifier was increased with increasing pressure even though the quality of the gas on a molar basis was poorer. Figure 3.2(B) also indicates that at high pressures using a shorter bed length will improve the HHV of the dry product gas.

Varying Initial Velocity and C_{RF}

The superficial gas velocity and the length of the gasifier bed determine the gas residence time within the bed. Figures 3.3 (A) and (B) show the model predictions for the gasifier temperature and dry gas HHV using different initial gas velocities.

Multiplying the superficial gas velocity by a factor of ten produced results almost equivalent to dividing the bed length by a factor of ten. The HHV of the dry product

gas reached an apparent maximum when the ratio $\frac{\text{Bed length}}{\text{Gas velocity}}$ was approximately 1 s.

The position of this maximum HHV depended on the C_{RF} , as a higher reactivity meant that more reactions occurred within a given residence time. It also depended upon the initial gas composition and temperature. Figures 3.4 (A) and (B) show the effects of varying the C_{RF} on the model predictions of temperature and dry gas HHV respectively.

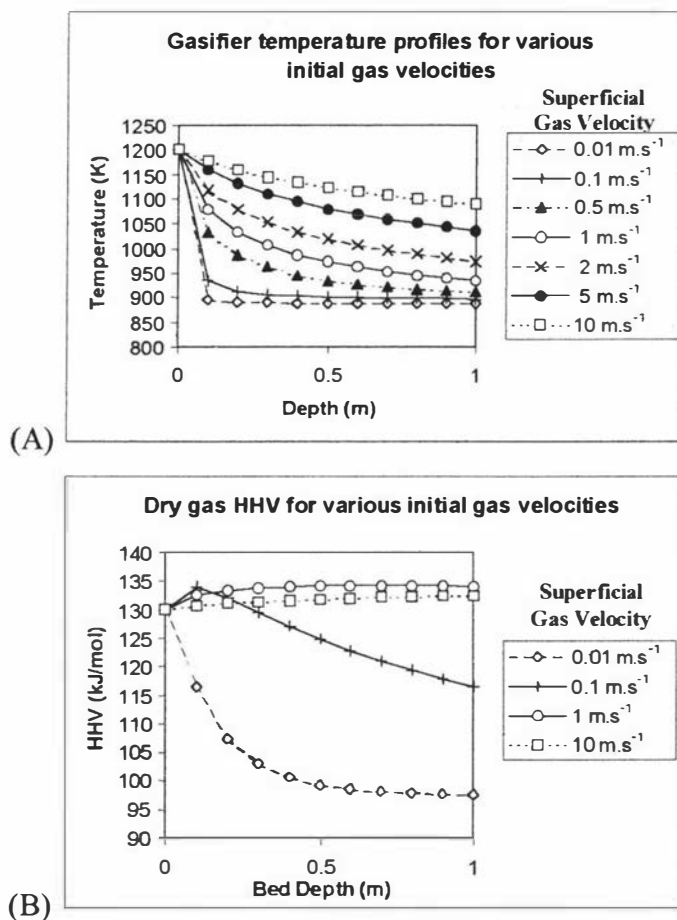


Figure 3.3: The effects of varying superficial gas velocity on (A) the gasifier temperature profile and (B) the dry gas HHV predicted.

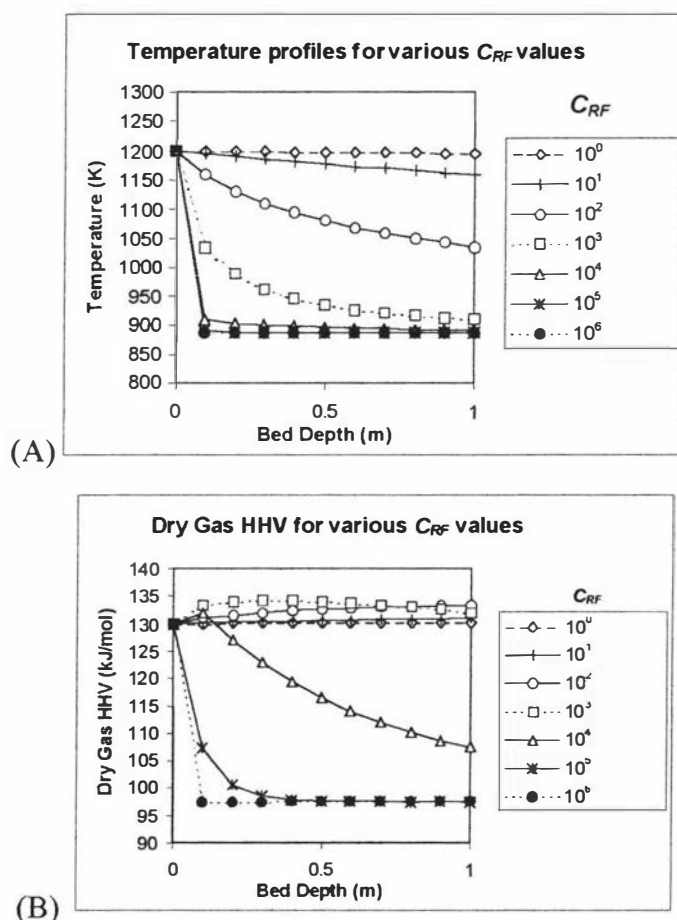


Figure 3.4: The effects of varying the C_{RF} on (A) the temperature profile of the reduction zone and (B) the dry gas HHV predicted.

Varying Initial CO_2

Figure 3.5 shows that increasing the initial amount of CO_2 in the gas resulted in an increased proportion of CO in the dry product gas (and hence a higher HHV product gas) and a lower temperature. This was due to the increased initial CO_2 increasing the initial rate of the endothermic Reaction 1.

CO_2 is initially formed in the gasifier by oxidation of the pyrolysis products. If air is used as the inlet gas then approximately four moles of N_2 will accompany every mole of O_2 into the system limiting the maximum CO_2 concentration possible. Higher initial CO_2 concentrations (which result in a higher HHV product gas) can be achieved by using pure oxygen or by adding extra CO_2 to the inlet gas.

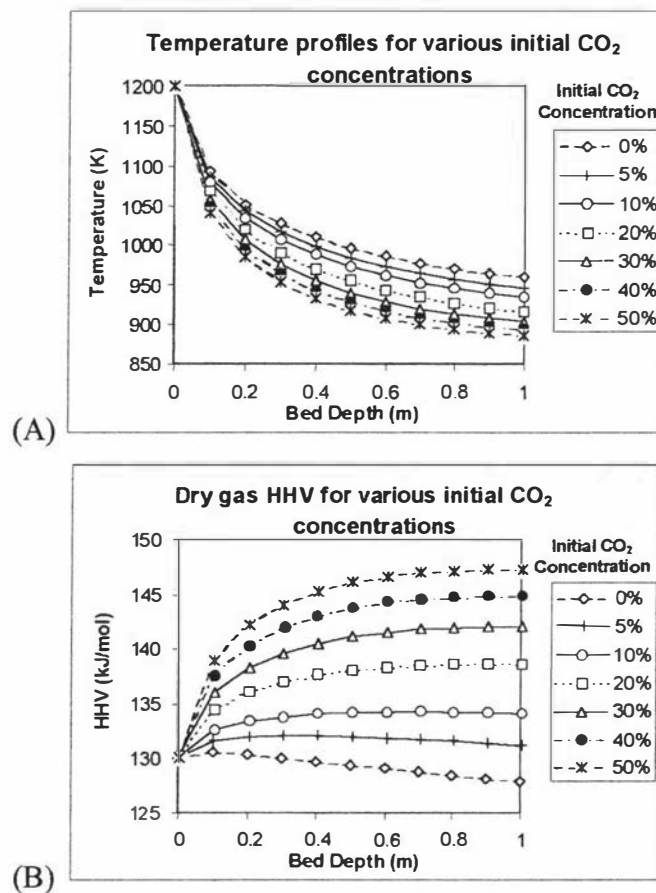


Figure 3.5: The effects of varying initial CO₂ concentration on (A) the temperature profile of the reduction zone and (B) the dry gas HHV predicted.

Varying Initial CO and CH₄

Both CO and CH₄ are combustible gases and therefore contribute directly to the HHV of the product gas.

Higher initial concentrations of CO will tend to slow down the rate of Reaction 1 (or even reverse it). Figure 3.6 (B) shows that for high initial CO concentrations the HHV decreased as the gas travelled through the bed (due to Reaction 1 operating in reverse) but for lower initial CO concentrations the HHV increased as the gas travelled through the bed (due to Reaction 1 acting in the forward direction). In all cases the temperature of the gas decreased as it travelled through the bed indicating that overall the endothermic reactions were dominant. The temperature gradient along the bed levelled off at a higher temperature for higher initial CO concentrations indicating that chemical equilibrium was obtained earlier.

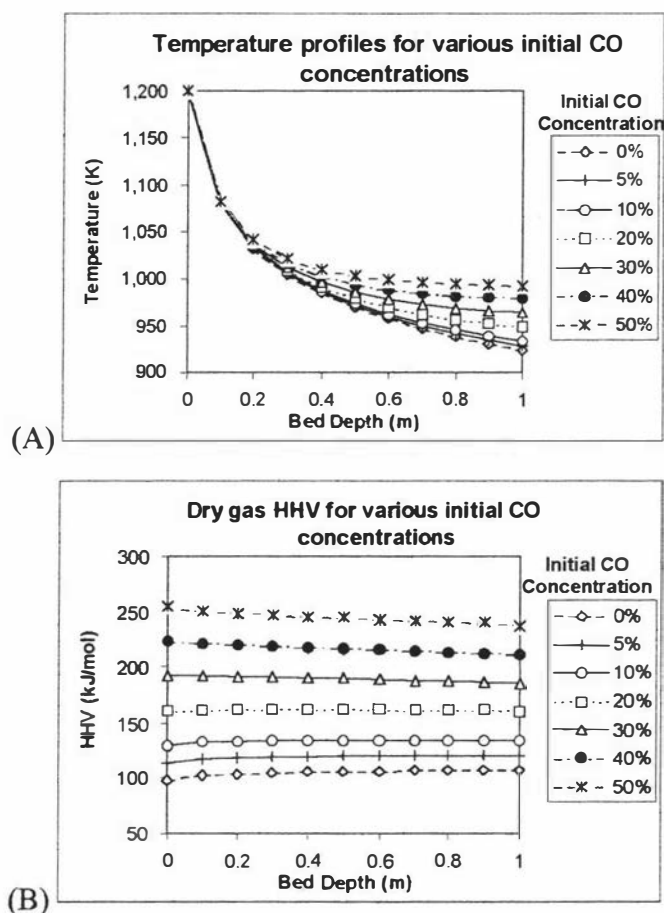


Figure 3.6: The effects of varying the initial concentration of CO on (A) the temperature profile of the reduction zone and (B) the dry gas HHV predicted.

Similarly low concentrations of CH_4 tend to drive Reaction 3 in the forward direction and Reaction 4 in the reverse direction. Both of these reactions rely on the presence of H_2 which was not included in the original gas composition but is formed within the gasifier by the reduction of H_2O (Reaction 2). Figures 3.7 (A) and (B) show the effects of varying the initial CH_4 concentration on the predicted temperature and dry gas HHV respectively.

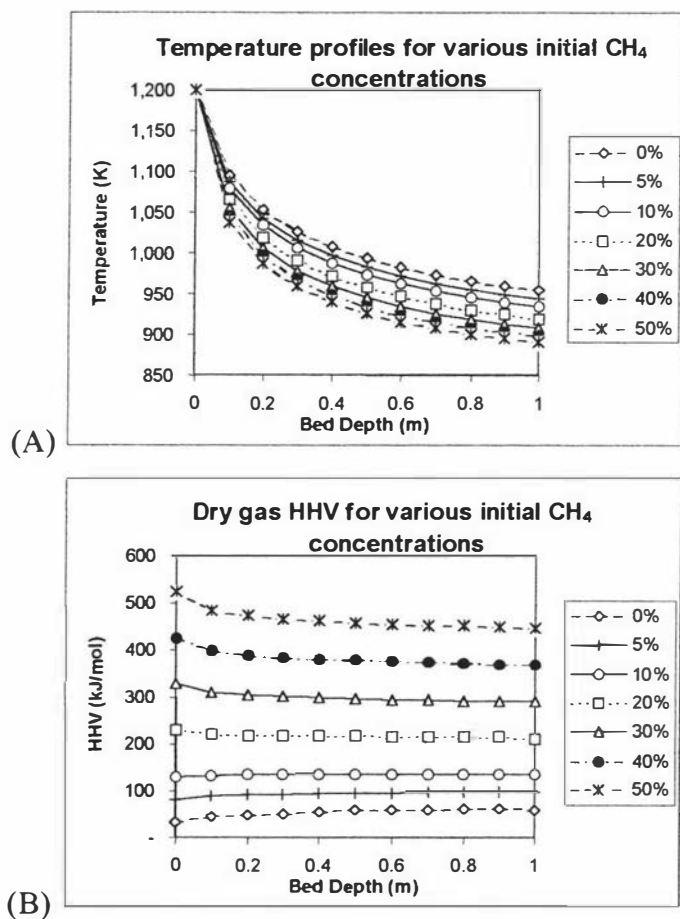


Figure 3.7: The effects of varying initial CH_4 concentration on (A) the temperature profile in the reduction zone and (B) the dry gas HHV predictions.

The initial CO and CH_4 originate from cracking of the pyrolysis products and are dependent on the properties of the fuel and the temperature.

Varying Initial H_2

H_2 is formed by reduction of water vapour by the char surface. Figure 3.8 shows the effects on the model prediction of temperature and HHV of altering the initial H_2 concentration. However, in practice the initial H_2 concentration is unlikely to be particularly high.

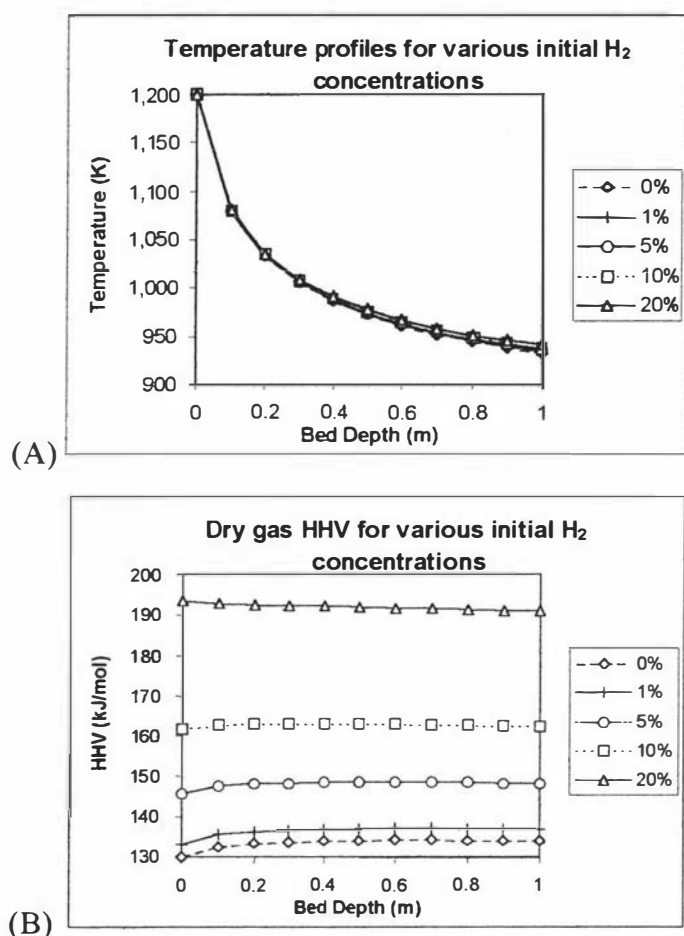


Figure 3.8: The effects of varying initial H_2 concentration on (A) the temperature profile of the reduction zone and (B) the dry gas HHV predictions.

H_2 plays a part in Reactions 2-4. Changing the initial H_2 concentration made very little difference to the temperature profile of the gasifier. Even at 20% initial H_2 Reactions 2-4 all still ran in the H_2 producing direction (the slight decrease in HHV with Bed Depth at 20% initial H_2 was due to decreasing CH_4 concentrations). Increasing the initial H_2 concentration increased the HHV of the product gas as H_2 is combustible and contributes directly to the HHV.

Varying Initial H_2O

Figures 3.9 (A) and (B) show the temperature profile and dry gas heating values predicted by the model as the initial H_2O concentration was varied. Increased H_2O concentration in the gas tends to increase the rate of Reaction 2, resulting in increasing H_2 content and lower temperatures as the gas progresses through the gasifier bed.

Figure 3.9(B) shows a dramatic increase in the HHV of the dry gas as the initial H_2O content was increased. Although increasing the H_2O content does lead to increased H_2 production, much of this apparent increase in HHV was an artefact of looking at the dry gas. When we increased the percentage of H_2O in the gas we did so at the expense of inert N_2 which led to a higher proportion of combustible gases in the dry gas. However the decrease in temperature down the bed was greater for higher initial H_2O concentrations indicating that the high initial H_2O concentration led to an increased rate of endothermic reduction reactions.

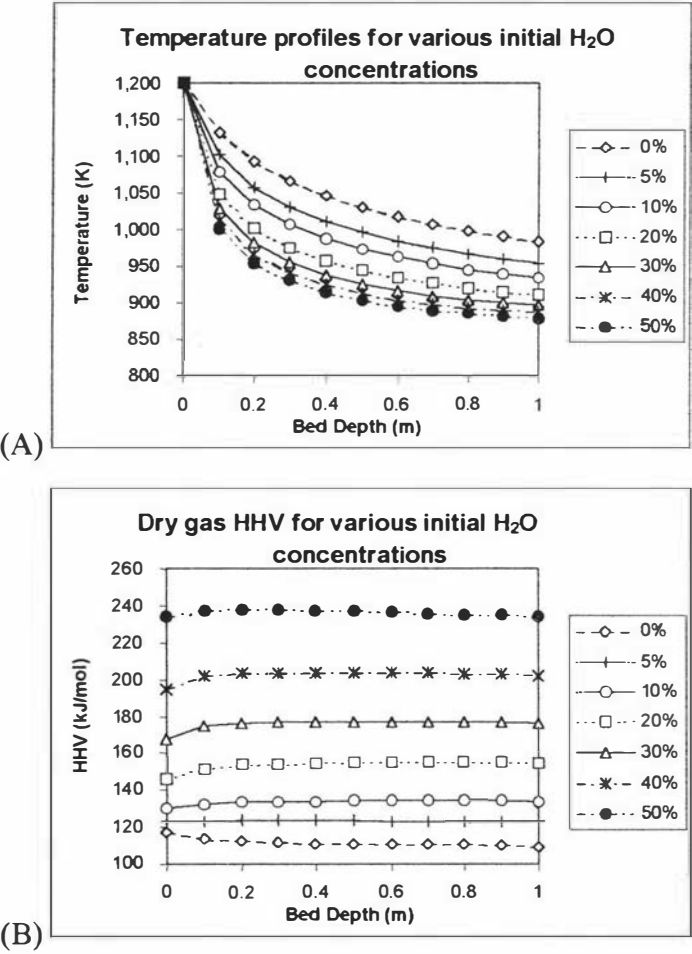


Figure 3.9: The effects of varying the initial H_2O concentration on (A) the temperature profile of the reduction zone, and (B) the dry gas HHV predictions.

H_2O enters the system as a product of hydrocarbon combustion and from evaporation of moisture in the fuel. Some gasifiers add extra steam at the gas inlets to enhance the

quality of the product gas. If the extra H_2O content came from the fuel moisture content then we would expect a lower initial temperature as energy would have been required to evaporate the moisture. These simulations assumed that the initial temperature was 1200 K for all runs.

(D) Initial Values

The model can predict the state of the gasifier anywhere within the reduction region given a complete set of measurements of the nine system variables at a single point. In practice, measurements are usually made at the exit point of the gasifier. However, as a predictive tool the model could be used to predict the gasifier output for a given initial state at the top of the gasifier. In this section we look for some reasonable estimates of the system variables at the top of the reduction zone.

Initial Gas Concentrations

We took as our starting position the point in the gasifier bed at which all the oxygen from the air inlet had been consumed by combustion reactions. It was also assumed that all the pyrolysis and cracking reactions had been completed by this point.

The gas at the top of the reduction zone comes from two different sources: from the inlet gas (usually air, but pure oxygen, steam or CO_2 are sometimes used) and from pyrolysis of the fuel. The exact proportion of each would depend upon the rate of air flowing into the gasifier relative to the rates of the combustion, pyrolysis and cracking reactions. Rather than attempt to calculate this directly we introduced the "pyrolysis fraction" variable (f_p), which can vary from 0 (no pyrolysis products) to 1 (pyrolysis products only).

The air flowing into the gasifier is a mixture of N_2 and O_2 . We assumed that all the O_2 from the air inlet had been consumed by combustion reactions with the char ($\text{C} + \text{O}_2 \rightarrow \text{CO}_2$), while the N_2 remained inert.

The pyrolysis products were assumed to have been cracked into an equivalent amount of CO , CH_4 and H_2O . We calculated this using the composition of pinus radiata shown in Table 3.3.

	Mass Percentage
C	50.26
H	5.98
N	0.03
O	42.14
S	0.01
Ash	0.3
Volatile Matter	80.45

Table 3.3: Composition of pinus radiata wood (Department of Energy, 2002).

The composition of the pyrolysis products was calculated by assuming that the 19.55% of the mass *not* included in the volatile matter consisted of all the nitrogen, sulphur and ash with the remaining mass consisting of carbon. Table 3.4 shows the calculated composition of the volatile matter both in terms of mass percentages and molar percentages.

Element	Mass Percentage	Molar Percentage
C	40.2	23.8
H	7.4	52.9
O	52.4	23.3

Table 3.4: Calculated composition of the volatile component of pinus radiata wood.

Assuming that the volatile matter ultimately ends up as a mixture of CO, CH₄ and H₂O and using the elemental composition in Table 3.4 we calculated the composition of the pyrolysis gas as 45.9% CO, 27.8% CH₄ and 26.3% H₂O (molar basis). This is assuming a dry feedstock. Additional moisture content in the feedstock can be accounted for by increasing the proportion of H₂O in the pyrolysis gas. Wet fuel will also lower the temperature within the gasifier as additional energy is required to vaporise the water.

Initial Gas Temperature

In the combustion region energy is required to dry the incoming fuel, drive the pyrolysis/cracking processes and to raise the temperature of the incoming gases. This energy is supplied by the exothermic combustion reactions. Thus the steady-state temperature at the top of the gasifier will be the temperature at which the rate of energy production matches the rate of energy consumption, and we expect lower temperatures for fuels with high moisture contents or large volatile fractions.

Senelwa (1997) found the average temperature just beneath the air inlets when gasifying an oven-dried biomass feedstock to be 955°C (1228 K). We therefore used an initial temperature of 1200 K to test our model.

Char Reactivity Factor (C_{RF})

The C_{RF} values for different chars were not known. However, the number of reactions occurring within a bed of fixed length L is related to L , the C_{RF} , the superficial gas velocity v , the reaction rate r_i and the cross-sectional area of the bed A . Figure 3.10 shows the temperature profiles as the C_{RF} value is varied using an f_P of 0.5, v of 1 m.s⁻¹, A of 3.14×10^{-2} m² and a starting temperature of 1200 K.

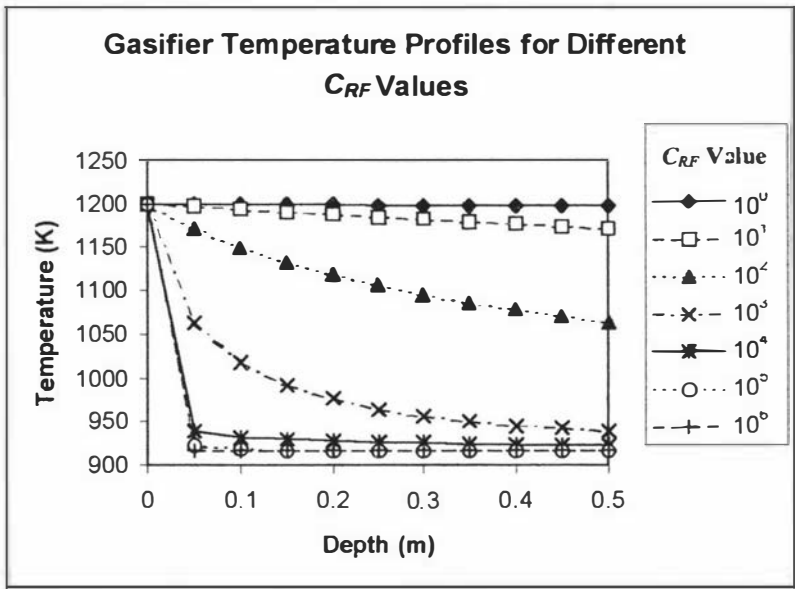


Figure 3.10: Gasifier temperature profiles predicted by the model using different C_{RF} values.

As the C_{RF} value increased, the temperature within the gasifier dropped more rapidly as the gas underwent more endothermic reactions in the time it took to travel the length of the gasifier. However, the temperature tended to stabilise at about 916K.

The outlet temperature found by Senelwa (1997) for a bed length of 0.275m was 1034 K. Comparing this with the results in Figure 3.10, a C_{RF} between 100 and 1,000 should produce a similar result.

Pyrolysis Fraction

The pyrolysis fraction f_p is the effective fraction of the initial gas that comes from pyrolysis and cracking reactions. The value of f_p will depend upon the proportion of volatile matter in the fuel, the rate at which air enters the system and the relative kinetics of the pyrolysis, cracking and combustion reactions. Rather than attempt to calculate this we examined the effect of different f_p values on the model output.

The air entering the gasifier is 79% N_2 by volume. No N_2 is produced by the reactions considered and it does not participate (significantly) in any reactions. So the N_2 concentration in the exit gas can be used to infer f_p . Figure 3.11 shows the N_2 concentration within the gasifier for different values of f_p using an initial temperature of 1200K, and a C_{RF} of 500.

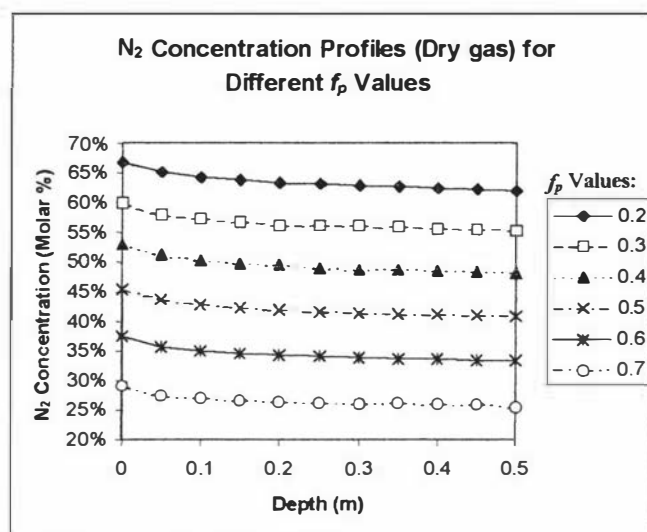


Figure 3.11: N_2 concentrations in dry gas predicted by the model using different f_p values.

Air-blown downdraft gasifiers typically produce gas containing ~50% N_2 (as a percentage of the dry gas volume). Therefore Figure 3.11 shows that f_p values between 0.3 and 0.4 produce results typical of downdraft gasification of biomass.

(E) Comparison with Experimental results

We tested our model against data collected from two different downdraft gasifiers (Chee, 1987, and Senelwa, 1997). Table 3.5 shows the parameters used in our model compared with those from the experiments. Figure 3.12 shows the composition of the dry product gas predicted by the model along with those found experimentally.

Parameter	Chee (1987) Data	Senelwa (1997) Data	Model
Bed Length	not stated	0.275 m	0.275 m
v	not stated	0.699 m/s	1 m/s
T initial	not stated	1228 K	1200 K
Moisture Content	5 wt %	"oven dried"	0
C_{RF}			500
f_P			0.4

Table 3.5: Parameters used in experimental downdraft gasification and in the model simulation.

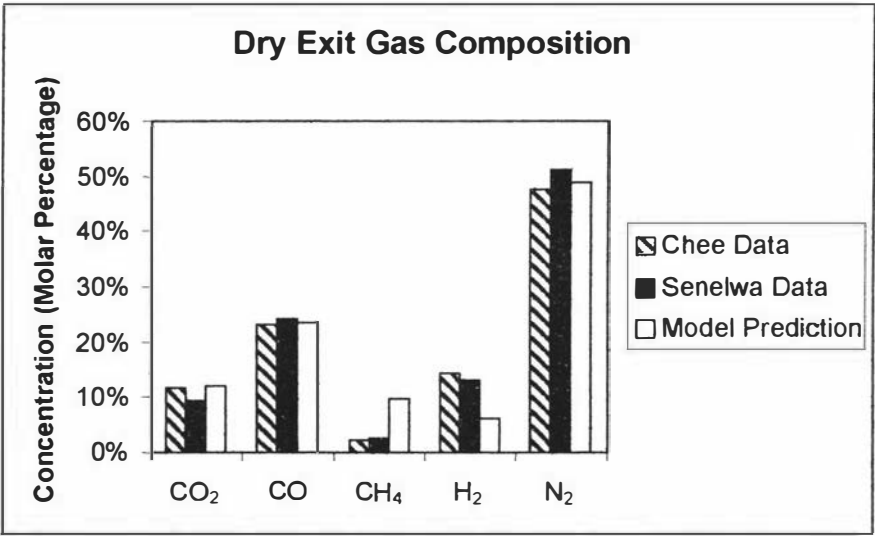


Figure 3.12: Dry exit gas composition predicted by the steady state model compared with the experimental results of Chee (1987) and Senelwa (1997).

The model produced reasonable agreement with the experimental results for CO₂, CO and N₂ but over-predicted CH₄ and under-predicted H₂. This over-prediction of CH₄ is most likely the result of the assumption that the O₂ in the air reacted only with the char. The pyrolysis products were cracked in a region of high temperature and in the presence of O₂, so it is probable that some of the CH₄ produced underwent combustion with O₂ ($\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$). The under-prediction of H₂ is likely to be a consequence of over-predicting CH₄.

We changed the initial conditions of the model using the new assumption that the O_2 from the air had reacted with some of the CH_4 from the cracking of pyrolysis gas. Figure 3.13 shows the gasifier output predicted given these new initial concentrations but otherwise using the conditions given in Table 3.5.

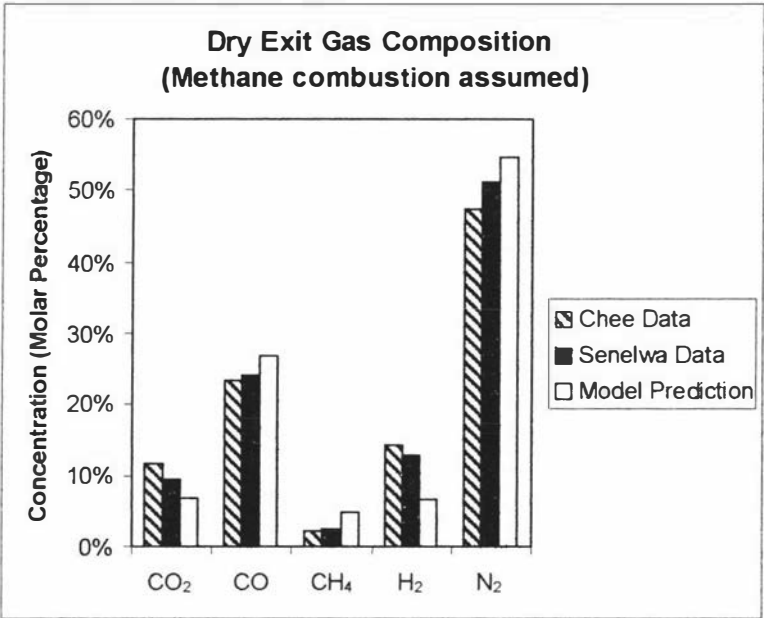
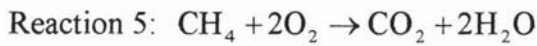


Figure 3.13: Dry exit gas composition predicted by the steady state model compared with the experimental results of Chee (1987) and Senelwa (1997). The initial conditions used for the model prediction assumed that the oxygen in the inlet air underwent combustion with some of the methane produced by pyrolysis of the fuel.

The change in the initial starting conditions improved the agreement between the model prediction and experimental results for the CH_4 concentration (and to a lesser degree the H_2 concentration), while the agreement between the model prediction and experimental results worsened slightly for the CO_2 , CO and N_2 concentrations. Overall the result is not too bad for a first approximation. Closer agreement could be obtained by refining the initial values and C_{RF} used.

3.2 1-Dimensional Steady State Model with Combustion Reactions

In the experiments carried out as part of this research project there was some evidence that not all the O_2 from the air supply had been depleted by the time the gas exited the gasifier (see Chapter 4). In Section 3.1 we assumed that the combustion reactions were sufficiently rapid that the initial O_2 from the inlet air could simply be replaced by the products of combustion. Therefore, we might get a more accurate model by including the kinetics of combustion reactions. Reaction 5 below was added to the reaction scheme developed in Section 3.1 to account for methane combustion. Char combustion ($C + O_2 \rightarrow CO_2$) was neglected.



This meant that an extra variable had to be tracked (the concentration of O_2 in the gas) and the following new reaction rate equation added:

$$(3.15) \quad r_5 = A_5 \exp\left(\frac{-E_5}{RT}\right) \left(P_{CH_4} \cdot P_{O_2}^2 - \frac{P_{CO_2} \cdot P_{H_2O}^2}{K_5} \right)$$

The activation energy for combustion of pine bark was found experimentally by Chen (1995) to be $22,028 \text{ J.mol}^{-1}$. This value was used to approximate E_5 . Graboski (1981) quotes an approximate relationship between the rate of combustion and the rate of gasification at 900°C as:

$$(3.16) \quad \left(\frac{r_{\text{combustion}}}{r_{\text{gasification}}} \right)_{900^\circ\text{C}} = 240$$

So we approximated the value of A_5 using the following relationship:

$$(3.17) \frac{A_5 \exp\left(\frac{-E_5}{RT}\right)_{900^\circ C}}{A_1 \exp\left(\frac{-E_1}{RT}\right)_{900^\circ C}} = 240$$

All the relationships from the original model that contained reaction terms were updated. Table 3.6 below shows the new formulae for the net rates of production of each gaseous species considered in terms of the rates of Reactions 1 to 5.

Species	R_x (mol.m ³ .s ⁻¹)
O ₂	$-2r_5$
N ₂	0
CO ₂	$-r_1 + r_5$
CO	$2r_1 + r_2 + r_4$
CH ₄	$r_3 - r_4 - r_5$
H ₂ O	$-r_2 - r_4 + 2r_5$
H ₂	$r_2 - 2r_3 + 3r_4$
Total number of gas molecules	$r_1 + r_2 - r_3 + 2r_4$

Table 3.6: Net rate of production of the different gaseous species by chemical reactions in terms of the rates of Reactions 1 to 5.

For the initial conditions we used the same composition for the pyrolysis products as used in Section 3.1 and assumed that the remainder of the gas was air (79% N₂, 21% O₂).

Figure 3.14 compares the gas composition predicted using a pyrolysis fraction of 0.4, C_{RF} of 500, initial velocity of 1 m.s⁻¹ and initial temperature of 1200 K with the experimental results of Chee (1987) and Senelwa(1997).

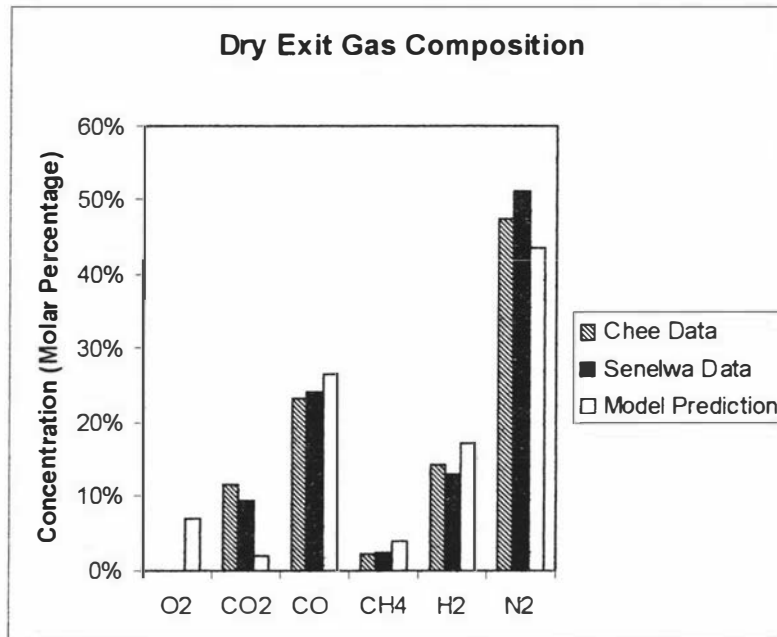


Figure 3.14: Dry exit gas composition predicted by model including methane combustion reaction compared with experimental results from Chee (1987) and Senelwa (1997).

Neither Chee nor Senelwa included O₂ measurements in their analysis, but it is likely that any O₂ in the product gas was not separated from the N₂. Adding the model O₂ concentration prediction to the N₂ concentration prediction brings the predicted N₂ level close to the experimental values. The model did significantly underestimate the amount of CO₂ produced. Several different values of C_{RF} and f_p were tried but in all cases the dry gas CO₂ concentration never increased beyond a couple of percent.

We tried increasing the initial CO₂ concentration by assuming that the pyrolysis gas was composed of CO₂, CH₄ and H₂O rather than CO, CH₄ and H₂O assumed earlier. Using the molar composition of pyrolysis gas from Table 3.4 above we recalculated the pyrolysis gas composition as 44.6% CO₂, 4.4% H₂O and 51.0% CH₄.

Figure 3.15 shows the dry gas composition predicted using the new pyrolysis gas composition with a C_{RF} of 2000 and an f_p of 0.3. The new model slightly over predicts the H₂ content of the dry product gas but is fairly close with respect to the other components.

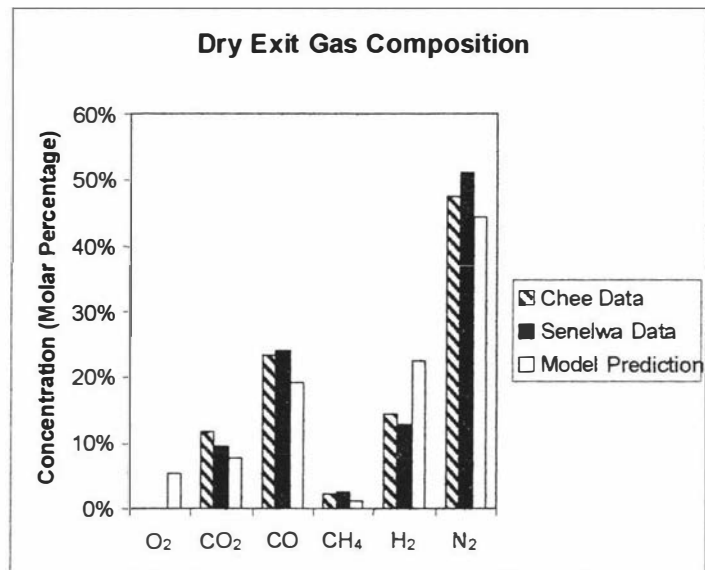


Figure 3.15: Dry exit gas composition predicted by the model including methane combustion reaction and assuming the pyrolysis gas consists of CO₂, CH₄ and H₂O, compared with experimental results from Chee (1987) and Senelwa (1997).

3.3 Time Dependent Model

The next step after constructing a steady-state model was to look at a time dependent model. A time dependent model could be used, for example, to see how long it takes the system to return to steady-state operation after some disruption.

(A) Model Construction

The mass and energy balance relationships for the time-dependent model are similar to the steady-state model except that mass and energy are able to accumulate over time within a volume element. We considered thin cross-sections of thickness Δz over a small time interval Δt . For each gaseous species i , the number of moles of this species accumulating within the cross-section is equal to the difference in the number of moles flowing into and out of the segment during the time interval Δt plus the net number of moles created by chemical reactions within the segment. This is expressed mathematically in Equation 3.18:

(3.18)

$$N_x(z, t + \Delta t) - N_x(z, t) = \int_t^{t+\Delta t} A n_x(z, \tau) v(z, \tau) d\tau - \int_t^{t+\Delta t} A n_x(z + \Delta z, \tau) v(z + \Delta z, \tau) d\tau + R_x(z, t) A \Delta z \Delta t$$

where $N_x(z, t)$ is the number of moles of gaseous species x at position z and time t .

A is the cross-sectional area of the gasifier bed (in m^2).

v is the superficial gas velocity (in m.s^{-1})

n_x is the molar density of gaseous species x (in mol.m^{-3}).

R_x is the net rate of formation of gaseous species x (in $\text{mol.m}^{-3}.\text{s}^{-1}$). R_x is given in terms of the rates of Reactions 1 to 5 in Table 3.6 above.

Dividing both sides by $A \Delta z$:

$$(3.19) \quad n(z, t + \Delta t) - n(z, t) = \frac{-\Delta(nv)}{\Delta z} \cdot \Delta t + R_x(z, t) \cdot \Delta t$$

Dividing both sides by Δt and taking the limit as $\Delta z \rightarrow 0$ and $\Delta t \rightarrow 0$:

$$(3.20) \quad \frac{\partial n_x}{\partial t} = \frac{-\partial(n_x v)}{\partial z} + R_x(z, t)$$

Similarly the energy accumulated in a small segment over time Δt will be the difference between the energy flowing into and out of the segment, plus the energy released by chemical reactions within the segment minus work done in moving the gas through the segment. We assumed that the energy accumulates as the thermal energy of the gas. The gas also had some kinetic and gravitational potential energy but these were small compared to the chemical and thermal energies of the gas. The thermal energy of the gas was:

$$(3.21) \quad Q = \sum_x n_x c_x T$$

where Q is the thermal energy of the gas (in J.m^{-3}),

x ranges over all gaseous chemical species,

n_x is the molar density of chemical species x (in $\text{mol} \cdot \text{m}^{-3}$),

c_x is the molar heat capacity of chemical species x (in $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$)

This gave us the following relationship:

$$(3.22) \quad A \int_z^{z+\Delta z} \left\{ \left(\sum_k n_k c_k T \right)(x, t + \Delta t) - \left(\sum_k n_k c_k T \right)(x, t) \right\} dx =$$

$$A \int_t^{t+\Delta t} \left\{ \left(v \sum_k n_k c_k T \right)(z, \tau) - \left(v \sum_k n_k c_k T \right)(z + \Delta z, \tau) \right\} d\tau$$

$$+ H_R A \Delta z \Delta t + A \int_z^{z+\Delta z} \left\{ (Pv)(x, t) - (Pv)(x + \Delta x, t) \right\} dx$$

where k ranges over all chemical species considered,

P is the total pressure (in Pa), and

H_R is the rate of energy released by chemical reactions (in $\text{J} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$).

Dividing both sides by A gave:

$$(3.23) \quad \Delta_t \left(\sum_k n_k c_k T \right) \Delta z = -\Delta_z \left(v \sum_k n_k c_k T \right) \Delta t + H_R \Delta z \Delta t - \Delta_z (Pv) \Delta z$$

Dividing both sides by $\Delta z \Delta t$ and taking the limits $\Delta z \rightarrow 0$, $\Delta t \rightarrow 0$ gave:

$$(3.24) \quad \frac{\partial \left(\sum_k n_k c_k T \right)}{\partial t} = H_R - \frac{\partial \left(v \sum_k n_k c_k T \right)}{\partial z} - \frac{\partial (Pv)}{\partial z}$$

This expanded to give:

$$(3.25) \quad \sum_k \frac{\partial n_k}{\partial t} c_k T + C \frac{\partial T}{\partial t} = H_R - \frac{\partial v}{\partial z} C T - v \sum_k \frac{\partial n_k}{\partial z} c_k T - v C \frac{\partial T}{\partial z} - v \frac{\partial P}{\partial z} - P \frac{\partial v}{\partial z}$$

where $C = \sum_k n_k c_k$

Restating Equation 3.7 in terms of partial derivatives:

$$(3.26) \quad \frac{\partial n_k}{\partial z} = \frac{1}{v} \left(R_k - n_k \frac{\partial v}{\partial z} \right)$$

Substituting into Equation 3.25 and rearranging:

$$(3.27) \quad \frac{\partial T}{\partial t} = \frac{H_R}{C} - v \frac{\partial T}{\partial z} - \frac{1}{C} \left(T \sum_k R_k c_k + v \frac{\partial P}{\partial z} + P \frac{\partial v}{\partial z} + \sum_k \frac{\partial n_k}{\partial t} c_k T \right)$$

Equations 3.20 and 3.27 together with the ideal gas equation (3.12) can be used to find the state of the gasifier at time $t+\Delta t$ given the state of the gasifier at time t . The MATLAB script 'TimeDepModel.m' included in Appendix C implements this model using forward differences to approximate the time derivatives and central differences to approximate the spatial derivatives. This implementation was unstable for time step sizes greater than 1 ms which makes it computationally expensive for time scales of the order of minutes. This could be improved by using a higher order approximation for the time derivatives. However, when the gasifier operation is changing with time then it is likely that other factors such as the rate of heat transfer between the gaseous and solid phases should also be considered.

(B) Agreement with Steady State Model

If the time dependent model is compatible with the steady-state model developed earlier then Equations 3.20 and 3.27 should yield the steady-state relationships when the time

derivatives are set to zero. Setting $\frac{\partial n_k}{\partial t} = 0$ in Equation 3.20 gave:

$$(3.28) \quad \frac{-v \partial n_x}{\partial z} + \frac{-n_x \partial v}{\partial z} + R_x = 0$$

Rearranging:

$$(3.29) \quad \frac{\partial n_x}{\partial z} = \frac{1}{v} \left(R_x - n_x \frac{\partial v}{\partial z} \right)$$

This corresponds to Equation 3.7. Similarly setting $\frac{\partial T}{\partial t} = 0$ in Equation 3.27 gave:

$$(3.30) \quad \frac{H_R}{C} - v \frac{\partial T}{\partial z} - \frac{1}{C} \left(T \sum_k R_k c_k + v \frac{\partial P}{\partial z} + P \frac{\partial v}{\partial z} + \sum_k \frac{\partial n_k}{\partial t} c_k T \right) = 0$$

We also have $\frac{\partial n_k}{\partial t} = 0$ for all chemical species. Rearranging:

$$(3.31) \quad \frac{\partial T}{\partial z} = \frac{1}{v \sum_k n_k c_k} \left(H_R - \sum_k R_k c_k T - v \frac{\partial P}{\partial z} - P \frac{\partial v}{\partial z} \right)$$

The heat released by reactions (H_R) is given by the formula:

$$(3.32) \quad H_R = - \sum_i r_i \Delta H_i$$

where r_i is the rate of reaction i (in $\text{mol.m}^{-3}.\text{s}^{-1}$),

ΔH_i is the change in enthalpy of reaction i (in J.mol^{-1}), and

i ranges over all chemical reactions considered.

Substituting Equation 3.32 into Equation 3.31:

$$(3.33) \quad \frac{\partial T}{\partial z} = \frac{1}{v \sum_k n_k c_k} \left(- \sum_i r_i \Delta H_i - \sum_k R_k c_k T - v \frac{\partial P}{\partial z} - P \frac{\partial v}{\partial z} \right)$$

which corresponds to Equation 3.20 in the steady-state model.

3.4 Conclusion

We developed a steady-state model of downdraft gasification that models some of the physical and chemical processes occurring in the reduction region. When compared with previously published experimental data the model was reasonably accurate in predicting the exit gas produced although the degree of accuracy depended upon the initial conditions assumed. The steady-state model was extended to include time dependence. The time dependent model wasn't tested against experimental data due to a lack of sufficient data including temporal and spatial information. It is likely that for non steady-state operation, some of the factors neglected in the steady-state model (such as heat transfer between the gaseous and solid phases) could be significant.

4. Experimental Results

4.1 Performance of Gasifier Run in Batch Mode

The downdraft gasifier used to gather experimental data was operated in batch mode rather than continuous mode. This meant that the gasifier operation was time dependent. However, we assumed that at some time between the initial start-up phase and the exhaustion of the fuel, the gasifier operation would behave as a close approximation to steady-state operation.

Figure 4.1 shows the exit gas temperature plotted against time for the gasifier operated using 9 ± 2 kg pine chips as fuel and a bed length of 10 ± 1 cm.

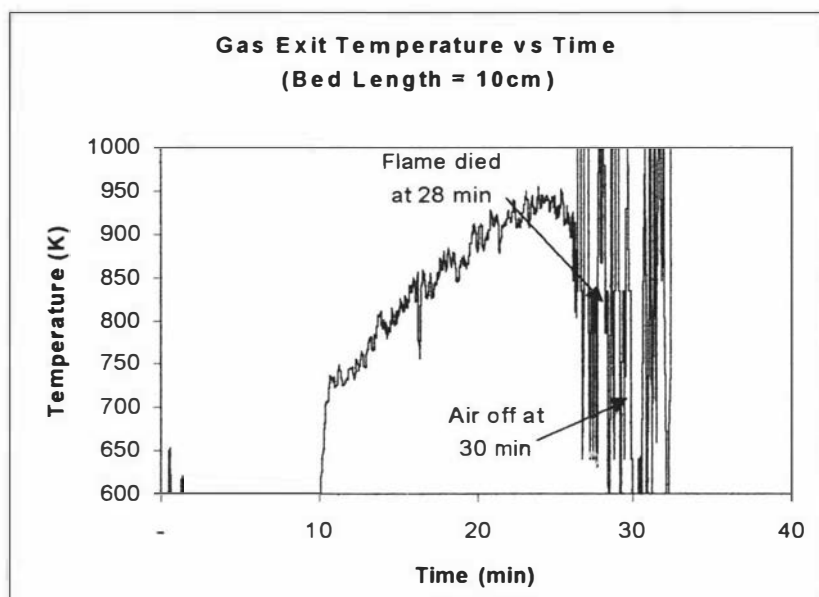


Figure 4.1: Exit gas temperature plotted against time for gasifier operated using pine chips as fuel and a bed length of 10 ± 1 cm. Thermocouple readings were collected every two seconds. A five point moving average of the thermocouple readings was used to calculate the temperature.

The start time was taken from when the burner unit was removed and the air supply switched to the vacuum cleaner. There was a delay of about ten minutes before normal

gasifier operation was established. This was because the air inlets used by the vacuum cleaner were in a lower position than the air inlet for the burner unit fan, so combustion had to be re-established at the new position. Also, the gasifier had been loaded with fresh fuel so the region between the grate and the air inlets was filled with fresh fuel rather than char (as would be the case with continuous operation). The exit gas would contain a high proportion of uncracked pyrolysis products until the fuel beneath the air inlets had been pyrolysed.

After 11 minutes the exit gas could be ignited, indicating the presence of significant amounts of combustible gases such as CO and H₂. The exit gas flame extinguished after 28 minutes indicating that the fuel supply was nearly exhausted. The thermocouple signal became very noisy after 27 minutes. This was probably the result of hot cinders falling onto the thermocouple as the fuel supply became depleted.

Figure 4.2 shows the composition of dry exit gas samples taken at different times throughout the gasifier run. The gas chromatograph column used for this analysis was only capable of separating CO₂, CO, CH₄ and H₂, so it was assumed that the remainder of the dry gas was N₂.

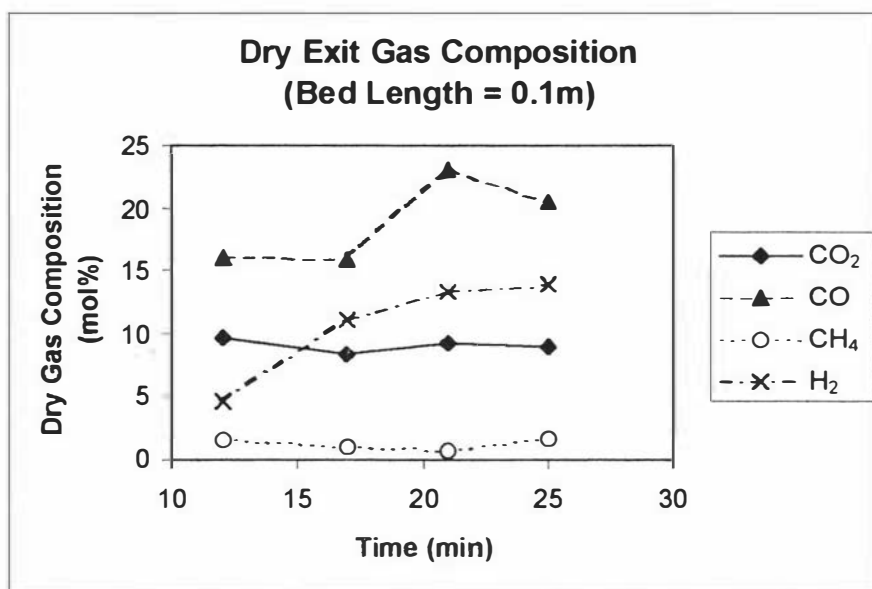


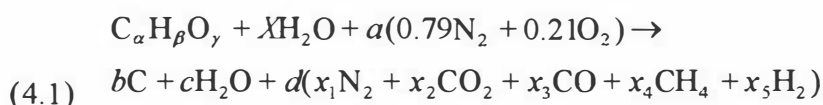
Figure 4.2: Composition (by volume fraction) of dry exit gas samples taken at various time intervals throughout the gasifier run.

From Figures 4.1 and 4.2 we can see that the gasifier operation was roughly stable between about 21 and 26 minutes from start-up.

(A) Mass and Energy Balances of Gasifier

It was not practical to attempt to test the mass and energy balances of the gasifier experimentally. There were too many sources of mass loss from the system that could not be accurately measured, such as the mass of entrained particles in the exit gas, small gas leaks in the system and the mass of tars condensing onto the interior surfaces of the gasifier. In addition the ash collection system was not perfect and some solid residue would get trapped inside the gasifier instead of falling into the ash bucket.

However, we can take the empirical formula for bone dry fuel as $C_\alpha H_\beta O_\gamma$ and assume that gasification in air is expressed by the following equation:



where the values x_1 to x_5 are the fractions of each of the components of the dry exit gas which have been measured and X is the moisture content of the fuel expressed as a molar fraction.

This expression, given the dry exit gas composition, the dry fuel composition and the fuel moisture content, can predict the moisture content of the exit gas, the fraction of carbon that remains in the solid residue, the amount of gas produced and the molar air:fuel ratio.

Values for α , β , and γ were available in biofuel databases. X and x_1 to x_5 were all measured experimentally. Therefore the unknown variables were the parameters a , b , c and d . By applying a molar balance to each element we obtained the following relations that can be solved for a , b , c and d :

$$(4.2) \quad \alpha = b + d(x_2 + x_3 + x_4)$$

$$(4.3) \quad \beta + 2X = 2c + d(4x_4 + 2x_5)$$

$$(4.4) \quad \gamma + X + 0.42a = c + d(2x_2 + x_3)$$

$$(4.5) \quad 0.79a = dx_1$$

The pine chips used had a moisture content of 18.7% (as a weight percentage of the dry fuel). Using the elemental analysis of pinus radiata from the Department of Energy Biofuels Database (Department of Energy, 2002) the empirical formula of the dry biomass was $\text{CH}_{1.42}\text{O}_{0.63}$ and the value of X was 0.244.

We took the average dry gas composition for the steady state region of the gasifier run using a 10 cm depth bed of pine chips and used these values to solve Equations 4.2 to 4.5 for the variables a , b , c and d . Table 4.1 shows these results.

Dry Gas Composition (mol%)	
N_2	$54.4 \pm 0.9\%$
CO_2	$9.1 \pm 0.2\%$
CO	$22 \pm 1\%$
CH_4	$1.1 \pm 0.5\%$
H_2	$13.6 \pm 0.2\%$
HHV Dry Product Gas (kJ/mol)	110.6 ± 0.8
a	1.2 ± 0.5
b	0.5 ± 0.2
c	0.69 ± 0.09
d	1.7 ± 0.7

Table 4.1: Values of parameters a , b , c , and d derived from experimental measurements of steady-state downdraft gasifier product gas.

The values of parameters a , b , c , and d were very sensitive to the composition of the exit gas. In Table 4.1 we used two samples taken during the same gasification run and the

small differences in the chemical compositions led to significant differences in the calculated parameter values. In order to use this method reliably the average composition of a large number of gas samples should be used.

The value of parameter b indicated that at least 30% of the carbon in the biomass should remain in solid form. When the solid residue from the gasifier was inspected it was black in colour suggesting a high carbon content.

Parameters c and d indicate that the moisture content of the exit gas could be between 20 - 40% (molar basis). It could also be possible that not all of the water vapour created went through the exit pipe. For example, as the fuel above the combustion region was dried it would be possible that the water vapour could rise and condense on the walls of the upper region of the gasifier. The moisture content of the exit stream was not measured as we were cooling the gas below the condensation point of water before we sampled it. An approximate value could be inferred by comparing the N_2 concentration in the dry outlet gas along with the measured volume flow rate of the exit gas to the known rate of N_2 entering through the air inlets. However, the uncertainties in the volume flow rate measurements led to very large uncertainties in the moisture content calculated by this method.

4.2 Effect of Varying Bed Length

We performed a series of gasification runs with bed lengths of 10, 13 and 24 cm (all bed length measurements were ± 1 cm). In each case the fuel was pine chips (moisture content 18.7% by weight, dry basis) and the air supply was provided by a vacuum cleaner operated as a blower. The vacuum cleaner was operated using mains electricity without the Variac variable transformer.

(A) Exit Gas Temperature

Figure 4.3 shows the exit gas temperature from the end of the start-up procedure for three different gasifier runs using different bed lengths but otherwise operating under

similar conditions. The temperature was sampled every 2 seconds and a 5-point moving average was used to smooth the graphs.

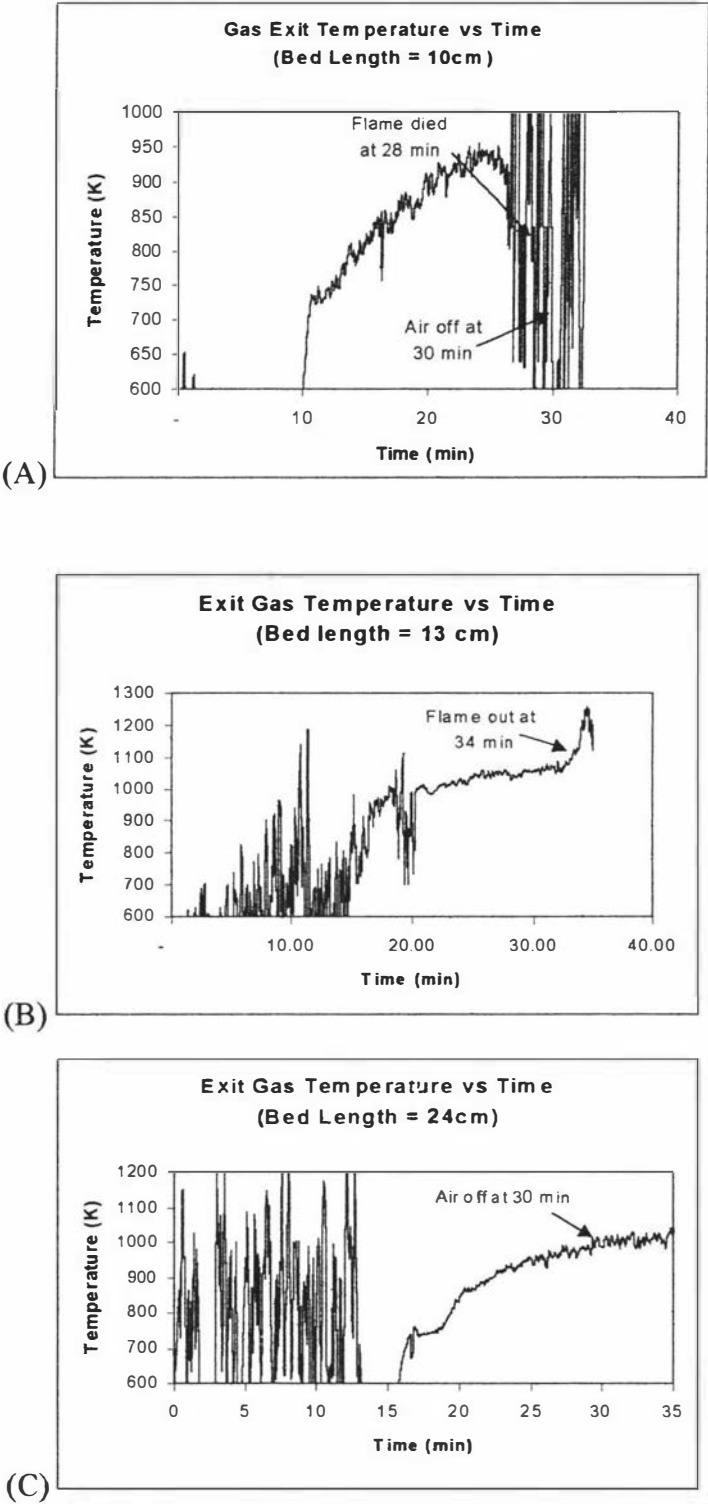


Figure 4.3: Exit gas temperature vs time for gasifier bed lengths (A) 10cm, (B) 13cm and (C) 24cm.

There are some regions in each of the graphs where the thermocouple signal was noisy. These noisy regions occurred at the beginning and/or end of the runs. This could be due to hot cinders falling onto the thermocouple as greater numbers of cinders were emitted from the exit pipe during the initial and final stages of gasifier operation.

Figures 4.3(B) and (C) both show relatively long periods of stable temperature, while Figure 4.3(A) has only a short period of steady temperature. The average temperature for these stable regions is plotted in Figure 4.4 below.

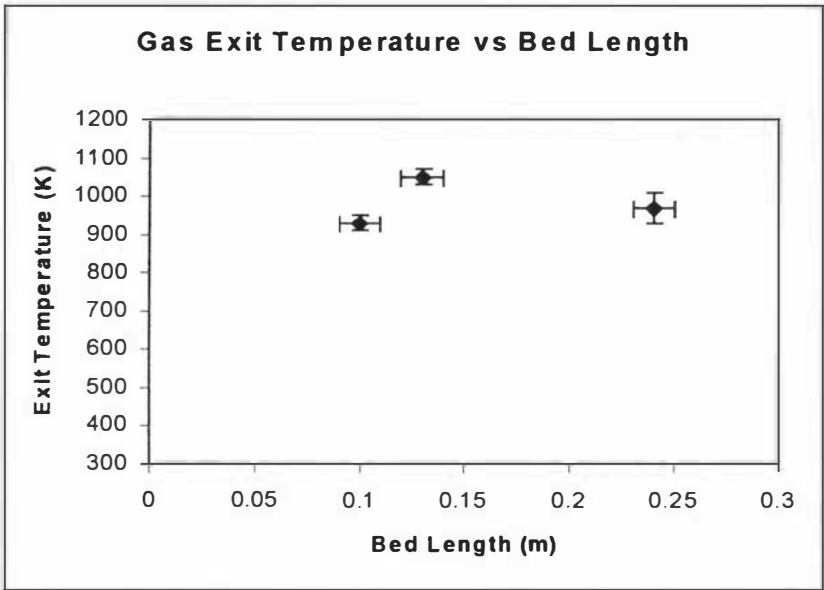


Figure 4.4: "Steady-state" exit gas temperature of gasifier vs bed length.

Increasing the bed length effectively increases the residence time of the gases within the gasifier bed. Given that the major reactions in the reduction zone are endothermic we expect that the exit gas temperature will decrease with increasing bed length to some lower temperature limit where the reaction rates approach zero. The increase in exit gas temperature between bed lengths of 0.10 and 0.13 cm suggests that there were some exothermic reactions occurring between these depths. Figure 4.5 below shows the oxygen concentration variation with time for a run performed by Sime (1998). There were still traces of O_2 in the dry exit gas at steady-state, so combustion reactions could still be occurring at this depth.

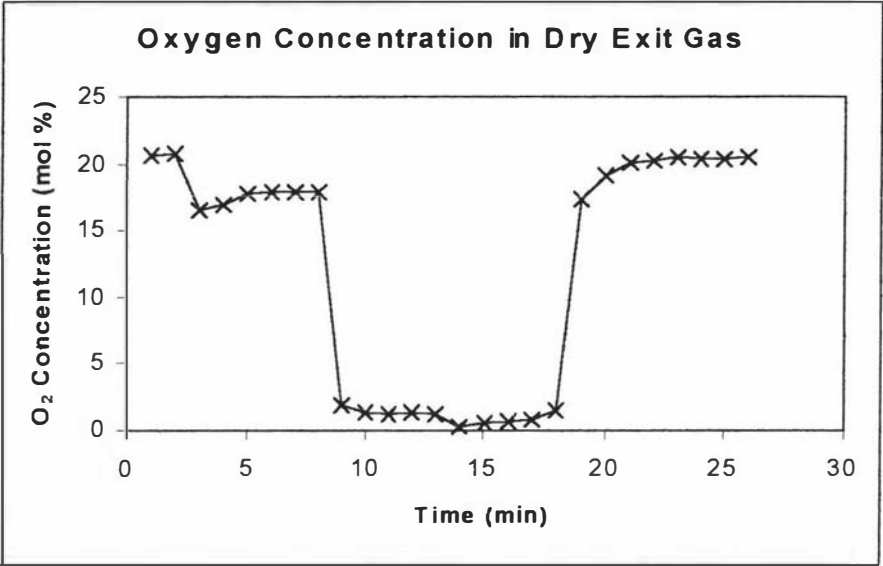
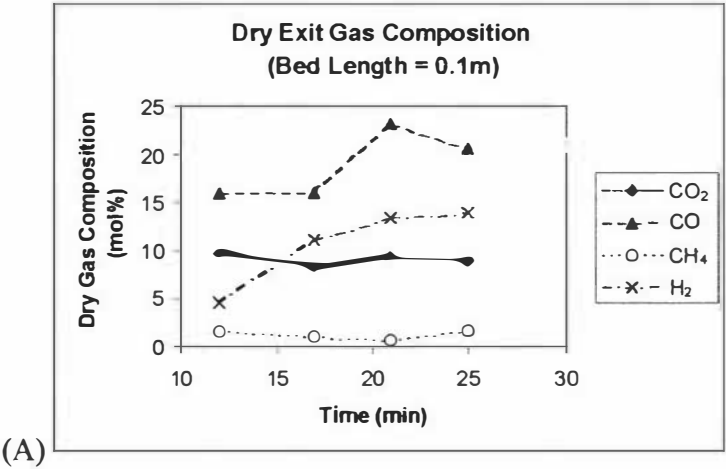


Figure 4.5: O₂ Concentration for gasifier running on pine chips at near atmospheric pressure (Sime, 1998)

(B) Exit Gas Composition

The composition of the dry exit gas vs. time is plotted for the different bed lengths in Figures 4.6 (A) to (C) below.



(A)

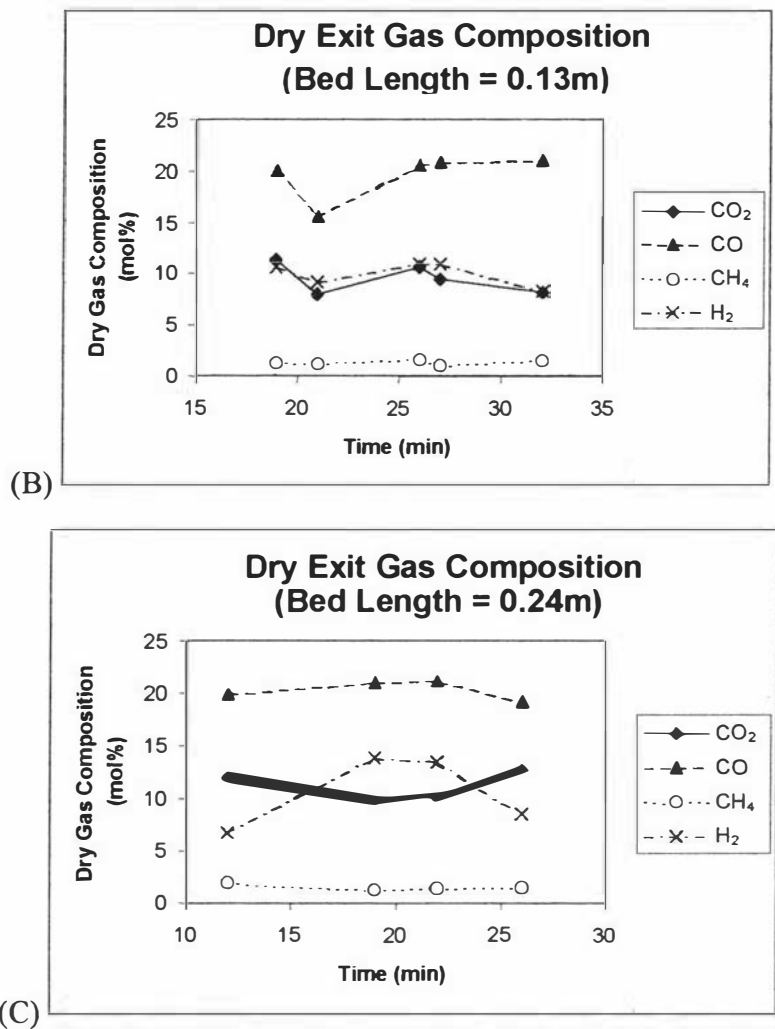


Figure 4.6: Composition of dry exit gas vs time for bed lengths (A) 0.10 ± 0.01 m, (B) 0.13 ± 0.01 m and (C) 0.24 ± 0.01 m.

From Figures 4.4 and 4.6 we determined the time intervals over which the gasifier operation was approximately steady-state for each run. The gas composition was taken as the average composition of the samples taken within the time interval of approximately steady-state operation. Figure 4.7 shows the variation of the dry exit gas composition plotted against the bed length.

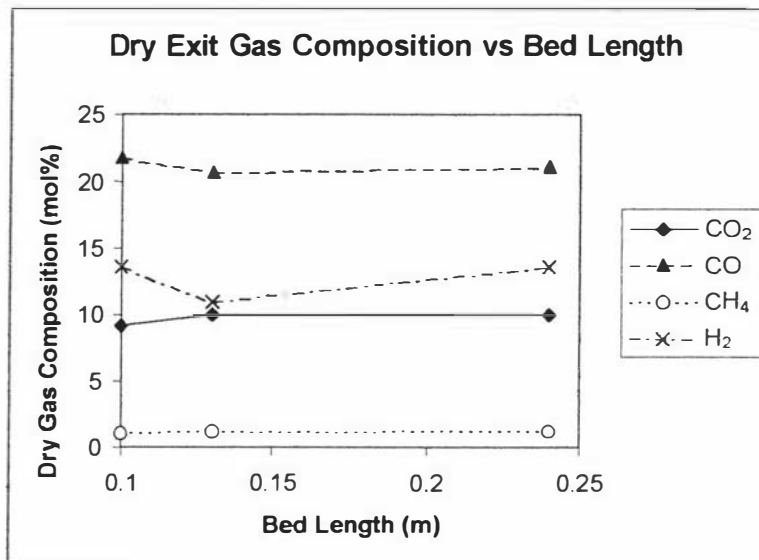


Figure 4.7: Average composition of the dry exit gas during "steady-state" operation vs gasifier bed length.

The CO₂ and CH₄ concentrations both increased with increasing bed length indicating that reactions producing these two products were occurring. The H₂ concentration fell between bed lengths of 0.10 and 0.13 cm then increased between bed lengths of 0.13 and 0.24 cm. In conjunction with the temperature measurements from Figure 4.4 this could represent a transition between a region where combustion reactions dominated to a region where reduction reactions dominated somewhere in the region between 0.10 and 0.24 cm below the air inlets.

(C) Mass and Energy Balance of Gasifier

Equations 4.2 to 4.5 were applied to the steady-state compositions of the dry exit gas for different gasifier bed lengths found earlier. Table 4.2 shows the dry gas compositions used and the calculated values of the parameters a , b , c and d .

Dry Gas Composition (mol%)	Bed Length = 0.10 m	Bed Length = 0.13 m	Bed Length = 0.24 m
N ₂	54.4 ± 0.9%	57.2 ± 0.6%	54.1 ± 0.1%
CO ₂	9.1 ± 0.2%	10.0 ± 0.6%	10.0 ± 0.2%

CO	$22 \pm 1\%$	$20.7 \pm 0.2\%$	$21.0 \pm 0.1\%$
CH ₄	$1.1 \pm 0.5\%$	$1.2 \pm 0.3\%$	$1.25 \pm 0.05\%$
H ₂	$13.6 \pm 0.2\%$	$10.95 \pm 0.05\%$	$13.6 \pm 0.2\%$
HHV of Dry Exit Gas (kJmol ⁻¹)	110.6 ± 0.8	100 ± 2	109.5 ± 0.2
<i>a</i>	1.2 ± 0.5	1.9 ± 0.2	1.4 ± 0.2
<i>b</i>	0.5 ± 0.2	0.2 ± 0.2	0.4 ± 0.1
<i>c</i>	0.69 ± 0.09	0.60 ± 0.07	0.63 ± 0.05
<i>d</i>	1.7 ± 0.7	2.7 ± 0.5	2.0 ± 0.3
Exit Gas Moisture Content (mol. basis)	$30 \pm 10\%$	$19 \pm 5\%$	$24 \pm 4\%$

Table 4.2: Values of parameters *a*, *b*, *c*, and *d* derived from experimental measurements of steady-state downdraft gasifier product gas for different gasifier bed lengths.

The uncertainty in the dry exit composition led to large uncertainties in the values of parameters *a*, *b*, *c*, and *d*. Altering the bed length between 0.10 m and 0.24 m did not make any detectable difference to the calculated parameter values given the large uncertainties involved.

(D) Summary

Increasing the bed length of the gasifier effectively increases the residence time of the gases within the gasifier. Within the reduction zone of the gasifier increased residence time means more time for reduction reactions to occur so it is expected that increasing bed length will lead to increased H₂ and CO concentrations in the exit gas and a lower exit temperature. However, the three experimental gasifier runs with different bed lengths did not follow this trend. One explanation is that there was still sufficient O₂ remaining at the bottom of the shorter gasifier beds that combustion reactions occurred and the assumption that only the reduction reactions were occurring did not hold.

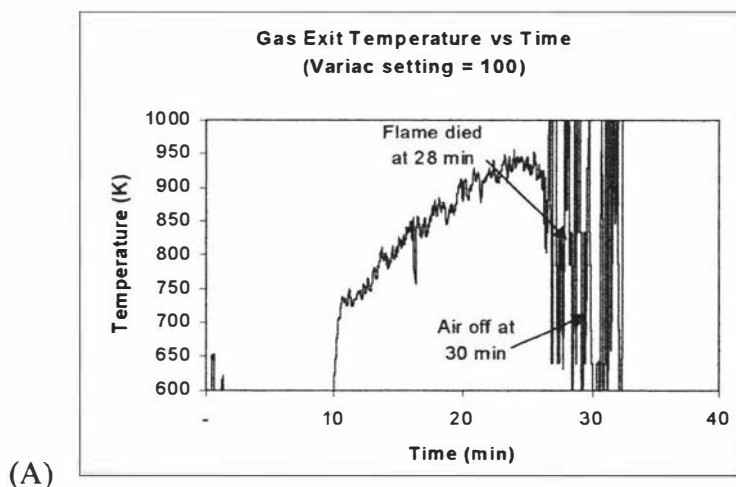
4.3 Effect of Varying Air Flow Rate

We performed a series of gasification runs using a 0.10 ± 0.01 m length bed of pine chips with different air flow rates. The air flow rate was controlled using a Variac variable transformer to limit the power supply to the vacuum cleaner used to pump air into the gasifier. In Chapter 2 we measured the volume flow rate and the inlet air speed of the vacuum cleaner as a function of the variable transformer setting.

(A) Exit Gas Temperature

Figures 4.8 (A) to (D) show the exit gas temperatures plotted against time for gasifier runs using different Variac settings. In all cases the fuel was pine chips and the bed length was 10 ± 1 cm.

During the start-up phase the vacuum cleaner was run at full power to speed up the establishment of combustion at the air inlets. Once combustion appeared to be well-established (when thick smoke emerged from the gasifier exhaust) the power to the vacuum cleaner (and hence the air flow rate) was reduced to the specified level.



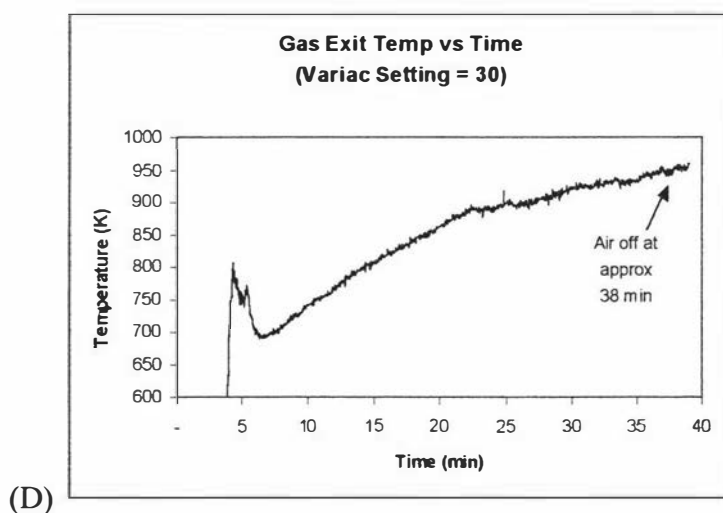
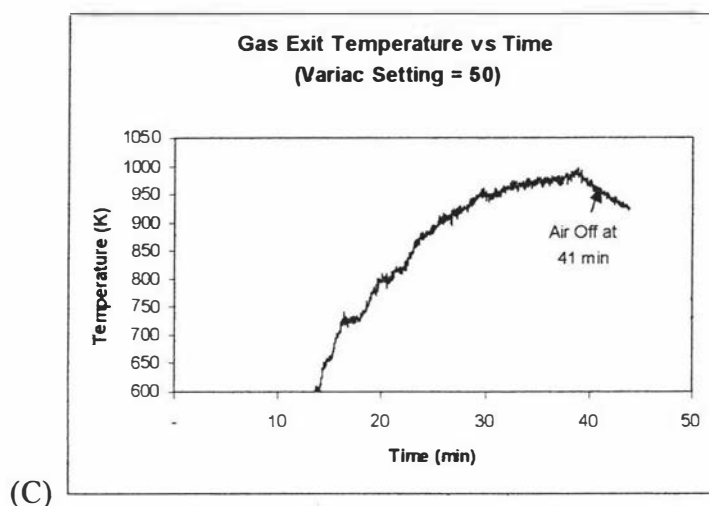
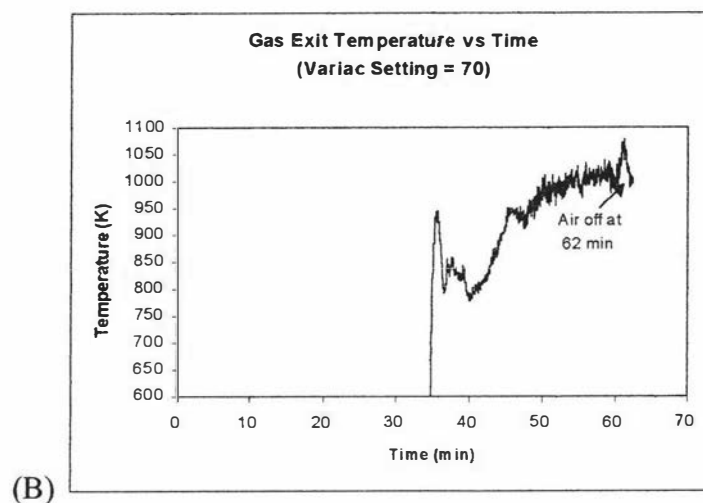


Figure 4.8: Gas exit temperature vs time for gasifier using pine chips as fuel. Bed length in all cases was 10 ± 1 cm. The molar flow rate of air (at vacuum cleaner inlet) was (A) 0.6 ± 0.1 mol/s, (B) 0.4 ± 0.1 mol/s, (C) 0.32 ± 0.06 mol/s and (D) 0.22 ± 0.03 mol/s.

In each case the exit gas temperature rose to some upper limit where it levelled off. In some of the plots the temperature started to fall as the fuel was depleted. We used these exit gas temperature plots to estimate the time interval during which the gasifier operation was approximately steady-state. Table 4.3 shows the time interval of approximate steady state operation and the corresponding steady-state exit temperature for each run.

Variac Setting	Air Flow Rate (mol/s)	Time interval of approximate steady-state operation	Exit gas temperature during steady-state operation (K)
100	0.6 ± 0.1	21-26 min	920 ± 30
70	0.4 ± 0.1	53-60 min	1000 ± 20
50	0.32 ± 0.06	31-39 min	970 ± 20
30	0.22 ± 0.03	27-36 min	920 ± 20

Table 4.3: Time intervals for which the gasifier operation was approximately steady-state and the average gas exit temperature over this time interval.

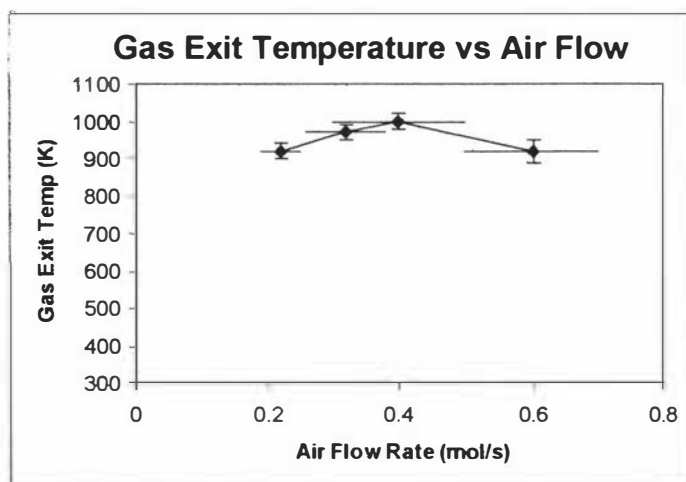
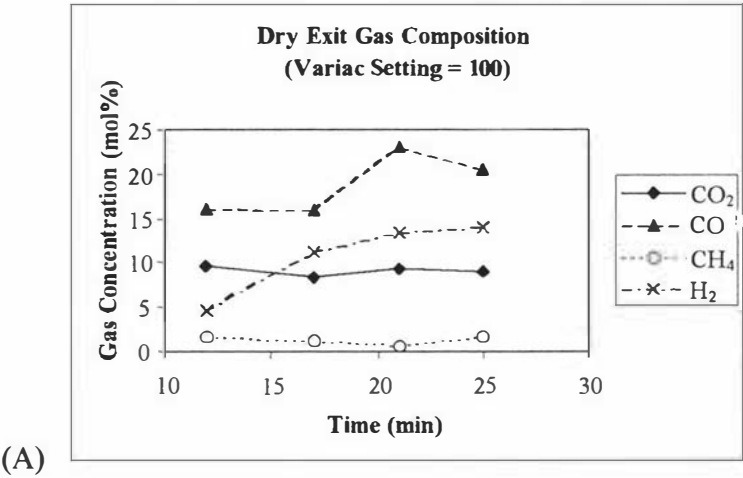


Figure 4.9: Exit gas temperature during steady-state operation vs the molar flow rate of air into the inlet.

Figure 4.9 shows the "steady-state" exit gas temperatures plotted against the rate of air flow into the gasifier. There was a small variation in the exit gas temperature over the range of air flow rates investigated with an apparent peak in the gas exit temperature around an air flow rate of 0.4 mol/s. The reactions of CO_2 and H_2O with the char surface are endothermic and will act to lower the gas temperature. Therefore at high air flow rates the higher oxygen concentrations in the combustion region lead to higher reduction reaction rates (and thus lower exit gas temperatures) due to higher initial temperatures and greater concentrations of CO_2 and H_2O being produced. However, below a certain air flow rate the exit gas temperature is lowered by the longer residence time of the gas within the gasifier that allows more reduction reactions to occur within the gas despite the reduced reaction rates.

(B) Exit Gas Composition

Figures 4.10 (A) - (D) show the composition of the dry exit gas at different times throughout the same gasifier runs used in Figures 4.8 (except for Figure 4.8(B) which was from a different run from Figure 4.10(B)). The molar percentages of CO , CO_2 , CH_4 and H_2 were measured using gas chromatography.



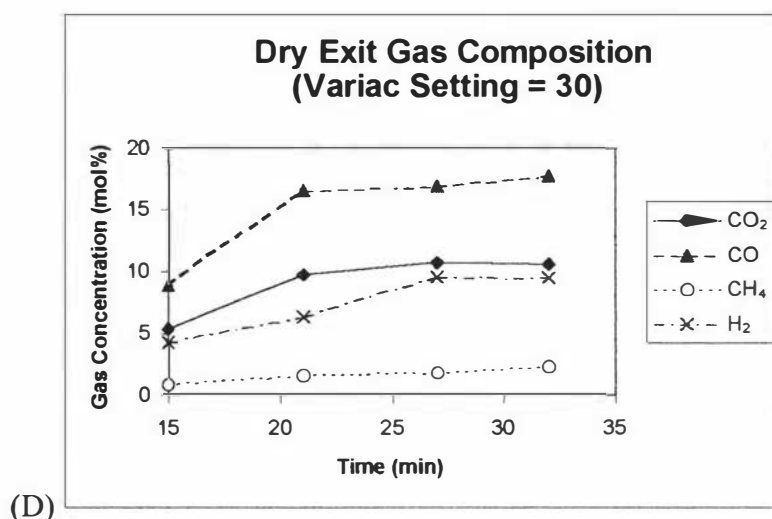
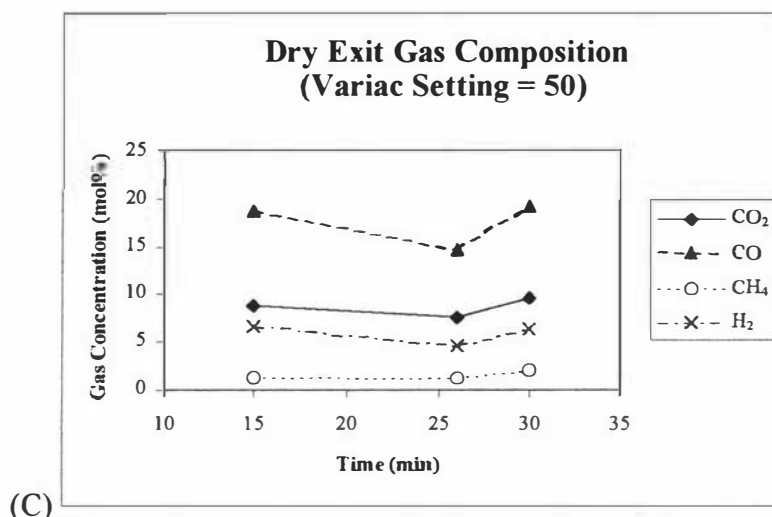
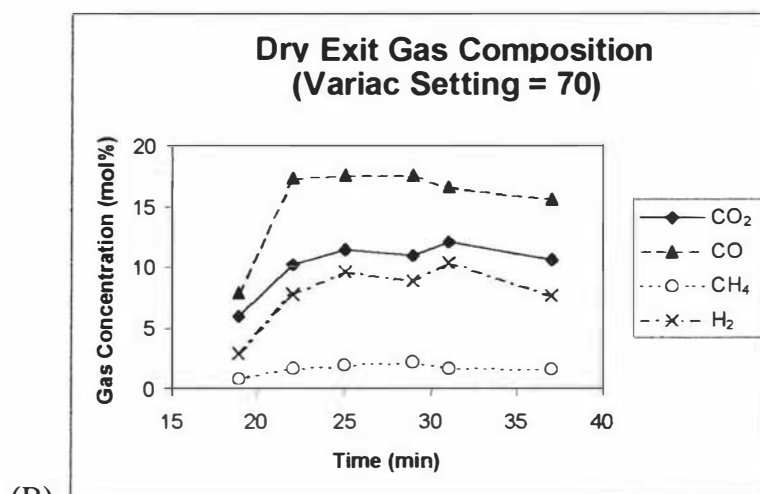


Figure 4.10: Measured gas concentrations (expressed as volume percentages) vs time for gasifier using pine chips as fuel. Bed length in all cases was 10 ± 1 cm. The molar flow rate of air (at vacuum cleaner inlet) was (A) 0.6 ± 0.1 mol/s, (B) 0.4 ± 0.1 mol/s, (C) 0.32 ± 0.06 mol/s and (D) 0.22 ± 0.03 mol/s.

Figure 4.11 shows the steady-state composition of the dry exit gas for the different air input flow rates. The gas compositions are the averages of all samples taken within the “steady-state” time intervals identified in Table 4.1.

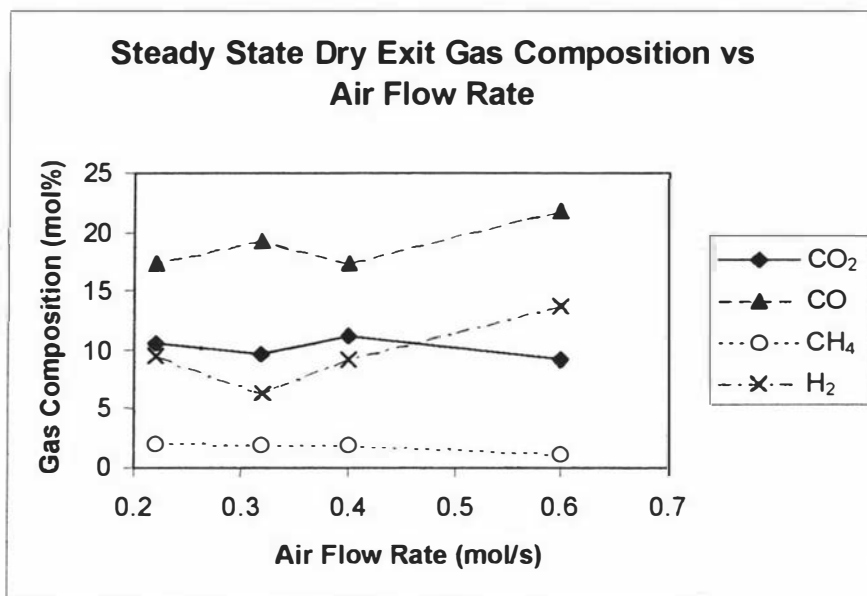


Figure 4.11: Steady-state composition of dry exit gas vs the flow rate of air into the gasifier.

The amount of CO in the exit gas generally increased with increasing input air flow both as a percentage of the total dry gas and relative to the amount of CO₂ in the gas. The increased air flow rate had the effect of both increasing the amount of carbon taken up by the gas and increasing the fraction of carbon within the gas that was in a combustible form.

The H₂ content of the gas appears to have a local minimum within this air flow range. There was also a local maximum in steady-state exit gas temperature around 0.4 mol/s. A decrease in H₂ formation would be consistent with an increased exit temperature as the major H₂ forming reaction is endothermic. However, the two local extrema do not exactly overlap.

(C) Mass and Energy Balances of Gasifier

Equations 4.2 to 4.5 were solved for the steady-state temperatures and exit gas concentrations found for the series of pine chip runs using different air flow rates. Table 4.4 shows the calculated values of parameters a , b , c and d .

Dry Gas Composition	Air Flow Rate (mol/s)			
	0.22 ± 0.03	0.32 ± 0.06	0.4 ± 0.1	0.6 ± 0.1
N ₂	60.7 ± 0.5%	63% ¹	60 ± 2%	54.4 ± 0.9%
CO ₂	10.6 ± 0.1%	10%	11.2 ± 0.9%	9.1 ± 0.2%
CO	17.3 ± 0.5%	19%	17.3 ± 0.1%	22 ± 1%
CH ₄	1.9 ± 0.2%	1.9%	1.9 ± 0.2%	1.1 ± 0.5%
H ₂	9.5 ± 0.1%	6.3%	9 ± 1%	13.6 ± 0.2%
HHV Dry Product Gas (kJ/mol)	93 ± 3	89	92 ± 6	110.6 ± 0.8
a	0.87 ± 0.03	1.2	1.1 ± 0.2	1.2 ± 0.5
b	0.66 ± 0.02	0.5	0.55 ± 0.09	0.5 ± 0.2
c	0.804 ± 0.009	0.80	0.76 ± 0.06	0.69 ± 0.09
d	1.13 ± 0.04	1.5	1.5 ± 0.3	1.7 ± 0.7
Exit gas moisture content (mol. percent)	42 ± 1%	40%	34 ± 6%	30 ± 10%

Table 4.4: Values of parameters a , b , c , and d derived from experimental measurements of steady-state downdraft gasifier product gas for various air flow rates.

Most of the mass balance parameter values calculated did not change significantly as the air flow rate into the gasifier was varied from 0.22 ± 0.03 mol/s to 0.6 ± 0.1 mol/s.

¹ Uncertainties for this run have not been calculated as only one sample was collected during the "steady-state" phase of this run.

However, the fraction of carbon remaining in solid form (parameter *c*) appeared to decrease slightly with increasing air flow rate.

The mass balance parameters were used to perform an energy balance on the gasifier. Energy can leave the gasifier in the following forms: the chemical energy of the exit gas, the thermal energy of the exit gas, the latent heat of vaporisation of the moisture content and the chemical energy remaining in the char (which we assumed to equal the heat of combustion of carbon). This was compared to the HHV of the original biomass and the thermal energy of the inlet air. Any differences were assumed to be "losses" from the system.

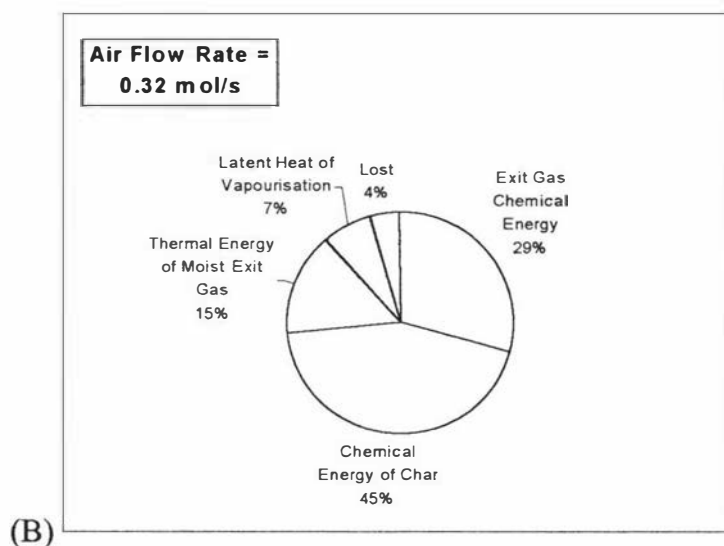
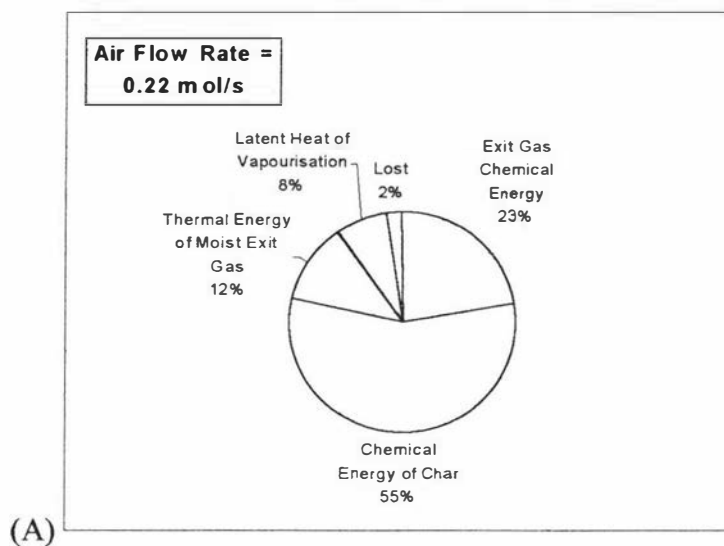
Air Flow Rate (mol/s)	0.22 ± 0.03	0.32 ± 0.06	0.4 ± 0.1	0.6 ± 0.1
Chemical Energy of Dry Product Gas	105 ± 7	137	140 ± 30	190 ± 70
Chemical Energy of Char ²	260 ± 8	207	220 ± 40	180 ± 90
Thermal Energy of Moist Product Gas	56 ± 2	71	70 ± 7	70 ± 20
Latent Heat of Vaporisation of Moisture in Exit Gas.	35.4 ± 0.3	35	34 ± 2	30 ± 4
HHV of wood ³	459	459	459	459

² Assuming the remaining carbon is in the form of graphite.

³ Department of Energy (2002)

Thermal Energy of Inlet Air	7.4 ± 0.2	10	10 ± 2	10 ± 4
Energy Lost	10	19	5	5

Table 4.5: Energy balance for gasification of a mole of pine chips with different air flow rates. All energies are quoted in kJ.



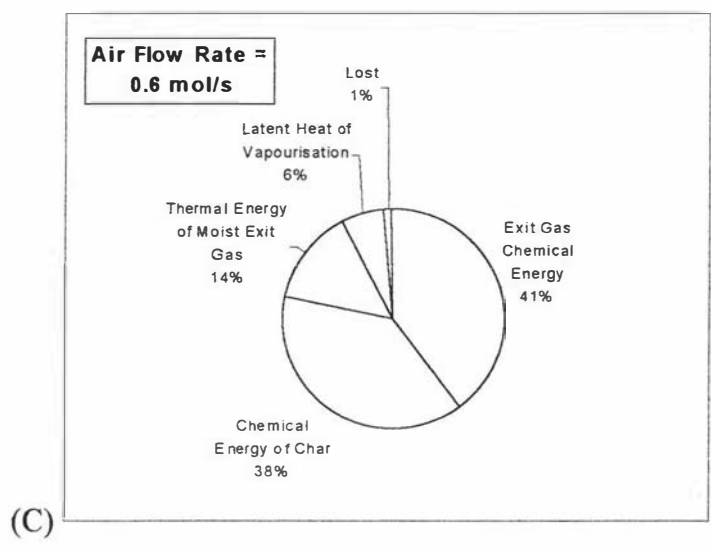


Figure 4.12: Energy balances for gasification of pine chips at air flow rates of (A) 0.22 ± 0.03 mol/s, (B) 0.32 ± 0.06 mol/s and (C) 0.6 ± 0.1 mol/s. All energies are quoted as percentages of the energy input (that is, the HHV of the fuel consumed and the thermal energy of the inlet air).

The major effect of increasing the air flow rate in terms of energy is that a greater proportion of the HHV of the fuel is converted to the chemical energy of the product gas, with a corresponding reduction in the chemical energy in the residual char. Generally the HHV of the dry product gas is the key factor in the utility of a gasifier. However, depending upon the application, some of the thermal energy of the exit gas and HHV of the char may also be recoverable.

The rate of energy production is important for applications, such as electricity production, where the product gas is used continuously rather than being stored for later consumption. As the moisture content of the product gas was not measured directly we calculated the rate of dry gas production using the steady state assumption that the molar flow rate of inert N_2 at the air inlet equals the molar flow rate of N_2 exiting the gasifier. Table 4.6 below shows the results of these calculations.

	Air Flow Rate (mol/s)		
	0.22 ± 0.03	0.32 ± 0.06	0.6 ± 0.1
N_2 inlet flow rate	0.17 ± 0.02	0.25 ± 0.05	0.47 ± 0.08

(mol/s)			
Dry Product Gas N ₂ Content (mol %)	60.7 ± 0.5%	63.0%	54.3 ± 0.9%
Dry Product Gas Flow Rate (mol/s)	0.28 ± 0.04	0.40 ± 0.08	0.9 ± 0.2
Rate of Exit Gas Chemical Energy Production (kW)	26 ± 5	36 ± 7	100 ± 20

Table 4.6: Rate of exit gas chemical energy production for different air flow rates.

Over the range of air flow rates measured, the rate of exit gas production increased with increasing air flow rate leading to an increased rate of chemical energy production.

(D) Summary

In conclusion, altering the air flow rate alters the composition and rate of production of the exit gas. Using a simple mass balance formula we calculated that over the range of air flows considered the amount of dry product gas produced per mole of fuel consumed increased with increasing air flow, while the fraction of carbon remaining in solid form decreased. The rate of dry gas production calculated by equating the rate of N₂ exiting the gasifier to the rate of N₂ entering the gasifier was found to increase with increasing air flow rates. Over the range of air flow rates measured the rate of chemical energy production was increased by increasing the air flow rate.

4.4 Effect of Different Fuel Types

Some gasification runs were made using walnut shells instead of pine chips as fuel. Walnut shells differ in both shape and composition from pine chips. In Section 2.2(B) we plotted the pressure gradient versus air speed for a bed of walnut shells and for a bed of pine chips. It was found that the pressure gradient was significantly lower for the bed of walnut shells, indicating that the walnut shells were providing less resistance to the air

flow. Walnut shells also have slightly less volatile components than pine chips (as a weight fraction).

(A) Exit Gas Temperature

A gasification run was performed using walnut shells as fuel with a bed length of 10 ± 1 cm. Temperature measurements were logged every 5 seconds. Figure 4.13 shows a five point moving average of the exit gas temperature plotted against time.

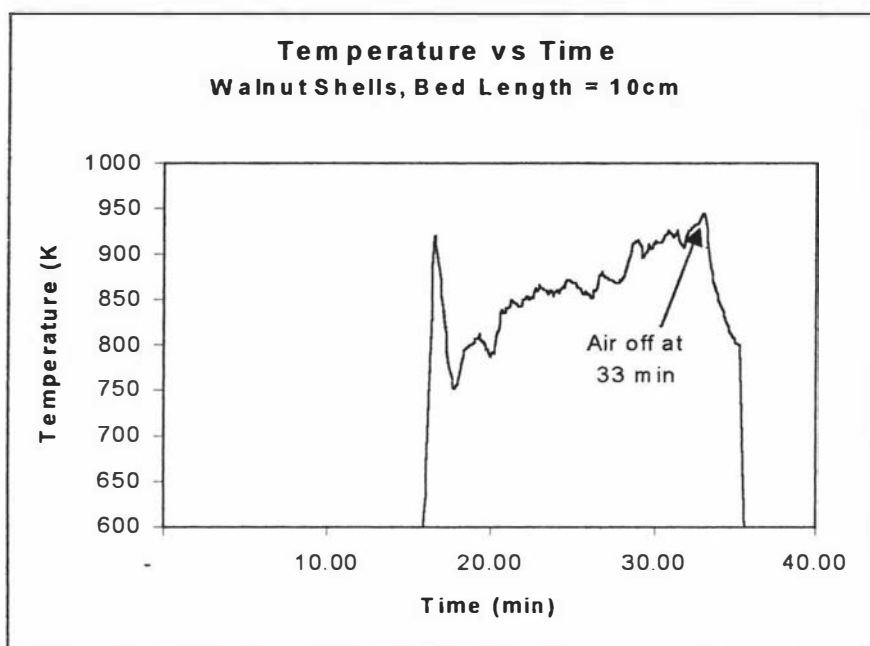


Figure 4.13: Temperature of exit gas vs time for gasifier operating on walnut shells. Bed length = 10 ± 1 cm.

The exit gas temperature in Figure 4.14 does not appear to reach a steady temperature before the air was turned off at 33 min. However, the exit gas composition for this run (see Section 4.4(B) below) showed that at 28 minutes the exit gas contained significant amounts of oxygen. This suggests that the fuel was nearly depleted by that time and that the time interval from 21-26 minutes was the closest approximation to steady-state operation. The average temperature over this time interval was 860 ± 20 K. This was lower than the steady-state exit gas temperature for pine chips gasified under similar conditions.

(B) Exit Gas Composition

Figure 4.14 shows the composition of the exit gas for the same run as plotted in Figure 4.13.

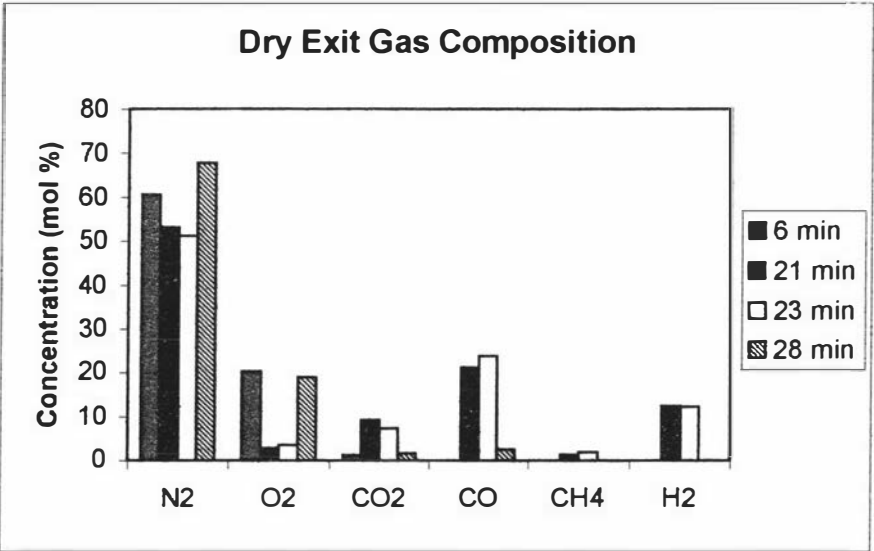


Figure 4.14: Composition of dry exit gas. Gasifier operating with walnut shells for fuel, bed length = 10 ± 1 cm.

These gas samples were analysed using the Alltech CRTI column in the gas chromatograph. This column, unlike the silica gel packed column, was able to separate N₂ and O₂ in the sample but could not detect H₂. The first and last sample taken (at 6 minutes and 28 minutes respectively) contained mostly air indicating that gasification was not occurring. The other two samples were quite similar to each other and were assumed to be representative of the steady-state product gas. In both the steady-state samples there was a small amount of O₂ detected (~3%). This adds to the plausability of the conjecture in Section 4.2(B) that there was some O₂ remaining in the gasifier at a depth of 10 cm.

The unaccounted for fraction of these two samples was assumed to consist entirely of H₂. The H₂ concentrations thus calculated represents the upper limit of H₂ in the exit gas. Figure 4.15 shows the steady-state composition of the exit gas produced using walnut shells compared to that produced using pine chips.

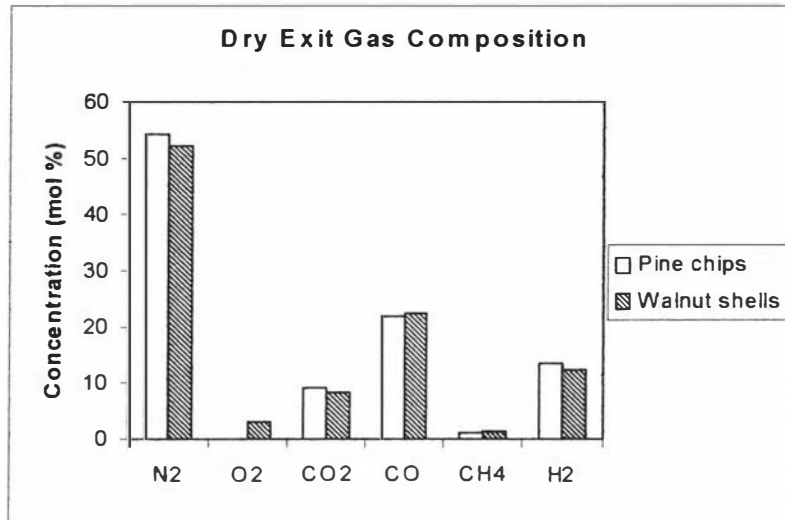


Figure 4.15: Composition of steady-state dry exit gas for gasifier run on pine chips and walnut shells. In both cases the air flow rate was 0.6 ± 0.1 mol/s and the bed length 10 ± 1 cm. For the pine chip run the N_2 concentration was assumed whereas for the walnut shell run the H_2 concentration was assumed.

The two results are very similar, especially when the fact that the O_2 concentration for the pine chips was assumed to be zero effectively making the calculated N_2 concentration the sum of the N_2 and O_2 concentrations. The walnut shell dry exit gas has an HHV of 112 ± 6 kJ/mol, similar to that of the dry exit gas produced by pine chips.

(C) Mass and Energy Balances of the Gasifier

Table 4.7 shows the composition of dry walnut shells obtained from the Phyllis Database for Biomass and Waste (Netherlands Energy Research, 2002):

	Composition (weight %, dry basis)	Composition (mol %, dry basis)
C	50	33.2
H	5.71	45.3
O	43.3	21.5
Volatiles	78.3	

HHV	20.180 MJ/kg	
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Table 4.7: Composition of walnut shells (Netherlands Energy Research, 2002).

The empirical formula for walnut shells can therefore be written as $\text{CH}_{1.36}\text{O}_{0.65}$. The moisture content of the walnut shells was measured as 12.3% as a weight percentage of the dry fuel. Therefore for every mole of dry fuel there are 0.162 moles of water.

Equations 4.2 to 4.5 were solved to find the value of parameters a , b , c , and d . Equation 4.6 below replaced Equation 4.4 to account for the presence of O_2 in the exit gas.

$$(4.6) \quad \gamma + X + 0.42a = c + d(2x_2 + x_3 + 2x_6)$$

where x_6 is the mole fraction of O_2 in the dry exit gas.

Dry Gas Composition (mol%)	
N_2	52.1%
CO_2	8.3%
CO	22.5%
CH_4	1.6%
H_2	12.3%
O_2	3.2%
HHV Dry Product Gas (kJ/mol)	112 ± 6
a	-1.00
b	1.49
c	1.08
d	-1.52

Table 4.8: Values of parameters a , b , c , and d derived from experimental measurements of steady-state dry exit gas composition for downdraft gasifier operated using walnut shells as fuel with a bed depth of 10 ± 1 cm.

The values of parameters a and d calculated were negative. This does not make sense physically, so there must be something wrong with the assumptions made. The most likely explanation is that the gasifier had not reached "steady-state" operation at the time the gas samples were taken. Other possible explanations include the moisture content and/or composition of the walnut shells changing during the start-up phase or processes occurring that were not accounted for in Equation 4.1.

(D) Summary

The walnut shell run had slightly less fuel (by volume) than was used for the pine chip runs. This meant that the fuel was exhausted quite quickly and that the gasifier was only operating in "steady-state" mode for a short time (or may not quite have achieved steady operation). The composition of the gas during the time interval that steady-state operation was very close in composition to that produced using pine chips as a fuel under similar conditions but the exit gas temperature was slightly lower. However, the mass balance equations did not produce a physically meaningful result using the composition of the dry product gas found and the composition of walnut shells listed in the Phyllis Database (Netherlands Energy Research, 2002). This indicated that some of the assumptions used in formulating these equations did not hold.

4.5 Conclusion

In the batch mode gasifier runs there was a short interval of time during which the gasifier operation was approximately steady-state. A simple "mass balance" relationship on the gasifier steady-state output indicated that a significant proportion of the carbon in the fuel remained in solid form. This was supported by the black colour of the "ash" collected after a gasifier run.

Altering the depth of the gasifier bed beneath the air inlets between 0.10 and 0.24 m only made a small difference in the temperature of the exit gas. However, the exit gas temperature did appear to increase when the bed length was increased from 0.10 to 0.13 cm. This is the opposite of what would be expected if only reduction reactions were occurring at these depths. However, if O_2 was still present at these depths then some

combustion reactions could also occur. The gas compositions were analysed but these analyses assumed that there was no O_2 in the exit gas. Analyses by Sime (1998) and of exit gas samples produced by gasifying walnut shells indicated that some (< 5 mol %) O_2 could have been present in the exit gas. This meant that the mass and energy balance equations were not accurate, but the amounts of CO_2 , CO , CH_4 and H_2 measured in the dry exit gas were not affected by this assumption.

Increasing the air flow into the gasifier generally increased both the rate of gas production and the heating value of the dry product gas over the range of flow rates investigated. Applying the mass and energy balance equations to these results indicated that a higher air flow rate results in a greater conversion of energy from the solid fuel to the product gas and less carbon left in the solid residue.

Some walnut shells were also gasified. The dry product gas was very close in composition to that produced using pine chips although the exit temperature was slightly lower. However, the fuel for this run was depleted quite quickly and it is possible that the gasifier had not completely stabilised before the fuel was exhausted. Solving the mass balance equations using the measured composition of the dry exit gas and the composition of walnut shells from the literature did not produce a physically meaningful result.

5. Comparing Experimental Results with Model Predictions

In Chapter 3 we developed a model of steady-state downdraft gasification that predicted dry gas compositions within $\pm 10\%$ of previously published experimental results (with the exception of the CH_4 and H_2 compositions or the CO_2 and H_2 compositions depending on whether or not methane combustion was included in the reaction scheme). In this chapter we compare the model predictions with the experimental results found in Chapter 4 to see whether the model correctly predicted the effect of varying the bed length and the air inflow.

5.1 Model without Methane Combustion

The fuel had a moisture content of 18.7% of the dry fuel weight. The pyrolysis gas composition calculated was 45.9% CO , 27.8% CH_4 and 26.3% H_2O (molar basis). The volatile fraction of pine wood comprised 80.45% of the dry wood mass (Department of Energy, 2002). Therefore for every 80.45 g of pyrolysis gas generated, 100 g of dry wood had been devolatilised and 18.7 g of additional water evaporated. In molar terms this translates to 0.284 extra moles of water for every mole of pyrolysis gas produced. We included the extra water as part of the pyrolysis fraction on the assumption that the proportional decrease in the other pyrolysis products reflected the loss of energy available to drive pyrolysis and cracking due to the requirement to evaporate the moisture content. The composition of the pyrolysis gas plus extra moisture was 35.7% CO , 21.7% CH_4 and 42.6% H_2O .

We used the same C_{RF} and f_p values that were used in Chapter 3 (500 and 0.4 respectively). We assumed that the temperature at the top of the reduction zone was 1200 K.

We used atmospheric pressure for the pressure at the top of the gasifier. The pressure inside the gasifier would actually have been slightly higher than atmospheric pressure. The effects of pressure on the gasifier performance were plotted in Figure 3.2. The

slight under-estimation of the pressure inside the gasifier should not have significantly effected the results.

Figure 5.1 below shows the model prediction of the dry gas composition for an air flow rate of $0.22 \pm 0.03 \text{ mol.s}^{-1}$ and bed length of $0.10 \pm 0.01 \text{ m}$ compared to the experimental results.

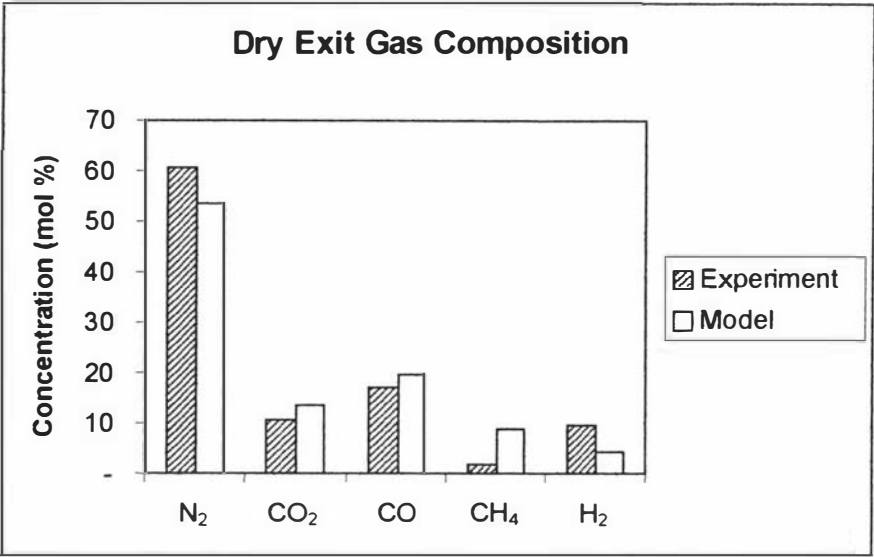


Figure 5.1: The dry exit gas composition found for a gasifier run using an air flow rate of $0.22 \pm 0.03 \text{ mol.s}^{-1}$ and bed length of $0.10 \pm 0.01 \text{ m}$ compared to the model prediction.

The major discrepancy between the model prediction and the experimental result is that the model over-predicted CH₄ and under-predicted H₂. The same was found in Chapter 3 when the model was compared to previously published experimental results.

(A) Effect of Varying Air Flow Rate

The superficial gas velocity was calculated by converting the volume flow rate of air into the gasifier into a molar flow rate. The total molar flow rate was calculated by dividing the molar flow rate of air by $(1-f_p)$ to account for the pyrolysis gases. The total molar flow rate was converted into a volume flow rate using the ideal gas law (Equation 3.12). Then the volume flow rate was divided by the cross-sectional area of the gasifier to obtain the superficial gas velocity.

Table 5.1 shows the initial values for the superficial gas velocities corresponding to the different air flow rates used.

Air flow rate (mol.s ⁻¹)	Superficial gas velocity at top of gasifier (m.s ⁻¹)
0.22 ± 0.03	1.1 ± 0.2
0.32 ± 0.06	1.7 ± 0.3
0.4 ± 0.1	2.1 ± 0.5
0.6 ± 0.1	3.1 ± 0.5

Table 5.1: Superficial gas velocities corresponding to the different air flow rates for an f_p of 0.4, temperature of 1200 K, pressure of 101,300 Pa and gasifier bed diameter of 0.2 m.

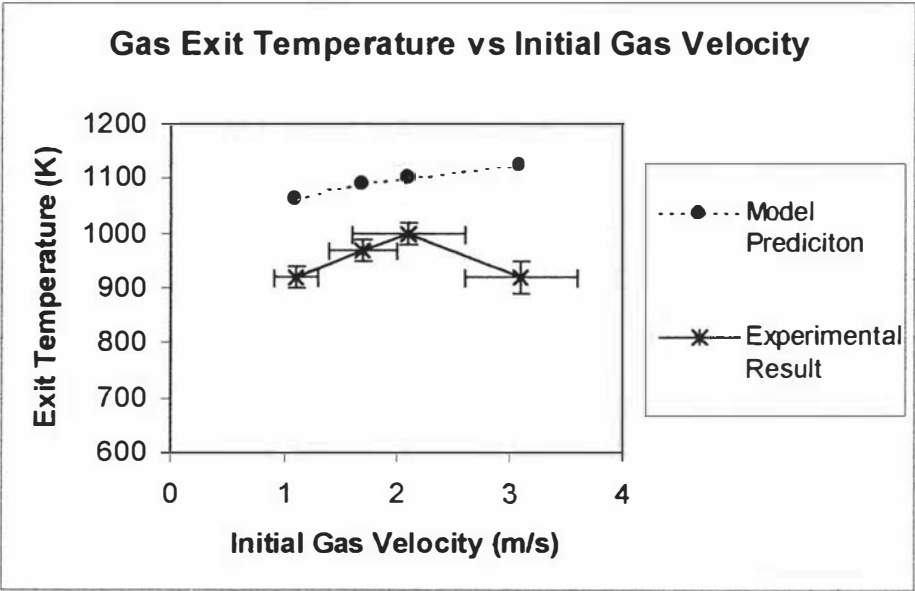


Figure 5.2: Experimental results and model predictions of the exit gas temperature vs initial gas velocity for a bed length of 0.10 ± 0.01 m.

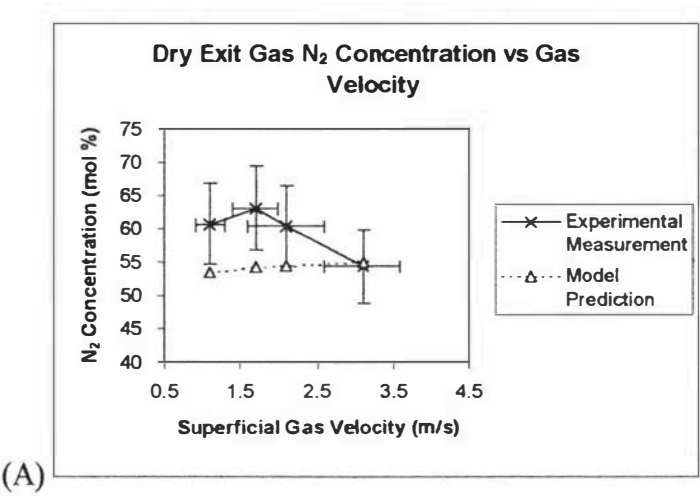
In Figure 5.2 the steady-state exit temperature was plotted against the initial gas velocity for the experimental results and for the model predictions using a C_{RF} of 500 and an f_p of 0.4. The model predicted an increase in exit gas temperature with increasing initial

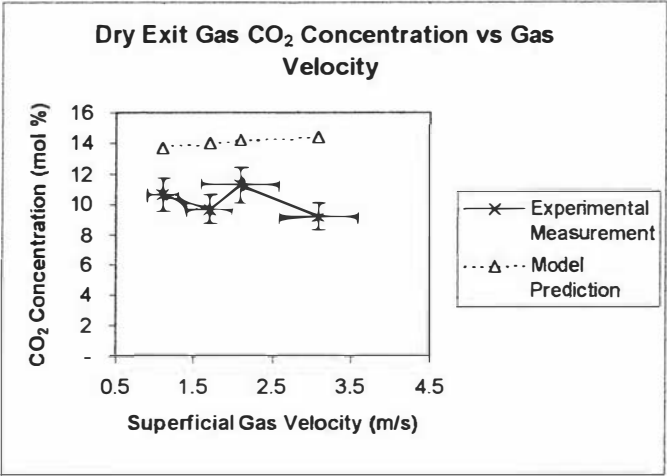
gas velocity. This was because the higher gas velocities corresponded to a lower residence time and therefore less time for the endothermic reduction reactions to lower the gas temperature.

The model temperature predictions were all slightly higher than the experimental results. This could be the result of the C_{RF} in the model being slightly too low and therefore fewer endothermic reactions occurring during the gas residence time.

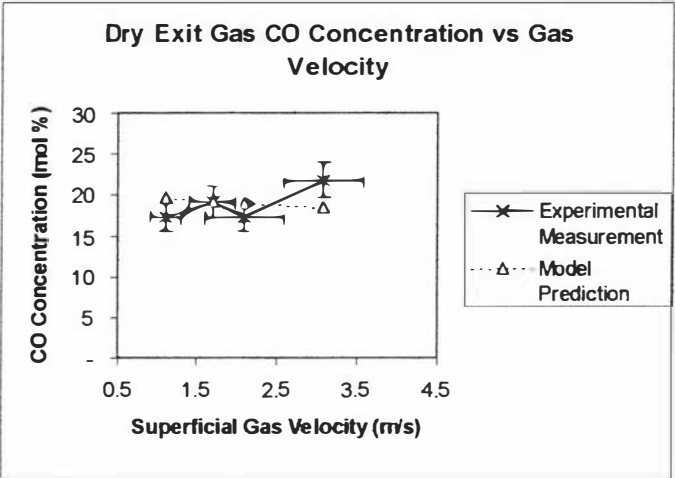
The first three experimental points also followed an increasing temperature trend (although the exit temperature was consistently lower than the model prediction). The experimental result at the highest gas velocity had a lower exit temperature than expected. The model assumed that the f_p and initial temperature remained constant for all air flow rates, however it could be the case that a higher rate of air flowing into the gasifier led to a change in the initial temperature or the relative amount of pyrolysis products produced.

Figures 5.3(A)-(E) below show the "steady-state" dry gas composition as the initial superficial gas velocity is varied.

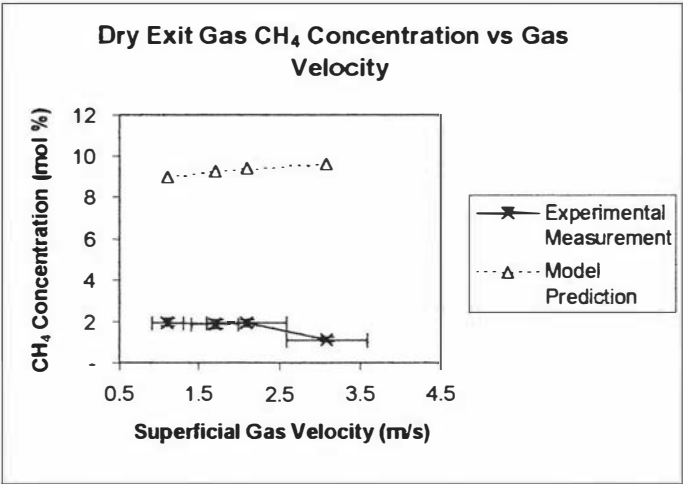




(B)



(C)



(D)

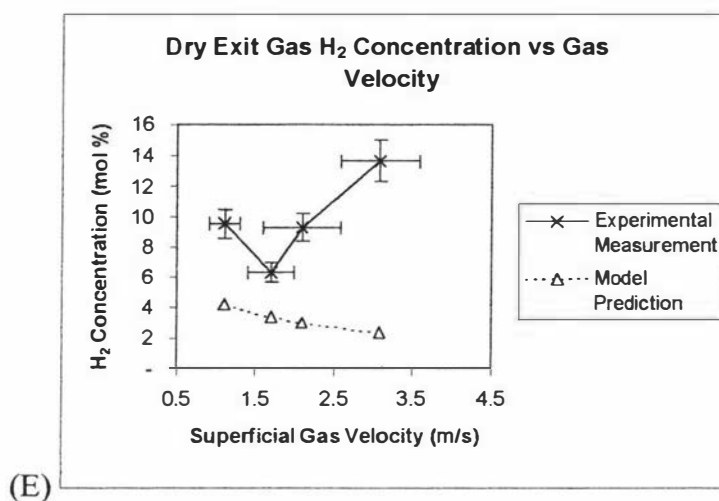


Figure 5.3: Model predictions and experimental measurements of the molar fraction of (A) N₂, (B) CO₂, (C) CO, (D) CH₄ and (E) H₂ in the dry exit gas as the initial superficial gas velocity is varied. The bed length was 0.10 ± 0.01 m.

The model predictions of the N₂ and CO concentrations in the exit gas were close to the experimental measurements within the uncertainties involved. However, the CO₂ and the CH₄ concentration predicted by the model were consistently higher than found experimentally. The model under-predicted the H₂ concentration.

In general the uncertainties in the experimental measurements were too large to see whether the trends predicted by the model were followed over the range of initial gas velocities examined. In all the experimental measurements the value at the highest initial superficial gas velocity diverged significantly from the other measurements. This could be because at high air flow rates the conditions at the top of the gasifier (for example, the temperature and the pyrolysis fraction) may have changed rather than remaining constant as the model assumed.

(B) The Effect of Varying Bed Length

A series of gasifier runs with varying bed lengths were made using an air flow rate of 0.22 ± 0.03 mol.s⁻¹. Figure 5.4 shows the steady-state exit gas temperatures plotted against the gasifier bed length.

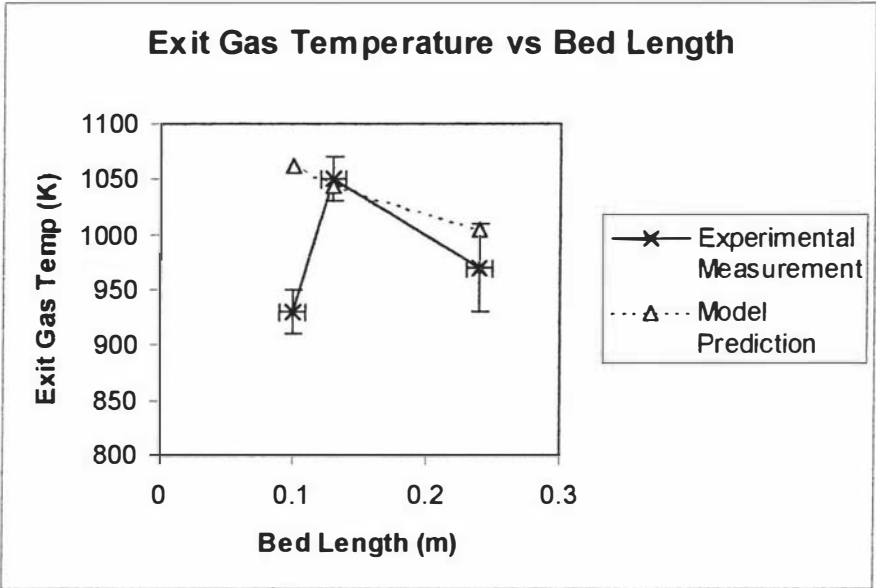
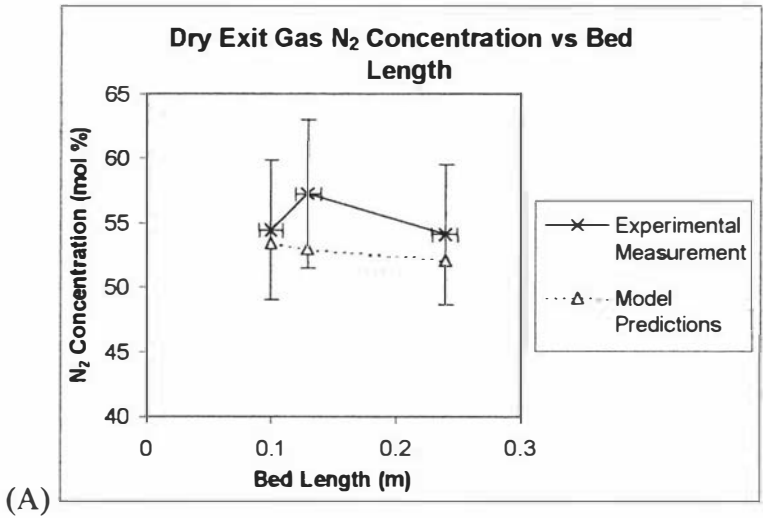
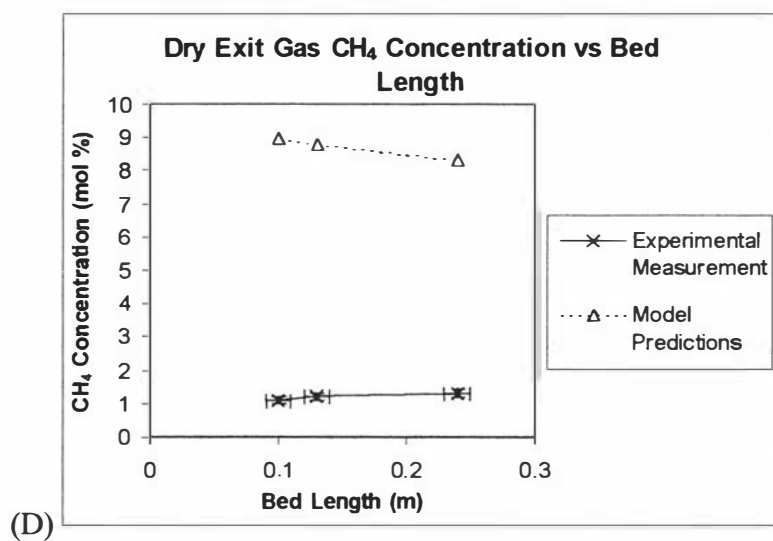
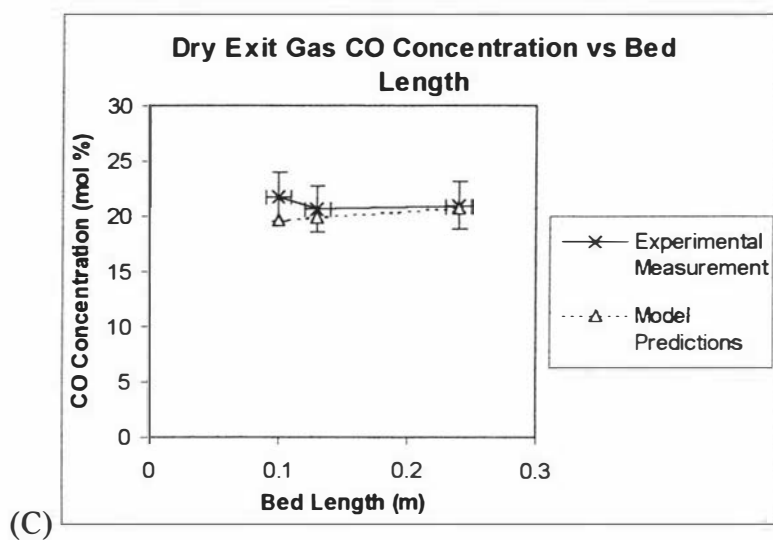
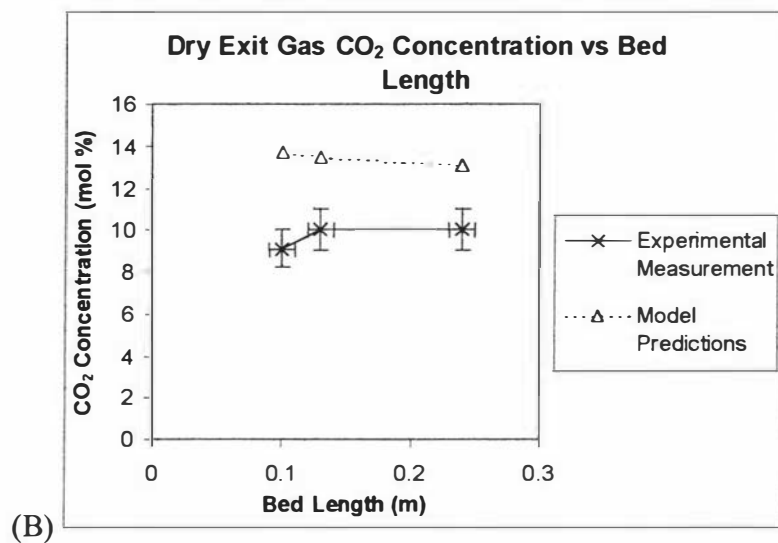


Figure 5.4: Experimental measurement and model prediction of the steady-state exit gas temperature vs gasifier bed length. The air flow rate was $0.22 \pm 0.03 \text{ mol.s}^{-1}$.

The model prediction agreed with the experimental results for the two longer bed lengths, but was slightly too high for the 0.1 m bed length.

The dry exit gas concentrations vs bed length were plotted in Figure 5.5 (A)-(E).





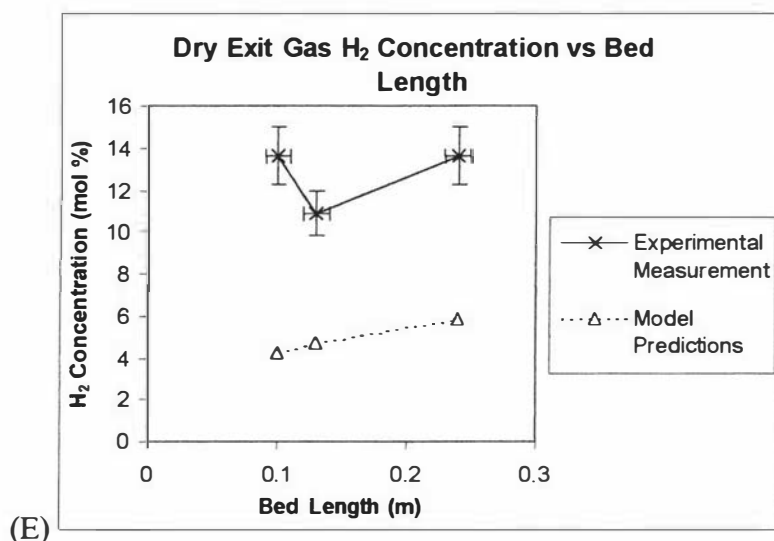


Figure 5.5: Model predictions and experimental measurements of the molar fraction of (A) N_2 , (B) CO_2 , (C) CO , (D) CH_4 and (E) H_2 in the dry exit gas as the bed length was varied. The air flow rate was 0.22 ± 0.03 m.

The model predicted the N_2 and CO concentrations in the dry exit gas to within the uncertainties of the experimental values. The model significantly over-predicted the CH_4 and under-predicted the H_2 produced when compared with the experimental findings. The model CO_2 predictions were slightly higher than the experimental results. So the differences between the model predictions and the experimental results as the bed length was varied were similar to the differences found when varying the air flow rate. Again some trends in the model predictions were visible as the bed length was varied but the uncertainties in the experimental results were too large to tell whether the experimental results were following the same trends.

(C) Summary

In both the series of runs that varied the initial gas velocity and the series varying the bed length there seemed to be one run that differed from the model prediction more than the others.

In the series where the initial gas velocity was varied it was the run corresponding to the highest initial gas velocity that deviated most significantly from the model predictions. One explanation is that the higher air flow rate into the gasifier resulted in a change in

the initial temperature and/or amount of pyrolysis products produced. The model assumed that the initial temperature and f_p were the same for all runs.

In the series where the bed length was varied the results for the shortest bed length were slightly anomalous. The gas residence time is proportional to the length of the gasifier bed. The model assumed that the combustion/cracking reactions were sufficiently fast that all the oxygen was effectively consumed at the air inlets. However, in reality oxygen combustion will continue down to a certain depth in the bed where either all the oxygen has been depleted or the temperature is too low to maintain combustion. The shorter the bed length the more likely it is that there are still unaccounted for combustion reactions occurring at the gas exit.

5.2 Model including Methane Combustion Reactions

In Section 5.1, it was found that the model that neglected methane combustion reactions resulted in an over-prediction of the methane concentration in the dry exit gas. In this section we compare the experimental results with the predictions from the model that included methane combustion reactions.

In Section 3.2 two different pyrolysis gas compositions were tried (one consisted of CO, CH₄ and H₂O, the other of CO₂, CH₄ and H₂O). In this section we used the second pyrolysis gas composition which over-predicted the dry gas H₂ concentration in Section 3.2 but overall produced a closer prediction of the dry exit gas composition. Allowing for the 18.7% moisture content of the fuel using the method in Section 5.1 above we obtained a pyrolysis gas composition of: 34.7% CO₂, 25.6% H₂O, and 39.7% CH₄ (molar basis). The C_{RF} and f_p values used were the same as used for this pyrolysis gas in Chapter 3 (2000 and 0.3 respectively).

(A) The Effect of Varying the Air Flow

Figure 5.6 shows the model predictions and experimental measurements of the exit gas temperature plotted against the initial superficial gas velocity.

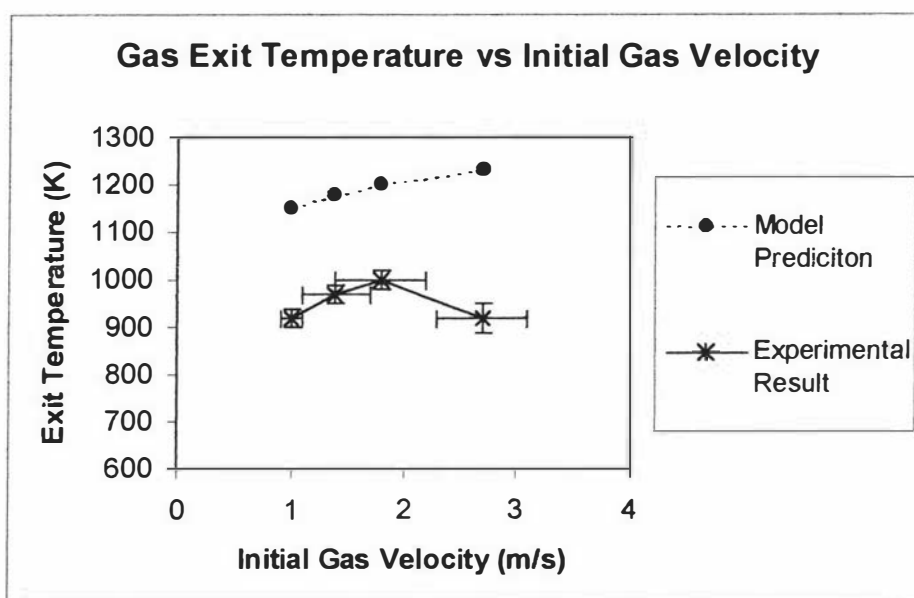
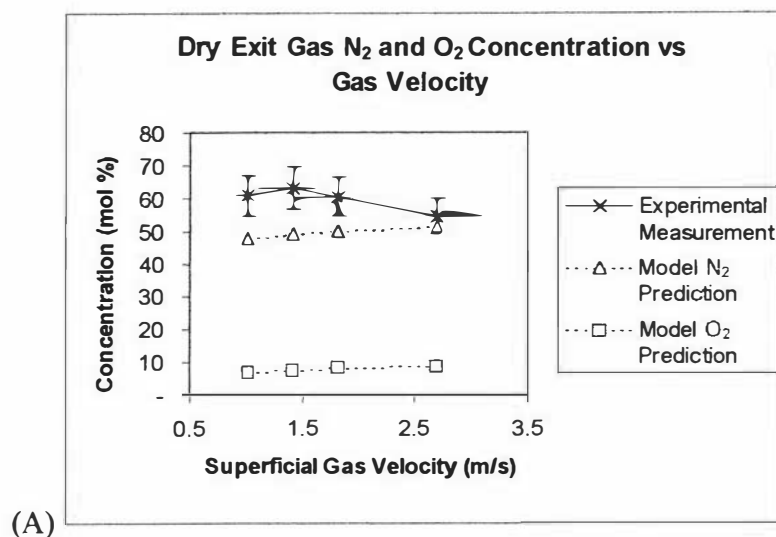


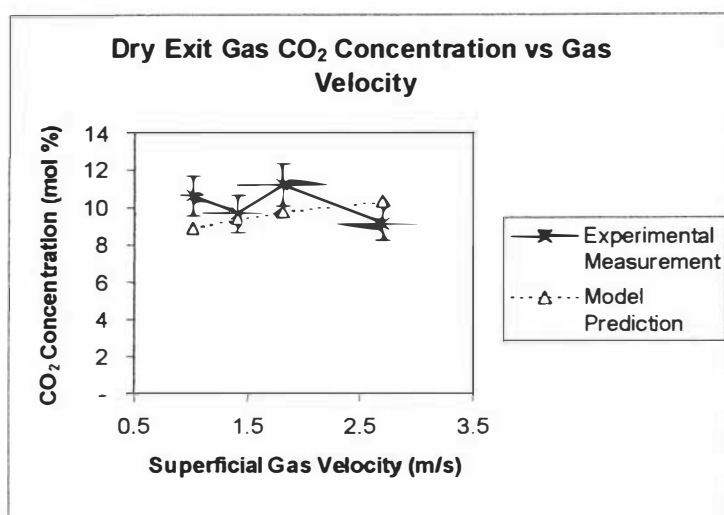
Figure 5.6: Experimental results and model predictions of the steady-state exit gas temperature vs initial gas velocity for a bed length of 0.10 ± 0.01 m.

The model temperature predictions were higher than the exit gas temperatures found experimentally. This could be due to the C_{RF} or initial temperature values selected for the model. At the highest initial gas velocity the model predicts an exit gas temperature higher than the initial temperature. This indicates that the exothermic combustion reactions were still significant at this point.

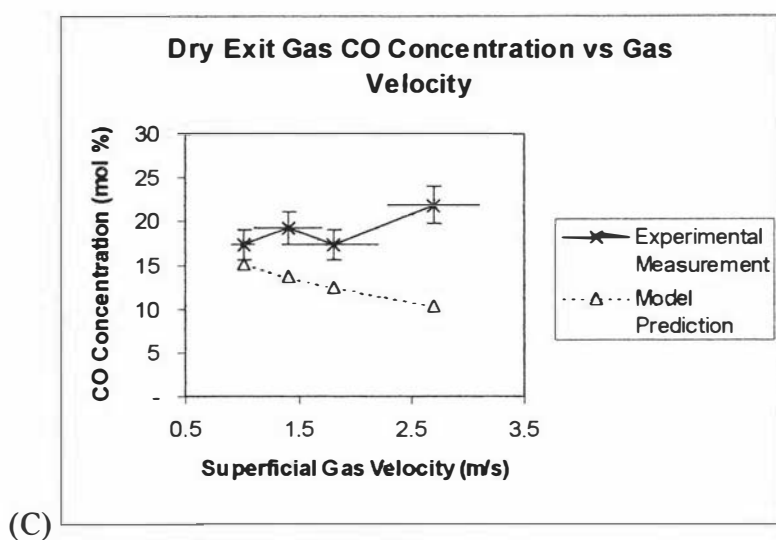
Figure 5.7 (A)-(E) show the concentrations of each gas component plotted against the initial superficial gas velocity.



(A)



(B)



(C)

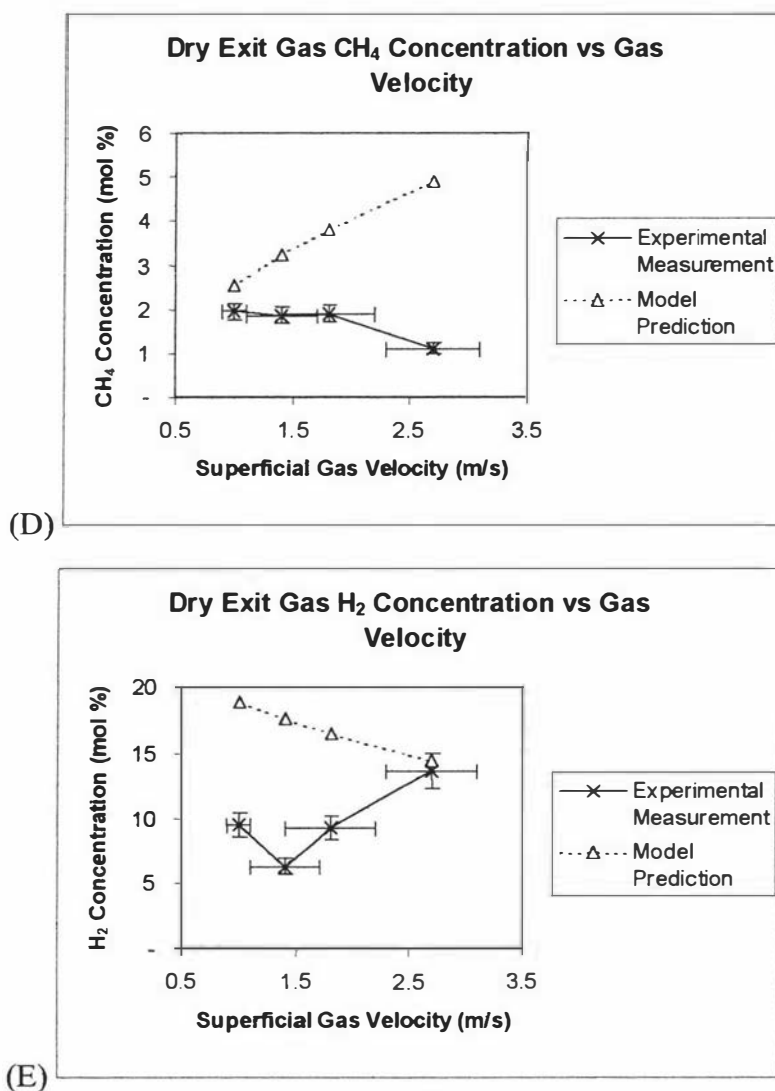


Figure 5.7: Model predictions and experimental measurements of the molar fraction of (A) N_2 , (B) CO_2 , (C) CO , (D) CH_4 and (E) H_2 in the dry exit gas as the initial superficial gas velocity is varied. The bed length was 0.10 ± 0.01 m.

The sum of the model N_2 and O_2 concentrations agreed with the experimental N_2 measurement¹. Similarly the model prediction of the dry exit gas CO_2 concentration agreed with the results within the experimental uncertainties involved. The model under-predicted the dry gas CO concentration and over-predicted the H_2 concentration.

¹ Note that the experimental N_2 mole fraction was found by subtracting the measured mole fractions of CO_2 , CO , CH_4 and H_2 in the dry exit gas from 1. Therefore any O_2 in the exit gas would have been included in the N_2 concentration.

The CH₄ concentration was still over-predicted by the model, but not as dramatically as the earlier model that neglected CH₄ combustion.

(B) The Effect of Varying Bed Length

A series of gasifier runs with varying bed lengths were made using an air flow rate of $0.22 \pm 0.03 \text{ mol.s}^{-1}$. Figure 5.8 shows the model predictions and the experimental measurements of the exit gas temperature plotted against bed length.

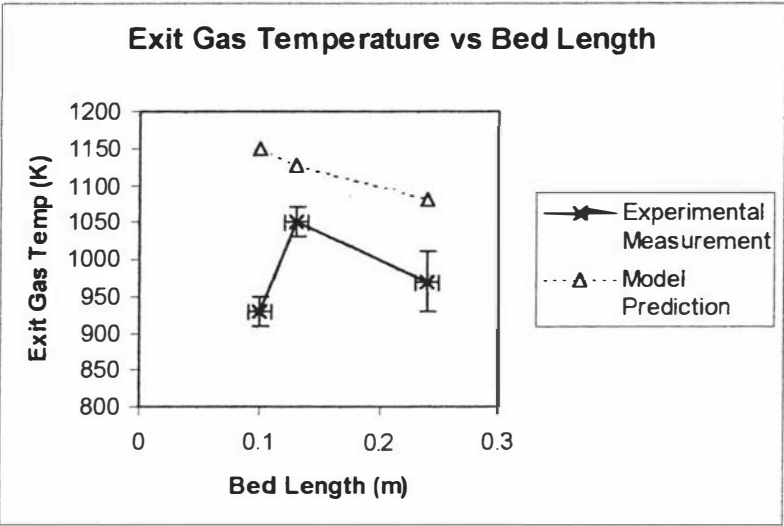
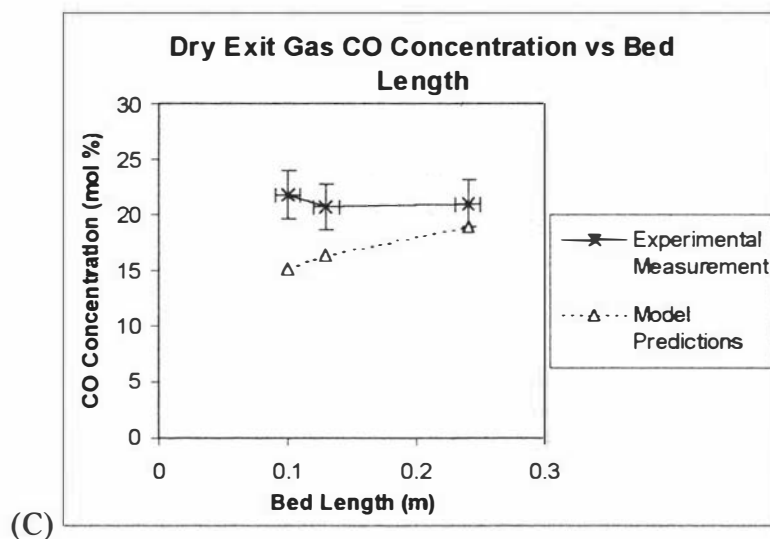
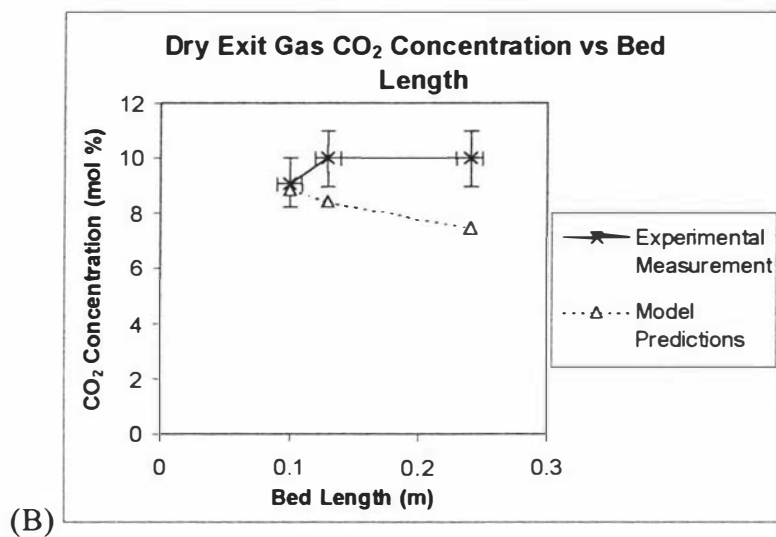
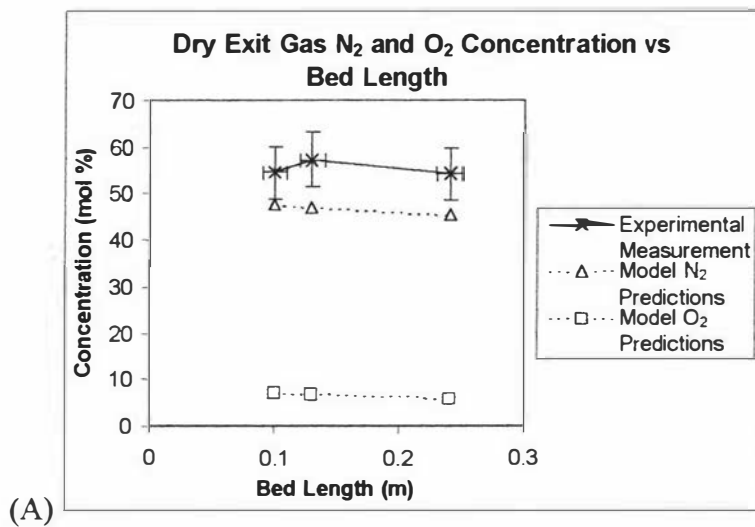


Figure 5.8: Experimental measurement and model prediction of the steady-state exit gas temperature vs gasifier bed length. The air flow rate was $0.22 \pm 0.03 \text{ mol.s}^{-1}$.

The experimental measurements and the model predictions for the concentrations of the dry exit gas components were plotted against the bed length in Figure 5.9 (A)-(E).



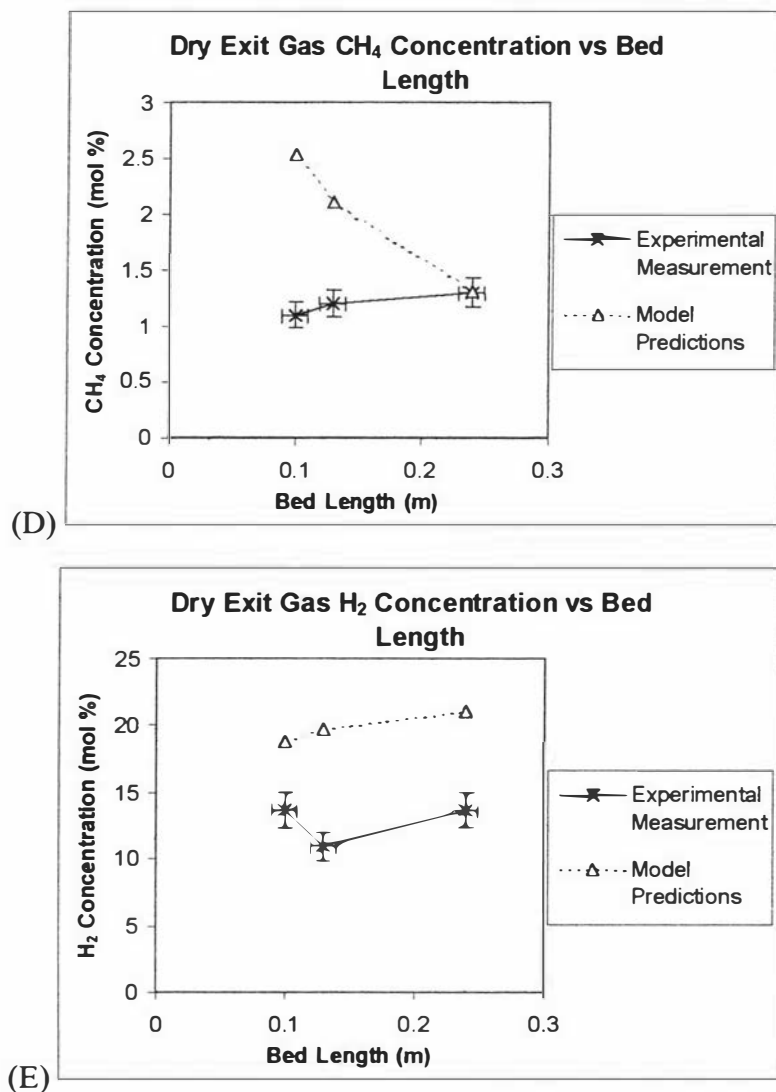


Figure 5.9: Model predictions and experimental measurements of the molar fraction of (A) N₂, (B) CO₂, (C) CO, (D) CH₄ and (E) H₂ in the dry exit gas as the bed length was varied. The air flow rate was 0.22 ± 0.03 m.

The sum of the model N₂ and O₂ predictions were close to the experimental N₂ concentration in the dry gas. The model slightly under-predicted the dry gas CO₂ and CO concentrations compared with the experimental results, while the H₂ concentration was over-predicted.

The CH₄ concentrations for the two shorter bed lengths were over-predicted by the model. The model also showed a marked decrease in the CH₄ concentration with increasing bed length that was not visible in the experimental results. One explanation

is that the CH_4 depleting reactions were actually faster than assumed in the model and had reached equilibrium by the time the gas had travelled 0.1 m through the bed.

(C) Summary

The model predicted gas exit temperatures which were significantly higher than those measured. This could indicate that the C_{RF} value used (2000) should have been higher, or that the initial temperature was lower than the 1200 K assumed.

Including the methane combustion reaction in the model made the model predictions of the dry gas exit composition closer to the experimental values, particularly with respect to the methane concentration. The model under-predicted the CO and over-predicted the H_2 and CH_4 concentrations in the dry product gas. The experimental N_2 concentrations were close to the sum of the model N_2 and O_2 concentrations. The general trend regarding which chemical species were under- and over- predicted by the model was the same for both the series of varying air flow rates and the series of varying bed lengths. In Section 3.2 the same model compared with previously published results under-predicted the CH_4 . The major difference between the results used in Section 3.2 and the results found in Chapter 4 was that the experimental results used in Section 3.2 were for a gasifier with a longer bed length and smaller superficial gas velocity (and hence longer residence times).

While the model did predict trends in the gas exit temperature and composition as the initial gas velocity and bed length were varied, in many cases the uncertainties were too large to determine whether these trends occurred in the experimental results over the range of values examined.

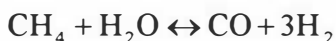
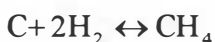
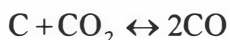
The model predictions were sensitive to the initial values and C_{RF} assumed. Overall the model gave a reasonable prediction of the exit gas composition given that many of the model parameters were estimates. A better understanding of the relationships between the initial temperature, the air flow rate, fuel moisture content and the amount (and composition) of pyrolysis gases produced could improve the model.

6. Conclusion

The aim of this study was to develop a model of downdraft gasification based on the chemical and physical processes occurring, that was general enough to be applied to different gasifiers running on different fuels and under different operating conditions. We also ran a series of experimental runs using a local downdraft gasifier in which the bed length, fuel type and air flow rate were varied.

We developed a simple, 1-dimensional steady-state model of a downdraft gasifier for the region of the bed beneath the pyrolysis/cracking zone. This allowed us to treat the pyrolysis/cracking reactions as a source of incoming CO, CH₄ and H₂O without having to model the complicated chemical reaction schemes involved.

The chemical reactions considered in the reduction zone were:



This was the same set of chemical reactions considered by Wang and Kinoshita (1993) in their kinetic model of gasification.

Two parameters were introduced to the model. The "Char Reactivity Factor" (C_{RF}) was a constant multiplier applied to all the chemical reaction rates that could be varied to account for differences in the reactivity of the different fuel types. The pyrolysis fraction (f_p) represented the molar fraction of the gases entering the modelled region of the gasifier that were derived from pyrolysis of the fuel. The values of these parameters were estimated by looking at the effect they produced on the model output. Initially it was assumed that all the oxygen from the air supply had been rapidly converted to carbon dioxide by reaction with the char surface.

The model predictions were compared to experimental results published by Senelwa (1997) and Chee (1987). The predicted exit gas compositions were quite close to the experimental results except that the model over-predicted the methane content. The

model was reformulated to include methane combustion ($\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$). This reduced the over-prediction of methane but the model predictions were quite sensitive to the initial gas composition assumed. The model also predicted that some oxygen would remain in the exit gas for the bed lengths used.

Sime (1998) found that the throughput of a downdraft gasifier could be improved by operating at higher pressures. We ran the model using pressures up to 20 atm. The model predicted that the rate of gas production would be increased at higher pressures leading to a higher rate of chemical energy output. However, the higher heating value of the dry product gas on a molar basis would be reduced. The model predictions assumed that the increase in pressure did not affect the initial temperature or the composition of the gas at the top of the reduction region.

The model was extended to include time-variation. However, due to a lack of sufficiently detailed experimental data this model was not tested or developed further.

The experimental work was performed using a downdraft gasifier at Massey University. The exit gas temperature was logged electronically while the pressure drop across the gasifier bed and exit gas velocity were recorded manually. The exit gas was also sampled and analysed to obtain the dry exit gas composition.

There was a fair amount of experimental uncertainty involved in the measurements. The size of the hopper limited the total gasifier run time while the gasifier approached "steady-state" operation quite slowly. This meant that there was a fairly narrow window of approximately "steady-state" operation during which to take measurements. Secondly the gas chromatograph used could only have one analysis column installed at a time. One was able to separate nitrogen and oxygen but unable to detect hydrogen while the other was able to detect hydrogen but unable to separate nitrogen and oxygen. The moisture content of the exit gas was not measured.

However, the experimental measurements made were sufficient to make some comparisons with the model. Again the model dry gas predictions were fairly close to the experimental results, although the model tended to over-predict the methane concentration. Better agreement was found when the methane combustion reaction was

included but the methane content was still over-predicted. A series of gasifier runs using different bed lengths and air flow rates were compared with the model. The model showed some trends in the exit gas composition with the air flow rate and bed length, but the uncertainties were too large to determine whether the experimental results followed similar trends.

Our model of steady-state downdraft gasification seemed to produce reasonable agreement with experimental results but methane production tended to be over-predicted. The model predictions were quite dependent upon the initial parameter values chosen. The model could be improved by combining it with a study of fast pyrolysis that could predict the initial temperatures and gas composition at the top of the reduction zone. A second method of determining the initial conditions would be to take measurements of the steady-state exit gas including H_2O and O_2 content then to run the model using $z = L$ (the bed length) as the starting position and calculating the conditions at $z = 0$. If the correct C_{RF} has been selected then the initial conditions should be the same for a series of runs that differ only in the bed length.

Appendix A: Justification of the Ideal Gas Approximation

In our treatment of the gases within the downdraft gasifier we have assumed that the ideal gas law ($PV=NRT$) holds. The ideal gas law is a good description for gases where the volume occupied by the gas molecules is effectively zero compared to the total volume available and the intermolecular attractive forces are negligible. That is the ideal gas law is a good approximation for gases at high temperature and low pressure, but needs some correcting terms as the gas approaches condensation. The Van der Waals gas equation contains correction terms to the ideal gas equation to account for the behaviour of "real gases" (a more detailed explanation can be found in Kondepuni and Prigogine (1998)):

$$(7.1) \quad \left(P + \frac{a}{V_m^2} \right) (V_m - b) = RT$$

where P is the total pressure in Pa,

R is the gas constant in $\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$,

T is the temperature in K, and

V_m is the molar volume ($=V/N$) in $\text{m}^3 \cdot \text{mol}^{-1}$.

The terms a and b are related to the critical constants by the following relationships:

$$(7.2) \quad V_{mc} = 3b, \text{ and}$$

$$(7.3) \quad T_c = \frac{8a}{27bR}$$

where V_{mc} is the critical molar volume in $\text{m}^3 \cdot \text{mol}^{-1}$, and

T_c is the critical temperature in K.

Rearranging Equation 7.1:

$$(7.4) \quad PV_m = RT + Pb - \frac{a}{V_m} + \frac{ab}{V_m^2}$$

Therefore the term $(Pb - \frac{a}{V_m} + \frac{ab}{V_m^2})$ acts as a correction to the ideal gas equation and can be neglected if small compared to RT . For convenience we shall denote this term as Y .

The gasifier was operating at temperatures between 900 - 1200 K and at a pressure slightly above atmospheric pressure. We evaluated the "real gas" correction term to the ideal gas equation at 900 K and 1 atm in Table 7.1 below. V_m was assumed to be $\frac{R \times 900 \text{ K}}{101,300 \text{ Pa}}$. Values for V_{mc} and T_c were taken from Kaye and Laby (1995).

Gas	V_{mc} (m ³ /mol)	T_c (K)	a (Jm ³ mol ⁻²)	b (m ³ /mol)	RT (J/mol)	Y (J/mol)	Y/RT
CO	3.50x10 ⁻⁶	132.9	4.36x10 ⁻³	1.17x10 ⁻⁶	7480	0.059	8x10 ⁻⁴ %
CO ₂	7.38x10 ⁻⁶	304.1	2.10x10 ⁻²	2.46x10 ⁻⁶	7480	- 0.036	-5x10 ⁻⁴ %
CH ₄	9.86x10 ⁻⁵	190.6	1.76x10 ⁻¹	3.29x10 ⁻⁵	7480	0.95	0.01 %
H ₂	6.50x10 ⁻⁵	33.2	2.02x10 ⁻²	2.17x10 ⁻⁵	7480	1.9	0.03 %
H ₂ O	5.60x10 ⁻⁵	647.1	3.40x10 ⁻¹	1.87x10 ⁻⁵	7480	-2.7	-0.04 %
N ₂	8.95x10 ⁻⁵	126.2	1.06x10 ⁻¹	2.98x10 ⁻⁵	7480	1.6	0.02 %
O ₂	7.34x10 ⁻⁵	154.6	1.06x10 ⁻¹	2.45x10 ⁻⁵	7480	1.0	0.01 %

Table 7.1: Correction terms to the ideal gas equation for gases with $T = 900 \text{ K}$, $V_m = 7.38 \times 10^{-2} \text{ m}^3 \text{ mol}^{-1}$, $P = 101,300 \text{ Pa}$.

The terms were also evaluated at 10 atm in Table 7.2 as there may be some future interest in operating downdraft gasifiers at high pressure.

Gas	V_{mc} (m ³ /mol)	T_c (K)	a (Jm ³ mol ⁻²)	b (m ³ /mol)	RT (J/mol)	Y (J/mol)	Y/RT
CO	3.50x10 ⁻⁶	132.9	4.36x10 ⁻³	1.17x10 ⁻⁶	7480	0.594	0.008%
CO ₂	7.38x10 ⁻⁶	304.1	2.10x10 ⁻²	2.46x10 ⁻⁶	7480	-0.357	-0.005%
CH ₄	98.6x10 ⁻⁶	190.6	1.76x10 ⁻¹	32.9x10 ⁻⁶	7480	9.63	0.1%
H ₂	65.0x10 ⁻⁶	33.2	2.02x10 ⁻²	21.7x10 ⁻⁶	7480	19.3	0.3%
H ₂ O	56.0x10 ⁻⁶	647.1	3.40x10 ⁻¹	18.7x10 ⁻⁶	7480	-27.0	-0.4%
N ₂	89.5x10 ⁻⁶	126.2	1.06x10 ⁻¹	29.8x10 ⁻⁶	7480	15.8	0.2%
O ₂	73.4x10 ⁻⁶	154.6	1.06x10 ⁻¹	24.5x10 ⁻⁶	7480	10.5	0.1%

Table 7.2: Correction terms to the ideal gas equation for gases in gasifier with $T = 900\text{ K}$, $V_m = 7.38 \times 10^{-3}\text{ m}^3/\text{mol}$, $P = 1,013,000\text{ Pa}$.

Even at a pressure of 10 atmospheres the difference between the real gas equation and the ideal gas approximation was less than 1%. The uncertainties in the experimental measurements were larger than the errors introduced by using the ideal gas approximation. Therefore using the ideal gas approximation was justified.

Appendix B: Equilibrium Constants for Reactions

Consider the reaction:



where the upper case letters represent gaseous compounds and the lower case letters represent the stoichiometric amounts of each compound.

The equilibrium constant for the reaction is defined as:

$$(B.1) \quad K_{eq} = \frac{P_{Y,eq}^c \cdot P_{Z,eq}^d}{P_{W,eq}^a \cdot P_{X,eq}^b},$$

where $P_{W,eq}$ - $P_{Z,eq}$ are the partial pressures of compounds W-Z at chemical equilibrium.

The equilibrium constant of a reaction changes with temperature (higher temperatures shift the equilibrium in the direction of the endothermic reaction) and pressure (higher pressures shift the reaction in the direction that produces the smallest total number of gaseous molecules).

Values for $\log_{10}K$ for the chemical compounds considered in this work were tabulated in Barin (1993) at 100 K intervals. These values assumed that all partial pressures were quoted in bars. The value of $\log_{10}K_{eq}$ for each reaction was found by adding the $\log_{10}K$ value of each compound multiplied by its stoichiometric coefficient (reactants were considered to have negative coefficients).

Figure 8.1 shows $\log_{10}K_{eq}$ for each reaction plotted against $1/T$ (where T is the temperature in K). The plots appear linear over this range of temperatures and the lines found using the method of least squares were used in the MATLAB scripts to calculate the equilibrium constants at a given temperature.

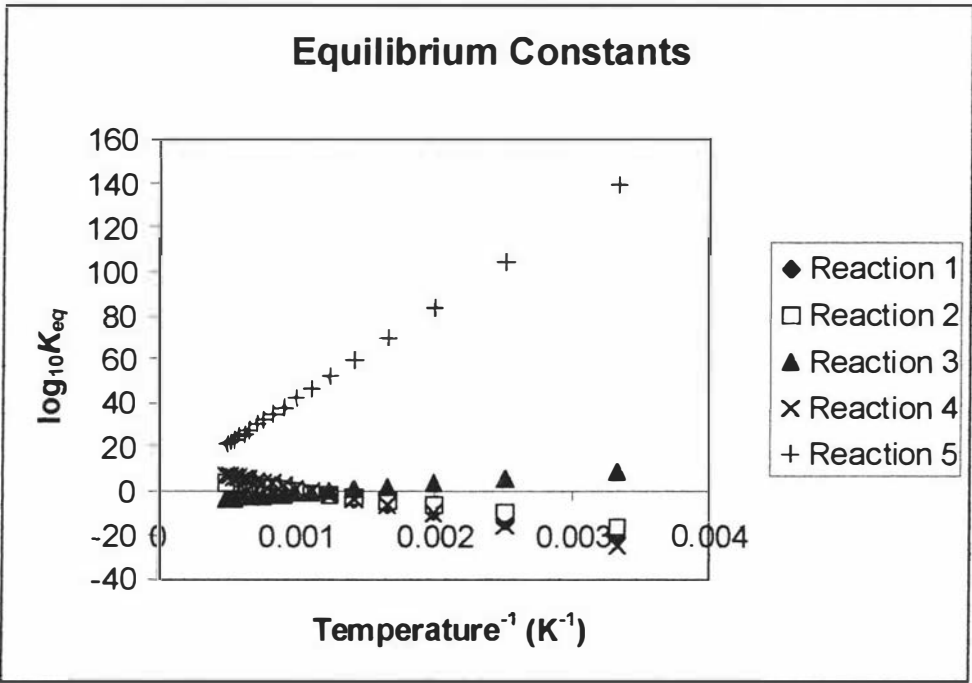


Figure 8.1: The log of the equilibrium constants for Reactions 1-5 plotted against the reciprocal of the temperature.

Reaction	Best fit line
Reaction 1	$\log_{10} K_{eq} = -8900/T + 9.1$
Reaction 2	$\log_{10} K_{eq} = -7000/T + 7.4$
Reaction 3	$\log_{10} K_{eq} = 4400/T - 5.5$
Reaction 4	$\log_{10} K_{eq} = -11370/T + 12.878$
Reaction 5	$\log_{10} K_{eq} = 41800/T - 0.08$

Table 8.1: Formulae used to calculate equilibrium constants of reactions at different temperatures.

Appendix C: MATLAB Scripts

The following MATLAB scripts were used to generate the model predictions used in Chapters 3 and 4. Several commonly used expressions were written as separate function calls to improve the clarity of the code.

```
% This function calculates the equilibrium constant of
% a gasification reaction at a particular temperature
% (temp) in K.
%
% rxn is a number that specifies the reaction
% that the equilibrium constant is to be calculated for
%
% rxn = 1:  C + CO2 -> 2CO
% rxn = 2:  C + H2O -> CO + H2
% rxn = 3:  C + 2H2 -> CH4
% rxn = 4:  CH4 + H2O -> CO + 3H2
% rxn = 5:  CH4 + 2O2 -> CO2 + 2H2O
% Any other value for rxn will give an erroneous result

function [eqk]=EqmConst(rxn, temp)

% Check to see which reaction is requested
%
if (rxn == 1)
    logk = -8.91807171624500e3./temp + ...
        0.00905163363023e3;
end;

if (rxn == 2)
    logk = -7.01021893134055e3./temp ...
        +0.00741310929237e3;
end;
```

```

    if (rxn == 3)
        logk = 4.37346352538647e3./temp -0.00547438215349e3;
    end;

    if (rxn == 4)
        logk =-1.13845220272271e4./temp + 0.0012888757407e4;
    end;

    if (rxn == 5)
        logk = 4.18318770608402e4./temp-0.0751343488;
    end;

    eqk = 10.^logk;

return;

```

The following five functions calculate the rates of Reactions 1 to 5 given the conditions at a certain point.

```

function x = r1(CRF, temp, PCO2, PCO)

R = 8.31434;

% Need to convert pressures from Pa to bar

PCO2 = PCO2./1e5;
PCO = PCO./1e5;

for i=1:length(PCO2)
% This section checks to make sure that the partial

```

```

% pressures are not negative.  If a negative partial
% pressure is found then it is set to zero.
    if PCO2(i) < 0
        PCO2(i) = 0;
    end
    if PCO(i) < 0
        PCO(i) = 0;
    end
end

x = (36.16*CRF*exp(-77390./(R.*temp))).*(abs(PCO2) -
PCO.^2./EqmConst(1,temp));

return

function x = r2(CRF, temp, PH2O, PCO, PH2)

R = 8.31434;

% Need to convert pressures from Pa to bar

PH2O = PH2O./1e5;
PCO = PCO./1e5;
PH2 = PH2./1e5;

for i = 1:length(PH2O)
% This section checks to make sure that the partial
% pressures are not negative.  If a negative partial
% pressure is found then it is set to zero.
    if PH2O(i) < 0
        PH2O(i) = 0;
    end
    if PCO(i) < 0
        PCO(i) = 0;
    end
end

```

```

    end
    if PH2(i) < 0
        PH2(i) = 0;
    end
end

x = (1.517e4*CRF*exp(-121620./(R.*temp))).*(abs(PH2O) ... -
    abs(PH2.*PCO)./EqmConst(2,temp));
return

function x = r3(CRF, temp, PH2,PCH4)

R = 8.31434;

% Need to convert pressures from Pa to bar
PH2 = PH2./1e5;
PCH4 = PCH4./1e5;

for i = 1:length(PH2)
% This section checks to make sure that the partial
% pressures are not negative. If a negative partial
% pressure is found then it is set to zero.
    if PH2(i) < 0
        PH2(i) = 0;
    end
    if PCH4(i) < 0
        PCH4(i) = 0;
    end
end

x = 4.189e-3*CRF*exp(-19210./(R.*temp)).*(PH2.^2 -...
    abs(PCH4)./EqmConst(3,temp));
return

```

```

function x = r4(CRF, temp, PCH4, PH2O, PCO, PH2)

R = 8.31434;

% Need to convert pressures from Pa to bar
PCH4 = PCH4./1e5;
PH2O = PH2O./1e5;
PCO = PCO./1e5;
PH2 = PH2./1e5;

for i=1:length(PH2)
% This section checks to make sure that the partial
% pressures are not negative. If a negative partial
% pressure is found then it is set to zero.
    if PCH4(i) < 0
        PCH4(i) = 0;
    end
    if PH2O(i) < 0
        PH2O(i) = 0;
    end
    if PCO(i) < 0
        PCO(i) = 0;
    end
    if PH2(i) < 0
        PH2(i) = 0;
    end
end

x = 7.301e-2*CRF*exp(-36150./(R.*temp)).*((PH2O.*PCH4)-...
    (PH2.^3.*PCO)./EqmConst(4,temp));
return

function x = r5(CRF, temp, PO2, PCH4, PCO2, PH2O)

```

```

R = 8.31434;

% Need to convert pressures from Pa to bar
PO2 = PO2./1e5;
PCH4 = PCH4./1e5;
PCO2 = PCO2./1e5;
PH2O = PH2O./1e5;

for i = 1:length(PCH4)
    if PO2(i) < 0
        PO2(i) = 0;
    end;
    if PCH4(i)<0
        PCH4(i)=0;
    end;
    if PCO2(i)<0
        PCO2(i) = 0;
    end;
    if PH2O(i)<0
        PH2O(i)=0;
    end;
end;

% Use rcomb/rgas = 240 (at 900 C)
x = 29.71*CRF*exp(-22028./(R.*temp)).*(PCH4.*PO2.^2 -...
    (PCO2.*PH2O.^2)./EqmConst(5,temp));
return

```

The following functions were used in the model calculations and were written as separate scripts to save retyping.

```
function x=cp(no2,nco2,nco,nh2o,nh2,nch4,nn2)
```

```

% Returns Heat Capacity of Gas (in J/K)

% Molar Heat Capacities in J/K/mol
% (at standard pressure and temperature)
% (Values from Aylward and Findlay)
cpco = 29;
cpco2 = 37;
cpo2= 29;
cph2= 29;
cpn2= 29;
cph2o= 34;
cpch4 = 36;

x = (nco*cpco+no2*cpo2 + nco2*cpco2+nh2*cph2 + ...
      nn2*cpn2 + nh2o*cph2o+nch4*cpch4);
return

function x = density(no2,nco2,nco,nh2o,nh2,nch4,nn2)
% Returns density of gas in kg/mol
x = no2*0.032 + nco2*0.044 + nco*0.028 + nh2*0.002 ...
    + nh2o*0.018 + nch4*0.016 + nn2*0.028;
return

function x = Hreact(CRF, temp, pressure, ngas, no2,...
    nco2, nco, nh2o, nh2, nch4)

% Note Hreact returns the heat _created_ by chemical
% reactions
% Hreact is positive for exothermic reactions and
% negative for endothermic reactions

% Standard temp and pressure delta H values for
% Reactions 1 to 5 in J/mol

```

```

deltaH1 = 171000;
deltaH2 = 131000;
deltaH3 = -75000;
deltaH4 = 206000;
deltaH5 = -888000;

```

```

x = - deltaH1*r1(CRF, temp, pressure.*nco2./ngas,...
    pressure.*nco./ngas) ...
    -deltaH2*r2(CRF, temp, pressure.*nh2o./ngas,...
    pressure.*nco./ngas, pressure.*nh2./ngas) ...
    -deltaH3*r3(CRF, temp, pressure.*nh2./ngas, ...
    pressure.*nch4./ngas) ...
    -deltaH4*r4(CRF, temp, pressure.*nch4./ngas,...
    pressure.*nh2o./ngas, pressure.*nco./ngas,...
    pressure.*nh2./ngas) ...
    -deltaH5*r5(CRF, temp, pressure.*no2./ngas,...
    pressure.*nch4./ngas, pressure.*nco2./ngas,...
    pressure.*nh2o./ngas);
return;

```

```

function x = RC(CRF, temp, pressure, ngas, no2, nco2,...
    nco, nh2o, nh2, nch4)
% RC is the change in the heat capacity of the gas due to
% chemical reactions changing the chemical composition of
% the gas (Units J/K/m^3/s).

```

```

% Molar Heat Capacities (in J/K/mol)
% (at standard pressure and temperature)
% (Values from Aylward and Findlay)
cpco = 29;
cpco2 = 37;
cpo2= 29;
cph2= 29;
cpn2= 29;

```

```

cph2o= 34;
cpch4 = 36;

x = r1(CRF, temp, pressure.*nco2./ngas, ...
    pressure.*nco./ngas).*(2*cpco-cpco2) + ...
    r2(CRF, temp, pressure.*nh2o./ngas, ...
    pressure.*nco./ngas, pressure.*nh2./ngas).*(cph2 + ...
    cpco - cph2o) + ...
    r3(CRF, temp, pressure.*nh2./ngas, ...
    pressure.*nch4./ngas).*(cpch4 - 2*cph2) + ...
    r4(CRF, temp, pressure.*nch4./ngas, ...
    pressure.*nh2o./ngas, pressure.*nco./ngas, ...
    pressure.*nh2./ngas).*(cpco + 3*cph2 - cpch4 - ...
    cph2o) + ...
    r5(CRF, temp, pressure.*no2./ngas, ...
    pressure.*nch4./ngas, pressure.*nco2./ngas, ...
    pressure.*nh2o./ngas).*(cpco2 + 2*cph2o - 2*cpo2 - ...
    cpch4);
return;

```

The script 'SteadyStateEqns.m' defines the set of ordinary differential equations used in the steady state model. This implementation includes the methane combustion reaction (Reaction 5). To simulate the model used in Section 3.1 that neglected methane combustion, replace any reference to r5 with the value 0.

```

function Y = SteadyStateEqns(z, StateVars)
% SteadyStateEqns contains the ODEs needed to determine
% the state of the gasifier in steady state operation
% Statevars contains initial values of [pressure, temp, v,
% no2, nco2, nco, nh2o, nh2, nch4, nn2, ngas]
%

```

```

pressure = StateVars(1);
temp = StateVars(2);
v = StateVars(3);
no2 = StateVars(4);
nco2 = StateVars(5);
nco = StateVars(6);
nh2o = StateVars(7);
nh2 = StateVars(8);
nch4 = StateVars(9);
nn2 = StateVars(10);
ngas = StateVars(11);

R = 8.31434;

% CRF is a special parameter used to represent the
% relative differences in reactivity of
% different fuel types.
    CRF = ; % Set this parameter to desired CRF value

% Formulae for the spatial derivatives of the state
% variables

dPdz = -1183.*density(no2, nco2, nco, nh2o, nh2, nch4,...
    nn2).*v.^2./1.2 -388.19.*v + 79.896;
% Note: v^2 term is multiplied by the ratio of the actual
% gas density compared to the density of air at std temp
% and pressure used for calibration.

dvdz = (1/(cp(no2,nco2,nco,nh2o,nh2,nch4,nn2) + ...
    ngas*R)).*(cp(no2, nco2, nco, nh2o, nh2, nch4,...
    nn2).*(r1(CRF, temp, pressure.*nco2./ngas,...
    pressure.*nco./ngas) + ...
    r2(CRF, temp,pressure.*nh2o./ngas,...
    pressure.*nco./ngas, pressure.*nh2./ngas)...)

```

```

-r3(CRF, temp, pressure.*nh2./ngas,...
pressure.*nch4./ngas) + ...
2*r4(CRF, temp, pressure.*nch4./ngas,...
pressure.*nh2o./ngas, pressure.*nco./ngas,...
pressure.*nh2./ngas))./ngas + ...
Hreact(CRF, temp, pressure, ngas, no2, nco2, nco,...
nh2o, nh2, nch4)./temp ...
-RC(CRF, temp, pressure, ngas, no2, nco2, nco,...
nh2o, nh2, nch4) ...
-v.*(1./temp +cp(no2, nco2, nco, nh2o, nh2, nch4,...
nn2)./pressure).*dPd);

dTdz = (1./(v.*cp(no2, nco2, nco, nh2o, nh2, nch4,...
nn2))).*(Hreact(CRF,temp, pressure, ngas, no2, ... nco2,
nco, nh2o, nh2, nch4) - v.*dPd - ... pressure.*dvdz -
RC(CRF, temp, pressure, ngas, no2,... nco2, nco, nh2o,
nh2, nch4).*temp);

dno2dz = -(2*r5(CRF, temp, pressure.*no2./ngas,...
pressure.*nch4./ngas, pressure.*nco2./ngas, ...
pressure.*nh2o./ngas) + no2.*dvdz)./v;

dnco2dz = (-r1(CRF, temp, pressure.*nco2./ngas,...
pressure.*nco./ngas) + r5(CRF, temp, ...
pressure.*no2./ngas, pressure.*nch4./ngas, ...
pressure.*nco2./ngas, pressure.*nh2o./ngas) ...
-nco2.*dvdz)./v;

dncodz = (2.*r1(CRF, temp, pressure.*nco2./ngas, ...
pressure.*nco./ngas) + ...
r2(CRF, temp, pressure.*nh2o./ngas,...
pressure.*nco./ngas, pressure.*nh2./ngas) + ...

```

```

r4(CRF, temp, pressure.*nch4./ngas,...
pressure.*nh2o./ngas, pressure.*nco./ngas,...
pressure.*nh2./ngas) - nco.*dvdz) ./v;

```

```

dnh2odz = (-r2(CRF, temp, pressure.*nh2o./ngas, ...
pressure.*nco./ngas, pressure.*nh2./ngas)- ...
r4(CRF, temp, pressure.*nch4./ngas, ...
pressure.*nh2o./ngas, pressure.*nco./ngas,...
pressure.*nh2./ngas) + ...
2*r5(CRF, temp, pressure.*no2./ngas,...
pressure.*nch4./ngas, pressure.*nco2./ngas,...
pressure.*nh2o./ngas) - nh2o.*dvdz) ./v;

```

```

dnh2dz = (r2(CRF, temp, pressure.*nh2o./ngas,...
pressure.*nco./ngas, pressure.*nh2./ngas) - ...
2*r3(CRF, temp, pressure.*nh2./ngas,...
pressure.*nch4./ngas) + ...
3*r4(CRF, temp, pressure.*nch4./ngas, ...
pressure.*nh2o./ngas, pressure.*nco./ngas,...
pressure.*nh2./ngas) - nh2.*dvdz) ./v;

```

```

dnch4dz = (r3(CRF, temp, pressure.*nh2./ngas, ...
pressure.*nch4./ngas) - ...
r4(CRF, temp, pressure.*nch4./ngas,...
pressure.*nh2o./ngas, pressure.*nco./ngas, ...
pressure.*nh2./ngas) - ...
r5(CRF, temp, pressure.*no2./ngas, ...
pressure.*nch4./ngas, pressure.*nco2./ngas,...
pressure.*nh2o./ngas) - nch4.*dvdz) ./v;

```

```

dnn2dz = (-nn2.*dvdz./v);

```

```

dngasdz = dno2dz + dnco2dz + dncodz + dnh2odz + dnh2dz ...
+ dnch4dz + dnn2dz;

```

```
Y = [dPdZ; dTdZ; dVdZ; dno2dZ; dnco2dZ; dncodZ; dnh2odZ;
dnh2dZ; dnch4dZ; dnn2dZ; dngasdZ];
```

```
return;
```

```
*****
```

The script 'STEADY_STATE.m' sets the conditions at the top of the gasifier then uses the ODE45 function to solve the set of ordinary differential equations defined in the 'SteadyStateEqns.m' script at intervals of size 'step' down the gasifier until the distance from the top of the gasifier is equal to the parameter 'length'.

```
% STEADY_STATE.m
```

```
% Steady State Model
```

```
% This model is intended to simulate the operation of a %
downdraft gasifier operating in a time stable manner.
```

```
% The ordinary differential equations are contained in a %
file called 'SteadyStateEqns.m'
```

```
% *****
```

```
% Reactions considered
```

```
% *****
```

```
%
```

```
% r1:  $C + CO_2 = 2CO$ 
```

```
% r2:  $C + H_2O = CO + H_2$ 
```

```
% r3:  $C + 2H_2 = CH_4$ 
```

```
% r4:  $CH_4 + H_2O = CO + 3H_2$ 
```

```
% r5:  $CH_4 + 2O_2 = CO_2 + H_2O$ 
```

```
% Note: SteadyStateEqns.m can be modified to remove r5
% from the reaction scheme.
```

```

clear;

% *****

% Constants
% *****

% Gas constant in J/K/mol, Source: SI Chemical Data
R = 8.31434;

% *****

% Discretisation Parameters
% *****

% Note: The values of these parameters can be changed
% as necessary.

length = 0.1;
step = 0.05;

% *****

% Initial Values
% *****

% Set these values as appropriate
v(1) = ;
temp(1) = ;
pressure(1) = ;
ngas(1) = pressure(1)/(R*temp(1));
fp = ; % Enter the pyrolysis fraction (from 0 to 1)
pyrmol = ngas(1)*fp;

no2(1) = 0.21*(ngas(1)-pyrmol);
nco2(1) = 0.347*pyrmol;
nco(1) = 0*pyrmol;
nch4(1) = 0.397*pyrmol;

```

```

nh2o(1) = 0.256*pyrmol;
nh2(1) = 0*ngas(1);
nn2(1) = ngas(1) - no2(1) - nco2(1) - nco(1) - nch4(1) -
    nh2o(1) -nh2(1);

[Z,Y] = ...
    ode45('SteadyStateEqns', [0:step:length], ...
    [pressure(1), temp(1), v(1), no2(1), nco2(1), nco(1),
nh2o(1), nh2(1), nch4(1), nn2(1), ngas(1)]);

pressure = Y(:,1);
temp = Y(:,2);
v = Y(:,3);
no2 = Y(:,4);
nco2 = Y(:,5);
nco = Y(:,6);
nh2o = Y(:,7);
nh2 = Y(:,8);
nch4 = Y(:,9);
nn2 = Y(:,10);
ngas = Y(:,11);

LHV = (nco*283080+nch4*889000+nh2*239960)./ngas;
HHV = (nco*282000+nch4*888000+nh2*285000)./ngas;

```

```

*****

```

The script 'TimeDepModel.m' implements a first-order time dependent model of downdraft gasification. The initial conditions were set so that the gasifier should be operating in steady state (the initial conditions could be altered to test other scenarios). A time step size of less than 1 ms was required for the conditions to remain stable over time. This is not particularly convenient for looking at timescales of the order of minutes. Using a higher order approximation of the time derivatives would allow larger timesteps to be used.

```

% TimeDepModel.m
% Time dependent model

clear;

% Gas constant in J/K/mol, Source: Aylward and Findlay
R = 8.31434;

%*****

% Discretisation Parameters
%*****

length = 0.5;
step = 0.05;
no_points = length/step + 1;

minutes = 1; %Total time of run
timestep= 0.001; %Time step in seconds

%*****

% Operational Parameters
%*****

CRF = 2000; %Char reactivity factor

airflowrate = 0.5; % Moles per second of air flow in
pyrfrac = 0.3; %Fraction of total incoming gas that is
               %derived from pyrolysis products (0-1)
pyrmol = airflowrate/pyrfrac;
pyrch4 =0.51*pyrmol;
pyrco2 =0.446*pyrmol;
pyrh2o =0.044*pyrmol;
pyrco = 0;

area = pi*0.1^2; %Cross sectional area of gasifier bed

```

```

% Create matrices of appropriate sizes
no2 = zeros(no_points,minutes);
nco2 = zeros(no_points,minutes);
nco = zeros(no_points,minutes);
nh2o = zeros(no_points,minutes);
nh2 = zeros(no_points,minutes);
nn2 = zeros(no_points,minutes);
nch4 = zeros(no_points,minutes);
ngas = zeros(no_points,minutes);

pressure = zeros(no_points,minutes);
temp = zeros(no_points,minutes);
v = zeros(no_points,minutes);

%Set initial conditions at top of gasifier
v(1,1) = 1;
temp(1,1) = 1200;
pressure(1,1) = 1.013e+005;

ngas(1,1)=pressure(1,1)./(R*temp(1,1));
no2(1,1) = 0.21*pyrfrac;
nco2(1,1) = 0.446*(1-pyrfrac)*ngas(1,1);
nco(1,1) = 0;
nch4(1,1) = 0.51*(1-pyrfrac)*ngas(1,1);
nh2o(1,1) = 0.044*(1-pyrfrac)*ngas(1,1);
nh2(1,1) = 0;
nn2(1,1) = ngas(1,1)-no2(1,1)-nco2(1,1)- nco(1,1)- ...
nch4(1,1)-nh2o(1,1)-nh2(1,1);

%Set the initial state of the gasifier to steady state
[Z,Y] = ode45('SteadyStateEqns', [0:step:length], ...

```

```

        [pressure(1,1), temp(1,1), v(1,1), no2(1,1), ...
        nco2(1,1), nco(1,1), nh2o(1,1), nh2(1,1), ...
        nch4(1,1), nn2(1,1), ngas(1,1)]];

pressure(:,1) = Y(:,1);
temp(:,1) = Y(:,2);
v(:,1) = Y(:,3);
no2(:,1) = Y(:,4);
nco2(:,1) = Y(:,5);
nco(:,1) = Y(:,6);
nh2o(:,1) = Y(:,7);
nh2(:,1) = Y(:,8);
nch4(:,1) = Y(:,9);
nn2(:,1) = Y(:,10);
ngas(:,1) = Y(:,11);

% Temporary results are stored in matrices with a 't'
% prefix. Column 1 = old results
% Column 2 is for results at t = t+1

tno2=zeros(no_points,2);
tnco2 = zeros(no_points,2);
tnco = zeros(no_points,2);
tnh2o = zeros(no_points,2);
tnh2 = zeros(no_points,2);
tnn2 = zeros(no_points,2);
tnch4 = zeros(no_points,2);
tngas = zeros(no_points,2);

tpressure = zeros(no_points,2);
ttemp = zeros(no_points,2);
tv = zeros(no_points,2);

```

```

% Set first column of temporary matrices to the initial
% state
tno2(:,1)=no2(:,1);
tnco2(:,1) = nco2(:,1);
tnco(:,1) = nco(:,1);
tnh2o(:,1) = nh2o(:,1);
tnh2(:,1) = nh2(:,1);
tnn2(:,1) = nn2(:,1);
tnch4(:,1) = nch4(:,1);
tngas(:,1) = ngas(:,1);

tpressure(:,1) = pressure(:,1);
ttemp(:,1) = temp(:,1);
tv(:,1) = v(:,1);

for k = 1:minutes
    for j = 1:timestep:60
        % Find the spatial derivatives at time t using
        % central differences
        dno2dz(1,1) = (tno2(3,1)-tno2(1,1))/(2*step);
        dno2dz(2:no_points-1,1)=(tno2(3:no_points,1)-...
            tno2(1:no_points-2,1))/(2*step);
        dno2dz(no_points,1) = (tno2(no_points,1)-...
            tno2(no_points-2,1))/(2*step);

        dnco2dz(1,1)= (tnco2(3,1)-tnco2(1,1))/(2*step);
        dnco2dz(2:no_points-1,1)=(tnco2(3:no_points,1)-...
            tnco2(1:no_points-2,1))/(2*step);
        dnco2dz(no_points,1) = (tnco2(no_points,1)-...
            tnco2(no_points-2,1))/(2*step);

        dncodz(1,1)= (tnco(3,1)-tnco(1,1))/(2*step);
        dncodz(2:no_points-1,1)=(tnco(3:no_points,1)-...
            tnco(1:no_points-2,1))/(2*step);
    end
end

```

```

dncodz(no_points,1) = (tnco(no_points,1)-...
    tnco(no_points-2,1))/(2*step);

dnh2odz(1,1)= (tnh2o(3,1)-tnh2o(1,1))/(2*step);
dnh2odz(2:no_points-1,1)=(tnh2o(3:no_points,1)-...
    tnh2o(1:no_points-2,1))/(2*step);
dnh2odz(no_points,1) = (tnh2o(no_points,1)-...
    tnh2o(no_points-2,1))/(2*step);

dnh2dz(1,1)= (tnh2(3,1)-tnh2(1,1))/(2*step);
dnh2dz(2:no_points-1,1)=(tnh2(3:no_points,1)-...
    tnh2(1:no_points-2,1))/(2*step);
dnh2dz(no_points,1) = (tnh2(no_points,1)-...
    tnh2(no_points-2,1))/(2*step);

dnch4dz(1,1)= (tnch4(3,1)-tnch4(1,1))/(2*step);
dnch4dz(2:no_points-1,1)=(tnch4(3:no_points,1)-...
    tnch4(1:no_points-2,1))/(2*step);
dnch4dz(no_points,1) = (tnch4(no_points,1)-...
    tnch4(no_points-2,1))/(2*step);

dnn2dz(1,1)= (tnn2(3,1)-tnn2(1,1))/step;
dnn2dz(2:no_points-1,1)=(tnn2(3:no_points,1)-...
    tnn2(1:no_points-2,1))/(2*step);
dnn2dz(no_points,1) = (tnn2(no_points,1)-...
    tnn2(no_points-2,1))/(2*step);

dnngasd = dno2dz + dnco2dz + dncodz + dnh2odz + ...
    dnh2dz + dnch4dz + dnn2dz;

dvdz(1,1)= (tv(3,1)-tv(1,1))/(2*step);
dvdz(2:no_points-1,1)=(tv(3:no_points,1)-...
    tv(1:no_points-2,1))/(2*step);
dvdz(no_points,1) = (tv(no_points,1)- ...

```

```

    tv(no_points-2,1))/(2*step);

dTdz(1,1)= (ttemp(3,1)-ttemp(1,1))/(2*step);
dTdz(2:no_points-1,1)=(ttemp(3:no_points,1)-...
    ttemp(1:no_points-2,1))/(2*step);
dTdz(no_points,1) = (ttemp(no_points,1)-...
    ttemp(no_points-2,1))/(2*step);

dPdz(1,1)= (tpressure(3,1)-tpressure(1,1))/(2*step);
dPdz(2:no_points-1,1)=(tpressure(3:no_points,1)-...
    tpressure(1:no_points-2,1))/(2*step);
dPdz(no_points,1) = (tpressure(no_points,1)- ...
    tpressure(no_points-2,1))/(2*step);

%Shorthand term to help calculate partial pressures.
partp = tpressure(:,1)./tngas(:,1);

% Calculating the time derivatives
dno2dt = -tno2(:,1).*dvdz -tv(:,1).*dno2dz - ...
    2*r5(CRF,ttemp(:,1),partp.*tno2(:,1), ...
    partp.*tnch4(:,1), partp.*tnco2(:,1), ...
    partp.*tnh2o(:,1)));
dnco2dt = -tnco2(:,1).*dvdz - tv(:,1).*dnco2dz -...
    r1(CRF, ttemp(:,1), partp.*tnco2(:,1),...
    partp(:,1).*tnco(:,1)) + ...
    r5(CRF, ttemp(:,1), partp.*tno2(:,1),...
    partp.*tnch4(:,1), partp.*tnco2(:,1), ...
    partp.*tnh2o(:,1)));

dncodt = -tnco(:,1).*dvdz - tv(:,1).*dncodz + ...
    2*r1(CRF, ttemp(:,1), partp(:,1).*tnco2(:,1),...
    partp(:,1).*tnco(:,1)) + ...
    r2(CRF, ttemp(:,1), partp(:,1).*tnh2o(:,1),...
    partp(:,1).*tnco(:,1), partp(:,1).*tnh2(:,1)) +...

```

```

r4(CRF, ttemp(:,1), partp(:,1).*tnch4(:,1),...
partp(:,1).*tnh2o(:,1), partp(:,1).*tnco(:,1),...
partp(:,1).*tnh2(:,1));

dnh2odt = -tnh2o(:,1).*dvdz -tv(:,1).*dnh2odz -...
r2(CRF, ttemp(:,1), partp(:,1).*tnh2o(:,1), ...
partp(:,1).*tnco(:,1), partp(:,1).*tnh2(:,1)) -...
r4(CRF, ttemp(:,1), partp(:,1).*tnch4(:,1), ...
partp(:,1).*tnh2o(:,1), partp(:,1).*tnco(:,1), ...
partp.*tnh2(:,1)) + ...
2*r5(CRF, ttemp(:,1), partp.*tno2(:,1),...
partp.*tnch4(:,1), partp.*tnco2(:,1), ...
partp.*tnh2o(:,1));

dnh2dt = -tnh2(:,1).*dvdz-v(:,1).*dnh2dz + ...
r2(CRF, ttemp(:,1), partp(:,1).*tnh2o(:,1), ...
partp(:,1).*tnco(:,1), partp(:,1).*tnh2(:,1)) -...
2*r3(CRF, ttemp(:,1), partp(:,1).*tnh2(:,1), ...
partp(:,1).*tnch4(:,1)) + ...
3*r4(CRF, ttemp(:,1), partp(:,1).*tnch4(:,1),...
partp(:,1).*tnh2o(:,1), partp(:,1).*tnco(:,1), ...
partp(:,1).*tnh2(:,1));

dnch4dt = -tnch4(:,1).*dvdz -tv(:,1).*dnch4dz + ...
r3(CRF, ttemp(:,1), partp.*tnh2(:,1), ...
partp.*tnch4(:,1)) - ...
r4(CRF, ttemp(:,1), partp(:,1).*tnch4(:,1), ...
partp(:,1).*tnh2o(:,1), partp.*tnco(:,1),...
partp.*tnh2(:,1)) - ...
r5(CRF, ttemp(:,1), partp.*tno2(:,1),...
partp.*tnch4(:,1), partp.*tnco2(:,1), ...
partp.*tnh2o(:,1));

dnn2dt = -tnn2(:,1).*dvdz - tv(:,1).*dnn2dz;

```

```

dngasdt = dno2dt + dnco2dt + dncodt + dnh2odt + ...
          dnh2dt + dnch4dt + dnn2dt;

```

```

dTdt = (Hreact(CRF, ttemp(:,1), tpressure(:,1), ...
              tngas(:,1), tno2(:,1), tnco2(:,1), tnco(:,1), ...
              tnh2o(:,1), tnh2(:,1), tnch4(:,1)) - ...
        RC(CRF, ttemp(:,1), tpressure(:,1), ... tngas(:,1),
          tno2(:,1), tnco2(:,1), tnco(:,1), ... tnh2o(:,1),
          tnh2(:,1), tnch4(:,1)).*ttemp(:,1) ... -
        tv(:,1).*dTdz.*cp(tno2(:,1), tnco2(:,1), ...
          tnco(:,1), tnh2o(:,1), tnh2(:,1), tnch4(:,1),...
          tnn2(:,1)) -tv(:,1).*dPdzt(:,1) - ...
        tpressure(:,1).*dvdz - ...
        ttemp(:,1).*(dno2dt*cpo2 + dnco2dt*cpco2 + ...
          dncodt*cpco + dnh2odt*cph2o + dnh2dt*cph2 + ...
          dnch4dt*cpch4 + dnn2dt*cpn2))./ ...
        cp(tno2(:,1), tnco2(:,1), tnco(:,1), ...
          tnh2o(:,1), tnh2(:,1), tnch4(:,1), tnn2(:,1));

```

```

%Calculate values at time = t + timestep

```

```

tno2(:,2) = tno2(:,1) + timestep*dno2dt;
tnco2(:,2) = tnco2(:,1) + timestep*dnco2dt;
tnco(:,2) = tnco(:,1) + timestep*dncodt;
tnh2o(:,2) = tnh2o(:,1) + timestep*dnh2odt;
tnh2(:,2) = tnh2(:,1) + timestep*dnh2dt;
tnch4(:,2) = tnch4(:,1) + timestep*dnch4dt;
tnn2(:,2) = tnn2(:,1) + timestep*dnn2dt;
tngas(:,2) = tno2(:,2) + tnco2(:,2) + tnco(:,2) ...
            + tnh2o(:,2) + tnh2(:,2) + tnch4(:,2) + tnn2(:,2);

```

```

ttemp(:,2) = ttemp(:,1)+timestep*dTdt;

```

```

tpressure(:,2) = tngas(:,2).*R.*ttemp(:,2);

```

```

%Keeping conditions at top of gasifier constant

```

```

tpressure(1,2)=tpressure(1,1);

% Calculate pressure gradients
dPdZ(1,1)= (tpressure(3,1)-tpressure(1,1))/(2*step);
dPdZ(2:no_points-1,1)=(tpressure(3:no_points,1)-...
    tpressure(1:no_points-2,1))/(2*step);
dPdZ(no_points,1) = (tpressure(no_points,1)-...
    tpressure(no_points-2,1))/(2*step);

dPdZ(1,2)= (tpressure(3,2)-tpressure(1,2))/(2*step);
dPdZ(2:no_points-1,2)=(tpressure(3:no_points,2)-...
    tpressure(1:no_points-2,2))/(2*step);
dPdZ(no_points,2) = (tpressure(no_points,2)-...
    tpressure(no_points-2,2))/(2*step);

d2PdZdt(:,1)=(dPdZ(:,2)-dPdZ(:,1))/timestep;

%Calculating dvdt
a = 1183*density(tno2(:,2), tnco2(:,2), ...
    tnco(:,2), tnh2o(:,2), tnh2(:,2), tnch4(:,2), ...
    tnn2(:,2)).*tngas(:,2)/1.2929;
b = 388*ones(size(tv(:,2)));

dvdt = d2PdZdt./(2.*a.*tv(:,1)+b);

tv(:,2) = tv(:,1)+timestep*dvdt;

%The following lines to keep values at top of
%gasifier constant. They can be commented out or
%replaced if necessary
tno2(1,2)=tno2(1,1);
tnco2(1,2) = tnco2(1,1);
tnco(1,2) = tnco(1,1);
tnh2o(1,2) = tnh2o(1,1);

```

```

    tnh2(1,2) = tnh2(1,1);
    tnch4(1,2) = tnch4(1,1);
    tnn2(1,2) = tnn2(1,1);
    tngas(1,2) = tngas(1,1);
    ttemp(1,2)=ttemp(1,1);
    tpressure(1,2)=tpressure(1,1);
    tv(1,2)=tv(1,1);

    %Replace the values at time t with the values at %t+1
    tv(:,1)=tv(:,2);
    ttemp(:,1)=ttemp(:,2);
    tpressure(:,1)=tpressure(:,2);

    tno2(:,1)=tno2(:,2);
    tnco2(:,1)=tnco2(:,2);
    tnco(:,1)=tnco(:,2);
    tnh2o(:,1)=tnh2o(:,2);
    tnh2(:,1)=tnh2(:,2);
    tnch4(:,1)=tnch4(:,2);
    tnn2(:,1)=tnn2(:,2);
    tngas(:,1)=tngas(:,2);
end;

% Store values in matrices
v(:,k+1)=tv(:,1);
temp(:,k+1)=ttemp(:,1);
pressure(:,k+1)=tpressure(:,1);

no2(:,k+1)=tno2(:,1);
nco2(:,k+1)=tnco2(:,1);
nco(:,k+1)=tnco(:,1);
nh2o(:,k+1)=tnh2o(:,1);
nh2(:,k+1)=tnh2(:,1);
nch4(:,k+1)=tnch4(:,1);

```

```
nn2(:,k+1)=tnn2(:,1);  
ngas(:,k+1)=tngas(:,1);  
end;
```

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