
Developments in modelling and simulation of coal gasification

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Abstract

In recent years, the considerable increase in the price of crude oil and natural gas and concerns about their security of supply focused attention on whether fuel for power production and feedstocks for the chemical industry could be obtained from the gasification of coal. The need to reduce greenhouse gas emissions has enhanced the prospects of power generation from Integrated Gasification Combined Cycle (IGCC) plant. However, the higher capital costs and concerns about reliability and availability of IGCC plant have limited their market penetration. The coal gasifier has been a significant source of operational issues.

A thorough understanding of the processes occurring in a gasifier is essential both for addressing existing causes of gasifier unavailability and improving designs for the future. Many complex processes take place in a gasifier and developing models of gasifiers results in a greater insight into these processes. Computational models in conjunction with plant data can be used to evaluate gasifier operation, solve operational problems, probe new designs and provide performance data for commercial scale-up.

This report has surveyed models which are currently available for modelling gasifiers. The report contains a brief description of the three types of gasifiers which are most commonly used. The models available for each type of gasifier are considered. Insight gained by modelling has advanced the design of gasifiers and can improve gasifier performance. In some cases, the results have been compared with plant data and it has been possible to choose model inputs to give reasonable fit with the measured data. However, there are fewer examples where modelling has directly solved operational problems.

Acronyms and abbreviations

AFT	ash fusion temperature
CCS	carbon capture and storage
CFBC	circulating fluidised bed combustion
CFD	computational fluid dynamics
CPD	chemical percolation devolatilisation
CSFMB	comprehensive simulator for fluidised and moving bed
HHV	higher heating value
IGCC	integrated gasification combined cycle
NETL	National Energy Technology Laboratory
PCC	pulverised coal combustion
US DOE	United States Department of Energy

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I Introduction

Power generators, oil refinery operators and producers of chemicals such as methanol and ammonia have turned in recent years to gasification to unlock the power of coal and other carbon-based fuels. Gasification involves reacting a carbonaceous fuel with a combination of air, oxygen and steam to produce gaseous products which can be used either as a source of energy or as a raw material for the synthesis of chemicals, liquid fuels or other gaseous fuels. The fuel is combusted with insufficient oxygen to convert all the energy contained in the fuel into thermal energy but instead to convert it into chemical energy in the syngas produced. The syngas contains gases such as carbon monoxide, hydrogen and light hydrocarbons rather than carbon dioxide and steam as in complete combustion. Gasification usually converts a solid or liquid fuel into a gaseous fuel which is easier to use. It also enables impurities in the fuel such as sulphur to be removed before combustion thus avoiding the need to remove them in the oxidised form from larger volumes of flue gas following combustion. In the recent past interest in coal gasification has increased significantly. The considerable increase in the price of crude oil and natural gas and concerns about their security of supply focused attention on whether fuel for power production and feedstocks for the chemical industry could be obtained from the gasification of coal. The need to reduce greenhouse gas emissions has enhanced the prospects of power generation from Integrated Gasification Combined Cycle (IGCC) plant.

There are three main types of coal gasifiers namely, moving (also known as fixed) bed, fluidised bed and entrained flow. In a moving bed gasifier, the coal is fed through the top of the gasifier and the oxygen and steam usually from the bottom. The gases flow upwards through the bed of coal and the slag is withdrawn through the bottom. In a fluidised bed gasifier, the coal is gasified in a bed of heated particles suspended in flowing air. In an entrained flow gasifier, the pulverised coal and the gases flow concurrently at high speed. The three types differ in relation to what rank of coals they are most suitable for, whether the ash conditions are dry or slagging, the size of coal feed, the type of feed system, whether the oxidant is oxygen or air, how the slag is handled, the operating pressure, temperature and the exit gas temperature. The operation of moving bed gasifiers is relatively insensitive to fluctuations in fuel, air or steam flow but they can produce large quantities of tar. This is the most mature technology for gasification. Fluidised bed gasifiers can gasify most types of coal but are particularly suited for reactive fuels. They utilise smaller coal sizes than fixed bed systems. Entrained flow systems use very finely ground coal. They are the most versatile in relation to the types of coal that can be gasified. Their high operating temperatures produce superior carbon conversions and the potential to use high temperature reject heat.

The development of IGCC plant in the 1980s was the result of integrating gasification technology with a combined cycle plant. Such IGCC plant can achieve high efficiencies and produce low emissions. The impetus for the interest in IGCC technology has included the adoption of increasingly stringent emission legislation, concerns about the security of natural gas supplies and the desire to retain coal as part of the national energy portfolio. Further impetus has resulted from increasing concerns regarding the emissions of CO₂ from the power plant. As the concentration and pressure of CO₂ in the shifted syngas in an IGCC plant is much greater than in the flue gas of a pulverised coal combustion (PCC) plant, CO₂ removal is considerably easier in the former. However, the higher capital costs and concerns about reliability and availability of IGCC plant have limited their market penetration. For plants without CO₂ capture, IGCCs are more expensive to build than PCC plant. The historic data from the existing coal-based IGCC plant show that they have not been able to achieve 85% availability on a sustained basis. These operational problems are not all caused by the gasifier itself and are frequently related to the more conventional plant. Nevertheless the gasifier is a significant source of operational issues. There have been relatively few improvements in gasifier design in the last decade.

A thorough understanding of the processes occurring in a gasifier is essential both for addressing

existing causes of gasifier unavailability and improving designs for the future. Gasifiers in future will require greater fuel flexibility, reliability, availability, maintainability, higher throughput and fuel conversion. They will also need to integrate with gas clean-up and CCS (carbon capture and storage) equipment. Many complex processes take place in a gasifier: pyrolysis of coal particles; devolatilisation of volatile material; char oxidation or gasification; gas phase reactions; soot formation, growth and destruction and slag interactions. Developing models of gasifiers results in a greater insight into these processes. Computational models in conjunction with plant data can be used to evaluate gasifier operation, solve operational problems, probe new designs and provide performance data for commercial scale-up. Models can be used to identify operational shortcomings and suggest possible solutions. This approach is faster and less expensive than building and testing demonstration plant at different scales prior to commercialisation. Models can be used to assess conditions which are difficult to simulate experimentally. They enable a much deeper understanding of the experimental results and can be used to optimise experimental procedures. Models can be refined as more experimental data become available. In order to model the processes taking place in gasifiers it will be necessary to have a thorough understanding of them (Guenther and others, 2012; De Souza-Santos, 2010a).

This report will survey models which are currently available for modelling gasifiers. It will update an earlier report *Modelling and simulation for coal gasification* (Moreea-Taha, 2000). The report will contain a brief description of the three types of gasifiers which are most commonly used. It will detail the fundamental processes that occur in gasifiers. The models available for each type of gasifier will be considered. The report will particularly focus on what assumptions are made, what processes are modelled, how the results compare with available rig or plant data and whether the modelling output has been able to improve the performance of the process.

2 Gasification systems

Though there are many different gasification reactors, each with their own design and operating characteristics, all are based on one of three generic types, namely moving bed (sometimes known as fixed bed), fluidised bed and entrained flow reactors. They differ on whether air or oxygen is used as the oxidant. The method of feeding the coal varies with the system. It is either fed in lump form, as granules, as a dry powder or in a slurry. The flow geometry which determines the way the fuel and oxidant are brought into contact differs between gasifiers. The operational pressures and temperatures in the gasifier and the temperature of the syngas produced varies between the systems. They differ as to whether the minerals in the coal are removed as dry ash or slag. The composition of the syngas depends on whether the oxidant used is air in which case nitrogen is present, or it is mainly oxygen, in which case nitrogen levels are low. It also depends on the amount of steam used, the temperature and pressure of the system and the type of coal used.

In a moving bed gasifier, relatively large particles of coal move slowly down the bed while reacting with oxygen and steam moving usually up the bed. Moving bed gasifiers are only suitable for solid fuels and can gasify biomass and waste as well as coal. The slag is withdrawn through the bottom. In the dry ash version, the temperature is kept below the ash-slugging temperature by the presence of the excess steam. In the slagging version much less steam is used and the temperature is maintained above the ash-slugging temperature. Coal in the size range 5–80 mm is fed into the top of the gasifier using a lock hopper system. The coal residence time is in the range 15 to 60 minutes for high pressure steam/oxygen gasifiers but can be several hours for atmospheric steam/air gasifiers. The pressure in the bed is typically 3 MPa. The oxidant requirements are relatively low. The gas exit temperature is typically 400–500°C. This is not sufficiently high for tars, phenols and other hydrocarbons produced in the pyrolysis zone to be removed by reaction. Methane formation is also very high. Moving bed gasifiers have high cold gas efficiency, compared with other types of gasifiers and a larger proportion of the heating value of the coal appears as chemical energy of the gas rather than thermal energy. These gasifiers do not require the high temperature heat exchangers as with entrained flow and fluidised bed gasifiers. Though moving bed gasifiers have been used less often in power plant than entrained flow gasifiers, they do have the advantage of being more mature technology. There are two main commercial versions of moving bed gasifiers, the dry ash Lurgi version and the slagging British Gas/Lurgi (BGL) version. The main requirement for the sound operation of moving bed gasifiers is the efficient transfer of heat and mass between the solids and gases in the bed. This involves good bed permeability and tight restrictions on the amount of fines present. It is also necessary to avoid coal caking as this increases the likelihood of gas channelling and unstable operation. For the dry ash version, there are limitations on the range of suitable ash fusion temperatures (AFT). A low AFT can result in the formation of large clinkers of fused ash which can cause similar problems as caking coals.

In a fluidised bed gasifier, the fuel is gasified in a bed of hot non-combustible particles suspended by an upward flow of fluidising gas. The coal enters the side of the reactor while the steam and air or oxygen enter at the bottom and fluidise the bed. The residence time of the feed in the gasifier is typically in the range 10–100 seconds but can be much longer. These gasifiers operate at temperatures well below ash fusion temperatures of 900–1050°C to prevent ash melting. They are usually air-based. The low operating temperatures can result in incomplete gasification and the char particles entrained in the raw gas leaving the gasifier are usually recovered by a cyclone and recycled back to the gasifier. Fluidised bed gasifiers differ in ash conditions as being dry ash or agglomerated. In the agglomerating process, there are localised regions of higher temperatures where limited agglomeration of the ash takes place. The agglomerated particles fall to the bottom and the preferential removal of low-carbon particles results in higher carbon conversion. The agglomerated ash operation improves its ability to gasify high-rank coals. Conventional dry ash operation is more suited for low-rank coals. This type of gasifier has the advantage of being able to operate at variable loads. They operate at a uniform and

moderate temperatures. Their oxygen and steam requirements are also modest. Commercial versions of the standard process include the High Temperature Winkler (HTW) and Kellogg, Brown and Root (KBR) designs. Technologies utilising the agglomerating process are the Kellogg Rust Westinghouse (KRW) and the U-gas process. Relatively few large fluidised bed gasifiers are in operation. The operation of fluidised bed gasifiers is affected by many factors including coal properties, in particular the reactivity of the char which must be sufficiently high. Hence reactive coals such as brown coals, lignites, subbituminous and to an extent high volatile bituminous coals and biomass are recommended for these gasifiers. In order to avoid agglomeration, coals with an AFT higher than the operating temperature of the gasifier are recommended.

In entrained flow gasifiers, fine coal particles react concurrently with steam and oxygen or air. Oxygen is the more common oxidant. Coal can either be fed into the gasifier dry or wet in a slurry. They are either single-stage or two-stage depending on how many points the coal is injected. They operate at high temperatures of 1200–1600°C and pressures in the range 2–8 MPa. The temperature must be above the slagging temperature so that the ash behaves like a liquid. The gases exiting the gasifier require significant cooling before being cleaned. The two methods of cooling the gas are either using a high temperature syngas cooler or by quenching the gas with water or recycled syngas. The short residence time of only a few seconds results in high load capacity but requires the coal to be pulverised to <0.1 mm. The reactor is either refractory lined or has a membrane wall. The refractory design typically consists of two or three layers with different materials for coal and oil gasifiers. If there is a membrane wall, boiling water is used to cool the membrane wall and a thin layer of refractory and slag layers protect the wall from erosion. There is a pressure vessel outside the wall and the annular space is pressurised with clean cooler syngas. For this type of construction, slag formation is required.

Entrained flow gasifiers are the most versatile type of gasifier in that they can gasify all coals regardless of coal rank, caking characteristics or amount of fines, though feedstocks with lower ash contents are preferred. They operate at a uniformly high temperature to ensure high carbon conversion and produce a syngas free of tars and phenols. The residence time in the gasifier is very short hence the coal must be very finely divided and homogeneous. The oxidant requirement is relatively large and there is a large amount of sensible heat in the raw gas. The high operating temperatures have an impact on burners and refractory life and require the use of expensive materials of construction as well as the use of sophisticated high temperature heat exchangers to cool the syngas. The differences in design among entrained flow gasifiers currently in operation include the feed system, the internal containment of the hot reaction mixture and the heat recovery configuration. This type of gasifier has been chosen by nearly all coal and oil IGCC systems currently in operation and under construction. Commercial entrained flow gasifiers include the GE gasifier, two versions of the Shell gasifier (one for coal, the other for oil), the PRENFLO gasifier, ConocoPhillips E-Gas (formerly Destec) and Siemens (GSP).

There is ongoing research and development work being undertaken to improve the reliability and efficiency of gasifiers, to reduce their costs and to increase the range of coals they can gasify. The feed injectors for slurry-fed gasifiers incur high failure rates. Both GE and ConocoPhillips experience significant maintenance costs for these injectors, which require replacing as often as every few months. It is desirable to improve the design of feed injectors to achieve a life of at least 8000 h. The feed injector life is not a major concern for dry-fed Shell gasifiers, whose injectors last for at least 16,000 h but these use lock hoppers to bring the pulverised coal up to gasifier pressure. These systems comprise high pressure components and require a large superstructure. They also consume high pressure nitrogen and need significant maintenance due to frequent pressure cycling of large valves exposed to solids. Interest in using water quench to cool the raw gas has increased in recent years as additional moisture in the syngas is beneficial for the water-gas shift reaction which is required prior to CCS. In the original GE gasification system, the radiant cooler mounted below the gasifier was followed by twin convective coolers. In the current design, the radiant cooler is retained but the syngas cooler is replaced by a water bath.

Fouling and plugging of syngas cooler systems have been a major cause of unplanned outages in slurry-fed IGCC plant. The syngas coolers used in IGCC plant in the USA are of fire tube design whereas those in European IGCCs are of water tube design. The former have tended to suffer loss of availability due to deposition, erosion and corrosion. Fouling and plugging reduce plant heat rates, place additional strain on solids handling and grey water circuits and reduce overall reliability of the gasifier. The primary cause of fouling is deposition of condensible solids and particulate matter on the heat transfer surfaces. It is important to understand how the presence of metallic elements such as iron and vanadium and their oxidation state impact slag velocity. Modelling can be utilised to simulate the flows, temperatures and condensation phenomena occurring in syngas cooling systems. Models can be used to predict conditions under which deposition would occur, the location of these deposits and enable designers to develop coolers that would minimise its occurrence.

Refractory developments are essential for improved gasifier performance. High temperature gasifiers use one of two techniques to protect the steel walls of their containment vessels from the high temperatures in the gasifier. Shell and Siemens use water-cooled membrane walls to produce a solidified slag layer on the wall surface. This system requires a complex and costly cooling and control system but does have an estimated life of 25 years. The other approach, adopted by GE and ConocoPhillips involves a multiple-layer refractory lining. This results in a significantly lower cost for the gasification vessel but repair and replacement of the refractory lining is frequent and expensive. Ongoing research into refractory operation has focused on the development of improved chrome-based refractory by the addition of aluminium and chrome phosphates. Modelling will facilitate the understanding and control of slag chemistry. The development of slag models will lead to a deeper understanding of the fundamental processes taking place and will help operators to control slag viscosity, maximise refractory service life and minimise downstream issues such as syngas fouling (Fernando, 2008; NETL, 2012a,b).

3 Fundamental processes

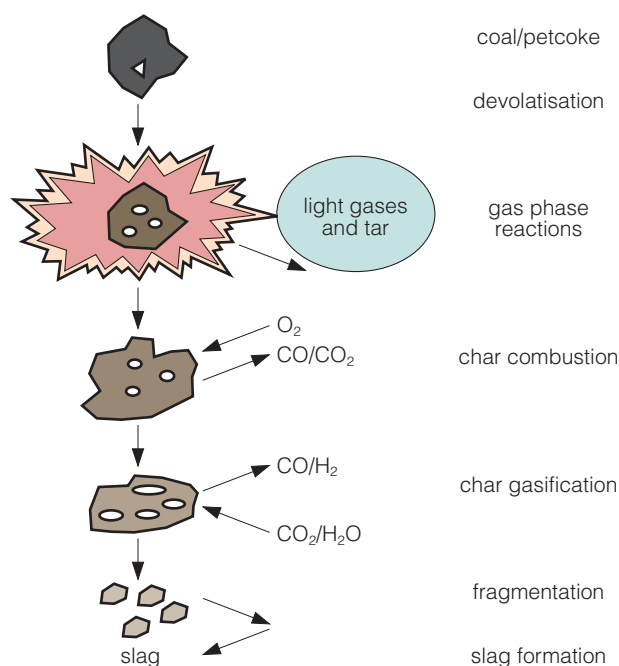


Figure 1 Processes occurring during gasification (Oshinowo, 2009)

Coal gasification involves several fundamental processes. Firstly, volatile components in the coal such as light gases and tar are released by pyrolysis (also known as devolatilisation). These species undergo homogeneous gas phase reactions forming CO, CO₂, H₂, H₂O which then combust and gasify the char. These are shown in Figure 1. Each process must be understood and modelled when modelling coal gasifiers.

3.1 Pyrolysis (devolatilisation)

Coal pyrolysis is the initial step in most coal conversion processes, accounting for up to 70% of the weight loss and 50% of the heating value of the coal. This process is the most dependent on the organic properties of the coal. When gasifying coal, the temperatures and product distributions are strongly influenced by pyrolysis. During pyrolysis, the labile bonds between the aromatic clusters in

the coal are ruptured, generating fragments of molecular weight much smaller than coal. Fragments with low molecular weight vaporise and escape from the particle to constitute light gases and tar. The fragments with high molecular weight and low vapour pressure remain in the coal and they reattach to the char lattice. This solid product is the char. The process starts at temperatures about 100°C with the desorption of gases such as water vapour, CO₂, CH₄ and N₂ which are stored in the coal pores. At temperatures above 300°C, the release of gaseous compounds is accompanied by the release of liquid hydrocarbons called tar. Methane formation is probably due to the decomposition of methyl groups at low temperatures and methylene bridges at higher temperatures. The amount of methane produced depends on several factors namely the coal, the gasifier type and the operating temperature and pressure. It is favoured by low temperatures and high pressures. Hence higher amounts of methane can be expected in moving bed gasifiers than in fluidised bed or entrained flow gasifiers. Tar formation at a particular temperature depends on coal rank and tar stability at that temperature. As the coal rank increases, the proportion of light gases in the volatile product increases in relation to the tar. The overall weight loss can be characterised by rapid initial release of 80–90% of the volatiles followed by the slow release of the remaining 10–20%. The early release consists primarily of tar, aliphatics, CO₂ and H₂O while the later releases include predominantly CO, H₂O with minor amounts of HCN, benzene and other compounds. At temperatures above 500°C, the coal particles become plastic and they undergo drastic changes in size and shape. They harden again and become char when the temperature reaches 550°C.

3.1.1 Devolatilisation modelling

There are several approaches to model devolatilisation. A single first-order model is commonly used in which the rate of devolatilisation is taken to be dependent on the amount of volatiles remaining in the particle. In its simplest form this rate is expressed as:

$$dV/dt = k (V^* - V)$$

and k is typically correlated with temperature by the Arrhenius expression:

$$k = k_0 \exp(-E/RT)$$

where V is the cumulative amount of volatiles produced up to time t and k is the rate constant. V^* represents the effective volatile content of coal. The single first-order model is strictly applicable only to homogeneous systems in which decomposition from source V^* results from a single chemical process with a single activation energy. A more realistic model assumes devolatilisation occurs through a series of parallel independent reactions. This model allows V^* to be somewhat inhomogeneous, so that instead of a single reaction, there are several. The rate expression for each volatile species is given by:

$$dV_i/dt = \sum k_{ij} \exp(-E_{ij}/RT) (V_{ij}^* - V_{ij})$$

This first-order kinetics approach for devolatilisation has limitations but has been found to give an adequate representation of hydrocarbon yield (Lee and others, 2011).

A more detailed representation can be derived by obtaining more accurate values for V_{ij}^* . This is possible utilising the FLASHCHAIN programme which predicts the complete product distribution and char characteristics for any coal under any operating condition, given the proximate and ultimate analysis of the sample and the process operating conditions. Coal is modelled as a mixture of chain fragments ranging from a monomer to the nominally infinite chain. These are constructed from four structural components: aromatic nuclei, labile bridges, char links and peripheral groups. The theory's central premise is that partitioning of the elements among aliphatic, heteroatomic and aromatic constituents largely determines the devolatilisation behaviour of any coal type. In the FLASHCHAIN model, population balances are used to account for the distribution of mass in each molecular weight size bin based on chain statistics, the flash distillation process and a crosslinking mechanism. The results from this model have been shown to compare well with a wide variety of experimental data from hundreds of coal samples although vapour pressure coefficients are determined empirically and do not correspond well with independent vapour pressure data.

Results from the FLASHCHAIN model can be incorporated to enable a more accurate representation of coal devolatilisation when using the single first order reaction for devolatilisation. The parameters k_0 , E and V^* are usually assigned from laboratory test data. Instead FLASHCHAIN can be used to synthesise simulation data that can subsequently be analysed for rate parameters just like test measurements. Firstly, dV/dt , $V(t)$ and V^* for the operating conditions of interest can be evaluated from FLASHCHAIN predictions. These values can be used to calculate k and then using data for different conditions to assign k_0 and E using the following equation:

$$k = (V^* - V(t))/dV(t)/dt = k_0 \exp(-E/RT)$$

Arrhenius diagrams can be produced by plotting $\log k$ against $1/T$. This has been undertaken in three cases: (i) a pf combustion case based on the mean thermal history of a simulation of a 1.7 MW pilot-scale flame at atmospheric pressure (ii) an entrained-flow gasification case based on 55 μm particles injected into gases at 1600°C at 2.5 MPa (iii) PFBC case having 2 mm particles heated to 850°C at 1.5 MPa. All cases are based on typical bituminous coal. The FLASHCHAIN (dashed lines) and linear fits are compared in Figure 2. It is apparent that the frequency factor of the Arrhenius expression (k) is greater at faster heating rates whereas the activation energies are hardly affected (Niksa and Kerstein, 1993; Niksa and others, 2003; Niksa, 2005).

The chemical percolation devolatilisation (CPD) model was developed to describe devolatilisation in terms of the chemical structure of the parent coal. Coal is visualised as a macromolecular array whose building blocks are clusters of fused aromatic rings of different sizes and shapes containing

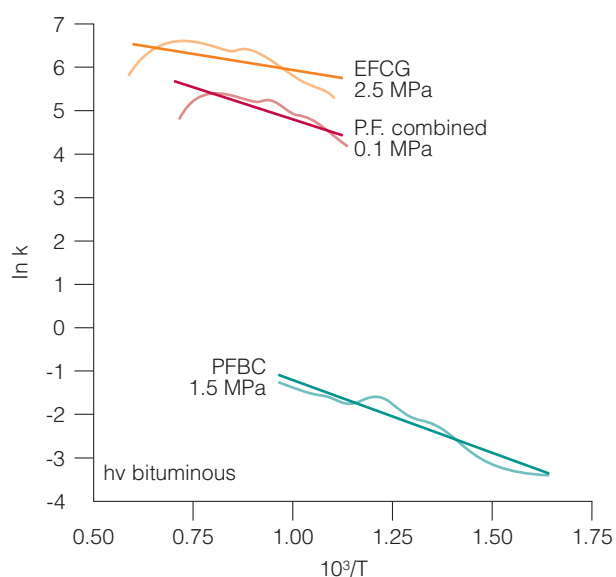


Figure 2 Arrhenius diagrams to fit FLASHCHAIN results (Niksa, 2005)

heteroatoms such as nitrogen and oxygen. These aromatic clusters are interconnected by a series of chemical bridges some of which are labile and break readily during pyrolysis while others continue to be stable depending on temperature. The bridges which remain intact throughout a given thermal process are referred to as charred bridges. Side chain attachments to the aromatic clusters include aliphatic (-CH-) and carbonyl (-CO₂-) groups which are the precursors of the light gases released during devolatilisation. Fragments that detach from the coal matrix consist of one or more of the aromatic clusters connected by labile and/or char bridges. Distributed activation energies are utilised and literature values for kinetic parameters are used whenever available in the model. The model incorporates ultimate gas yields and chemical structural data from solid state NMR measurements to fix input parameters. The model exploits the features of percolation theory to specify the total yield and mass distribution of tar species for a given degree of bond rupture. The approach that was applied was to obtain chemically dependent input parameters, partly from NMR data, to reflect the chemical diversity found in coals of different rank and type. Lattice statistics with explicit mathematical functions were used. The distribution of tar molecular clusters of varying sizes as well as the fraction of material in the infinite array were provided by expressions from percolation theory. The published values for the activation energy for tar release were used as were the activation energies and frequency factors for light gas release from the weighted averages of available data. A simplified method was used to calculate the distributed activation energies for both tar and light gas release. The model allows the distinction between (a) low molecular weight aromatic fragments that vaporise as tar and (b) high molecular weight fragments that remain with the char in a liquid or solid state as metaplast. A new vapour pressure

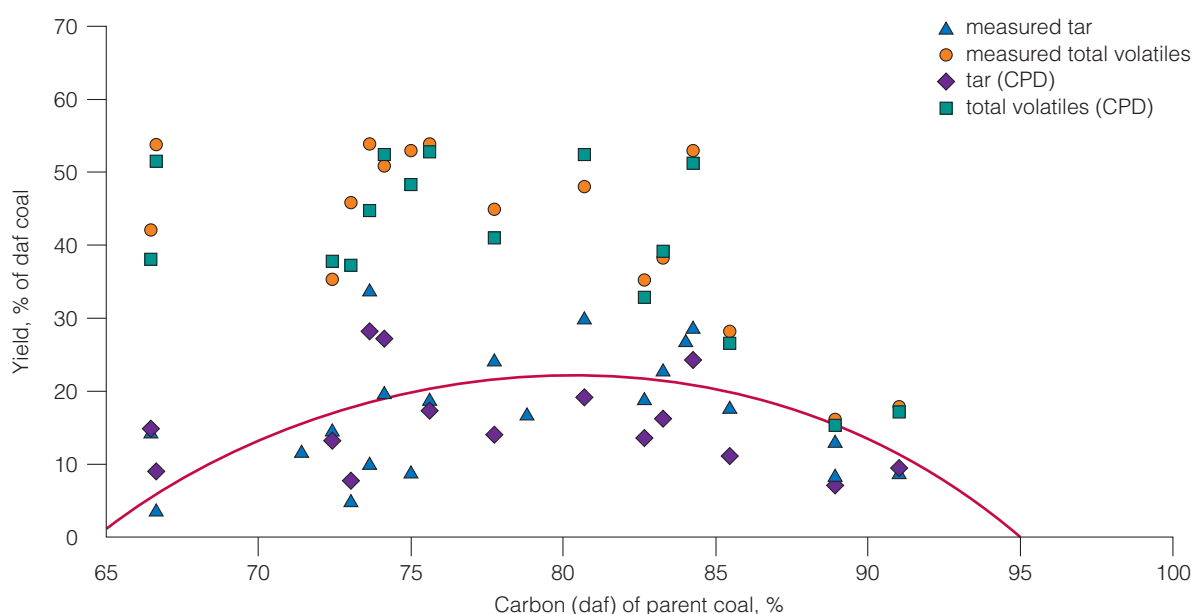


Figure 3 Measured and predicted tar and volatile yields (Fletcher and others, 1992)

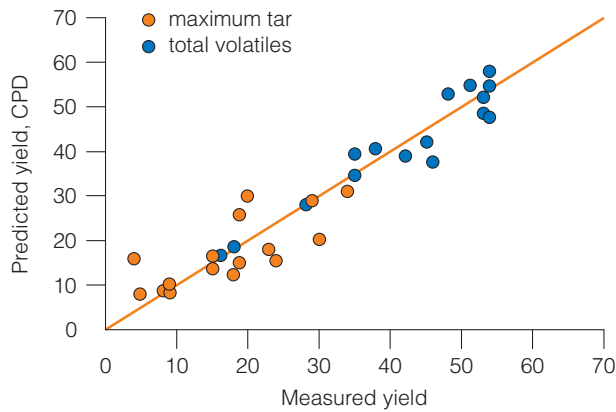


Figure 4 Comparison of predicted and measured tar and volatile yields (Fletcher and others, 1992)

premium coal samples; (b) in rapid heating experiments for three coals at heated tube reactor and (c) in a laminar flow reactor for five coals at high heating rates. The experimental data are compared with CPD predictions in Figure 4. The general trend is that low rank coals produce similar total volatile yields as high volatile bituminous coals then the volatile yield decreases for high rank coals. The model results not only confirm the trend but give quantitative agreement. The tar is underpredicted for high tar yields from high volatile bituminous coals but is probably within the uncertainty in the data (Fletcher and others, 1992).

correlation was developed from data on coal liquids that enabled predictions of tar molecular weights and yields as a function of residence time, temperature and pressure. In contrast to other models in which model parameters are chosen to fit experimental data, in CPD the coal-dependent structural coefficients for the model are taken from analyses of the parent coal. The predictions of tar and volatile yield as function of coal type, temperature, heating rate and pressure are a true test of the model rather than a curve-fitting exercise. CPD model predictions for tar and total volatile yields are compared with several sets of experimental data in Figure 3. The data shown were obtained for (a) at low heating rates in TGA for eight Argonne

3.2 Homogeneous reactions

The volatile components released from the coal undergo homogeneous reactions with the oxygen present on the gasifier. These can be modelled as large numbers of detailed reactions involving radicals or based on a global reaction. The former approach is too complex given the number of processes that need to be modelled in a gasifier hence it is more usual to adopt global reactions. The following Arrhenius expression is utilised for the homogenous reactions.

$$\text{Rate} = A_i \exp(-E/RT) [X]^a [Y]^b$$

Typical reactions considered are given in Table 1. Most of the available O_2 reacts during volatiles

Table 1 Typical chemical reactions occurring during gasification (Lee and others, 2011)	
Homogeneous reactions	ΔH , kJ/mol
$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$	-519.5
$C_2H_6 + 2.5O_2 \rightarrow 2CO + 3H_2O$	-862.4
$C_6H_6 + 4.5O_2 \rightarrow 6CO + 3H_2O$	-1471.3
$CO + 0.5O_2 \rightarrow CO_2$	-283.1
$H_2 + 0.5O_2 \rightarrow H_2O$	-242.0
$CO + H_2O \rightarrow CO_2 + H_2$	-41.2
Heterogeneous reactions	
$C(s) + 0.5O_2 \rightarrow CO$	-110.5
$C(s) + H_2O \rightarrow CO + H_2$	131.3
$C(s) + CO_2 \rightarrow 2CO$	172.5
$C(s) + 2H_2 \rightarrow CH_4$	-74.6

combustion and oxidative pyrolysis. While volatiles are being released, O_2 does not react with the char as the reactions with the volatiles are more rapid. The heat released by these exothermic reactions constitute a major heat source of heat and these reactions take place throughout the gasifier.

3.3 Char gasification

Following pyrolysis, the char residue contains the remaining mineral matter and carbon. At temperatures above 700°C , char gasification takes place. As the rate of char gasification is much slower than devolatilisation, the design and operation of gasifiers is primarily

dependent on the gasification of char. This process can be summarised by following five simple basic chemical reactions (Adams and others, 2009):

Gasification with oxygen (partial combustion):



Combustion with oxygen:



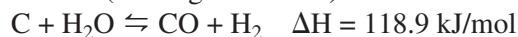
This is the most effective reaction for gasification and produces the heat necessary to dry the coal, break chemical bonds in the coal, to raise the products to reaction temperature and to drive the other gasification reactions.

Gasification with carbon dioxide (Boudouard reaction):



This reaction is endothermic and, in the absence of a catalyst, takes place several orders of magnitude slower than the reaction with oxygen. It is very slow below 730°C and is inhibited by its product.

Gasification with steam (water-gas reaction):



The endothermic reaction with steam is favoured by elevated temperatures and reduced pressures and, in the absence of catalysts, occurs slowly at temperatures below 930°C. The uncatalysed reaction is inhibited by its product but is generally faster than the reaction with CO₂ under the same conditions.

Gasification with hydrogen:



This reaction is very slow except at high pressure.

The following two reactions change the composition of the syngas. The water-gas reaction alters the CO/H₂ ratio. The methanation reaction increases the calorific value of the syngas but is very slow except at high pressure and in catalytic reactions.

Water-gas shift reaction:



Methanation:



The gasification reactions occur at the char surface. Under gasification conditions, most of the surface area is present in the pores of the particle. Hence the overall gasification process involves a series of steps:

- 1 External mass transfer of the reactant from the main gas stream to the char particle surface.
- 2 Adsorption of the reactant onto the surface.
- 3 Diffusion of the reactant within the pores of the char.
- 4 Reaction of the adsorbed gases and the solid.
- 5 The diffusion of the product gases through the pores of the char.
- 6 Desorption of the product gases
- 7 Mass transfer of the product gases from the particle surface to the main gas stream (Adams and others, 2009; Bell and others, 2011).

The reactivity of coal chars is affected by several factors and these will be described below.

3.3.1 Particle temperature and pressure

In gasification, chemical reaction and transport processes both have a role in the overall process. The rate limiting step is either the chemical reaction (4) or the diffusion process (3 and 5). At relatively low temperatures, the surface reaction is the slowest step and controls the overall rate of reaction. As the temperature increases, the surface reaction rate rapidly increases and the diffusion becomes rate-limiting. Laboratory studies have shown that, for gasification with both CO₂ and H₂O, at temperatures below 1000°C, the rate was chemically reaction controlled. Katijani and others (2006) measured CO₂ gasification rates for four coal chars and found that the mass transfer rate affected the overall reaction rate when the temperature exceeded 1200–1300°C. Below this temperature, the char particle size did not affect gasification rates but at higher temperatures, the rates for smaller particles were faster than for larger particles. The transition temperature from chemically to transport-controlled kinetics is usually carried out using an Arrhenius plot. This temperature is much lower for lignites than for bituminous coal which in turn is lower than for anthracites. This is due to their different reactivities. Since non-slugging gasifiers typically operate at temperatures less than 1100°C, they are probably in the surface reaction rate limited regime. Slugging gasifiers operating at higher temperatures are most likely affected by mass transfer rate limitations. Low rank coals, such as lignites, are better suited for non-slugging gasifiers than high rank coals. Entrained-flow gasifiers, with their high operating temperatures can gasify low reactivity fuels such as petroleum cokes (Bell and others, 2011).

3.3.2 Pore structure

During the gasification of char under chemically controlled conditions, the porosity changes and the reactivity changes as a result of the changes in the total number of active sites per given amount of carbon present. The processes taking place are: the widening of existing pores; the creation of new pores and the opening of previously inaccessible pores. Initially, as the pores become larger, the surface area increases. Later, as the pores merge and the walls dividing them disappear, there is a loss of surface area. These processes can be modelled by the random pore model. The rate of reaction is described in terms of the extent of reaction:

$$dx/dt = (1 - X) \sqrt{1 - \psi \ln(1-X)}$$

where X is the extent of reaction and ψ a dimensionless quantity related to structural properties. ψ is related to measurable quantities but cannot be determined absolutely and hence must be regarded as a parameter used to fit experimental data. Figure 5 contains a prediction for the random pore model of how the extent of reaction increases with time. Initially, the rate of reaction increases because the pores become larger. Later, as the pore surface disappears, the rate slows down. The random pore model can be modified to account for the fact that the surface reactivity is more accurately proportional to the number of active sites which is not necessarily directly proportional to the surface area (Zhang and others, 2010; Bell and others, 2011).

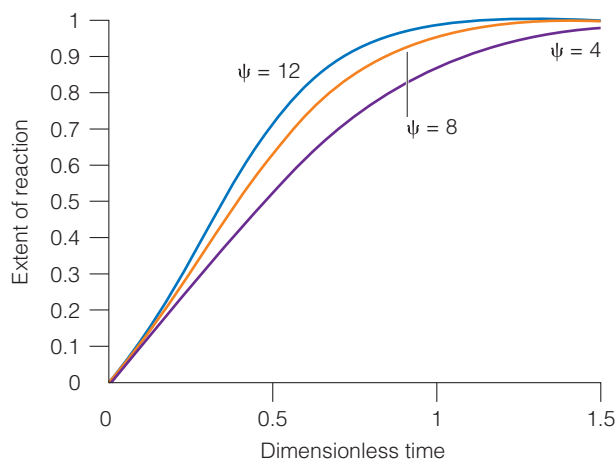


Figure 5 Extent of reaction predicted by random pore model (Bell and others, 2011)

3.3.3 Shrinking core model

At very high reaction rates, the overall reaction rate is not determined by the surface reaction rate or the rate of diffusion in the pores but by the rate of mass transfer to and from the exterior of the particle. In this case the rate of reaction can be modelled by the shrinking core model. Whereas in the random pore model, as the reaction proceeds, the particle diameter is unchanged but the porosity increases until there is nothing left but ash, in the shrinking core model, the porosity remains constant but the particle diameter decreases. In the case of the shrinking core model, the particle mass is taken to be proportional to the volume and the reaction rate to be proportional to the external surface area. The volume of the particles is proportional to the mass which is dependent on the proportion of char remaining.

$$\frac{4}{3}\pi r^3 \propto (1-X) \text{ where } X \text{ is the extent of reaction}$$

The rate of reaction is proportional to the surface area of the char.

$$-dX/dt \propto 4\pi r^2$$

$$\rightarrow -dX/dt \propto (1-X)^{2/3}$$

As in the random pore model, the shrinking core model also predicts that the rate falls as the particles react. The shrinking core model, however, does not predict the initial acceleration but there is often enough scattering in the measured results for either model to fit the data. While the two models give similar predictions, their base assumptions are very different. The random pore model assumes a surface reaction determined mechanism whereas the shrinking core model assumes a mass transfer determined one. In non-slagging gasifiers, the reaction is normally surface reaction limited hence the random pore model is preferred. The high reaction rates of slagging gasifiers are more likely to be mass transfer limited hence the shrinking core model is more appropriate (Bell and others, 2011).

4 Approaches to gasifier modelling

Modelling complex systems such as gasifiers involves solving two types of equations:

- Fundamental equations such as laws of thermodynamics, conservation of mass and momentum.
- Auxiliary equations, usually based on empirical and semiempirical correlations.

The combination of fundamental equations and empirical correlations may mean that the model is only valid within the same range as the correlations. There are several degrees of complexity that can be incorporated in the model. First is the number of space dimensions considered; three levels are possible. Secondly, whether time is included. If it is, the model is dynamic, otherwise it is steady state. In the latter case, for a given set of space co-ordinates, it has to be assumed that the control surface does not deform or move. Furthermore, the mass flows and the average properties of output streams are constant. The rates of heat and energy transfer between the control volume and the surrounding space are constant and though conditions may be different at different points in the control volume, they remain constant. Many industrial processes, after an initial period, work at or near steady state but some degree of fluctuations regarding variables such as temperatures, concentrations and pressures are inevitable. However, these are normally within a narrow range and can be treated as constant (De Souza-Santos, 2010a).

4.1 Zero-dimensional models

In zero-dimensional models, the output variables are evaluated in relation to the input variables without considering the details of the processes occurring inside the control volume. There is no evaluation or description of temperature, velocity or concentration inside the equipment. In spite of the limitations, these models may be useful if only an overall analysis is required. They will generally need to assume that chemical and thermodynamic equilibrium is present at the output streams. Rigorously, this will require infinite residence times. The assumption will not be valid for gasifiers for which residence times are in the range of seconds to minutes. Furthermore, in gasifiers where gas-solid interactions occur, a certain level of fuel conversion will have to be assumed as the model cannot evaluate heat and mass transfer. The internal temperature may be much higher than that of the exiting stream. Choosing some average temperature is arbitrary and will cause misleading results. These models cannot model pyrolysis or devolatilisation. For these reasons, these models are not suitable for modelling gasifiers (De Souza-Santos, 2010a).

4.2 One-dimensional models

These models assume that all variables inside the equipment vary along one space co-ordinate. They constitute a considerable improvement compared with zero-dimensional models. Equilibrium hypotheses are no longer necessary and profiles of variables such as temperature, pressure and compositions can be evaluated throughout the system. Of course, they will not be adequate to model systems where there are large variations of parameters in more than one direction (De Souza-Santos, 2010a). One-dimensional models have been used successfully to model all types of gasifiers.

4.3 Two-dimensional models

Two-dimensional models are necessary where the variation of an important property of the system in a second dimension can no longer be neglected. For example, considering a reactor in which an exothermic reaction is taking place and heat is exchanged with the environment through an external wall. The examples of plug-flow and laminar-flow are shown in Figure 6. The variations of

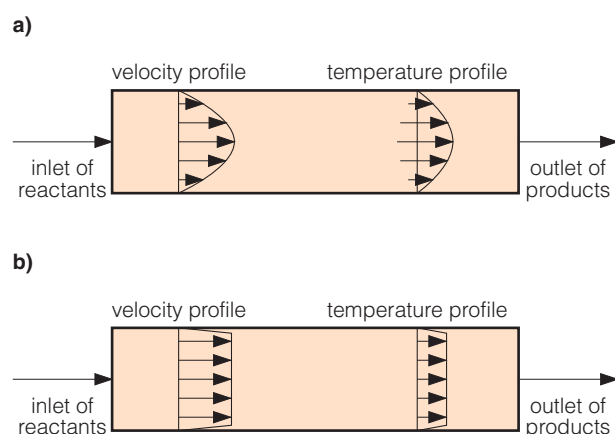


Figure 6 Schematic representation of laminar and plug flow (De Souza-Santos, 2010a)

temperature and composition in the axial and radial directions are shown. In the case of plug flow which will occur if the flow is highly turbulent or there is packing in the reactor, it would probably be adequate to compute temperature, velocity and concentration averages at each cross-sectional position along the reactor length. Though there is a large change in temperature or velocity in a thin layer near the wall, this layer is not representative of the flowing mass. Compared with the variations of composition and temperature in the axial direction it would be adequate to neglect variations in the radial coordinate. Hence a 1-D model would probably suffice in this case. However, in the laminar flow case, both the velocity and temperature change in the radial direction.

This will result in a non-uniform concentration of chemical components and a 2-D model will be required to predict the exit conditions (De Souza-Santos, 2010a).

4.4 Three-dimensional modelling

Three-dimensional modelling entails considerable mathematical and computational complexity but in many situations is necessary for a realistic representation. If the model and simulation are successful a great deal of valuable information about the process can be obtained. If the process to be modelled has cylindrical symmetry, a two-dimensional model may be adequate but for asymmetric geometries, 3-D models are necessary. In order to set up a 3-D model for a complex process such as coal gasification, the complete Navier-Stokes or momentum conservation equations need to be solved. These solutions have to be combined with equations for energy and mass conservation for all chemical species. All these equations must be formulated in three dimensions and solved throughout the reactor. Such a system of equations also requires a large number of boundary conditions. Frequently, these consist not only of the values at interfaces but also derivatives. Moreover, the specification of boundary conditions may entail complex geometric descriptions. For example, the injection of the reactant streams at the feeding section may be made by such a complex distribution system that even setting the boundary conditions would be complex. When auxiliary correlations and equations for the computation of all parameters are included, the final set of mathematical equations will be very large. However, commercially-available computational fluid dynamic programmes have been developed to solve such systems of equations, which are described in the following section. Very good agreement in some cases has been obtained, particularly for single-phase systems. Nevertheless, modelling combustion and gasification of solid fuels poses considerable difficulties given the large number of processes involved.

When developing models, it is instructive to consider what information is necessary for good design and optimisation. Is it essential to predict details of velocities, concentrations and temperature profiles in all directions inside the equipment? Another issue is whether the greater predictive ability between simulation and real operation justifies the resources required to upgrade a model for 2-D to 3-D. Furthermore, which parameters need to be measured experimentally to validate the model. Though temperatures, pressures, mass flows and composition of streams entering and leaving a gasifier can be easily measured, the measurement of these variables inside the gasifier is very much more difficult to determine with a reasonable degree of accuracy. Sometimes only average values at some points are possible. This illustrates how important it is that those involved with modelling are well acquainted with its real operation (De Souza-Santos, 2010a).

4.5 Computational fluid dynamics (CFD)

In the last few decades, CFD modelling has played an important role in improving the performance of pf plant. Similarly, CFD modelling can provide insights into the flow field within a gasifier and can lead to improved performance. Used correctly, a CFD model is a powerful tool that can be used to investigate many types of plant. These models incorporate gasifier geometry, operating conditions and the gasification processes. The outputs or predicted values from a CFD model can provide localised information about hundreds of thousands of points within the gasifier. This can lead to a better understanding of the operation of the gasifier and indicate solutions to potential problems (Bockelie and others, 2002).

When a system simpler than a gasifier is modelled with CFD, the continuity equations and the equations of motion can be discretised using a finite element method. In this method, the continuous equations are approximated by dividing the flow problem into a three-dimensional mesh. Each mesh element is assumed to have uniform properties and the mesh size is chosen such that the solution will approximate the continuously varying fluid properties. Equations are written to describe the geometry of the system and appropriate boundary conditions are chosen. This generates a large matrix of simultaneous equations whose solution describes the fluid flow in the system.

Using CFD models to describe gasifier operation requires the addition of several layers of complexity. Firstly multiple phases are present as gasifiers contain solids in addition to the gas phase. The solid particles have a range of shapes and sizes and their organic components are consumed while passing through the gasifier. In a slagging gasifier, liquids are also present. The phases in the reactor are complex and contain changing chemical mixtures. Both homogeneous and heterogeneous reactions must be considered. In addition to the continuity equation and the equation of motion, the energy equation and mass transfer equations must be solved as coupled equations. Both the latter equations contain reaction terms. To accurately model the gasifier, the modeller needs to have complete knowledge of relevant phenomena including solid properties, reaction rates, mass transfer rates, heat transfer rates, gas viscosities and equation of state data. These models require total knowledge of the system. Unfortunately, much of the necessary data is rarely available. It has been estimated that 90% of what is needed to model combustion systems is known whereas only 20% is known for gasifiers. Key areas requiring further research include heterogeneous reaction kinetics, the behaviour of the ash/slag and the interactions with the gasifier wall.

CFD modellers incorporate accurate, measured data as much as possible. Where this is not possible, it will be necessary to obtain approximations from reasonable sub-models. Hence a typical CFD model can contain a large number of unknown parameters and assumed equations. The modeller will attempt to validate the model by comparing model results with the available measured data. Since the model contains a large number of assumed parameters, it is often possible to adjust these parameters to fit the experimental data. Even with a purely empirical model, having no fundamental information, it is sometimes possible to match system performance accurately over a limited set of conditions. The difficulty with empirical models is that they usually cannot be extrapolated to a new set of conditions. Empirical models cannot be used to predict conditions at points within the system that cannot be readily measured. A CFD model based on a combination of known, fundamental information and assumed data should be regarded as a semi-empirical model. These are better than purely empirical models but not as reliable as a model based on recognised fundamental data. Heterogeneous reaction kinetics are particularly difficult to model but it may be possible to obtain satisfactory overall model results as heterogeneous reactions can have little impact on overall reaction rates. Non-slugging gasifiers, on the other hand, are more likely to be surface kinetically limited. In these gasifiers it is more important to understand heterogeneous reaction kinetics than mass transfer in the gas phase. Slugging gasifiers operate in a coupled regime where both heterogeneous kinetics and mass transfer strongly affect overall reaction rates (Bell and others, 2011).

4.5.1 Recent developments

New gasifiers coming on-line will require greater fuel flexibility, reliability, availability, maintainability and higher throughput and conversion. To achieve these aims, one requirement is better mathematical models for gasifiers. The existing CFD models for gasifiers include MFIX, ANSYS-FLUENT and BARRACUDA. The accuracy and validity of CFD models depends on the kinetic models used to describe the homogeneous and heterogeneous reactions that take place in the gasifier. There is a need for sophisticated models for coal devolatilisation, combustion and gasification at various operating conditions and for a wide variety of coal. Kinetic models invariably have limitations in operating condition range and fuel types. Kinetics packages such as PC Coal Lab, CPD and FGDVC are currently utilised with CFD codes. PC Coal Lab is a mathematical model developed by Niksa and his group (Niksa, 2006). It predicts kinetics and composition of products from devolatilisation, tar cracking with secondary pyrolysis and gasification reactions for over 2000 coals and biomass and petcoke. The input data required are based on the proximate and ultimate analysis of the coal. The model predicts the yields of all major primary devolatilisation products as well as the elemental compositions of tar and char. It also predicts the subsequent secondary pyrolysis of the primary volatiles. It can predict the effect of pressure, temperature and heating rate on devolatilisation. The CPD (Chemical Percolation Model) was developed by Sandia National Laboratories and describes the devolatilisation behaviour of rapidly heated coal based on the chemical structure of the parent coal (Fletcher and others, 1992). The current version can only predict devolatilisation of coal. The CPD model successfully predicts the effects of pressure on tar and total volatile yields in heated grid experiments for coal. Predictions of the amount and characteristics of gas and tar from many different coals compare well with available data. The FG-DVC model is a comprehensive code for predicting yields and compositions of coal pyrolysis products. It can model coal as well as biomass and waste material. The FG-DVC model combines two previously developed models: the Functional Group (FG) model which predicts gas evolution functional group and the Depolymerisation, Vaporization and Cross-linking (DVC) which predicts the quantity and molecular weight of macromolecular fragments (Soloman and others, 1992).

Until recently, there was no software platform that enabled the user to access the information from kinetic packages and easily convert their predictions into usable, correctly formatted, reaction expressions that could be used subsequently to run CFD codes. NETL (National Energy Technology Laboratory) have developed C3M to facilitate the use of multiphase CFD models. The development of C3M has centred on two central goals: to provide a platform to perform virtual kinetic runs that elucidate the effect of operating conditions and to provide a tool that directly imports kinetic information into CFD models and other types of software. C3M provides the user with the necessary kinetic information for processes occurring in the gasifier such as moisture release, devolatilisation, tar cracking, char gasification, heterogeneous char and soot combustion and homogeneous combustion. C3M interfaces with kinetic packages PC Coal Lab, CPD, FG-DVC and NETL's in-house kinetic data. The kinetic models can be coded in any CFD software by the user. The C3M software directly exports the kinetic models to: NETL's open-source multiphase CFD software MFIX; commercial CFD software ANSYS FLUENT and BARRACUDA. These features enable C3M to incorporate gasifier chemistry into multiphase CFD and other computational models. Computational models can be used in industry to assess new gasifier designs quickly and to predict system response to changes in fuel type and operating conditions. The developers of C3M claim that by incorporating appropriate chemical reaction mechanisms into multiphase CFD models, C3M effectively opens a window into the actual operation of a gasifier. It should result in considerable reduction in man hours and computational hours and hence cost of the development and implementation of reacting CFD models (Chaudhari and others, 2011,2012; Guenther and others, 2012).

5 Modelling gasifiers

5.1 General considerations

As has been described in Chapter 2, in a moving bed gasifier, the solid carbonaceous fuel is fed at the top of the reactor and slowly flows to the base where the residual solid is removed. The gasification agents are injected most commonly at a position near the base or less commonly near the top. The syngas that is produced, composed mainly of CO, H₂, CO₂ and nitrogen is withdrawn at the top or in the downdraft design at the bottom. They are widely used because of their simplicity and degree of controllability. Many processes take place in the gasifier such as drying, devolatilisation, gasification and combustion. These include combined processes for example, homogeneous and heterogeneous chemical reactions; heat, mass and momentum transfers; and particle attrition. Though the system is inherently complex, several models have been developed which are able to reproduce the processes taking place and make predictions under industrial-scale operational conditions. In the case of moving bed gasifiers many models have been based on one-dimensional representations. This level of sophistication has been found adequate to provide information needed for engineering design and process optimisation.

The gasifier can be schematically represented by a model chart as shown in Figure 7. There are two basic streams: the solid flowing downwards and the gas upwards. The two streams exchange heat and mass through their common interface. This can be imagined as a single continuous surface with an area equivalent to the real area separating the two phases. This area would be given by the total surface area of all solid particles in the bed. Regarding the hydrodynamics of each phase, the simplest model is to assume each phase, gas and solid, flows through the reactor in plug-flow regimes. This assumption is reasonable for any fluid which percolates along the main direction. As the gas percolates up the bed, it is forced to pass through narrow channels between the particles. Irrespective of whether the flow is laminar or turbulent, the overall combination of these small streams mimics a plug-flow for the gas phase. If the gas velocity can be assumed to be even throughout the bed cross-section, the temperature and concentration profiles can also be modelled as flat profiles. Hence the gas-solid reaction rates would not vary significantly in the horizontal direction. This leads to an almost uniform consumption of coal at a given cross-section of the bed. The solid phase flows in similar downward movement and can also be assumed to be plug-flow. Another factor which allows one-dimensional treatment is the relatively large difference between the reactor cross-section diameter and the particle diameter. Steady-state operation is also assumed which is common when modelling most industrial reactors. Clearly, this is not so during start-up and shut-down but moving-bed gasifiers operate for long periods without the need for interruptions. The rates of solid feeding and gas production are relatively constant.

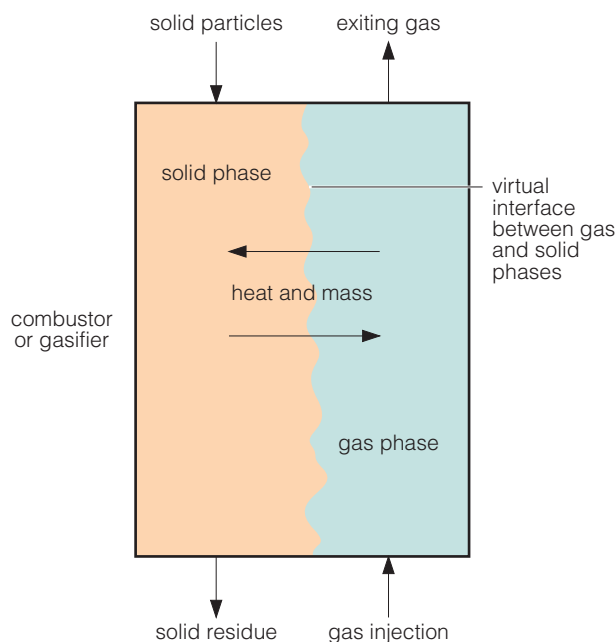


Figure 7 Schematic of idealised updraft moving-bed reactor (De Souza-Santos, 2010a)

When considering mass exchange between phases, the simplification of plug-flow requires further discussion. As oxygen, water and other gaseous species react with the carbonaceous

fuel, mass is transferred to the solid phase. At the same time, CO_2 , CO , H_2 and other gaseous components leave the solid phase and migrate to the gas phase. This establishes a crossflow perpendicular to the main, vertical direction of the gas and solid streams. Gases enter and leave the particles, which are more or less evenly distributed in the bed. In the model, radial components of the variables must be included in the source or sink terms. This approach preserves the integrity of mass and energy balances while requiring only ordinary differential equations without needing partial differential equations. Momentum transfers between the phases can be assumed to be negligible. Thus the velocity profile in one phase is not affected by the flow of the other phase. This assumption is reasonable since velocities of both components in the gasifier are relatively small.

The temperature and concentration profiles can be assumed to be flat but different for each phase resulting in heat and mass transfer. Strictly speaking, the difference in temperatures between the gas and solid phase at each position in the bed would lead to a non-flat temperature profile within each phase. For example, where the solid at a given axial position is hotter than the gas, at points near the particle surface, the surface solid temperature would be lower than in the bulk and the adjacent gas temperature would be higher than further from the surface. However, if the cooler layer within the particle is relatively thin compared with the particle diameter, the temperature profile will remain close to flat for most of the particle volume. Effectively, the heat transfer within the particle is assumed to be fast enough to equalise the temperature throughout its volume. For the gas phase also, flat temperature profiles can be assumed because of the thin layers between the gases. Heat transfer by radiation inside each phase and between phases can also be neglected in this first approach. Similarly secondary terms such as dissipation of energy due to viscous effects and coupling amongst various transport phenomena are also neglected (De Souza-Santos, 2010a).

5.2 Models for moving bed (fixed bed) gasifiers

Unlike entrained-flow and fluidised bed gasifiers, relatively few modelling studies have been

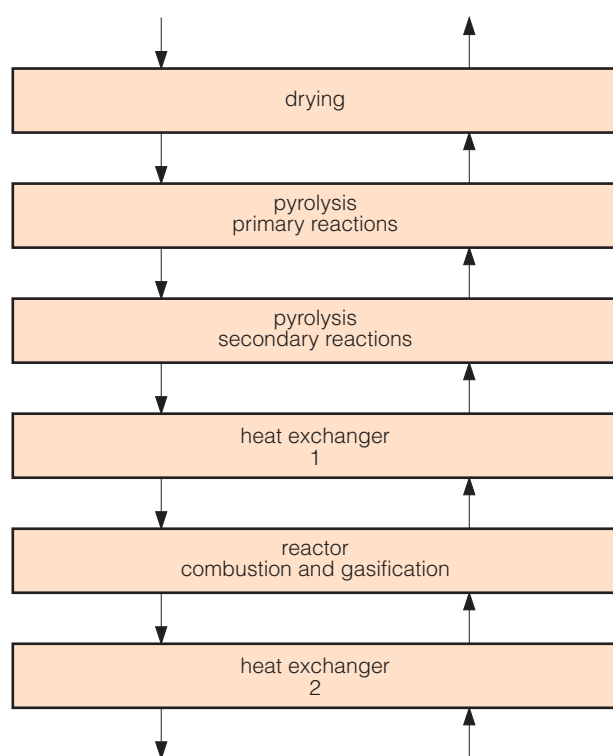


Figure 8 Moving bed gasification model steps (Brundu and others, 2009)

performed on moving-bed coal gasifiers. Recent work has tended to focus on biomass gasifiers. An early model for coal was the FBED-1 model developed by Radulovic and others (1995). This model included an advanced devolatilisation sub-model which could predict the evolution rates and yields of tar and individual gas products. This model was later modified and improved by Monazam and Shadle (1998). The results of this gasifier have been compared with an experimental gasifier and the predicted values for gas temperature and composition compared fairly well with the experimental data. Overall, the model was considered to be suitable as a design tool for new gasification units and as an analysis tool for the optimisation of existing ones (Morea-Taha, 2000).

A more recent simplified model of a fixed-bed countercurrent gasifier has been developed by Brundu and others (2009). In this model, the four steps making up the gasification process, namely drying, pyrolysis, gasification and combustion were considered separately. The whole reactor was divided into six different

steps, four of which were the reaction steps as shown in Figure 8. These steps were described by steady state, zero-dimensional, sub-models. Each step was assumed to take place in an ideal agitated reactor comprising of two separated phases: one gas and one solid. The whole gasification process has been modelled referring to the six steps evolving one after another. As can be seen in the figure, solid and gas move in countercurrent manner. Fuel was fed at the top of the gasifier and the ash removed at the bottom. Steam and air were fed at the bottom of the reactor and the syngas left at the top. In the model, the process was assumed to be in steady state. Each section was connected, at the most, to two sections by means of two solid and two gas streams moving in opposite directions. Mass and energy balance equations were included for each section and were assumed to be adiabatic. A CSTR (Continuous Stirred-Tank Reactor) model was assumed for the sections where chemical reactions take place. The solid fuel was assumed to be composed of four components: coal, ash, moisture and sulphur.

The fuel was fed to the top step where the drying process takes place. The gas and solid were assumed to be in local thermal equilibrium and the drying process was taken to be described by first-order reaction kinetics, Primary pyrolysis reactions took place in the next step where the dried fuel converts to char, tar and gas. The pyrolysis products were taken to be composed of CO, CO₂, H₂, H₂O, CH₄ and C₂H₆ and tar. The sulphur was released as H₂S, COS, CS₂, C₄H₄S. The coal particle was assumed to be homogeneous and the reaction:



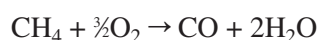
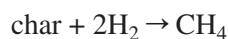
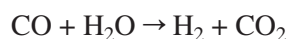
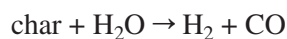
The heating rate was assumed to be sufficiently slow such that the reaction kinetics could be represented by first or second order kinetics. The sulphur was released in a similar reaction following first order kinetics.

In the next step, tar reacted to form gaseous compounds and char by the following reaction:



This reaction was assumed to be homogeneous and follow first order dependence on tar concentration.

The gasification and combustion were assumed to involve the following reactions:



The shrinking core model was used to model external mass transfer and internal diffusion is used to describe char conversion.

The model formulated the following equations based on the assumptions described above: mass

balance in each subsystem for each component, enthalpy balances for both solid and gas, congruence equations and equations defining solid and gas velocities. This led to 152 equations having the same number of unknown parameters. The model was utilised to simulate a theoretical fixed-bed reactor of 1.98 m diameter and 3.6 m height. A fuel rate of 0.284 kg/s was used in all simulations with an air/fuel ratio of 2.5 and a steam/fuel ratio of 0.31. The specific rate of solid stream passing through the reactor, measured at the exit of each subsystem was calculated and the predicted mass fractions of coal, char and ash are shown in Figure 9. The plot clearly shows that most of the coal transformed into char in the first pyrolysis reactor and most of the char reacts and converts to ash in the gasification and combustion section. The predicted mass fraction of the gaseous components was also shown in Figure 10. As this was a counter current reactor this figure must be read from right to left. As air was used as the oxidant as opposed to oxygen, the nitrogen concentration was high in the stream leaving the gasifier. The presence of water at the exit was due to the drying of the fuel. The majority of the oxygen reacted in the gasifier. The model predicted that the syngas was composed mainly of CO (>20%) and low amounts of hydrogen and light hydrocarbons (~1%). The model was used to simulate the effects of changes in air/fuel and steam/fuel ratio. The model clearly adequately simulated the broad features of the variation of the concentrations of the components in a coal gasifier. But as the results have not been compared with experimental data from a rig or actual gasifier, it is difficult to assess its predictive capabilities in a real situation (Brundu and others, 2009).

Brundu and Mura (2009) have also developed a model to simulate the transient behaviour of a fixed-bed countercurrent gasifier. As in the earlier model, coal was fed at the top in the first section of the gasifier where it was warmed by the heat exchanged with the countercurrent hot gas product. As

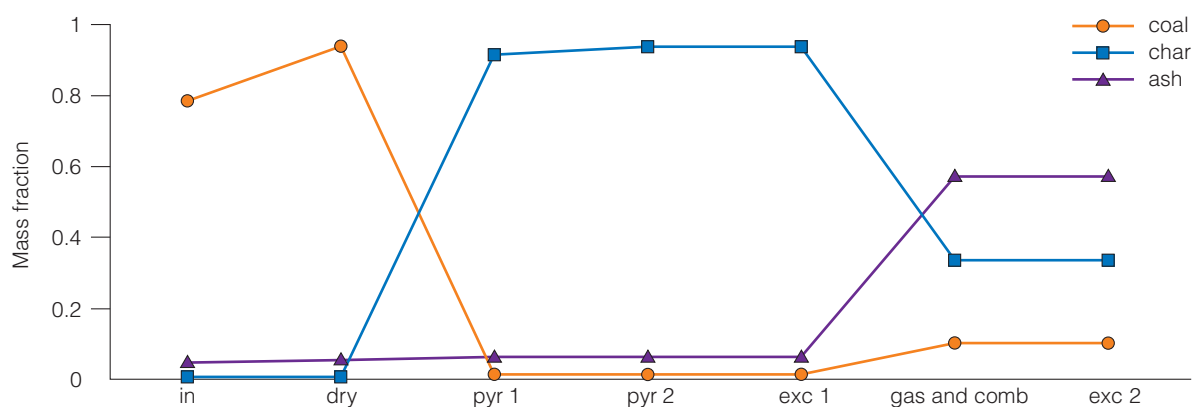


Figure 9 Model predictions for coal, char and ash concentrations (Brundu and others, 2009)

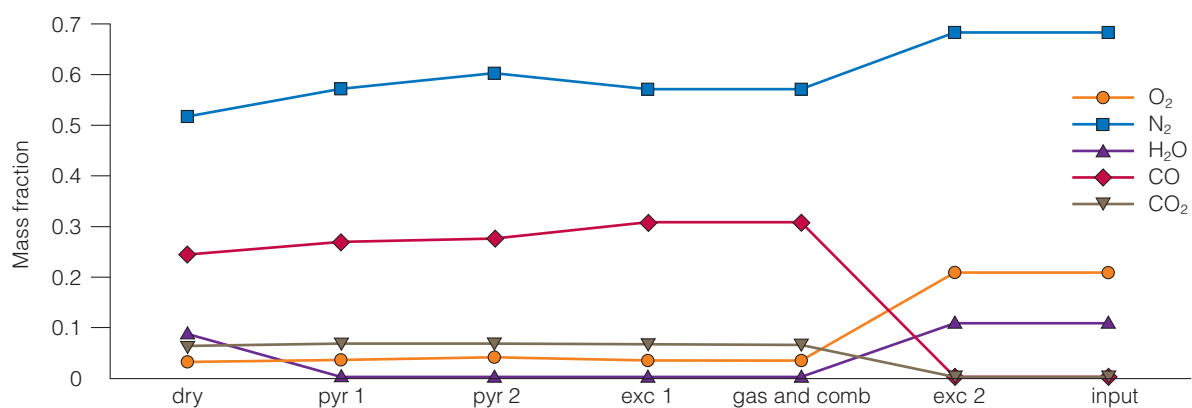


Figure 10 Model predictions for gaseous concentrations (Brundu and others, 2009)

the bed temperature was higher than 100°C, drying occurred very rapidly. As the coal descended along the reactor, it heated up and decomposed to produce a solid char phase and a gaseous mixture consisting of CO, CO₂, H₂, H₂O, CH₄ and a small amount of heavier hydrocarbons and tar. The char was further gasified as it proceeded down the gasifier and more syngas was produced. The oxidant, either air or oxygen with or without steam, was introduced at the bottom of the reactor.

The model was based on microscopic energy and mass continuity equations. It was a pseudo-homogeneous one dimensional model with a kinetic approach to some of the processes taking place. The heterogeneity of the system was taken into account when developing the equations, especially for heat balances. Heat was produced by the combustion reactions and was then transferred to the upper part of the gasifier by the gas flow. The transferred heat resulted in the drying and pyrolysis of the coal. It was necessary to consider the heat balances for both the gas and the solid phase. Both convective and radiative heat exchange between the gas and the solid phase were considered. Heat was transferred by conduction in the solid phase while gas phase heat transfer involved conduction and convection. As the reactor had a cylindrical shape, plug flow with variable axial velocities was considered for both gas and solid phase. The variation of solid and gas phase properties as a function of temperature, axial velocity and particle dimension was considered along the gasifier. The difference in void fraction between the top and the bottom of the gasifier was small and was due to pyrolysis. The solid proceeding down the reactor was compressed and the porosity of the bed tended to remain constant. To allow for the small variation in void fraction, the porosity was considered constant only during the gasification and combustion process. The velocity of the solid was also taken constant during the drying and pyrolysis process. The gas phase velocity was calculated by using the continuity equation for the gas phase and the ideal state equation.

One feature of this model was that a kinetic approach was adopted for some gas phase processes unlike the more common equilibrium treatment. Drying was thermally driven and the amount of moisture leaving the fuel depended on the temperature and the ability of the molecules to diffuse inside the particle. In the model, the drying process was modelled by a single first order reaction depending on the solid moisture content. The rate constant was calculated by an Arrhenius-type expression. Pyrolysis was also treated with a pseudo-homogeneous kinetic model while the shrinking

core mode was adopted for gas-char reactions. The model has been developed such that given some initial information, it was capable of simulating the evolution of the system from the initial state until a new steady state was reached. The model required initial conditions of the gasifier such as temperature, solid and gas phase composition and flow rate. The output of the model were temperature, concentration and velocity profiles for both gas and solid phases inside the reactor for each time step.

The model has been used to investigate the dynamic behaviour of a system with the operating parameters given in Table 2. At the start, the reactor was assumed to be filled with char. A linear temperature profile was assumed for the bed ranging from 820°C at the bottom and 25°C at the top. The gas phase was assumed to be nitrogen with a linear temperature profile ranging between 850°C at the bottom and 400°C at the top. When the simulation started, air and steam were fed at

Table 2 Operating conditions for the reference case (Brundu, 2010)

Parameter	Value
Inside diameter	0.3 m
Bed height	0.5 m
Bed pressure	0.1 MPa
Coal feed	0.01 kg/s
Particle diameter	1.0 cm
Void fraction	0.4
Moisture content	10% (weight)
Solid feed temperature	25°C
Air feed temperature	287°C
Steam feed temperature	287°C
Wall temperature	100°C
Air-solid feed ratio	4.0 (weight)
Steam-solid feed ratio	0.2 (weight)

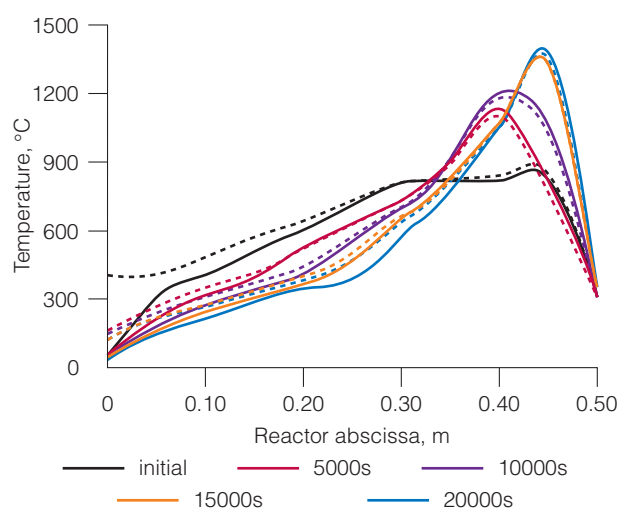


Figure 11 Gasifier temperature profile (Brundu, 2010)

the bottom and coal at the top. The dynamic changes in temperature for both the gas and solid phases are shown in Figure 11. The evolution of the combustion peak was predicted. The temperature in the reactor decreased with time until the gas phase temperature became higher than the solid phase temperature. The temperature peak became higher while the temperature decreased in the rest of the reactor. The peak temperature increases as the gasification process becomes established. Once the peak temperature reached a maximum, the temperature depletion stop in the rest of the gasifier and the gas temperature became higher than the coal temperature except in the combustion section. Sensitivity analyses were performed to model changes in air to fuel ratio, steam to fuel ratio and coal flow rate.

The solid phase conversion was found to depend on air to fuel ratio while the gas composition was mainly affected by steam to fuel ratio (Brundu and Mura, 2009; Brundu, 2010).

Grana and others (2010) have developed a general mathematical model of a fixed bed gasifier in which both transport phenomena and chemical kinetics were included. The mathematical description included solid devolatilisation, gas phase reactions and gas-solid interactions. The kinetics of the devolatilisation of solid particles was considered as a linear combination of pure component devolatilisation processes. The char gasification and combustion reactions are summarised in Table 3. The volatile components released during pyrolysis underwent successive decomposition or combustion reactions in the gas phase. An existing kinetic scheme for pyrolysis and oxidation of hydrocarbon species was extended to describe successive gas phase reactions of released species. Due to the modularity of the detailed kinetic scheme, it was only necessary to describe the primary initiation, decomposition and H-abstraction reactions of the new species. The model consisted of two models: one on the particle scale and the other on the reactor scale. The particle model provided an internal description to account for interparticle heat and mass transfer. The particle model was embedded into the reactor model. The reactor was taken to be a series of elemental units which exchanged mass and heat with each other. Each unit accounted for gas-solid interactions with particular attention to inter-phase resistances. More than 100 equations were obtained to model ten to fifteen solid species, 100 gas-phase species and ten reactor layers. The results for a counter-current fixed bed coal gasifier are shown in Figure 12. The model characterised the solid and gaseous streams and considered secondary gas phase reactions of tar and gas components. The predicted molar composition of the syngas was typically about H₂ (11–15%), CO (13–17%), CO₂ (10–12%), H₂O (15–20%), CH₄ (1–3%). The authors reported that the models required several hours of CPU time, due both to the stiff nature of the gas-phase kinetics and to the dynamic approach to the steady state solution. The model has not been validated by comparing with rig or plant data. Before doing so, in order to reduce CPU time, the authors considered that the treatment of both the solid and gas phase will need to be simplified (Grana and others, 2010).

Table 3 Char gasification and combustion reactions (Grana, 2010)

	k (kmol, m ³ , K, kcal, s)
Char + O ₂ → CO ₂	5.5x10 ⁹ exp(-38200/RT) [O ₂] ^{0.78}
Char + ½O ₂ → O	5.7x10 ¹¹ exp(-55000/RT) [O ₂] ^{0.78}
Char + H ₂ O → O + H ₂	7.9x10 ⁹ exp(-38200/RT) [H ₂ O] ^{0.78}

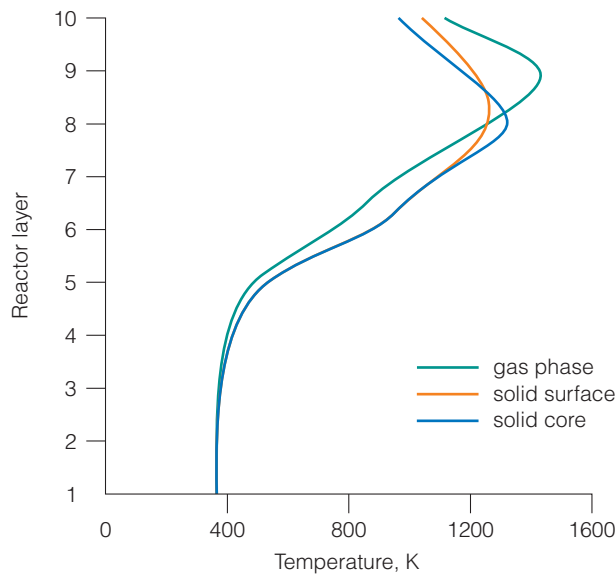


Figure 12 Gas and solid temperature profiles
(Grana and others, 2010)

Kulkarni and Ganguli (2012) have presented a process simulation of a moving bed gasifier using low rank, subbituminous, Usibelli coal from Alaska, USA. Alaska contains extensive coal reserves and the feasibility of gasifying the coal for power generation and chemical production has been assessed. Initially, only entrained-flow and fluidised bed gasifiers were studied and the objective of this paper was to evaluate the suitability of moving bed gasifiers for Alaskan coal. All the processes occurring in moving bed gasifiers such as drying, devolatilisation, gasification and combustion were included. The Aspen Plus simulation codes were the foundation of the model. Aspen Plus is the leading process simulation software provider which can model engineering systems involving solids, liquids and gases. The Aspen reactor blocks are described in Table 4. Developing the Aspen Plus model required knowledge of reaction

stoichiometry, reaction rates, mass and heat transfer. The Aspen Model required the following input conditions:

- component attributes and heating value of coal;
- yield of pyrolysis gases, tars and char in devolatilisation step;
- operational parameters including coal, steam and air flow rates, pressures, and temperatures;
- gasifier parameters such as dimensions and pressure;
- FORTRAN code for reaction kinetics.

The model made the following assumptions:

- the system was in a steady state;
- coal and gas flowed as plug flow. This assumed constant velocity across the cross section with no back mixing;
- the residence time of the coal in drying and pyrolysis sections was negligible compared to that in combustion-gasification section;
- pressure drop in gasifier was neglected;;
- volumetric reaction represented all gas-solid reactions except char combustion which followed shrinking-core model;
- gas temperature was same as solid temperature at every point in the gasifier.

The process flowsheet for the model is given in Figure 13. The wet coal was first fed to the R-Yield

Table 4 Description of reactor blocks used in model (Kulkarni and Ganguli, 2012)		
Process	Reactor block	Description
Coal drying	RYield	Simulates coal drying by considering the moisture content and proximate analysis of the coal
Coal pyrolysis	RYield	Simulates coal pyrolysis
Char decomposition	RStoic	Char decomposition is modelled in RStoic
Char gasification and combustion	RCSTR	Simulates char gasification and combustion using kinetic data for reactions occurring in reactor

Component	CO	H ₂	CO ₂	CH ₄	H ₂ S	N ₂	Tar, kg/h
Experimental results, mol%	20.2	36.4	28.7	13	0.4	1.3	270.8
Simulation results, mol%	20.3	40.2	28.8	8.4	0.2	1.13	114.2

The model predictions were compared with available experimental results from the Lurgi gasification plant in Westfield, Scotland for a similar Rosebud subbituminous coal. Table 5 compares the product gas composition predicted by the model with the experimental data. It should be noted that the simulated gasifier attained a temperature of 1182°C while the experimental value was 1000°C. The model results were in very good agreement with the experimental values for CO and CO₂, in reasonable agreement for H₂ but the agreement was poor for CH₄, H₂S and tar. The discrepancy could be attributed to the fact that the model predicted a higher temperature than the experimental value. The higher temperature increased the ratio of H₂/CH₄. The simulations were used to investigate the effect of oxygen to coal ratio, steam to coal ratio and pressure on product gas composition and carbon conversion efficiency. The results revealed that steam to coal ratio and oxygen to coal ratio were the

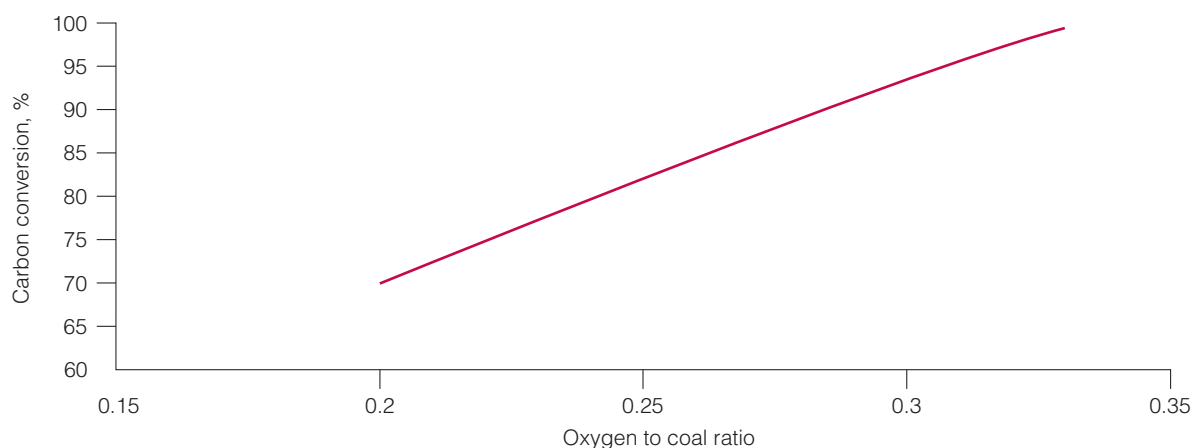


Figure 15 Effect of oxygen to coal ratio on carbon conversion (Kulkarni and Ganguli, 2012)

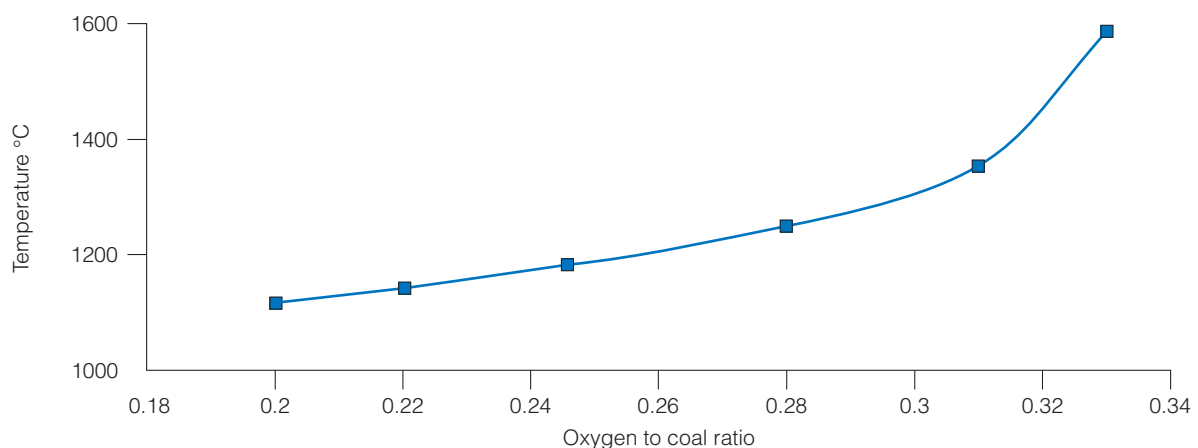


Figure 14 Effect of oxygen to coal ratio on gasifier temperature (Kulkarni and Ganguli, 2012)

governing factors controlling both carbon conversion and product gas composition. The effects of oxygen on gasifier temperature and carbon conversion are shown in Figures 14 and 15. Increasing the oxygen concentration resulted in further oxidation of char and increased temperature carbon conversion. An oxygen to coal ratio of 0.33 was necessary to obtain a carbon conversion of 99.9%. The results demonstrated that it should be possible to design a full-sized moving bed gasifier using Usibelli coal (Kulkarni and Ganguli, 2012).

Tola and Cau (2007) also developed a model using ASPEN Plus codes for a pilot-scale (5 MWth) fixed-bed updraft gasifier which was under construction at the Sotacarbo Research Centre in Sardinia. The simplified scheme for the gasification process is shown in Figure 16. The ASPEN model represented the gasifier as the following zones: coal preheating and drying, devolatilisation, gasification and combustion, steam and oxidant preheating. The model evaluated the mass and energy balance in each zone and the syngas characteristics for given coal composition and coal, steam and oxidant mass flows. In the gasification and combustion zone, the model calculated the syngas composition and equilibrium temperature by minimising Gibbs free energy. The model calculated the syngas temperature by considering the countercurrent heat exchange processes between the syngas and the coal inside the different sections, assuming a suitable difference in temperature. The gasifier manufacturer's expected syngas composition and the calculated values are compared in Table 6. The agreement was fairly good. The effect of the main process parameters was also investigated. The study showed that gasifier performance was extremely sensitive to air/coal and steam/coal mass ratios and to thermal energy losses and minimum difference in temperature between the syngas and the coal. The authors considered that the accuracy of the predictions could be improved by optimising the

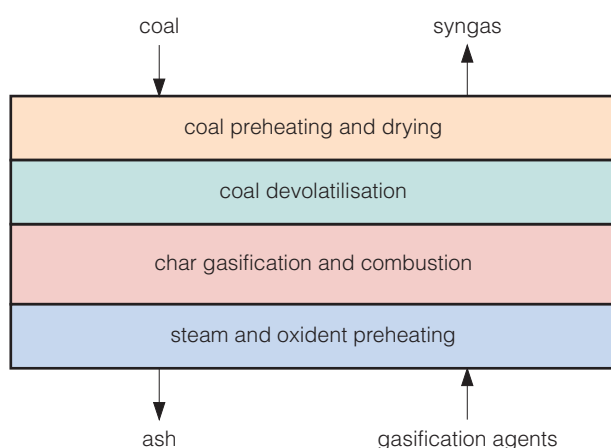


Figure 16 Simplified scheme of moving bed gasification process (Tola and Cau, 2007)

adjustable parameters such as the coal/syngas temperature difference, the amount and distribution of thermal energy losses and carbon conversion rate.

A comprehensive CFD model has been developed to simulate the gasification process in an air-blown updraft coal gasifier. Though simplified models, such as non-dimensional ones, are useful for preliminary gross mass and energy balance, they are unable to correctly simulate the overall gasification process. This CFD model was able to describe the space and time-dependent behaviour of the gasification process including the non-continuous loading of coal and the extraction of ash. Given the high volume fraction of the solid phase, close to packing conditions, the

Table 6 Expected and calculated syngas compositions (Tola and Cau, 2007)						
Syngas composition, %vol	Sulcis coal			South African coal		
	Expected	Adiabatic	5% thermal energy losses	Expected	Adiabatic	5% thermal energy losses
CO	31	30.1	25.8	28	31.3	27.9
CO ₂	4	3.44	6.7	5	2.7	5.3
H ₂	18	18.7	13.6	18	19.8	15.9
N ₂	45.5	42	44.7	46.5	43.9	46.1
CH ₄	1.5	3.7	7.1	2.5	1.6	4.2

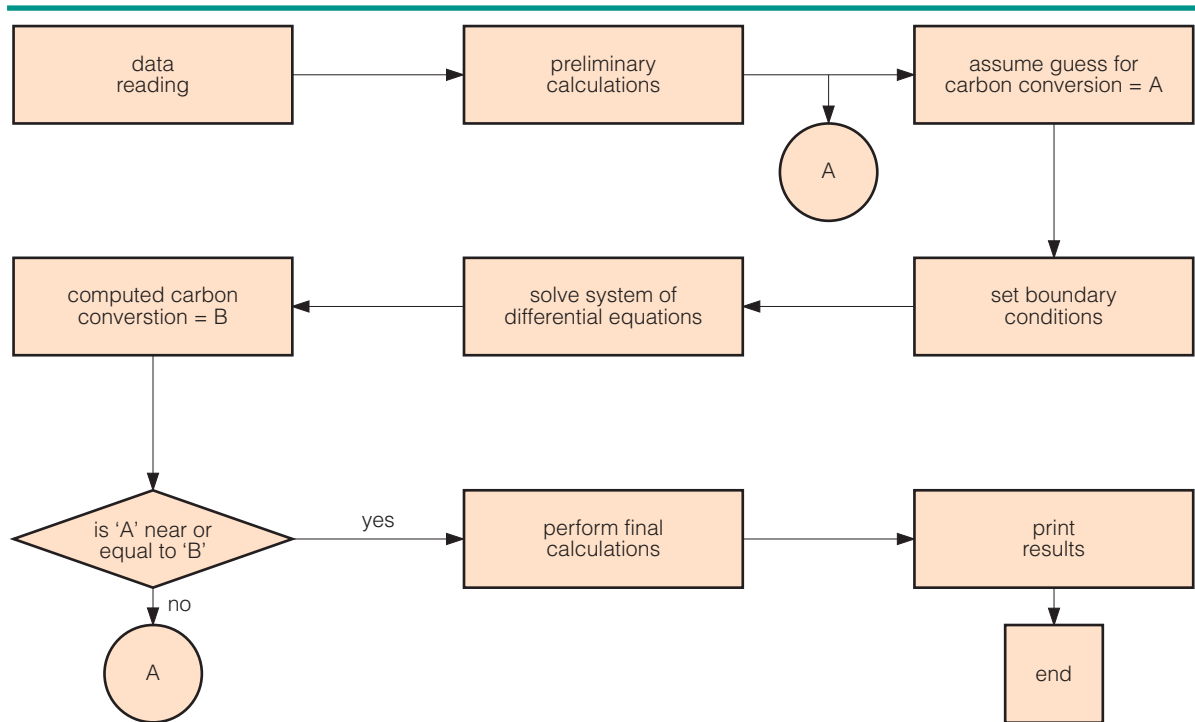


Figure 17 Programme chart for updraft gasifier (De Souza-Santos, 2010a)

Euler-Euler approach was required to model the multiphase flow. The solid was considered as a continua according to the kinetic and plastic theory of granular flows. This approach was used to model the non-continuous loading of a Wellman-Galusha updraft coal air-blown coal gasifier. The average syngas composition was compared to experimental data available in the technical literature giving encouraging agreement. The main drawback was the extremely long computational time required but this could be reduced by optimising the code parallelisation (Murgia and others, 2012).

De Souza-Santos has developed a Comprehensive Simulator for Fluidized and Moving Bed equipment (CSFMB) modelling (De Souza-Santos, 2010b). This has been mainly used for fluidised bed systems and is described in Section 5.3. For moving beds, the model required data for the physical characteristics of injected flows (mass flows, temperatures and compositions of both solid and gas flows) and a description of the physical geometry of the equipment. The programme chart for the model is shown in Figure 17. The computational strategy began with a guessed value for the fractional conversion of carbon (A). B indicated the computed value for value for the conversion. An iterative process then follows in which the equations for mass, momentum and energy continuity were solved given the stated boundary conditions. Equations for gas phase reactions, heterogenous reactions, drying and devolatilisation were also included. Once convergence was achieved, the simulation results were printed. The model was used to simulate a charcoal updraft moving bed gasifier (0.5 m dia, 4 m high) operating at steady state. There was excellent prediction for the concentration of hydrogen in the exiting gas stream but significant deviations for carbon monoxide and dioxide. Possible error sources were considered to be measurement errors or catalytic effects of impurities.

The sound operation of dry ash fixed bed gasifiers requires utilising coals with suitable ash properties. If the ash fusion temperature is too low, ash clinkering can take place which causes channel burning, pressure drop problems, unstable gasifier operation and even give rise to potential safety issues. These gasifiers can handle coals with quite high ash contents as long as the ash properties are suitable. The ash fusion temperature (AFT) indicates the average temperature at which the bulk minerals start to become soft and melt. It is an indication to what extent agglomeration or clinkering is likely to occur. The AFT is frequently used to assess the average slagging properties of coal sources. Historically, the

fusibility of a given coal has been assessed from the content of principal oxides such as SiO_2 , Al_2O_3 , TiO_2 , Fe_2O_3 , CaO , MgO , Na_2O and K_2O . The acid/base ratio is the most frequently used parameter for correlating ash fusibility with its composition. Van Dyk and others (2005) have reported how Sasol have used a combination of high temperature X-ray diffraction (HT-XRD) and FactSage modelling to understand mineral matter processes occurring in a Sasol-Lurgi Fixed Bed Dry Bottom gasifier. FactSage is a software package which can be used to calculate and manipulate phase diagrams. The database contains critically evaluated thermodynamic data for the SiO_2 - CaO - Al_2O_3 - Cu_2O - FeO - MgO - MnO - Na_2O - K_2O - TiO_2 - Ti_2O_3 - Fe_2O_3 - ZrO_2 - CrO - Cr_2O_3 - NiO - B_2O_3 - PbO - ZnO system. The particular modules in the package which were most relevant for Sasol's investigation were 'Equilib' and the Phase Diagram modules. The 'Equilib' module is the Gibbs energy package for FACTSAGE. It calculates the concentrations of chemical species when specific elements or compounds react or partially react to reach a state of chemical equilibrium. The Phase Diagram module is a generalised module which allows the user to calculate, plot and edit unary, binary, ternary and multi-component phase diagrams where the axes can be various combinations of T, P, V, composition, activity and chemical potential. Several runs have demonstrated the applicability of FACTSAGE calculations for the prediction of AFT as well as blending strategies.

For the base coal sample, the HT-XRD showed that the phases present were quartz, muscovite, calcite, dolomite, hematite, anhydrite, rutile and kaolinite. The FACTSAGE model supported the HT-XRD findings that slag formation would occur around 1000°C . No slag formation was observed in the drying or devolatilisation zones, as predicted. Although the amount of melt was fairly low at 1000°C , a degree of melting was taking place at temperatures not predicted by the AFT analysis. Sasol considered that the specific value of using FactSage with HT-XRD was that it was possible to analyse equilibrium conditions for reactions occurring inorganic and organic materials and provide an insight into mineral transformation and slag formation (Van Dyk and others, 2005). The FactSage modelling approach was improved by combining the drying, devolatilisation and gasification zones in the zones in the gasification process. This could speed up and improve the interpretation of mineral matter transformations and flow properties of reacted mineral matter in coal and assist identifying and quantifying slag formation. The updated model compared favourably with the original model and with HT-XRD results. It predicted feldspar formation correlated with slag formation at temperatures around 1000°C . Feldspar is one of the mineral species having one of the lowest AFT causing most slag-liquid formation. In the gasification zone, it was clear that slag-liquid formed at 1000°C but with lower feldspar content (Van Dyk and Wanders, 2008).

Models have also been developed to address ash issues in moving bed gasifiers. Alkali metals such as Na and K evaporate at the high temperatures in gasifiers. Their subsequent condensation at low temperatures can cause problems. In particular, the formation of deposits at the raw gas outlet, heat exchangers and refractory lining can cause blockages and reduce efficiency. Guhl and Meyer (2007, 2009) have developed a thermodynamic model of the BGL-gasification process with particular consideration of alkali metals. The BGL gasifier consists of a double-walled cylindrical reactor and coal is fed at the top. The coal was dried and devolatilised in the upper zone of the gasifier. It was gasified in the middle zone and combusted in the lower zone. The temperature in the gasifier was high enough to melt the ash which is tapped off at the bottom and quenched. In the gasifier, volatile elements in the coal ash such as Na, K, Pb and Zn reacting with S and Cl can lead to operational problems. For example, a deposit rich in alkali chlorides is sometimes formed at the raw gas exit and causes blockages. The formation of deposits on the reactor wall reduces the effective diameter of the vessel. Such accumulations can also damage the refractory lining.

The model was developed to describe the behaviour of volatile ash components in the BGL-process. Process data and measurements of feedstock, deposits and slag were used to optimise the model. A simplified flow diagram of the model is given in Figure 18. Two isobaric-isenthalpic equilibrium stages were defined. The upper one represented the devolatilisation zone and the lower one represented the gasification zone, the combustion zone and the slag bath. The stages were connected by material streams such that the gaseous stream from the upper stage left the model. This represented

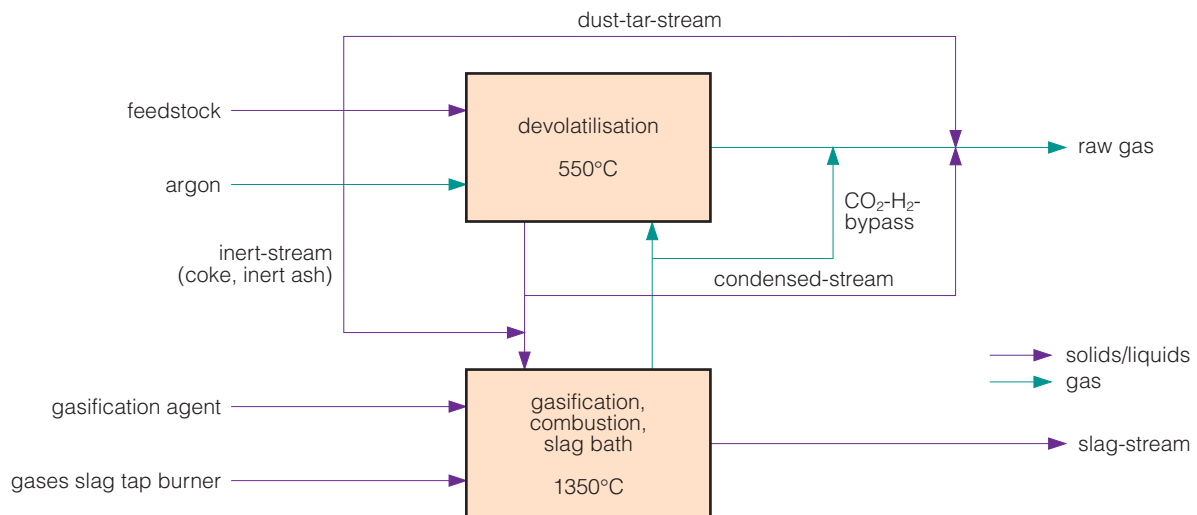


Figure 18 Flowsheet for BGL model (Guhl and Meyer, 2009)

the dust-free raw gas. Solid and liquid phases from the upper stage flowed down to the lower stage as the coke in the fixed bed. The condensed phase left the lower stage as slag. The gas phase of the lower stage entered the upper stage. This flow pattern described the counter flow fixed bed gasifier. The focus of the model was the cycle of volatile ash components which evaporated in the lower combustion stage and condensed in the upper pyrolysis stage. The process data for the model was obtained from the 200 MW BGL gasifier at Schwarze-Pumpe in Germany.

The following elements were considered: Al, C, Ca, Cu, Cl, Fe, H, K, Mg, N, Na, O, P, S, Si, Ti, Zn, Pb. The thermodynamic calculations required temperature dependent heat capacity and the standard enthalpy and entropy data for each substance. Additionally, parameters were needed to take account of interactions between species and non-ideal behaviour. The thermodynamic datafile was created with the software FactSage using data retrieved from FACT 5.3, FACToxide, FACTmisc and FACTsalt. The thermodynamic data were used to calculate the equilibrium state based on the Gibbs energy minimisation principle. The model was put together with SimuSage which is a ChemApp-based facility for process simulations. The model enabled the partitioning of the volatile ash components into condensed and gaseous species in the raw gas and into the slag to be assessed. The main volatile elements were K, Zn, Pb, Cl, Na, and S. The evaporation of these elements from the slag bath and their condensation in the devolatilisation zone resulted in the accumulation of the salt phases in the fixed bed with KCl as the dominant compound. The presence of phosphorous in the slag combined with iron was also predicted.

It is evident that the relatively few models developed recently to simulate moving bed gasifiers have tended to regard the system as consisting of several zones at steady state in which a particular process takes place. Many of the models utilise the Aspen Plus coding. The comparisons that have been made of model results with plant or rig data have indicated reasonable agreement.

5.3 Models for fluidised bed gasifiers

Fluidised bed gasifiers can be considered to consist of two phases: a bubble and an emulsion phase. Bubbles entering the bed expand as they pass up through the bed, hence the bubble size increases with bed height. Each bubble can be assumed to consist of a bubble volume which is surrounded by a bubble cloud. The size of the cloud depends on bubble velocity and the minimum fluidisation velocity. Following the bubble is the bubble wake or trail, which entrains solid particles through the bed.

Recirculation of these solids occurs within the emulsion phase and in systems with large internal bed recirculation, the gas velocity through the bed can become negative and thus flow down through the bed. Transport processes occur between the bubble phase, the cloud and the emulsion phase (Moreea-Taha, 2000).

Yan and others (1997) developed a 1-D isothermal model for FBG (fluidised bed gasification) using the two-phase theory of fluidisation. This assumed that the emulsion phase remained fluidised whilst the excess gas flowed as bubbles through the bed. The model was later modified to incorporate an overall energy balance to improve simulations. Yan and others (1998) then introduced the 'net flow' concept for modelling fluidised bed gasifiers. Net flow is different from the excess gas flow concept defined by two-phase theory and refers to the net generation of gas in the emulsion phase due to coal devolatilisation and homogeneous and heterogeneous reactions. The net flow concept is particularly important when low rank coals are gasified because of the large amount of volatiles released in the bed. Ross and others modelled a laboratory-scale bubbling fluidised bed gasifier with feeds of both char and propane. The model contained a comprehensive representation of a scheme of important chemical reactions occurring in the gasifier and the non-isothermal behaviour in the fluidised bed. The model was capable of predicting competition for oxygen between char and gas combustion, fluidisation states, mass transfer (by net flow and interface exchange), variations of bubble fraction, coalescence and bubble growth, gas product concentrations and gasification rates along bed height. The model was successfully used to simulate three pilot-scale and one full-scale fluidised bed gasifier (Ross and others, 2004).

De Souza-Santos has developed a comprehensive mathematical model and computer programme (CSFB) to simulate the operation of bubbling and circulating bed boilers and gasifiers. The model is

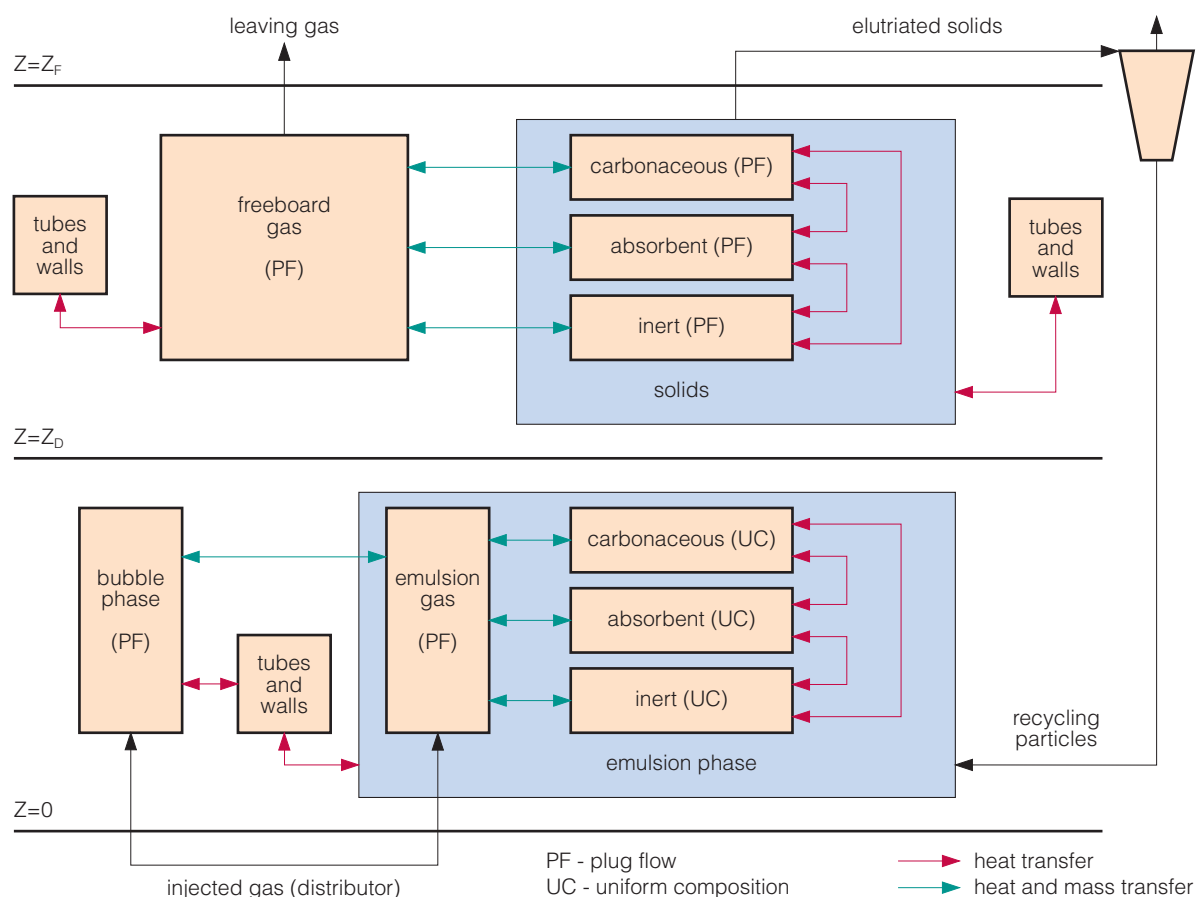


Figure 19 Schematic of bubbling fluidised bed model (De Souza-Santos, 2007)

considered to be comprehensive as it includes the conservation equations for the emulsion phase and bubbles, empirical equations for hydrodynamics and a thorough mass balance which considers that both drying and volatilisation are not instantaneous. The basic model was developed as part of a doctoral thesis in 1989. Since then, it has been upgraded significantly. It was a one-dimensional model and assumed that the system was at steady state and is schematically represented in Figure 19. The system was represented by two main regions: bed and freeboard. The bed was divided into bubble and emulsion. The solid phase consisted of three components: fuel, inert and sulphur absorbent. The ash, which eventually detached from the spent fuel constituted part of the inert solids. The emulsion was assumed to be composed of solid particles and percolating gas. The reacting emulsion gas passed through the bed following axial or vertical plug-flow regime. During their traverse, the gaseous part of the emulsion was assumed to exchange mass and heat with bubbles and particles. In addition, heat transfer occurred between all phases and the vessel walls. The total area for heat and mass transfer was equivalent to the surface area of all bubbles in the bed. The diameter and velocity of the bubbles varied in the axial direction.

The model did not assume an overall stirred-tank approach. Only the composition of the solid particulate phases in the bed was assumed to be well-mixed. The same was not assumed for the temperatures. These were obtained for each phase at each point by a detailed energy balance which considered all heat exchange processes between each solid and all others. In addition, the differential energy balances for each phase also took into account a large number of heterogeneous chemical reactions, heat and mass exchanges with emulsion gas and the gas in the freeboard region. The model considered the change in initial particle size distribution due to attrition between the particles and particles. The model also considered other processes affecting the particle size distribution: entrainment of fines to the freeboard, withdrawals from the bed and recycling to the bed particles collected in the cyclones. The freeboard contained particles and gases. The reacting gas phase passed through the freeboard following axial plug-flow. Particles also flowed in the axial or vertical direction, with the heavier ones returning to the bed. The homogeneous and heterogeneous reactions which occurred in the freeboard were considered. Thus all compositions, flows and size distributions of every solid species were computed at each point. Heat and mass transfers in the vertical direction within each phase were considered negligible compared with the respective transfers in the horizontal direction between one phase and another.

The programme performed successive iterations and, at each, boundary conditions for the three solid phases (carbonaceous, sulphur absorbent and inert) were obtained by solving differential energy balances for conduction, convection and radiative heat transfers between the distributor surface and the various phases. The temperature and composition profiles in the bed were obtained by iterative computation throughout the system. For the first iteration, a carbon conversion was assumed. Having solved a system of coupled non-linear differential equations describing mass and energy balances for all phases and chemical species, a new carbon conversion was calculated as were the conversions of all other solid phase components. The results contained the temperature and composition profiles of the species in the emulsion and bubble phases and the average composition and the temperature profile of solid phases in the bed. In addition, the values of a variables related to heat transfer were obtained. Though the model was one-dimensional, regardless of the apparent simplicity, the solution of the governing, non-linear and tightly coupled system of differential equations provided a complete and detailed representation of all significant processes occurring in the gasifier.

The original model has been successively improved. A more realistic model and calculations of circulation rates have been incorporated. More accurate models of pyrolysis and devolatilisation combining DISKIN-DISCHAIN and FG-DVC are now used. This has allowed the model to be applied to a wider rangel of fuels. The data used for reaction kinetics have been revised. In the case of bubbling fluidised beds, more reliable correlations for bubbling diameters have been used. The calculation of bubbling diameters is pivotal for the simulations as it influences all aspects of the process including heat and mass transfer. Correlations for the segregation among solid phases have been included. This allows for the prediction of unfavourable operation which can result in

carbonaceous fuel floating in the bed. This can result in devolatilisation at the bed surface and tar carry over with the syngas. The model is capable of predicting operations using slurries for feeding particulate solids into highly pressurised beds (De Souza-Santos, 2007).

The model results have been compared with operational results obtained from several pilot plants. One study involved comparing model results with those from a wood gasifier at the Institute of Gas Technology, Chicago, USA. A comparison of the rig and model results showed that the composition of H₂, CO, CO₂ and CH₄ differed by less than 10%. Another study involved comparing with data produced by the gasifier at the National University of Colombia. This gasifier had an internal diameter of 0.22m and height of 2m. It operated at an average operational pressure of 101.3 kPa and gasified Colombian coal with the ultimate analysis C(75.3%), H(5.4%), N(1.8%), O(15.6%), S(0.4%) and ash (1.5%). The experimental and simulation results for the product gas composition are compared in Table 7. Initially the predicted concentration of CO was too low and that of hydrogen too high. It was suspected that there was an impurity poisoning the shift reaction. Hence the pre-exponential factor of the shift reaction was reduced by a factor of 30. Following this arbitrary change, the calculations were repeated. The comparisons for H₂, and CH₄ were now reasonable but those for CO and CO₂ were poor. The prediction for bed temperature was good in one case and poor for the other. The model was also used to predict profiles of operational parameters such as bed temperature and concentrations of the chemical species in the system. These were reasonable. Overall, the comparison of model results with rig data can only be described as mixed. The model, however, was a useful tool for understanding the processes taking place in the gasifier and for predicting, in general terms, how changes in operational conditions might affect process parameters (De Souza-Santos, 2010b).

The results from this model were compared by Engelbrecht and others (2012) when gasifying high-ash South African coal in a gasifier pilot plant. This was part of project launched by CSIR to assess the feasibility of BFB technology for the gasification of high-ash coals. The atmospheric plant has a furnace height of 4 m (2 m bed and 2 m freeboard) and had bed temperature of 860–890°C and fired Grootegeluk coal from the Waterberg coalfield. The model required input data for the gasifier design such as gasifier diameter and height, height at which coal and reactants were injected and height at which syngas was withdrawn. Operational data such as the feedrates for coal, air, oxygen, steam, the temperatures of air, oxygen, steam gasifier pressure were also required. The model predicted: bed and freeboard temperatures; fixed and total carbon conversions; syngas output flow and composition, concentration of all gases as a height and gas velocity in the gasifier. The fixed carbon

Table 7 Comparison of experimental and simulation results (De Souza-Santos, 2010b)

Species, mol%	Test 1		Test 2	
	Experimental	Simulation	Experimental	Simulation
A Without any correction				
H ₂	8.53	12.45	10.1	15.1
CO	10.94	6.89	11.36	7.54
CO ₂	19.31	19.75	20.27	20.17
CH ₄	0.84	0.87	0.77	1.38
B With modification on shift correction				
H ₂	8.53	8.59	10.1	10.08
CO	10.94	11.83	11.36	16.93
CO ₂	19.31	16.04	20.27	13.11
CH ₄	0.84	0.77	0.77	0.84

Table 8 CaSFaMB model predictive capability		
Deviation between measured and predicted output variables, %	New Vaal	Grootegeluk
Mid bed temperature	2.1	2.4
Fixed carbon conversion	3.6	3.4
Gasifier exit temperature	3	13.4
CO	6.3	11
H ₂	11.7	39.5
CH ₄	38.5	27.1
CO ₂	4.6	8.6

conversion was found to increase with an increase in coal reactivity, temperature and residence time of the char particles in the gasifier. The results of the model and the rig data were compared for two sets of gas kinetic data for the two coals. The comparison is shown in Table 8. The agreement was clearly better for one set of input kinetic data than the other. For both, there were significant discrepancies for the predicted concentration of H₂ and CH₄. The discrepancies were attributed to elemental mass balance non-closures produced by the programme. The model predicted a significantly higher fixed carbon conversion for a scaled-up 15 MW gasifier (Engelbrecht and others, 2011,2012).

Chejne and others have investigated several models for simulating coal gasification in fluidised beds (Chejne and Hernandez, 2002; Chejne and others 2011). Initially, a steady state, one-dimensional model and algorithm was developed. The model included two fluids: emulsion and bubble; and two phases: gas and solid. The emulsion was formed by gas and solid. The bubble was considered free of solid particles and only contained gas. The solid was assumed to be isothermal and its consumption uniform through the bed depth. The mass and heat transfer between the solid and gas in the emulsion were considered as was the mass transfer between the emulsion and the bubble but the solid/bubble transfer was not. Attrition, elutriation and drag of the solid phase was included. Reaction models were used for homogeneous (gas-gas) or heterogeneous (gas-solid) chemical reactions. Devolatilisation and drying were considered to be instantaneous in the feed zone. This assumption was not made by De Souza-Santos but Chejne considered that the experimental data indicated that drying and volatilisiation take place very quickly. Either steam or CO₂ was used to gasify the coal. The partial differential equations for mass and heat transfer for each component in the gas and solid phases were derived and solved. Experimental correlations for the fluid-dynamic parameters were used. Chemical reactions and equations for convection and diffusion were included. The energy equations for both phases were coupled by convection on the surface of the particles.

The above model was applied to solid particles submerged in a fluidiser gas of an atmospheric gasifier as shown in Figure 20. The solids (coal, limestone, inert materials) entered the reactor at the feed point. The type of coal, initial particle size distribution and the composition of the solids were

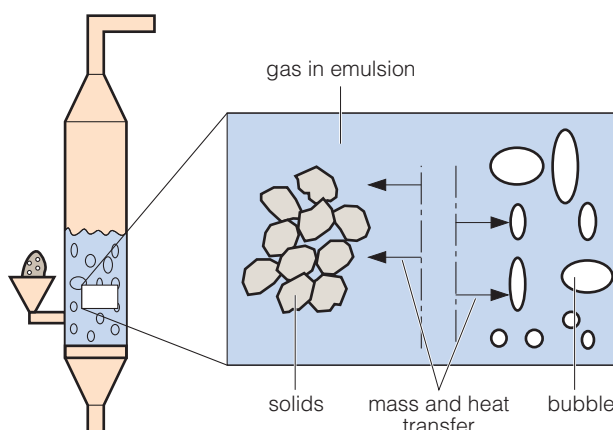


Figure 20 Schematic of coal gasification model (Chejne and others, 2002)

specified at this point. The gas (air, steam, carbon dioxide) entered through the bottom of the reactor with the inlet composition and temperature specified. At the feeding point, a Gaussian particle size distribution was assumed for the solid material. Inside the reactor, the shape of the distribution was assumed to be conserved but the average diameter changed due to attrition, elutriation, consumption and drag. The bubble was considered a fluid which increased the energy and mass transfer inside the reactor. The gas in the emulsion acted as a bridge between the solid and the bubble because it exchanged mass and energy with both solids and bubble while these exchanged mass and energy with the gas. A system of chemical reactions for the

solid and gaseous phase were included. The drying, devolatilisation and limestone reactions were assumed to have taken place instantaneously at the feeding point. The properties of the solid phase were considered to be unaffected by the axial co-ordinate. Consequently the temperature, consumption fraction and composition of the solid were assumed to be constant in the reactor. The gaseous phase changed along the bed height allowing mass and energy transfer to take place. The mass and heat transfer coefficients were calculated using experimental correlations from several references. The specific heat, conductivity, viscosity and binary diffusion coefficients for each component in the gas phase were calculated as a function of temperature at each point and the mixture's properties were then calculated. A system of 29 differential equations and ten non-linear equations, derived from mass, energy and momentum balances for each phase, at any point along the bed height were solved by the Gear and Adams method. The model predicted, temperature, converted fraction and particle size distribution for the solid phase. For the gaseous phase, in both emulsion and bubble, the model predicted temperature, gas composition, velocities and other fluid-dynamic parameters.

The model results were compared with those from a pilot fluidised bed gasification plant at the Universidad Nacional-Medellin in Bogota, Columbia. The reactor had an internal diameter of 0.22 m, a height of 2 m and consisted of three main modules. Different coals were gasified and input conditions, such as, inlet gas flowrate, composition and temperature were changed. The rig measurements were compared with the model predictions for six cases in Figure 21. The dashed lines represent 20% prediction error and most results were within this range. The greatest discrepancy was for the prediction of H₂ molar composition. This was due to the fact that the same devolatilisation rates for all coals and measured values for Columbian coals were not available. The results were considered to be satisfactory. The model was also used to optimise the gasification process by varying several parameters such as excess air, particle size distribution, coal type and geometry of the reactor (Chejne and Hernandez, 2002).

The model has been modified more recently to model a pressurised fluidised bed gasifier (Chejne and others, 2011). The main modifications were to incorporate high pressure effects in transport phenomena, bed fluid-dynamics, physical properties and kinetic models for heterogeneous reactions. The model structure was the same, as the mass and energy balance equations were assumed not to change at high pressure. The authors reviewed the information available in the literature on the reactivity of coals at elevated pressures. They concluded that though many mathematical models were available for coal gasification in fluidised beds at atmospheric pressure, literature about this process at high pressures was quite limited due to the high costs of experimentation and difficulty in operating at high pressures. The model results were compared with experimental data for a pressurised fluidised bed gasifier published by Chejne and others, 2011. These are shown in Figure 22. The dashed line represent the 20% error limits. The comparisons were reasonable for the mole fractions of hydrogen and the gas temperature. There were some discrepancies for the mole fractions of CO and CO₂ and this was attributed to inadequacies in the kinetic data used in the model.

Gräbner and others (2007) have also reported a numerical simulation for the modelling of a pressurised circulating fluidised bed gasifier. The applied gasification principle was the Power High-Temperature Winkler (PHTW) process which was developed at the Institute of Energy Process Engineering and Chemical Engineering of TU Bergakademie Freiberg. Unlike in the standard Winkler process, PHTW contains a slag bath at the bottom of the reactor. The PHTW gasifier can gasify a broad variety of feedstock ranging from hard and brown coals, biomass and wastes. These are gasified in a stationary fluidised bed using oxygen and steam as gasifying agents. These enter the reactor through radially arranged nozzles at two different levels. At the bottom of the gasifier vessel, an integrated natural gas-fired slag tap controls the molten slag flow. The liquid slag drains into the slag quench chamber. Above the slag bath and below the fluidised bed, a moving bed replaces the fixed bed of the BGL gasifier. In the zone of the moving bed, about 20% of the incoming carbon is converted. The gasification gases rise upward through the moving bed and fluidise the fluidised bed. The system contains a second level of nozzles above the moving bed

through which 75% of the gasifying agents are introduced. Pyrolysis and char gasification occur in the fluidised bed zone.

The modelled region of the reactor, its basic dimensions, the operating conditions and entering mass flows are shown in Figure 23. In the right part of the figure, the rotational and simplification of the reactor is shown, having one uniform inlet for all solid particles. All inlets located on the surface are annular gaps and the surface has a set uniform temperature of 800°C. The inclined pipes through which particles enter the reactor were modelled by velocity vectors at the same angle. For every fluid inlet a turbulence intensity of 10% was assumed. The simulation was accomplished in a step-by-step

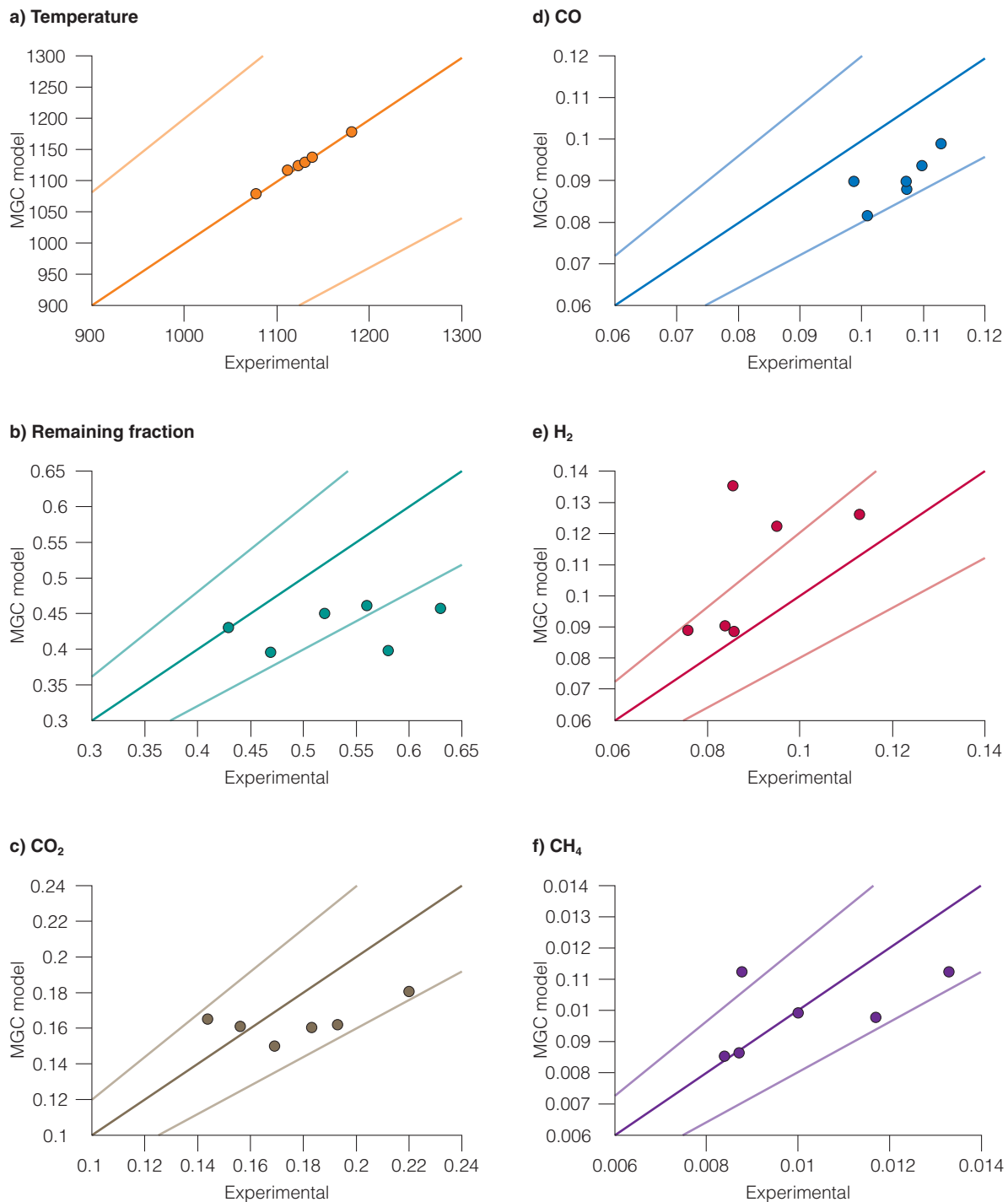


Figure 21 Comparison of model and experimental data (Chejne and Hernandez, 2002)

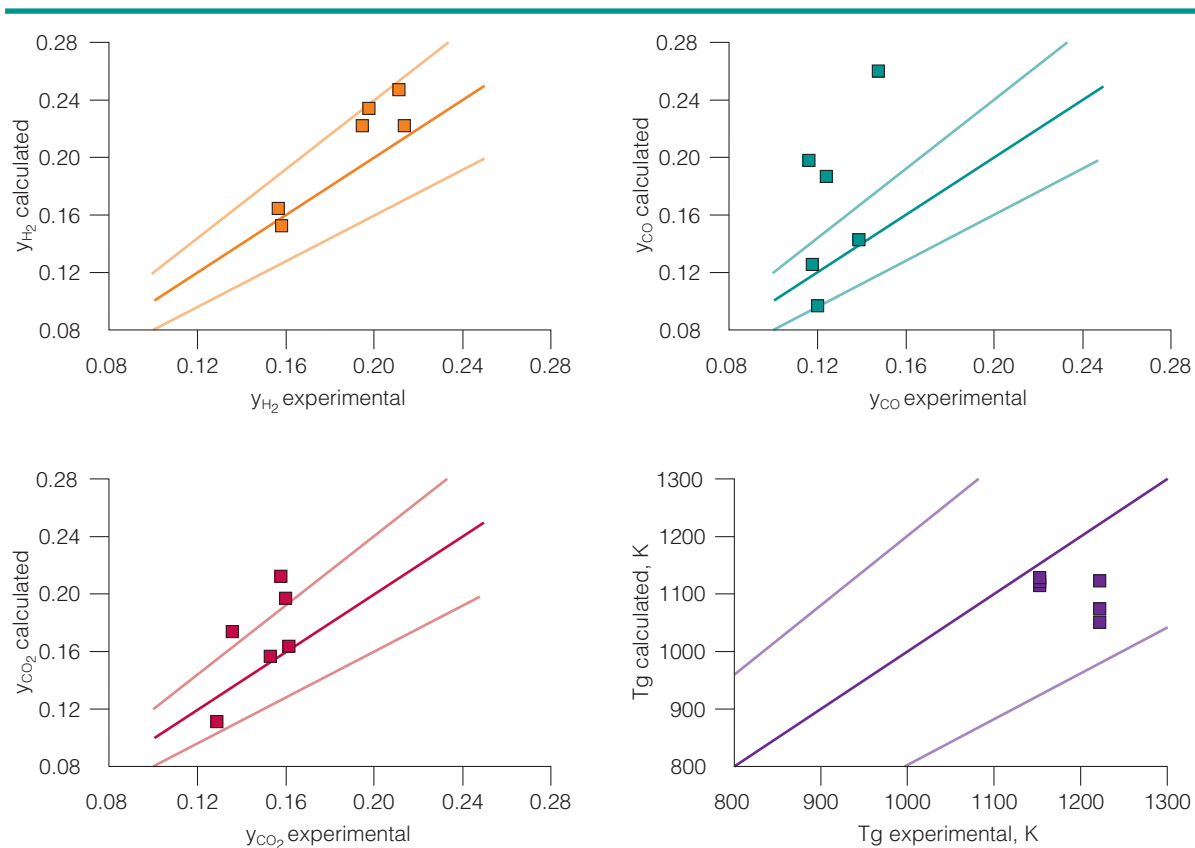


Figure 22 Comparison of model and experimental results (Chejne and others, 2011)

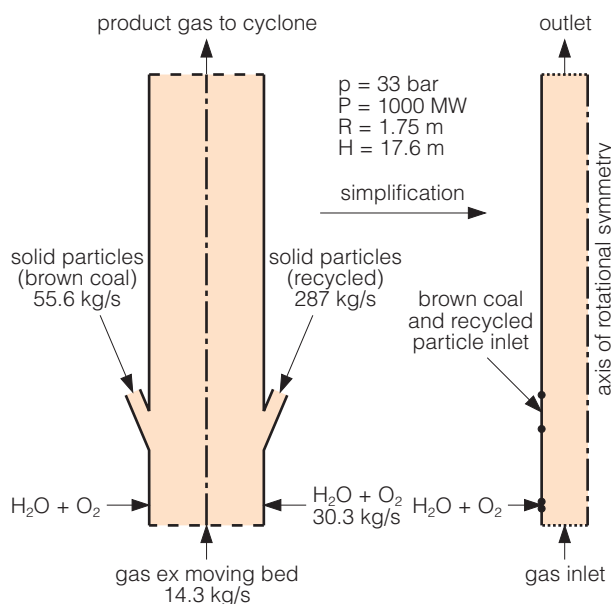


Figure 23 Schematic of modelled region of PHTW gasifier (Gräbner and others, 2007)

procedure gradually increasing the level of complexity especially concerning the amount of particles introduced to the reactor. The maximum particle loading that can be modelled was 10% hence the incoming particle flow was increased in stages. Initially results were obtained for an incoming particle mass flow rate of 55.6 kg/s containing reactive coal particles only. Later the solid flow was increased to 342.6 kg/s including inert reactive material as well as the reactive coal particles.

The model contained the basic set of equations for continuous phase flow computation comprising of equations for mass, momentum and energy conservation. All three additional source terms for particles could be included. Apart from the energy conservation term, radiative heat transfer was included. The transport equations included terms for turbulent kinetic energy. Under the assumption of equal diffusivities, the species equations

were reduced to a single equation for a given mixture fraction. Thus the modelling of the chemistry within the reactor was done by three mixture fractions, one for brown coal, one for the gasifying agent and one for the raw gas exiting the moving bed. The coal particles were modelled by an Eulerian-Lagrangian approach in order to include effects like shrinking particle size coupled with transport of

mass, energy and momentum from the particle into the fluid. The discrete-phase-model allowed tracking the trajectories of a representative group of particles moving through the continuous phase of the fluid. In order to convert these physiochemical processes into CFD, all mathematical models were codified using a finite volume method as discretisation procedure. The numerical calculations were accomplished on a stationary timescale. A two-dimensional, orthogonal, Cartesian co-ordinate and basis vector system was identified as the most suitable basis for calculation. A structured grid was generated at the beginning. Later the grid was partly refined adapting the magnitude of velocity gradients across the cell. A new block-structured grid consisted of 12,978 individual cells. The equations were solved using the commercial code FLUENT 6.2.

The model results showed that a core-annular-flow regime developed up to at least half of the reactor's height. This flow pattern was characterised by a fast, upward and dilute core flow and by a slow, downward and concentrated annular flow. Increasing reactor diameter resulted in an upward expansion of the circulation cells. Decreasing the diameter caused contraction of the circulation cells. The highest turbulent kinetic energy appeared in the transitional region between core and annular flow. The highest rate of dissipation occurred close to the tuyere nozzles. The highest temperature in the reactor was predicted to be 2600°C in a small region near the tuyere nozzles introducing the steam and oxygen. All other areas exhibited a homogeneous temperature of 970°C. The radiation absorption of gaseous H₂O and CO₂ was found to be two orders of magnitude lower than that for particles. The results demonstrated the change of particle diameter due to pyrolysis and surface reactions. The pressure drop, which is particularly important for recycling systems of cyclones, was calculated dependent on the total particle mass flow. The main inaccuracies of the simulation occurred in gas modelling and instabilities of the two phase flow. Another possible source of error was the limitation of the two phase model to 10% vol solid loading. By assuming rotational symmetry, all physical properties moving toward the axis of the reactor were concentrated. In turn, the maximum loading was exceeded quickly near the axis. To minimise this problem, the solid mass flow was increased in a step-by-step procedure. The simulation was reliable up to a mass flow of 200 kg/s. At higher solid mass flows, regions occurred where the limit loading of 10% solid matter was exceeded. However, the model was capable of being utilised as an effective tool for gasifier design evaluation and prediction of operating performance for proposed gasifier designs.

Nayak and Mewada (2011) extended an existing model for combustion of coal in a (circulating fluidised bed combustion) unit by using four Aspen Plus reactor models and several subroutines. The different modules in Aspen Plus which were incorporated to model the overall gasification process were decomposition of feed, volatile reactions, char gasification and gas-solid separation. The following assumptions were made:

- The process was at steady state and isothermal.
- Coal devolatilisation was instantaneous and the volatile products consisted mainly of H₂, CO, CO₂, CH₄ and H₂O.
- Char only contained carbon and ash.

The Aspen Plus yield reactor, was used to simulate the decomposition of the feed. In this step the coal was converted into its constituent components including carbon, hydrogen, oxygen, sulphur, nitrogen and ash by specifying the yield distribution according to the ultimate analysis. The Aspen Plus Gibbs reactor, RGIBBS, was used to model the volatile combustion assuming the volatile components were at Gibbs equilibrium and the mass consisted mainly of C, H, N, O, S, Cl, ash and moisture. The carbon partly devolatilised; the rest remained as char and subsequently gasifying. A SEPARATION COLUMN module was used before RGIBBS to separate the volatile materials and the solid. The amount of volatile material was specified in the coal proximate analysis. The Aspen Plus stoichiometric reactor, RSTOIC, simulated the char gasification process by including the char gasification reactions. In this reactor, char gasification took place. The principal components of the syngas were H₂ and CO as well as other components such as H₂O, N₂, S, SO₂, SO₃, Cl₂, HCl, CO₂, CH₄ and ash which needed to be separated. The outlet stream of RSTOIC were the products, some of which are in the gas phase others in the solid phase. The model separated the two phases in the

CYCLONE SEPARATOR module. The model was used to determine the effect of parameters such as steam to coal ratio and oxygen flow rate on the product gas composition. As expected, increasing the oxygen flow rate increased the concentrations of CO and CO₂ and reduced the concentration of H₂. Simulation runs were also conducted by varying the steam flow rate and changing the steam to coal ratio. The concentrations of H₂, CO, CO₂ and CH₄ all decreased with increasing steam to coal ratio and the reduction were more significant at high steam flow rates. At higher steam flow rates reforming reactions were favoured hence the reductions in the concentrations of CO and CO₂ were expected but the H₂ concentration would have been expected to increase.

Singh and others (2013) have reviewed CFD modelling of fluidised bed combustion and gasification. They contend that reliable CFD models were essential for the optimisation of fluidised bed design and predicting many parameters such as inert material concentration in the bed, fuel mixing efficiency, temperature profiles of solid and gaseous species present in the bed, temperature profile of the furnace and heat flux. Simulation using CFD was one of the most appropriate approaches for predicting critical parameters needed to control efficient operation of gasifiers. These multidimensional models bridge the gap between sub-scale testing and the operation of fluidised beds by providing information about gasification processes that experimental data alone cannot provide. The framework for CFD modelling of fluidised bed combustors and gasifiers is shown in Figure 24. CFD is a type of numerical simulation that combines fluid mechanics with numerical methods and algorithms to solve and analyse problems that involve fluid flow. These are coupled with the models required modelling combustion and gasification.

There are three approaches for the numerical solution of multiphase flow. These are the Euler-Lagrange, Euler-Euler TFM (E-E TFM) and the Discrete Element Method (DEM-CFD) within the Eulerian-Lagrangian concept. DEM is computationally time consuming hence it is complemented by a Discrete Phase Model (DPM). In the Eulerian-Lagrangian approach, the primary phase is treated as a continuum by solving the time-averaged Navier-Stokes equation. The behaviour of the dispersed phases are obtained by following a large number of particles through the calculated primary phase flow field. Particle trajectories are calculated in given intervals during primary phase flow

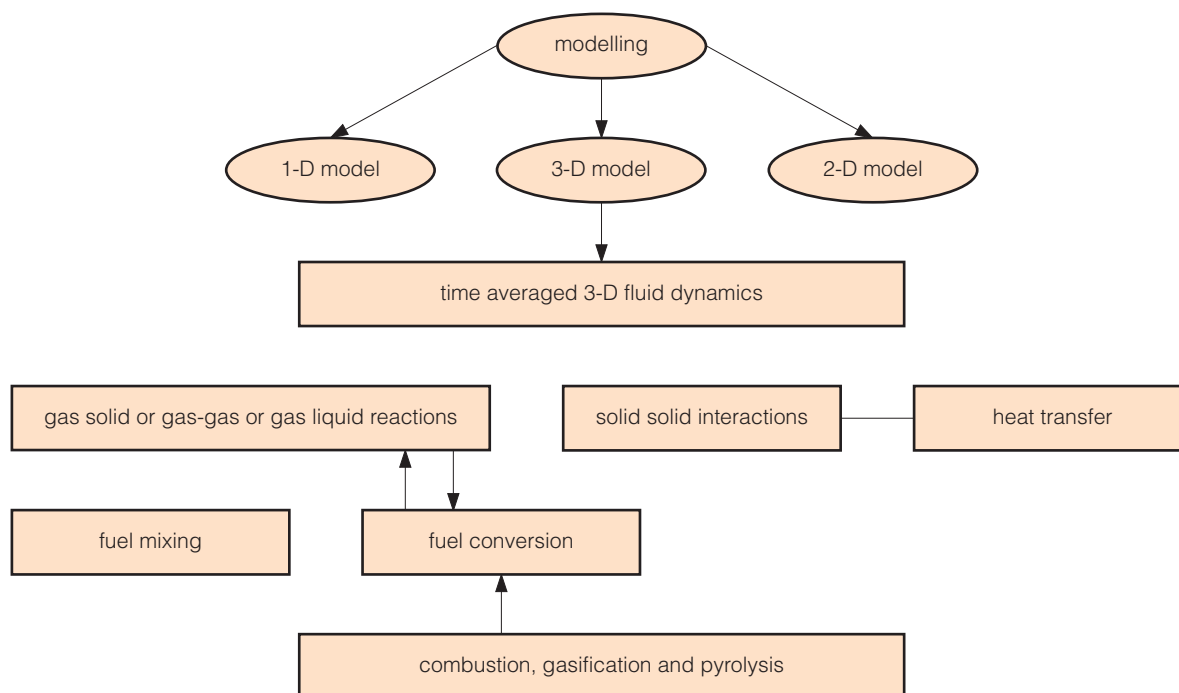
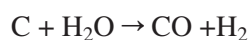
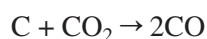


Figure 24 Framework for CFD modelling (Singh and others, 2013)

calculations. Dispersed and primary phases can exchange mass, momentum and energy. In the Euler-Euler approach, the different phases are considered as an inter-penetrating continua. Conservation laws are applied to each phase. Most of the gasification studies on gasification in dense beds have been undertaken with the Euler-Euler TFM approach and relatively simple system geometries. The Eulerian-Lagrangian DPM technique with single particle or particle parcel and a group of particles is mostly used in the freeboard region above the dense bed where diluted particle conditions are present. Different authors have adopted different approaches. Some have applied CFD to study combustion and gasification of solid fuels, their emissions and operational parameters. A few have used CFD to investigate flow patterns, temperature and main species in the reactor using their own code and Fluent. Others have tried to study ash deposition and produce deposition maps with positions of high probability of deposition. Many have modelled the freeboard using a probability density approach. They considered the fuel to be in the gas phase above the bed. The tracking of the fuel particle in a discrete phase with DPM was done by integrating the force balance on the particle which was written in a Lagrangian reference frame.

All CFD codes for modelling systems have to solve the basic fundamental equations for mass, momentum, energy and species transport. They also need to incorporate the basic equations of CFD to simulate the actual combustion and gasification processes in fluidised beds. Many devolatilisation models have been developed: some are one step, others, multi-step. The simplest ones calculate devolatilisation rates with single or two-step Arrhenius schemes. The important gas-phase reactions are included with kinetic parameters obtained from the literature. The char reactions are commonly simplified to the following three:



Models to simulate these char surface reactions are available in the literature. The models also need to include sub-models in the literature to simulate turbulence, heat transfer with radiation, mass transfer and diffusion. Eulerian-Eulerian TFM CFD models with chemistry models incorporated are needed to model solid fuel particles in the dense bed. CFD modelling of combustion and gasification of solid particles in the freeboard using discrete particle modelling and tracking of particles is undertaken using the Lagrangian approach. The conventional approach for modelling combustion or gasification in the freeboard in fluidised bed systems is the same as in pulverised furnaces.

CFD models have been used to study the physical and chemical behaviour of fuels in the fluidised bed gasification process. These models can present detailed information about the gasification processes and bridge the gap between large-scale commercial beds and small-scale rigs. Most of these have incorporated the Euler-Euler approach in two dimensions. For example, Deng and others (2008) have investigated the effect of various parameters on the gasification of coal in fluidised beds. They found that increasing pressure caused the CO level to increase in the system though temperature had no effect. Yu and others (2007) have undertaken 2-D numerical simulations of a bubbling fluidised bed gasifier. The model results gave much more accurate predictions for the distribution of pressure, temperature, velocity, volume fraction, of the phases and gas composition along the reactor than was possible with one-dimensional models. Cornejo and Farias (2011) undertook similar modelling of a fluidised bed reactor and Yu and others with more simplifications. Their chemical model involved five heterogeneous and five homogeneous chemical reactions tracking seven species in the gas phase and one in the solid phase. They assumed that coal entered the gasifier in the dried state and no ash was considered in the system. The results were found to be in good agreement with experimental data, for example, for temperature distribution and species concentration.

CFD has been used to investigate the effects of parameters which control gasification in fluidised beds

such as fuel properties, particle size, species concentration and bed material. Armstrong and others (2011) studied the parametric process of BFB gasification using CFD. They studied the effect of bed height on gas species. A lower bed height with an increased area of freeboard provided more space for the relevant species, namely CO, CO₂, H₂ and H₂O to compete in the water-gas shift reaction thus suggesting that equilibrium could be attained in a small-scale reactor provided the freeboard was sufficiently tall. The result showed that bed temperature had considerable effect on the gasification process. Fluidised bed combustors and gasifiers have been used for many to reduce emissions of pollutants such as SO₂, NO_x and CO and modelling has been undertaken; CFD modelling of emissions formation is still developing. It is difficult to describe chemical processes adequately with the E-E TFM method. CFD modelling of dense bed and freeboard/riser in combustion and gasification systems has usually been studied separately. In general, E-E TFM has been used for the dense bed and the Lagrangian model with DPM for the freeboard. The majority of studies have used the Ansys Fluent software. CFD model results are satisfactory when compared with experimental data in many cases. However, simulations still have many approximate sub-models as well as some assumptions. CFD modelling of commercial systems using the E-E TFM method are yet to be undertaken and the use of Eulerian technique with thermo-chemical reactions is still in the development stage. At present application of the DPM Lagrangian technique to model freeboard with thermochemical reactions seems to be sufficient to identify factors which affect the performance of industrial-scale fluidised bed systems. There are at present limitations on modelling large-scale sophisticated plant with CFD due to limitations of computer hardware but with the inevitable progress of computer power and the development of chemical and physical models The application of CFD to fluidised bed gasification will inevitably be more widely applied in the future (Singh and others, 2013).

A different approach has been adopted by Chavan and others (2012) for modelling the fluidised bed gasification process. They considered that gasification was a complex and non-linear process which is difficult to model by conventional ‘first principles’ models expressed in terms of mass, momentum and energy balance equations. The particular difficulties they suggested were:

- Existence of complex, non-linear and interactive relationships between process input-output variables and the throughput dependent process dynamics lasting many hours.
- Numerous, costly experiments are required to study the effect of influential process variables and parameters on the process output.
- There was insufficient knowledge of the physiochemical phenomena such as reaction kinetics, heat and mass transfer mechanisms underlying the gasification process since they depended on the quality of the raw coal which varied significantly.
- Time-intensive simulation effort was needed to arrive at a reasonable model.

The approach they suggested for modelling gasification utilised classical regression methods to formulate empirical models. These models essentially represented the dependency of gasification process output variables such as product gas generation rate and heating value on the key process operating parameters and coal quality parameters. In the regression-based modelling, the data fitting function must be specified a priori before estimating the function parameters. This was complex since in the gasification process multiple variables influence the non-linear gasification phenomena and the precise interactions between them were not fully known. These difficulties associated with regression based empirical modelling could be overcome by using artificial intelligence (AI)-based modelling formalism known as Artificial Neural Networks (ANNs). These networks are simplified systems simulating the intelligent behaviour exhibited by animals by mimicking the physical connections in their brain. The principal features on ANN-based models are:

- These are constructed exclusively from the representative process data pertaining to the independent (casual/input) and dependent (response/output) variables of a process. Subsequently, the model can be used predict process performance under varying process performance under varying operating conditions.
- The detailed knowledge of the mechanistic phenomena underlying a process is unnecessary for model development.
- A properly-developed model is able to predict accurately outputs for a new set of inputs which

- are not included in the example set.
- Multiple input-multiple output (MIMO) non-linear relationships can be fitted easily and simultaneously.
- An ANN approach uses generic non-linear function for fitting the example set of data and hence it is not necessary to pre-specify the form of data-fitting function explicitly.

The most commonly used ANN paradigm is known as multilayer perception (MLP). This network usually consists of a hierarchical structure of three layers (input, hidden and output) and a number of processing nodes. In addition, two standard multivariate regression (MVR) models have also been constructed. In the study, MVR and MLP neural network-based models have been developed to predict product gas generation and product gas heating value using coal properties such as fixed carbon, volatile matter, ash content and process parameters; namely air feed, steam feed and bed temperature. Process data from 18 fluidised bed coal gasification plants in India and other countries have been used to develop the stated MVR and ANN models. In the study, 81 data points were used for constructing (training) the models and 25 for testing the models.

Initially, multivariate regression (MVR) was used to develop two non-linear models predicting gas generation and product gas heating value from the six model inputs specifying coal properties and gasification process parameters. The magnitudes for the correlation coefficient (r), root mean squared error (RMSE) and average percentage error (APE) for the experimental and predicted values for gas generation (I) and heating value are given in Table 9. It is evident that the correlation coefficient for both MVR models had satisfactory predictive accuracy with r values of 0.96 and 0.86 for the training sets but were lower (0.95 and 0.82) for the test sets. This indicated that MVR models were not ideal for different process conditions. The MLP models had higher correlation conditions for both training (0.99, 0.97) and test (0.97, 0.95) and lower RMSE and APE values. The MLP models were more accurate for different conditions. A sensitivity analysis demonstrated that air feed rate had the greatest influence on gas production rate and gas heating value. This was not surprising given that the air feed determines the extent of gasification and combustion. The authors concluded that the model could be used to optimise gasifier design and chose the most suitable operating conditions for a particular type of coal.

Several new models for modelling fluidised bed gasifiers have been developed in the past decade. These have generally assumed steady state. A detailed CSFMB model which was produced by Souza-Santos and his co-workers can model both moving bed and circulating bed gasifiers. CFD modelling has also been extensively used for modelling fluidised bed gasification. These have been applied to multi-dimensional systems. The results of the models have been compared with plant and rig data. The comparisons have generally been satisfactory. There is little indication that modelling results have been utilised to solve particular plant problems.

Table 9 Statistical analysis of model performance (Chavan and others, 2012)						
Model	Training set			Test set		
	r	RMSE	APE	r	RMSE	APE
A Performance of MVR models						
I	0.956	0.221	6.52	0.949	0.216	6.01
II	0.859	0.523	10.55	0.823	0.435	11.32
B Performance of MLP models						
I	0.99	0.109	2.66	0.971	0.162	4.49
II	0.968	0.238	4.964	0.945	0.25	6.405

5.4 Models for entrained flow gasifiers

Entrained flow gasification technology is the most widely used gasification technology but modelling this process is more complicated than modelling fluidised bed gasifiers due to the need to model ash slugging. Unlike FBG modelling for which the motion of the coal particles is generally described by an Eulerian approach, in entrained flow gasifiers which are more lightly loaded, the Lagrangian approach is more suitable. Early models for entrained flow gasifiers are described in Moreea-Taha (2000). More recent models range from 1-D steady state equilibrium models to sophisticated dynamic 3-D CFD models which simulate coupled gas-solid hydrodynamics, heat and mass transfer and reaction kinetics within a complex gasifier geometry.

5.4.1 1-D models

Kasule and others (2011) have developed a 1-D, steady state model of a single-stage, downward-firing, oxygen-blown, slurry-fed, entrained-flow gasifier for use in context of IGCC process simulation. The model included a detailed energy balance model for the reacting phases and the gasifier wall, which incorporated the energy loss to the environment. A heuristic mixing and recirculation model was included to enhance the initial energy transfer in the model and to promote a stable flame-zone within the initial section of the gasifier. Mass, momentum and energy balance equations for solid (char) and gas phases were considered. When the coal was fed to the gasifier, the initial processes involved the evaporation of coal moisture and coal devolatilisation which released volatile components such as CO, H₂, CO₂, CH₄, H₂O, H₂S, tar and other hydrocarbons. The moisture evaporation and devolatilisation were modelled using standard expressions. Following the coal devolatilisation, the model assumed that the residual char underwent the reactions given in Table 10. The table also contains the main homogeneous reactions which are included in the model. The unreacted-core shrinking model was used for calculating the rates of heterogeneous reactions. A detailed model of radiative heat transfer was developed which considered the interactions between all internal surfaces of the gasifier and the solids as well as the interactions between the surfaces themselves. In slurry-fed gasifiers, recirculation near the inlet is promoted for rapid mixing of the slurry with the hot reaction products. This mixing results in a significant rise in temperature which facilitates evaporation of water and devolatilising the coal. In the model this process was included and

Table 10 Solid phase and gaseous reactions (Kasule and others, 2012)

A – Solid phase reactions	
Char combustion	$C + 1/\phi O_2 \rightarrow \{2-2/\phi\}CO + \{2/\phi - 1\}CO_2$
Steam gasification	$C + H_2O \leftrightarrow CO + H_2$
CO ₂ gasification	$C + CO_2 \leftrightarrow 2CO$
H ₂ gasification	$C + 2H_2 \leftrightarrow CH_4$
ϕ is a factor that gives the ratio of CO ₂ to CO in the reaction products.	
B – Gaseous reactions	
$CO + \frac{1}{2}O_2 \rightarrow CO_2$	
$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$	
$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$	
$CO + H_2O \leftrightarrow CO_2 + H_2$	
$CH_4 + H_2O \leftrightarrow CO + 3H_2$	
$\frac{1}{2}N_2 + \frac{3}{2}H_2 \leftrightarrow NH_3$	

Table 11 Comparison of gasifier model results with TECO data (Kasule and others, 2011)

	Gasifier results, %vol	TECO data, %vol
CO	41.9	41
CO ₂	19.6	17.5
H ₂	29.2	36.1
H ₂ S	1.05	0.91
CH ₄	1.59	0.07

the conservation equations were appropriately modified. The system of highly non-linear equations generated was discretised using the first order backward finite difference method and then simultaneously solved by the Aspen Custom Modeler using a Newton-type method with appropriate boundary conditions and a good initial guess.

The model was used to simulate the entrained-flow gasifier of the Tampa Electric Polk plant. A comparison of the syngas composition is shown in Table 11. The plant data came from the exit stream of the radiant syngas cooler (RSC) hence it was necessary to model the

processes occurring in the RSC. This was undertaken with an existing model. The results show that there was satisfactory agreement for the predictions of CO, CO₂ and H₂S. The mismatch in CH₄ was attributed to the devolatilisation model which considered higher molecular hydrocarbons to be CH₄. The predicted H₂ level was also somewhat low and this was probably due to the low CH₄ reforming rates used in the study. But overall the agreement was considered to be reasonable. The model was used to predict the effect of coal type on the syngas composition. There was noticeable variation in gaseous product distribution depending on the type of coal but CO, CO₂ and H₂ were always the dominant species. The concentration profiles of all the major gas phase species were predicted along the length of the reactor and the wall temperature profile was also predicted but there were no plant data with which to compare (Kasule and others, 2011).

Kasule and others have extended the steady state, 1-D model and developed a dynamic model of a downward-fired GE/Texaco entrained-flow gasifier. As in the steady state model, the dynamic model contained mass, momentum and energy balances for the gas and solid phases. As before, the model considered the initial gasification processes of water evaporation and coal devolatilisation. The key heterogeneous and homogeneous chemical reactions have been modelled. The defining equations for the dynamic model were similar to those of the steady state model except that transient terms were included. The dynamic simulation resulted in a highly non-linear system of partial differential algebraic equations. These were solved by the Aspen Custom Modeler using the Method of Lines approach. This discretised the space domain and left the time domain continuous, thereby converting the partial differential algebraic equations to differential algebraic equations with respect to time. This system of equations was solved using a variable-step implicit Euler integrator to obtain a transient response. The dynamic response of the gasifier to particular changes commonly undertaken during the practical operation of commercial gasifiers was investigated. These operational changes include ramp and step changes to input variables such as coal flowrate, slurry flowrate, oxygen-to-coal ratio and water-to-coal ratio. The predicted transient response of the scaled exit gas temperature to a stepwise ramp turndown of gasifier slurry flowrate is shown in Figure 25. This was consistent with the observed performance at the Coolwater plant (Kasule and others, 2012).

Tremel and Spliethoff (2013) have developed a one-dimensional plug flow model to simulate laboratory-scale Pressurised High Temperature Entrained Flow Reactor (PiTER). The model consisted of different submodels for fuel devolatilisation, intrinsic char gasification, surface area evolution, char thermal annealing, pore diffusion, boundary layer diffusion and particle size and density variation. The submodels were partly derived from experimental measurements and partly from theoretical derivations. The devolatilisation model was derived from experimental data and the rate was described by a single first-order rate equation. The intrinsic reactivity at the char was modelled by an nth order rate equation $-r_{\text{intr}} = k_0 \cdot \exp(-E_A/RT) \cdot p^n$ where p is the pressure of the reactant gas. The initial char surface area after devolatilisation was described by an empirical linear approximation of the experimental data. The char deactivation model was based on experimental data and described by a

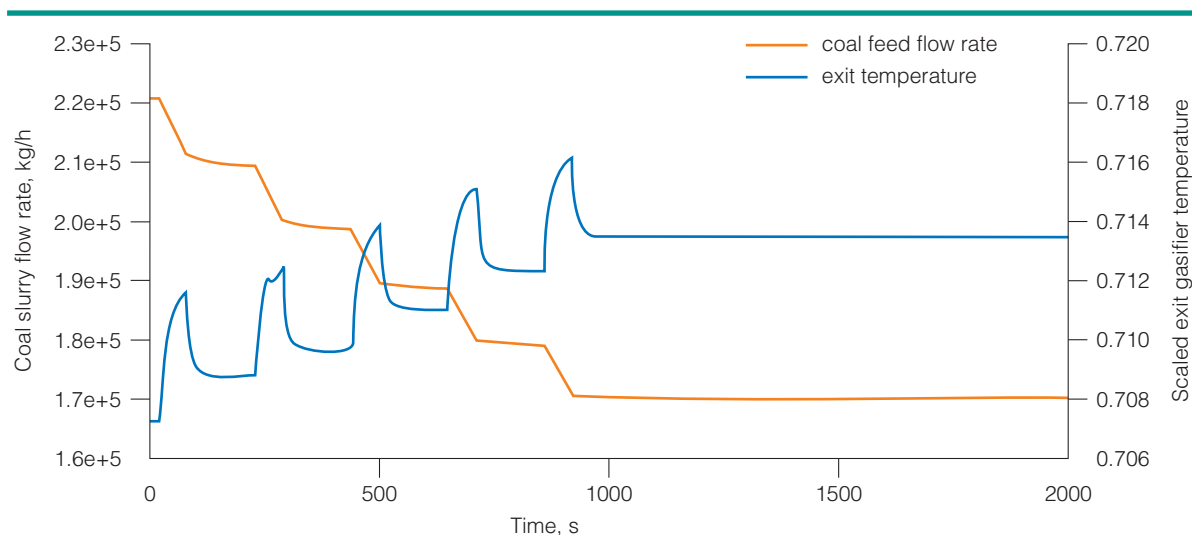


Figure 25 Gasifier temperature transient response (Kasule and others, 2012)

first-order Arrhenius type expression. The analysis of pore diffusion was based on that for heterogeneous catalysis. The calculation of reaction rate in the pore diffusion regime required knowledge of the gaseous concentration at the particle outer surface. The surface concentration was related to the bulk gas concentration by the mass transfer in the boundary layer of the char particle and this was modelled by a simple form of Fick's law. The change in particle size during devolatilisation was modelled by a swelling index which is the ratio of the char particle diameter after devolatilisation and the initial fuel particle diameter.

The model results were compared with measurements from the PiTER gasifier. In this the reactant gases were fed to the top of the reactor. The pulverised fuel was fed by a gravimetric dosing system with a highly controllable feed rate from 0.2 kg/h to 5.0 kg/h. The gas mixture was heated in a preheating tube and then entered the main reaction tube that had an internal diameter of 70 mm and a length of 2.3 m. The maximum operating temperature was 1800°C and maximum operating pressure was 5 MPa. The gas flow rate was used to adjust the gas residence time. In all experiments a constant stoichiometry of an O/C ratio of 1.0 was applied. The PiTER operated with a mass flow 1.25 kg/h in the temperature range 1200–1600°C and the pressure range 0.5 to 1.0 MPa. Experiments at lower pressures were carried out in a smaller BabiTER reactor. Both the overall and char conversions increased rapidly with particle residence time. The temperature was found to have a significant effect. However, the difference in conversion between 1200°C and 1400°C was small and decreased further between 1400°C and 1600°C. In the early stages of conversion there was a sharp increase in char conversion indicating a fast reaction rate. The reaction rate slowed down at higher residence times and conversions. There was no significant effect of total pressure on reaction rate. The experimental results were compared with model simulations. As the model contained several submodels which incorporated process parameters that were not constant during conversion, such as gas concentration, numerical methods were used to combine the submodels and calculate fuel conversion. The PiTER was assumed to be a one-dimensional plug flow reactor and was divided into cells in the gas flow direction. At the cell outlet the main gas concentrations were calculated assuming chemical equilibrium. The comparison of simulation and experimental data for char conversion and overall conversion is shown in Figure 26. The differences between the model and experimental data were small and the results demonstrate that the fuel conversion can be predicted by numerical calculation based on the different submodels. One objective of the model development was to predict the gasification behaviour in larger-scale entrained flow gasifiers. The model was applied to a one-dimensional plug flow reactor that represented a simple approach to a 500 MWe entrained flow gasifier. The concentrations of gaseous species and temperature profiles within a 500 MW gasifier were predicted and cold gas efficiencies and fuel conversions were calculated. Based on the model

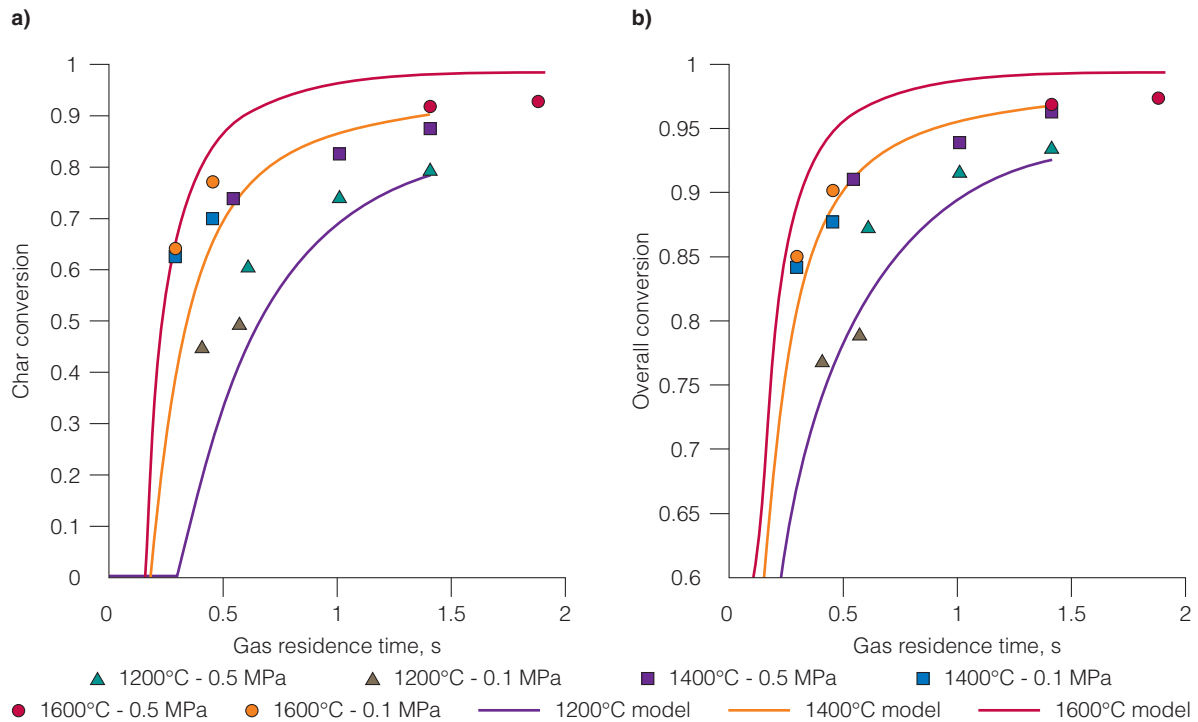


Figure 26 Comparison of model prediction and experimental data for char conversion and overall conversion (Tremel and Spliethoff, 2013)

predictions, the reaction regime of char conversion in entrained flow reactors was analysed. At very high temperatures in the burner zone, char gasification approached Regime III where the overall rate is controlled by mass transfer between the bulk and the particle surface. In the medium stages of char conversion, the reaction occurs under Regime II where the reaction is diffusion controlled within the pore and then approached Regime I conditions at high conversions and lower temperatures where the rate is determined by the reaction rate at the char surface. As all three regimes can apply, fuel properties that impact on diffusion such as particle size and pore structure as well as intrinsic char reaction such as intrinsic reactivity and thermal annealing have to be considered to determine entrained flow kinetics (Tremel and Spliethoff, 2013).

Lee and others (2011) have developed a simple process for modelling a dry-feed entrained flow gasifier. Their purpose was to develop a model that could analyse chemical processes in the gasifier when varying the oxygen to coal ratio, steam to coal ratio and operating pressure. The approach is different from a standard CFD analysis. The chemical processes in terms of coal gasification and combustion were interpreted along gasifier height. The degree of reaction was obtained at variable operating conditions. The gasifier modelled was a Shell-type, dry feeding entrained-flow gasifier with up-flow of feeding stock. The residence times of coal particles and other gases was about 3–4 s. The average operating conditions were 1800K and 4.2 MPa. The gasifier is schematically represented in Figure 27. The authors suggested that though a 3-D model was required for a detailed model of the gasifier, it was not necessary from the point of process analysis because heat and mass transferred across the reactor radially are more dominant than along the axial direction. From earlier CFD simulations, the recirculation pattern was known. A simplified flow pattern was adopted based on rough assumptions in a pseudo-2D model. The geometry of the gasifier was divided into five sections. The mixed feedstocks flow as 1-D plug flow in sequence and in each designated section of the pseudo 2-D model through the 2-D effective cross-section of each zone. The behaviour of the coal could be described in terms of devolatilisation, heterogeneous reactions at the solid particle surface and homogeneous reactions of gaseous components.

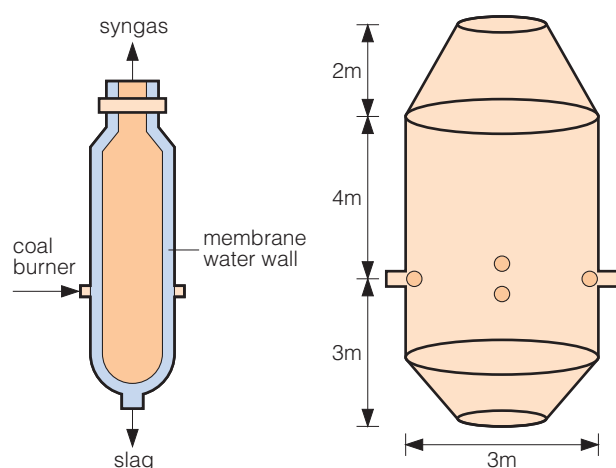


Figure 27 The Shell gasifier and a schematic of the gasifier model (Lee and others, 2011)

The gaseous species were assumed to be CO, CO₂, CH₄, C₂H₆, H₂, H₂O and C₆H₆. The kinetics of product formation were modelled by a set of first-order, parallel reactions with an Arrhenius-type rate constant. Though modelling devolatilisation by first-order kinetics has limitations, it has been found to give an adequate representation of hydrocarbon yield. Regarding the homogeneous chemical reactions of the gaseous species, one can either consider the overall global reaction or consider the kinetics of individual reactions including intermediate species. In this study, a simple global reaction was utilised as it had the advantage of simulating the overall coal reaction rate by considering many chemical reactions. Considering the heterogeneous reactions, it was assumed that the overall char reaction rate

was proportional to the n th power of the partial pressure of the gasifying agent and followed an Arrhenius-type expression. In modelling the solid-phase reaction, it is necessary to consider chemical reactions occurring on the internal surface but estimating the surface area is difficult because of large numbers of micro-pores. The random pore model was used. This predicted the reaction surface area at a given conversion as a function of initial pore structure parameter. The chemical reactions considered in the model are listed in Table 1. Performing the pseudo 2-D model enabled the carbon conversion, cold gas efficiency and gas temperature to be calculated. The main conclusions were:

- (i) As the concentration of oxygen was increased, adequate carbon conversion took place and a reactor length shorter than 6 m was adequate to get maximum carbon conversion at a given oxygen to coal ratio.
- (ii) The peak temperature increased as oxygen to coal ratio was raised.
- (iii) Although the rate of increase of temperature was higher during the early stages of reaction, the peak temperature was lower. This was because the higher pressure resulted in the higher reactivity of endothermic gasification reactions. As the pressure increased, the partial pressure of the gasifying agents, CO₂ and H₂O, increased. As a result carbon conversion and coal gas efficiency also increased.

The authors acknowledged that as a simplified model, it contained uncertainties. It relied on rate constants that were difficult to measure at high temperatures and pressure. There were few data in the open literature on the process analysis of a commercial gasifier for benchmarking, so validation of the model was not easy. Hence the model results should be used to evaluate trends rather than to provide exact predictions (Lee and others, 2011).

Gazzani and others (2013) have developed a reduced order model (ROM) as an alternative to comprehensive CFD to simulate a Shell-Prenflo entrained flow gasifier. ROM is computationally very efficient taking about 1 minute in typical desk-top or laptop computer, hence enabling integration of the gasifier model and the overall power plant flowsheet simulation. The ROM approach allows a reasonably accurate prediction of the gasification process as part of a plant simulation model. In the ROM the gasifier was represented by a reactor network model (RNM) which was based on idealised 0-D or 1-D chemical reactors to simulate different parts of the gasifier. The ROM simulation may require some input data from CFD. The RNM representation of the Shell gasifier consists of four zones:

- Internal Recirculation Zone (IRZ);
- Jet Expansion Zone (JEZ);
- External Recirculation Zone (ERZ);
- Downstream Section Zone.

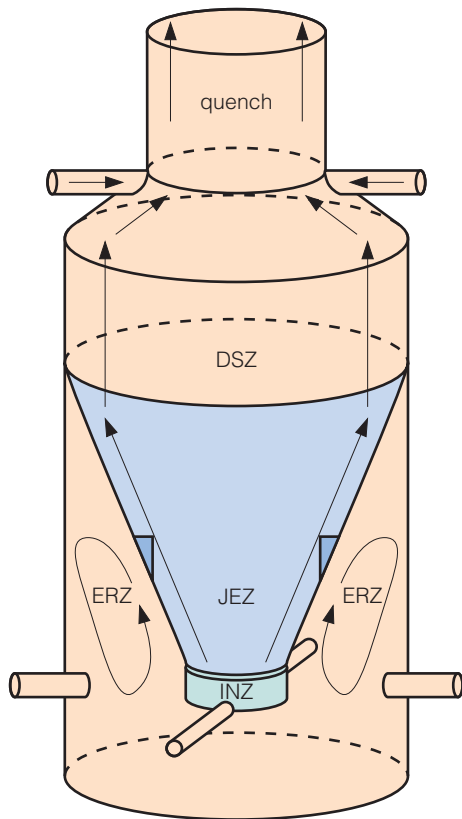


Figure 28 Shell gasifier physical macro areas representation (Gazzani and others, 2013)

These are shown in Figure 28. The organisation of the ROM model after the gasifier design was defined and the reactors were sized and linked is shown in Figure 29. Each reactor had its own conservation equations which required several submodels to perform the simulation. The parameters for these models were chosen based on experience and some modelling. The recirculation of gases between JEZ and ERZ was one of the most important parameters that needed to be assigned and ideally would be provided by CFD simulations. Because of the gasifier complexity which included these gas recirculation loops and a membrane wall, particular attention was paid to the two-phase heat exchange process in the gasifier wall and the syngas quench process. The modelling was undertaken using Aspen Custom Modeller. Aspen Plus and GS were utilised to model water scrubbing and the overall gasification process simulation. GS was an existing simulation software for energy conservation. The overall gasification process was represented by three different zones placed at the outlet of the gasifier reactor, the quench exit and the scrubber exit. The ROM provided detailed information for both the gasifier

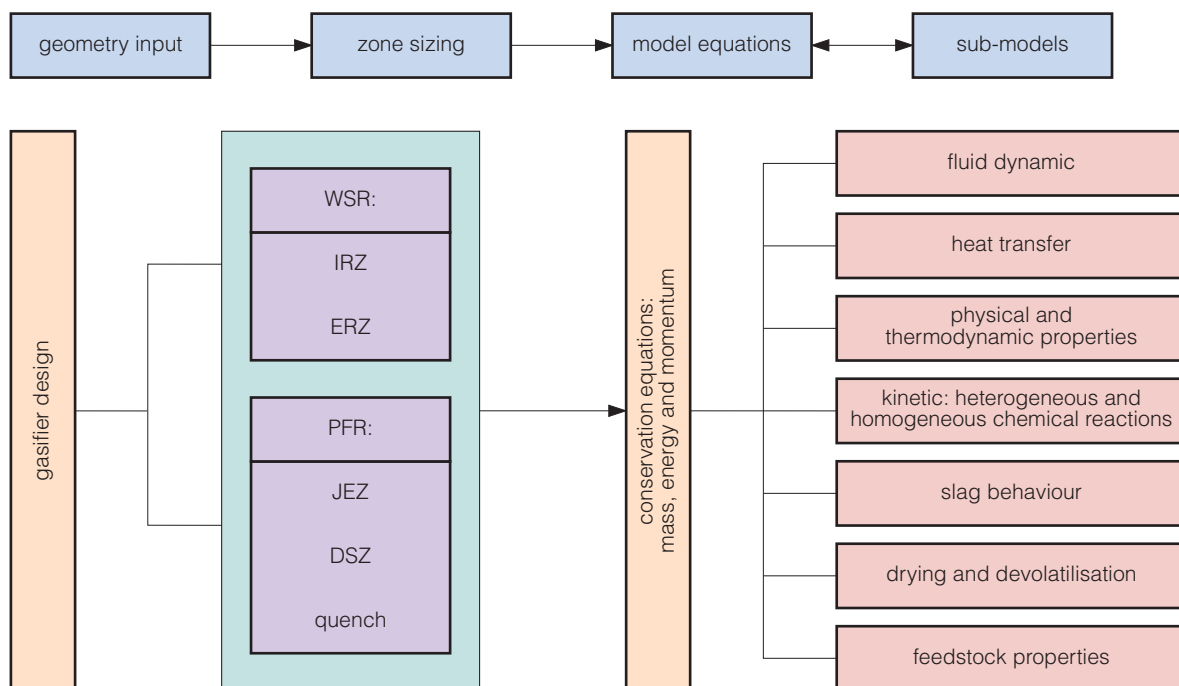
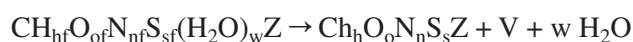


Figure 29 Shell gasifier ROM model layout (Gazzani and others, 2013)

Table 12 Comparison of model results and Shell data (Gazzani and others, 2013)							
	T°C	MPa	CO, mol%	H ₂ , mol%	CO ₂ , mol%	H ₂ O, mol%	H ₂ S, mol%
Kinetic ROM model							
Gasifier exit	1588	4.38	62.3	25.9	1.05	1.78	0.17
Quench exit	932	4.38	58.2	24.3	0.99	7.5	0.15
Scrubber exit	161	4.11	51.9	21.7	0.84	16.7	0.13
Equilibrium model							
Gasifier exit	1536	4.38	62.1	25.9	1.16	1.87	0.19
Quench exit	1001	4.38	55.3	27.7	4.32	3.59	0.18
Scrubber exit	154	4.11	49	24.5	3.65	13.96	0.15
Shell data							
Scrubber exit	165	4.10	48.7	22.4	2.34	17.97	0.13

reactor and the quench while the scrubber process was simulated in Aspen Plus. Table 12 contains the model results for temperature, pressure and molar composition for the gas phase at the outlet of the above mentioned sections. The equilibrium model was limited to the gas phase and did not consider solid-particle behaviour. The Shell data were only available for the scrubber exit. At the gasifier outlet, the equilibrium simulation produced data close to ROM. This resulted from rapid, complete char conversion in the gasifier. Larger differences arose at the outlet of the quench as the equilibrium calculations were affected by the higher conversion of CO due to the water-gas shift reaction. When comparing with the Shell data at the scrubber exit, the equilibrium model overpredicted CO₂ and H₂. The ROM model predicts lower CO₂ and H₂ due to WGS reaction rate. The cold gas efficiency predicted by ROM (82.5%) was very close to the Shell value (82.8%). Overall, the ROM predicted the syngas conditions at the scrubber outlet quite accurately. In addition, ROM could be applied to a variety of coals or under different operating conditions (Gazzani and others, 2013).

An earlier model to simulate the PRENFLO gasifier at the Puertollano IGCC plant was developed by Usón and others (2004). As the gasifier was already in operation, a CFD model was considered to be unnecessary and a chemical model to model the reaction chamber was produced which simulated the gasification of a fuel particle. The process was divided into three stages: volatilisation and volatiles combustion; char combustion and char gasification. In each stage, the products were calculated by mass balances and the kinetics of the processes were studied. The kinetics investigations of the first two stages were used to calculate their duration. Subtracting this time period from the overall residence time determined the degree of gasification possible. Volatilisation was represented by the following reaction:



where CH_{hf}O_{of}N_{nf}S_{sf}(H₂O)_wZ was the molecular formula of the fuel and Ch_hO_oN_nS_sZ was the molecular formula of the char and V are the volatiles. To simulate this stage, existing correlations and kinetic expressions were used. As the volatiles were released, they were combusted. For the char combustion and gasification stages, the shrinking core model was utilised. The model assumed that chemical reactions took place on a spherical surface that separated the core that had not reacted with the ash cover where non-mineral matter had already been consumed. In the model, mass convection around the particle, diffusion through the ash layer and reaction kinetics on the core surface were considered. During the combustion stage the particle reacted with O₂, CO₂ and H₂O which had flowed

through the ash layer from the gas to the core. The end of the presence of oxygen determined the end of the combustion stage and the commencement of gasification. In this third stage, the particle reacted with CO_2 and H_2O . At the same time, the shift reaction and CH_4 and COS forming reaction took place.

The reaction chamber was divided into two isothermal zones: combustion and gasification. Volatilisation, volatile combustion and char combustion took place in the first and char gasification in the second. In each zone, the temperature was calculated by an energy balance. In these balances, the heat transfer between the two zones and the heat transfer from the gasification zone to the reactor walls were considered. The model simulated the processes in the reaction chamber and provided the composition of the gases leaving the chamber. In reality, the quench due to mixing with the cold gas stream was not instantaneous and the concentrations of species in the gas phase changed before the cooling locked them. The model contained an additional stage to allow for this. To tune and validate the model, information provided by a Thermo-economic Diagnosis (TDG) system was incorporated. This diagnosis consisted of comparing two situations identifying the causes that determined which case is more efficient or generates more power than another and quantifying how much each of these causes was responsible for the deviation in efficiency or power production. TDG connected with the plant information system, detected steady state operating periods and mass and energy balances and data reconciliation to calculate the thermodynamic state of the plant. The information from 2874 real operating periods was filtered and processed by this system and used to tune the model. Measured coal conversions were used to adjust the particle residence time and the gas composition was used to adjust the equivalent lock temperature. The model was used to simulate gasifier operations with new fuels, optimise operation and develop a deeper understanding of the gasifier. The co-gasification of coal with biomass was investigated with the model. The simulations showed how the operating conditions should be modified as the fuel mixture varied and enabled the production of plant operation maps for a wide range of fuels (Usón and others, 2004).

5.4.2 3-D models

Chen and others (2000a,b) have developed a comprehensive 3-D model for entrained flow gasifiers. They used an extended coal/gas mixture fraction model with the Multi Solids Progress Variables (MSPV) method to model gasification reactions and the reactant mixing process. This allowed for an arbitrary number of coal off-gas components whereas the earlier Single Solid Progress Variable (SSPV) was based on the assumption that coal off-gas had a constant elemental composition and a constant heating value. Four mixture fractions were considered to model syngas from coal devolatilisation, char- O_2 , char- CO_2 and char- H_2O reactions separately. The following physical and chemical processes were included in the model: turbulent flow of gas and mixing of gaseous reactants; entrainment of particles and their turbulent dispersion; coal devolatilisation and volatile combustion; heterogeneous char reactions and convective and radiative coal/char/ash particle heating and cooling. The model was developed for simulating practical gasification facilities. Chen and others performed a series of numerical simulations of a 200 t/d, two-stage, air-blown, entrained flow gasifier developed for an IGCC process. They modelled variations of heterogeneous reaction rates, coal types, particle sizes and air/coal partitioning in the two stages. The predicted gas temperature profile and exit gas composition were in general agreement with the measured values. The MSPV model resulted in a combustion zone, a gasification zone and a devolatilisation zone in the two-stage gasifier. The results showed that coal devolatilisation and char oxidation were responsible for most (80%) of the carbon conversion. The predicted carbon conversion was independent of devolatilisation rate, sensitive to the chemical kinetics of heterogeneous reactions on the char surface and less sensitive to a change in coal particle size. The model predicted that increasing the air ratio lead to increased CO_2 and decreased CO and H_2 levels. The carbon conversion and the heating value of the product gas were found to be nearly independent of the air/coal partitioning between the combustor and the reductor and also of the feed rate of recycle char. The model also predicted that increasing the average coal particle size decreased the carbon conversion which resulted in an increase in the exit gas temperature and lower heating

there was sufficient ash deposition and heat flux to form a molten slag layer. To build confidence in the model, it was used to simulate a single stage, up-fired, dry feed gasifier similar to the Puertollano gasifier and the model results were compared with two other existing models. There was good agreement between the results produced by the three models. They all predicted liquid slag thicknesses of a few millimetres and solid slag thicknesses varying between 10 and 20 mm.

The model was used to simulate a generic, two-stage, up-flow gasifier based on the data contained in the studies by Chen and others (2000a,b). The quantities of particular interest to model were the composition of the syngas, temperature, heating value, the carbon conversion and the cold gas efficiency of the gasifier. The model results were compared with those of a existing DOE funded study that employed an ASPEN analysis for an IGCC plant with an IGCC plant with a similar two-stage gasifier. The systems modelled were not identical and some adjustments were needed to the DOE to make the predictions comparable. When this was done, there was good agreement for the predictions for syngas temperature, mass flow, heating value and syngas composition. A similar procedure was followed for a generic, single-stage gasifier based on the data for a pilot-scale facility. There was acceptable agreement between the predicted values of the two models (Bockelie and others, 2002).

As CFD-based models require significant computational time to produce a steady state solution, Bockelie and others developed a simpler model that could be used for rapid calculations and to narrow the range of operating conditions for a CFD model. This model consisted of three submodels: a zonal, equilibrium sub-model with heat transfer; a carbon burn-out sub-model and a model of the quench zone downstream of the gasifier. The zonal sub-model incorporated the equilibrium gas phase reactions and enthalpy balances for the gasifier and calculated exit gas concentration and temperature. Heat loss through the walls and heat absorbed by the ash were accounted for. The ash viscosity

Table 13 Comparison of model results with plant data (Bockelie and others, 2003)

A Cool Water gasifier												
Case	1		2		3		4		5		6	
Species, mole, fraction	CW	model	CW	model	CW	model	CW	model	CW	model	CW	model
CO	0.45	0.47	0.44	0.49	0.43	0.42	0.44	0.44	0.43	0.42	0.44	0.4
H ₂	0.38	0.34	0.39	0.33	0.38	0.37	0.38	0.37	0.38	0.36	0.37	0.35
CO ₂	0.15	0.17	0.15	0.15	0.18	0.2	0.17	0.19	0.19	0.2	0.18	0.22
HHV, kJ/m ³	9911	9840	9959	9806	9664	9419	9750	9561	9553	9344	9609	9664

B Shell gasifiers									
Case	1		2		3		4		
	Shell	model	Shell	model	Shell	model	Shell	model	
CO	0.63	0.63	0.64	0.65	0.65	0.65	0.63	0.63	
H ₂	0.26	0.26	0.27	0.27	0.26	0.27	0.28	0.29	
CO ₂	0.02	0.01	0.016	0.01	0.016	0.012	0.015	0.019	
N ₂	0.09	0.089	0.065	0.063	0.065	0.064	0.062	0.062	
HHV, MJ/kg	11.52	11.77	12.06	12.3	12.11	12.26	12.5	12.53	

sub-model developed for the CFD gasifier flowing slag model was used to calculate representative ash viscosity and critical ash temperature. The burn-out sub-model calculated the carbon combustion efficiency for chars of different reactivity. The fuel burn-out and char recycle were necessary inputs to the zonal sub-model and were obtained from the burn-out sub-model. The gas and radiation temperatures were necessary inputs for the burn-out sub-model and were obtained for the zonal sub-model. The quench model allowed for the reactions between the exit of the gasifier and the temperature at which the reactions were quenched.

Model results were compared with three sets of measured data from three working gasifiers. The first set was from the Cool Water demonstration plant using a Texaco, oxygen-blown gasifier designed to process 1000 t/d of coal fed as a water slurry. The syngas composition and heating values were compared with those from the process model and shown in Table 13. It is evident that excellent agreement, within 2%, was obtained for the calculated and measured heating values. The agreement between the two sets of gas composition data was also very satisfactory in three cases. In all cases, the predicted H₂S and COS concentrations were higher than the measured values as the measured ones were after cleaning whereas the model results were for initially formed components. The second set of results which were compared with the model were from three Shell gasifiers in Germany, the USA and the Netherlands. The calculated syngas compositions, lower and higher heating values and cold gas efficiencies were compared with measured values and in all cases the agreement were satisfactory. The model results were also compared with measured results from the Wabash River plant. Here the comparison was more difficult as the plant oxidant flowrate data were not reported hence an adjusted value had to be used. In spite of this there was reasonable agreement between the measured and predicted syngas composition values (Bockelie and others, 2003). The model was further developed to allow for modifications of process conditions, burner characteristics, fuel type, slurry composition and gross geometry. There were further refinements in the submodelling of reaction kinetics, slag, ash, soot, tar and air toxics. The model was used to investigate one- and two-stage gasifier designs based on commercial systems. The model provided information on, for example, gas flow field, wall conditions, carbon conversion, cold gas efficiency, unburnt carbon and syngas properties. This allowed for an evaluation the impact on carbon conversion, slag and ash properties and the refractory due to changes in fuel, oxidant properties (O₂ concentration, amount of pre-heat) and feed characteristics (wet/dry, solids loading, amount of pre-heat). The simulations were targeted towards understanding and improving gasifier performance (Bockelie and others, 2005).

In a slagging gasifier, high slag removal efficiency at the walls is needed. Modelling this requires tracking the particles to the wall and, knowing the viscosity of the slag, calculating the flow down the wall. It is hence necessary to understand and model the vaporisation and condensation of the mineral matter in the coal. This mineral matter forms submicron ash particles that can blind filters. The transformation of mineral matter is dependent on many factors including the size distribution of coal, the local gasification conditions, the forms and occurrence of elements in coal and the interaction of different elements. Ash vaporisation is most likely at the high temperatures (>3000°C) found near the injector in a gasifier. Bockelie and others have modelled slagging by incorporating an existing model for vaporisation and condensation, developed for PCC boilers. The mass of the submicron particles is dominated by the major constituents of the coal mineral matter such as iron, silicon, aluminium and alkali and alkaline earth elements. These elements are present in the coal partly as included mineral matter, partly as atomically dispersed elements and partly as extraneous mineral particles. During coal conversion, most of the mineral matter distributed within the particle is exposed on the surface of the char particle as it recedes during oxidation. A small amount of the mineral matter, of the order of one percent of the ash, will vaporise and subsequently recondense to form submicron particles that are in the size range in which penetration through filters is high.

The ash vaporisation process was modelled by developing the necessary mathematical representation of the transformational pathways shown in Figure 31. Part of this vaporisation occurred during devolatilisation when elements that are present in organo-metallic form were released. The refractory oxides were vaporised by the reduction of the oxides to the more volatile suboxide or metal, followed

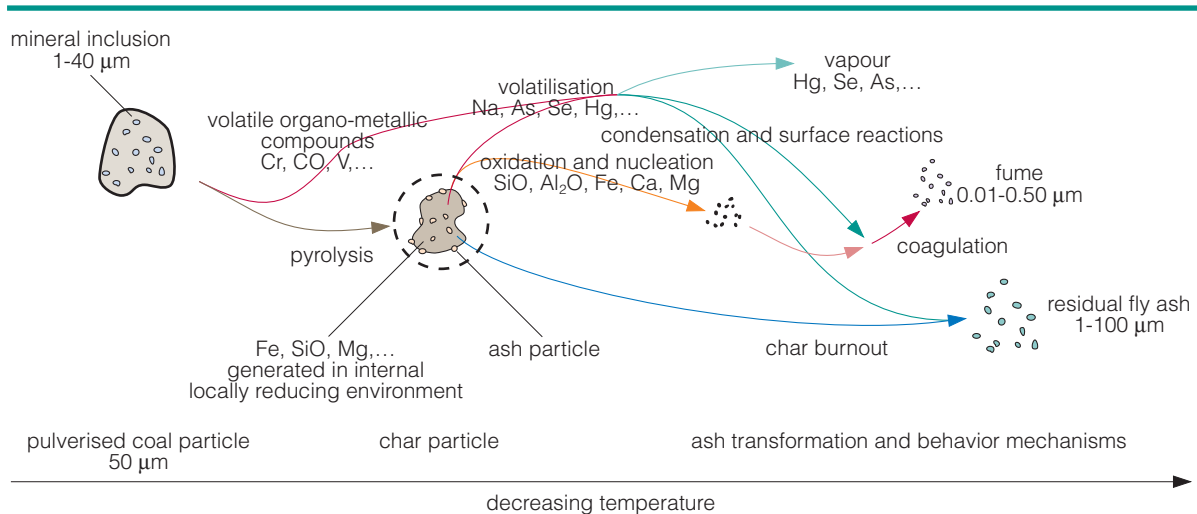
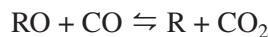


Figure 31 Schematic of mineral matter conversion during pulverised fuel conversion (Bockelie and others, 2008)

by the diffusion of the suboxide or the metal to the particle boundary layer where they were reoxidised and condensed to form a submicron aerosol. The vapour pressure of the vaporising suboxide or metal was determined at higher temperatures by the equilibrium of the reaction between the refractory oxide and CO inside the particle.



The vapour R of the reduced species was transferred from the surfaces of the mineral inclusion to the surface of the char particle. This process determined the vaporisation rate. The reduced species, once oxidised to oxygen in the particle boundary layer, was reoxidised and condensed to form the submicron particles. The size distribution of the submicron particles was calculated from established theories on aerosol dynamics. In addition, as shown in Figure 31, the more volatile salts of the alkali metals and volatile trace metals vaporised. These would condense downstream of the combustion zone when the combustion products had cooled to their condensation temperatures. The ash vaporisation model was run as a post-processor to the gasifier model as the feedback from ash vaporisation to the local gas temperature, gas composition and velocity fields were minimal. The model calculations were

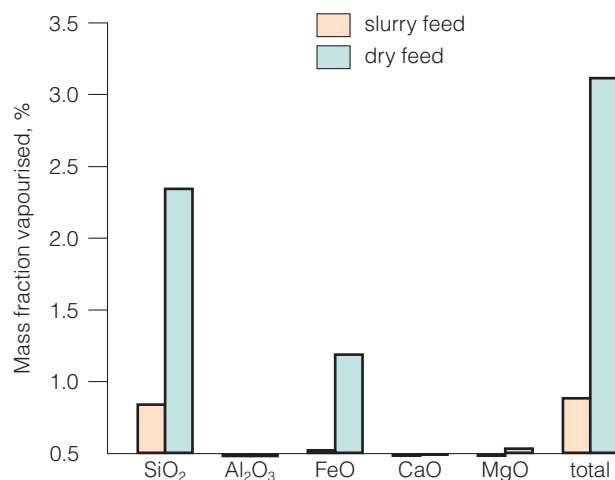


Figure 32 Component mass fractions of vaporised inlet ash (Bockelie and others, 2010)

performed along the trajectory for each cloud of particles contained in the model. Calculations that required local gas properties, for example, temperature and partial pressure, used values interpolated from the local flow field. This model could be used for evaluating the performance of one or two stage coal gasifier with either slurry or dry feed (Bockelie and others, 2008, 2010). Typical results for the proportion of ash vaporised is shown in Figure 32.

More recent modelling has addressed syngas cooler plugging and fouling. The syngas cooler is a fire tube heat exchanger located after the gasifier and before the turbine. Problems with the syngas cooler typically result in ash deposits developing on surfaces upstream of the syngas cooler, breaking loose,

then lodging in the syngas cooler causing plugging or increased erosion in the tube. It is also possible for deposits that form on the fireside surface of the syngas cooler tubes could lead to fouling of the cooler. The occurrence of either process can result in reduced system availability and increased maintenance costs. Methods to mitigate fouling include periodic tube cleaning and targeted soot blowing and the use of surface coatings that inhibit deposit buildup and provide for easier removal. The US DOE has joined with REI to explore ways to mitigate and manage syngas cooler plugging and fouling. The project involves laboratory-scale testing, model development and field testing of technologies developed under this project.

The CFD modelling part of the project used the existing REI Fouling and Deposit Growth model. Originally, generic syngas cooler models consisted of modelling the transition duct, tube sheet face and a tube bank with tubes 20 diameters long. Preliminary modelling results indicated that a smaller CFD model that modelled only a subsection of the syngas cooler could provide useful guidance on deposition with less computational time. Hence, a model for a 3 x 3 set of tubes was developed and used for most calculations. The model inputs such as syngas flow and composition were generated by the existing gasifier model. Two improvements to the basic fouling and deposit growth model were incorporated. Firstly, the particle cloud model used in the Eulerian-Lagrangian formulation for two phase flow was replaced with a stochastic particle tracking model to compute particle trajectories that include the effect of turbulent fluctuations in the syngas flow field on the trajectories of the fine particles. Secondly, the deposit build-up portion of the model now included a ‘pseudo steady state’ representation of the deposit surface geometry for regions in which the deposit thickness is large compared to the local syngas cooler design features. The CFD model employed an Eulerian-Lagrangian formulation in which a large number of gas-phase iterations were performed (Eulerian

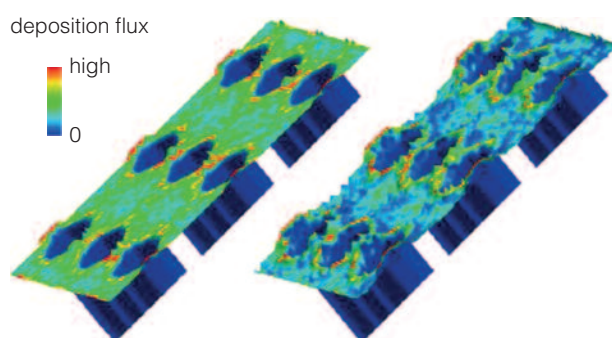


Figure 33 Ash deposition patterns (Bockelie and others, 2012)

calculation) followed by a Lagrangian particle phase calculation to compute particle trajectories, particle reactions, and deposition onto surfaces. This enabled the deposition patterns shown in Figure 33 to emerge. The model could assess the impact of ash properties (individual particle composition, particle size), presence of minerals (for example, Pyrite), local conditions (gas composition, temperature and heat flux) and deposit properties (composition, temperature, viscosity). The model could predict the properties of the particles exiting the gasifier, the deposition rate, properties of the deposits, the impact of the deposits in the gas phase

properties and the emissions of elements that could form a submicron fume. Model results indicated that most of the deposition occurs on uncooled surfaces upstream of the syngas cooler and on the tube sheet face of the cooler. There was little, if any, deposition on the tubes after the tube entrance region. This type of behaviour is reported by plant operators (Bockelie and others, 2010, 2012; NETL, 2013).

Silaen and Wang (2005) have developed models for entrained-flow gasifiers in order to help industry resolve problems and improve gasifier operation. They were particularly interested to investigate the effects of (i) slurry versus dry coal feed, (ii) oxygen versus air-blown, (iii) different arrangements for coal feeding and (iv) effects of wall cooling. They conducted numerical simulations of the coal gasification process in a generic two-stage entrained flow gasifier using the commercial CFD code FLUENT. The study focused on a two-stage entrained flow gasifier. The geometry of the gasifier and the operating conditions were based on the information contained in Bockelie and others (2002) and Chen and others (2000a). The gasifier was divided into two regions: a combustion region (combustor) in the first or lower stage and a reduction region (reductor) in the second or upper stage. It had three levels of injectors that were positioned symmetrically with two in the first stage and the other in the second stage. The oxidant and a proportion of the coal-slurry mixture were injected through the lower

injectors and the remaining mixture was injected through the upper injectors. The physical characteristics of the system were: the flow was three-dimensional, buoyancy force was considered, varying fluid properties were calculated and the walls were impermeable. It was assumed that the flow was steady, no-slip conditions applied on wall surfaces and chemical reactions were faster than the timescale of turbulent eddies. The equations for the conservation of mass, momentum and energy were applied. The standard k - ϵ turbulence model was used as it was robust, economic for computation and accurate for a wide range of turbulent flows. The chemical reaction model contained the following species: C, O₂, N₂, CO, CO₂, H₂O and H₂. All the chemical species were assumed to mix at the molecular level. The chemical reactions inside the gasifier were modelled by calculating the transport and mixing of the chemical species. This involved conservation equations which described convection, diffusion and the reaction of each component species. The 3-D Navier-Stokes equations and the seven species transport equations were solved by adopting the eddy-dissipation approach. This approach assumed that the chemical reactions were faster than the timescale of the turbulent eddies. The reaction rate was determined by the mixing of the species with the reactions assuming to occur instantaneously when the reactants met. The CFD solver used was the commercial FLUENT code. This is a finite-volume-based CFD solver which has the ability to solve systems involving fluid flow, heat transfer and chemical reactions in complex geometries. The segregated solution method was used. This approach solves the governing equations of continuity, momentum, energy and species transport sequentially. The non-linear governing equations were linearised implicitly with respect to dependent variables. The second order discretisation scheme was applied for momentum, turbulent kinetic energy, turbulent kinetic dissipation, the energy and all chemical species. A grid sensitivity study was conducted using three different grids: a coarse grid (35,168 grids), medium grid (95,182 grids) and a fine grid (160,170 grids). The difference in results between the medium and fine grids was only a few per cent hence the medium grid was used for the study as it gave acceptably good results with reasonable computational time.

The objective of the study was to investigate the effects of different parameters on the performance of a two-stage entrained-flow gasifier. The parameters of most interest were:

- (i) Coal mixture – coal slurry or coal powder;
- (ii) oxidant – oxygen or air;
- (iii) first and second stage mass flow rates – 75/25%, 50/50% and 100/0%;
- (iv) wall cooling (adiabatic, 1800K/1600K).

The base case was oxygen-blown, slurry-fed with a 75/25% coal distribution between the first and second stages. For this case the model predicted a carbon efficiency (ratio of carbon converted to CO) of 86% and fuel efficiency (ratio total mass of syngas to initial mass of carbon, water and oxygen injected) of 79% with a heating value of 12.5 MJ/kg. The model results when varying the parameters indicated that slurry-fed was preferred to powder-fed to produce hydrogen. However, powder-fed was preferable to produce CO. Air-blown operation yielded poor fuel conversion efficiency and lower syngas heating values. The effect of wall cooling was found to be insignificant on exit gas composition and heating value. The fuel conversion efficiency was better with a coal distribution of 75% (first stage) / 25% (second stage) than with 50/50 coal distribution. The results showed that the two-stage design had an advantage of flexibility to adjust parameters to optimise performance (Silaen and Wang, 2005). Further studies were undertaken to investigate the effects of fuel injection angles on the performance of the gasifier. The gasifier had three levels of injectors which were positioned axisymmetrically with two levels in the first stage and the other in the second stage. To create swirling inside the gasifier, lower injectors were placed tangentially. The upper injectors were aimed directly at the centre of the gasifier. All the oxidant and a fraction of the coal slurry were injected through the lower injectors, the remaining coal slurry was injected through the upper ones. In the base case all the injectors were placed horizontally. As a strong swirl motion was produced by the low level injectors, it was postulated that the fuel injector angles affected the fuel residence time and hence the performance of the gasifier. Model simulations were conducted to investigate the effects of coal slurry injection angles on performance. Operating the lower injectors pointing 30° downwards yielded a carbon fuel conversion 17% lower than with horizontal injectors but more hydrogen. Raising the injectors upward

improved performance but still lower than the base case. Altering the upper (second stage) injector directions or eliminating half the first stage injectors appeared to have an insignificant effect on gasifier performance. Overall, the results indicated that fuel conversion efficiency could be considerably affected by the flow pattern and gasifier injection angle (Silaen and Wang, 2006).

Silaen and Wang undertook additional investigations on the effects of different assumptions and parameters on predicted gasification performance including turbulence models, devolatilisation models, finite reaction rates and solid coal sizes. In the previous studies described above, the instantaneous gasification model of solid coal particles was used, which would result in the solid-gas reaction faster than the actual process. In this study, the particle combustion model using a finite rate was incorporated as the char particle surface reaction was involved. The transport of CO and heat from the surface layer to the surrounding gases would depend on the thermal-flow behaviour. Therefore, turbulence modelling and stochastic tracking of fluctuating particles would affect simulated results. In addition, the variation of coal particle sizes would affect coal surface/volume ratio and result in changes in gasification performance. To assess the implications of these considerations, this study investigated the effects of turbulence models, devolatilisation models, coal particle diameters, reaction heat and stochastic tracking time constant on the simulation results. The investigation showed that the choice of turbulence models significantly affected the simulated results. The five turbulence models tested were the standard $k-\epsilon$, the RNG (Re-Normalised Group) $k-\epsilon$, standard $k-\omega$ model, the SST (Shear Stress Transport) $k-\omega$ model and the RSM (Reynolds Stress Model). The standard $k-\epsilon$ and the RSM model gave the most consistent results. The various turbulence models were based on time-averaged equations. Using this flow velocity to trace the droplet results in an average trajectory. In reality, the instantaneous velocity fluctuations make the droplet oscillate around the average track. A way of simulating the effects of turbulence was to use stochastic tracking. This calculated droplet trajectories using instantaneous velocity rather than average velocity. The modelling showed that the timescale adopted for stochastic time tracking of particles affected model results. In the study, a time constant value of 0.015 and 0.00015 s produced consistent results. The four devolatilisation models assessed were the Kobayashi model, the single rate model, the constant rate model and the Chemical Percolation Devolatilisation (CPD) model. Of these, the Kobayashi model produced slower devolatilisation than the others. The constant rate model produced the fastest devolatilisation rate. The single rate and the chemical percolation models produced moderate and consistent devolatilisation rates. Slower devolatilisation produces lower CO, but higher exit gas temperature, H₂ and CO₂ and hence both the heating value and gasification efficiency are lower. Though smaller particles, having a higher surface-to-volume ratio, normally react faster than larger ones, the gasifier modelling suggested than in this case the larger ones react faster. The explanation was that larger particles possessed higher inertia after injection. Higher inertia produced higher slip velocities which increased higher convective transport and hence higher reaction rates. Higher inertia could also propel particles across the gas streamlines and increase particle-gas mixing which resulted in enhanced reaction rates. Such particles could impinge on the opposing jet and change the thermal-flow field (Silaen and Wang, 2008).

Silaen and Wang conducted further investigations comparing three different gasification reaction models: instantaneous gasification, global equilibrium and finite-rate models. The main purpose was to determine if the simplified instantaneous gasification model could be used to rapidly produce acceptable approximations of gasifier performance that could be used as a preliminary screening tool for new design ideas to improve gasifier performance. The models used were the same as those used by Silaen and Wang (2008). The time-averaged steady state Navier-Stokes equations as well as mass and energy conservation equations were solved. Species transport equations were solved for all gas phase species. The standard $k-\epsilon$ turbulence model was used. In the finite-rate model, the fluid flow was solved in Eulerian form while the particles were solved in Lagrangian form as a discrete phase. A stochastic model was utilised to model the effects of turbulence on the particles. The continuous phase and the discrete phases were connected through drag forces, lift forces, heat transfer, mass transfer, and species transfer. The finite-rate combustion model was used for the heterogeneous reactions but both the finite-rate and eddy dissipation models were used for the homogeneous reactions. The finite-

rate model calculated the reaction rates based on kinetics, while the eddy-dissipation model calculated based on the turbulent mixing rate of the flow. For solid particles, the rate of depletion due to surface reaction was expressed as a function of kinetic rate, solid species mass fraction on the surface and the particle surface area. For the chemical reaction rates, the finite rate used in the study implicitly applied a local equilibrium. The reaction rate of the water-shift reaction ($\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$) was adjusted to match the syngas composition with what is normally measured in commercial entrained-flow gasifiers.

In the Instantaneous Gasification Model, the exchange of mass, momentum and energy were assumed to be infinitely fast. The carbon particles were made to gasify instantaneously, so that the solid-gas reaction process could be modelled as homogeneous combustion reactions. This approach effectively modelled the overall combustion process and produced results without considering the complications of heterogeneous particle surface reactions, heat transfer, species transport and particle tracking in turbulent reacting flow. The eddy-dissipation model, which assumed that chemical reactions were faster than turbulence eddy transport, was used. Thus the reaction rate was controlled by flow characteristics. Regarding the water-shift reaction, two rates were used, the faster one with a catalyst and a slower one without. This approach could significantly reduce computational time but could only provide qualitative trends of the gasification process. Although the approach was very approximate, it captured the effect of the thermal-fluid field on chemical reactions, which was readily available from the equilibrium method. In the Global Chemical Equilibrium Model, four homogeneous and four heterogeneous chemical processes were considered. A CFD scheme was not utilised. The C-H₂O gasification reaction was assumed to consume steam first before the water-shift took place to use up the remaining steam.

The models were used to investigate a one-stage entrained flow coal gasifier. Initially, a simplified 2-D geometry was adopted to perform a parametric study of the effect of coal particle sizes on gasification performance. Using the 2-D results, a fixed coal particle size and one coal slurry model were selected to conduct 3-D simulations. The geometry of the gasifier was adopted from Bockelie and others (2002). The results showed that reactions using the instantaneous gasification model occurred fast and finished quickly whereas the reaction in the finite-rate model, which includes gas-solid reactions, occurred slowly. Varying the coal particle size in the finite-rate model showed that the syngas heating value of the smaller particle size was closer to the instantaneous gasification model results. The water shift reaction played an important role in predicting the syngas composition. The syngas composition using a fast water shift rate was close to that calculated from the global equilibrium method. The overall result showed that the instantaneous gasification approach could provide an overall evaluation of relative changes of gasifier performance in terms of temperature, heating value and gasification efficiency corresponding to parametric variations but did not predict gasification processes adequately at the local level in most parts of the gasifier as predicted by the finite rate model (Silaen and Wang, 2009).

Silanen and Wang (2010) undertook further modelling investigations in which the 3-D Navier-Stokes equations and eight species transport equations were solved with three heterogeneous global reactions, three homogeneous reactions and a two-step thermal cracking equation for volatile production. The CPD model was used for devolatilisation. Finite rates were used for heterogeneous solid-to-gas reactions. Both the finite rate and eddy-break-up combustion models were calculated for each homogeneous gas-to-gas reaction, and the smaller of the two was used. The water-shift reaction rate was adjusted to match the available syngas composition from existing operational data. This model was used to investigate the effects of different operational parameters such as coal mixture (dry or slurry), oxidant (oxygen or air) and different coal distributions in a two-stage gasifier on the gasification process. In the base case the coal was fed as slurry and the fuel distribution was 75–25% between the first and second stages. The second case investigated was dry coal input, oxygen-blown and 75–25% distribution in the two stages. The third was oxygen-blown, coal slurry, 50–50% coal distribution in the two stages. The fourth was oxygen-blown, coal slurry and 100% coal in the first stage. The fifth was air-blown, coal slurry, 75–25% coal distribution in the two stages. The five cases

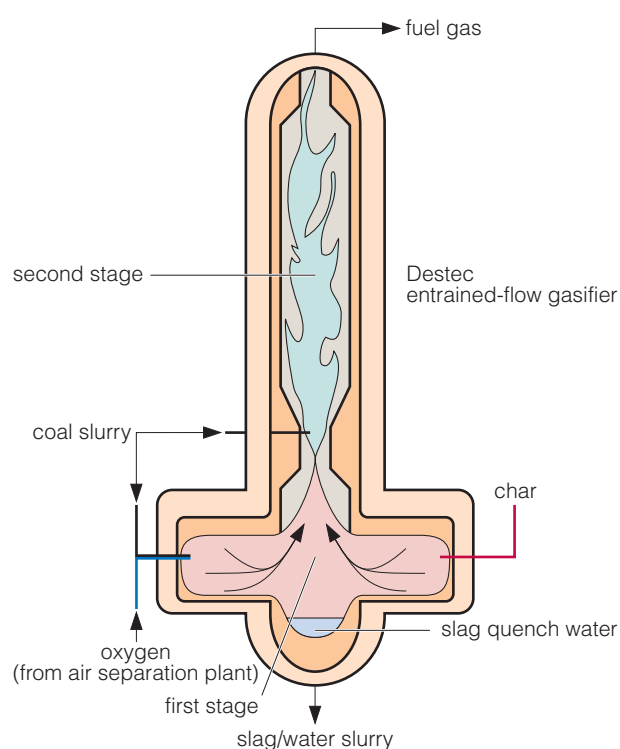
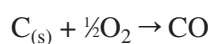


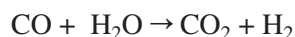
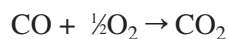
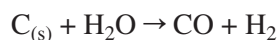
Figure 34 E-gas gasifier (Chyou and others, 2012)

distribution between the two stages showed that reducing the fuel feed in the first stage resulted in higher gas temperatures in the first stage due to less water being present to absorb the heat. One-stage operation yielded higher combined H_2 , CO and CH_4 than in two-stage operation but with lower syngas heating value. The 50–50% coal distribution case yielded the highest syngas HHV (higher heating value) but lowest syngas exit temperature among the cases studied. The syngas produced by single-stage operation contained the most unreacted char, highest exit temperature and lowest heating value. When comparing the effect of the oxidant, the gas temperature inside the gasifier for the air-blown case was lower than for the oxygen-blown gasifier due to the abundant presence of N_2 . The carbon conversion efficiency of the air-blown case also was lower (77.3%) than for the oxygen-blown case (99.4%). The lower carbon conversion was due to a lower gas temperature in the gasifier which resulted in less energy being available to drive the endothermic gasification reactions. The syngas heating value for the air-blown case was 4.40 MJ/kg which was about half that for the oxygen-blown case (8.24 MJ/kg). It was lower even when allowing for the presence of N_2 . This was the result of the lower carbon conversion efficiency (Silaen and Wang, 2010).

Chyou and others (2010, 2011) have adapted the instantaneous gasification model approach developed by Silaen and Wang to simulate the oxygen-blown coal gasification process within a cross-type, two-stage (E-Gas) gasifier with the commercial CFD solver ANSYS FLUENT. The gasifier consisted of two stages, a slagging first stage and an entrained-flow, non-slugging second stage. The exact dimensions of the E-gas gasifier were not known. The geometry of the gasifier was based on Figure 34 and information published in the open literature. The chemical reaction times were assumed to be faster than the timescale of turbulent eddies. All the species were assumed to mix at the intermolecular level. The 3-D Navier-Stokes equations for conservation of mass, momentum and energy and species transport equations with the eddy-breakup reaction model were incorporated. The standard $k-\epsilon$ turbulence model was applied. The chemical reactions included were:



were simulated with the model. The results showed that the temperature in the first stage for the dry-fed case was 400°C higher than the slurry-fed case. This occurred as in the dry-fed case, unlike in the slurry-fed case, it did not have substantial quantities of water to absorb the heat released by char combustion. Nor did much steam react with char through the $char-H_2O$ gasification. This higher gas temperature resulted in the fuel injectors and refractory walls in the first stage experiencing higher thermal loading than in coal slurry operation. The heating value syngas in the dry case (9.45 MJ/kg) was higher than with a slurry (8.24 MJ/kg). The higher syngas temperature in the dry case would result in lower IGCC plant thermal efficiency because the syngas needed to be cooled before it passed through the gas clean-up system downstream of a gasifier. Hence a significant quantity of energy would be downgraded through the waste heat exchanger though part of this energy could be recovered to produce superheated steam to generate electricity through the steam turbine. The comparison of changing the fuel



The instantaneous model assumed that the coal vaporised very fast into the gas phase without passing through the heterogeneous finite-rate reaction process. The equilibrium constants for the chemical reactions were incorporated into the CFD simulation. The interphase exchange rates of mass, momentum and energy were assumed to be infinitely fast. Carbon particles instantly gasified hence the solid-gas reaction could be modelled as a homogeneous combustion reaction. The eddy dissipation model was used to model the chemical reactions. This assumed that the chemical reactions were faster than turbulence eddy transport so that the reaction rates were controlled by the flow motions. The instantaneous gasification model could effectively model the overall combustion process without involving the complexities of heterogeneous particle surface reactions, heat transfer, species transport and particle tracking in turbulent reacting flow. The CFD solver used in the study was the commercial code FLUENT V.12.

The results showed that when the slurry concentration (carbon to water ratio) increased, the temperature of the exit syngas was higher. Reducing the slurry concentration increased the concentrations of H_2 and CO_2 and reduced CO . Under conditions of maximum gasification, low slurry concentration was preferred if more H_2 and lower syngas temperature was required whereas higher slurry concentration was preferable for producing more CO and higher syngas temperature and less CO_2 . The flow behaviour in the gasifier, especially the single stage design in the second stage was investigated. This design induced large recirculation regions which resulted in inefficiencies and reduced syngas production by trapping part of the flow and thereby decreasing the residence time of the main flow. The authors concluded that the simplified instantaneous gasification model could be used as a tool for preliminary examination of the overall effect of thermal-flow and turbulence in a cross-type, two-stage gasifier (Chyou and others, 2010).

Chyou and others have developed their model to replace the instantaneous gasification model with the more realistic heterogeneous finite-rate reactions using the discrete phase model (DPM) to track each coal particle. They also wanted to examine and improve the understanding of the gasifier thermal-flow behaviour and gasification process in an E-gas gasifier. In this version, the 3-D, steady state, Navier-Stokes equations were solved in an Eulerian-Lagrangian frame of reference. The coal particles were treated as a discrete secondary phase dispersed in the continuous phase by the DPM with stochastic tracking to consider the turbulent dispersion effect. The P1 radiation model was used and the gravitational force was considered. The standard $k-\epsilon$ model was used to simulate turbulence. The species transport equations were solved using the Finite-Rate-Eddy-Dissipation model. In this both the finite rate and the eddy-dissipation rates were calculated and compared and the slower rate was selected to compute the continuous phase reactions. The dimensions of the E-Gas gasifier were taken from an earlier NETL modelling study described by Zitney and Guenther (2005). Another chemical reaction was included: $\text{CH}_4 + 1.5\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2\text{O}$. The results of the base case showed good agreement with NETL's modelling results. A series of parametric studies was conducted. Increasing the O_2/coal ratio led to higher exit gas temperature and CO_2 concentration but lower CO levels. The syngas HHV and cold gas efficiency both also decreased. Higher oxygen levels resulted in more combustion to produce heat but poorer gasification performance to produce fuels. The model also showed that as the amount of coal in the coal slurry increased, the amount of H_2 , CO_2 and H_2O decreased but the CO level increased. The results were very sensitive to the water gas reaction rate. When the proportion of coal slurry mass flow in the first stage was increased, the exit temperature and

the concentrations of H₂ and CO₂ increased while that of CO decreased. However, as the space inside the E-Gas gasifier was sufficiently large enough to allow reactions to go to completion, changing the fuel distribution did not significantly influence gasification performance (Chyou and others, 2011). Further modelling was undertaken to investigate the suitability of a cold flow study, injection design in the second stage and the use of lignite. Cold flow studies have often been performed either experimentally or computationally as a rapid, first step to study the flow patterns in a gasifier. The modelling showed that the cold flow has a similar overall pattern to the hot flow field but the flow speed of the cold flow is much slower than that of the hot flow. This difference was caused by the change of fluid volume. Overall, the cold flow pattern provided a coarse view of the scaled-down hot flow field by catching the flow impingement in the first-stage of the horizontal cylinder and the large circulation zone but with significantly reduced flow velocity. In the original single, lateral injection design, an undesirable, large, recirculation design formed above the second stage injector. Modelling was undertaken to consider two dual-jet arrangements either opposing-jet or tangential-jet. The modelling showed that the recirculation region was significantly reduced in the case of the opposing jets and almost completely eliminated with the tangential jets. This would improve gasifier performance. Furthermore, as the tangential injection design made the average temperature reach equilibrium more rapidly, the height of the E-Gas could be shortened. The model was also used to compare the gasification of North Dakota lignite with Illinois No 6 bituminous coal. Lignites contain a lower heating value hence gasifying with the same feedstock mass flow rate as coal generated a syngas with a lower heating value (7.56 MJ/kg cf 10.54 MJ/kg for bituminous coal). Increasing the lignite flow rate such that the input heat content was the same as coal only increases syngas heating value slightly. However, when the lower cost of the lignite was considered, the feedstock price per unit syngas HHV for lignite was about 1.19 \$/GJ compared with 2.66 \$/GJ for coal (Chyou and others, 2012).

Lee and others (2010) have assessed how well commercial codes developed for simulating overall IGCC systems modelled processes occurring in the gasifier. Aspen Plus is a widely used chemical process simulator, which is used to predict plant performance, based on mass and heat balance, phase and chemical equilibrium at steady state. The Aspen model consisted of flow sheets of the important sections of the IGCC system. Each flowsheet consisted of unit operation blocks and the gasifier model is included in one of them. Gasification was simulated by two reactor blocks, RYield and RGibbs. RYield specified the yield distribution based on the ultimate analysis of the coal. RGibbs calculated the gas composition at equilibrium between reactants and products of the chemical reactions. In real gasifiers, coal gasification takes place simultaneously whereas commercial codes treat it as a sequence of blocks. In a real gasifier a number of sub-processes occur such as feedstock mixing, pyrolysis, combustion, gasification, heat transfer, coal swelling, diffusion, chemical reactions and slagging. In the commercial simulation codes, gasification processes are represented by simplified, lumped parameters. Considering the chemical reactions, the chemical equilibrium approach should be regarded as a one-step approach to determine gas composition and properties at the gasifier exit. This approach also does not incorporate the reactivity or kinetics of the coal reaction. The reactivity of an individual coal should be considered as should the kinetics, diffusion rates and local concentrations of individual reactants. Although the equilibrium model gives useful information, the interaction between chemical processes is not considered. In the case of entrained-flow reactors, as the residence time is 3–4 s, there may not be sufficient time for the reactants to attain chemical equilibrium due to slow char burn-out and incomplete gaseous mixing.

The authors concluded that though coal gasification models in commercial process analysis simulators were useful for interpreting the whole plant cycle, they could be improved. The conventional equilibrium model allowed a better understanding of the underlying thermodynamic principles governing coal gasification, but it was not sufficiently detailed to embody the actual phenomena. Devolatilisation should not be modelled simply as decomposition as in commercial codes because it influenced the following gasification steps such as homogeneous and heterogeneous reactions. They suggested incorporating a two-stage equilibrium model which did not solve all solid-gas and gas-gas reactions simultaneously. In the two-stage model, the solid-gas reactions were considered as the first

stage and gas-gas reactions as the second stage. Carbon conversion should be calculated at the first stage and the final gas composition calculated in the second stage with the products of the first stage. This should result in a more accurate prediction of carbon conversion and gasification performance (Lee and others, 2010).

One goal of modelling is to develop an integrated suite of software tools to enable engineers to simulate and visualise advanced plant design concepts. This requires integrating predictive tools for plant level cycle analysis with component models used for simulating individual items of equipment in the cycle. The Advanced Process Engineering CoSimulator (APECS) sponsored by the US Departments of Energy's NETL sought to bridge the gap by integrating plant modelling and equipment modelling software, for example those based on CFD. Process simulation and CFD are highly complementary technologies and combining these affords the opportunity to analyse overall system performance with respect to fluid flow, mass and heat transfer, chemical reactions and related phenomena. In APECS, the widely used, steady state process simulator Aspen Plus has been run with various equipment models including CFD models based on FLUENT. In one case, the entrained-flow

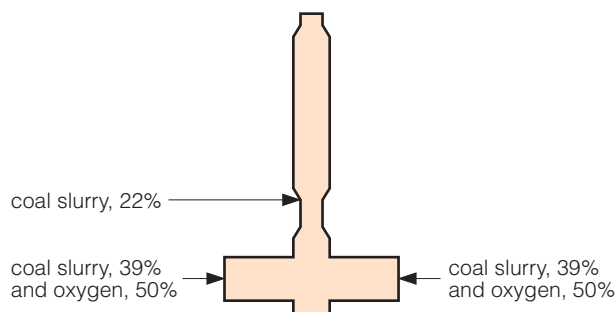


Figure 35 Gasifier feed streams (Zitney and Guenther, 2005)

gasifier CFD model was coupled into an Aspen Plus steady state process simulation of a potential, coal-fired, IGCC and hydrogen production plant for the US DOE's FutureGen project. The entrained-flow, coal-slurry gasifier considered was a two-stage, up-flow gasifier consisting of a horizontal first stage and a vertical second stage as shown in Figure 35. The oxidant and 78% of the coal slurry were introduced in the first stage which was mainly a coal combustor and provided hot gases to the second stage in which the remaining 22% of the slurry was injected. Most of the gasification occurred in the second stage. This was a prototype design which was

not meant to represent any existing design.

The entrained-flow gasifier was modelled using the steady state, 3-D CFD model described by Shi and others (2004). The continuous gas phase conservation equations included the continuity equation, momentum equations, energy equation, turbulence equations and radiation transfer equation. The gas phase reactions were modelled using the eddy dissipation model and the Arrhenius rate law. The discrete phase model (DPM) was used to simulate the coal slurry flow as two separate particle types, water droplets and coal particles. The assumption of two particle types was justified given that the water evaporated quickly on entering the gasifier. The particle trajectories, and the transfer of mass and energy to and from the particles were computed with a Lagrangian formulation. The physical and chemical processing of the coal slurry was undertaken by using user-defined functions for moisture release, vaporisation, devolatilisation, char oxidation and gasification. The coupling between the continuous gas phase and the distinct particle phase was solved by tracking the exchange of mass, momentum and energy. The gasifier CFD simulation with over 12,000 hexahedral computational cells was converged using approximately 50,000 gas phase iterations in FLUENT. The overall plant was modelled by the steady state process simulator, Aspen Plus which was based on several NETL reference case IGCC systems with CO₂ capture. This highly integrated flowsheet contains over 250 unit operation models comprised all the major plant sections including gasification, air separation unit, cold gas cleanup, gas turbine and steam cycle. The model results relating to temperature contours for the gasifier are shown in Figure 36. The hot gas generated from the combustion in the first stage provided the energy for gasification in the second stage. The char conversion was 100% in the first and 86% in the second stage. The mole fractions of some of the major chemical species are contained in the figure. Dark red represents the highest concentration and dark blue the lowest concentration of the product. The result suggested that practically all the oxygen is depleted in the first stage and the

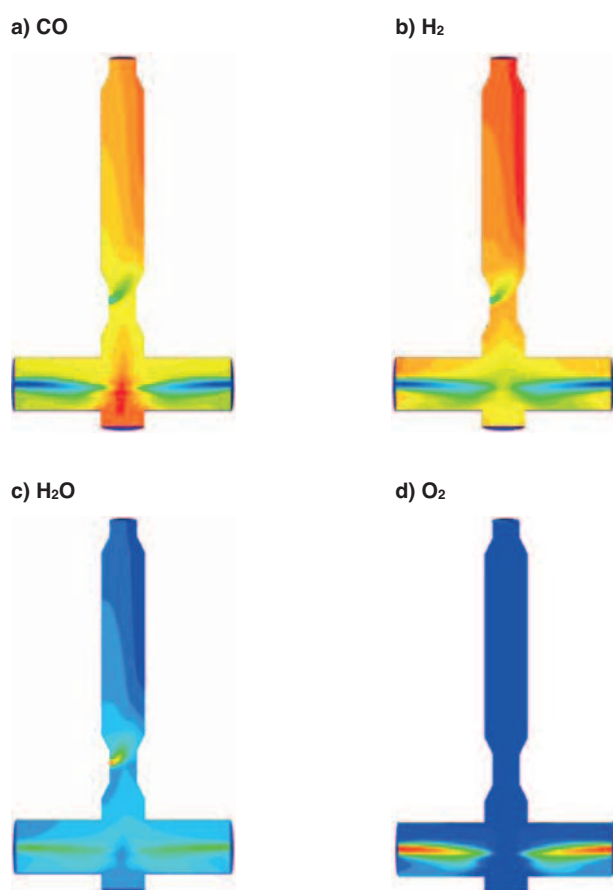


Figure 36 Species mole fraction contours
(Zitney and Guenther, 2005)

hydrogen is formed mainly in the second. The authors concluded that APECS technology could help engineers better understand and optimise gasifier fluid dynamics and related phenomena that affect overall plant performance (Zitney and Guenther, 2005).

Due to the complexity of physical and chemical processes involved in gasification, it is very challenging to simulate all of them accurately in a comprehensive CFD model. Ma and Zitney (2012a,b) have considered the existing Lagrangian discrete phase based CFD models and improved the accuracy of sub-models. They firstly focused on the coal moisture release model. Moisture release is the first process a coal particle experiences when it is injected into a gasifier. Even though the process is relatively straightforward, inaccurate formulation could result in incorrect prediction of gas temperatures near a fuel injector. Conventionally, moisture release is modelled by an Arrhenius expression. This approach was improved by considering convective outward flow (Stefan flow), high mass transfer corrections at high vaporisation rates and, if the particle temperature is very close to the boiling point, the limitation of vaporisation rate due to heat transfer rate. The treatment of devolatilisation has also been

improved. The volatile yield is conventionally measured by a drop-tube experiment and for a high volatile coal could be as high as 60%. The volatile yield in an entrained-flow gasifier could be higher because of the higher heating rate. Hence, without knowing the particle heating rate, the volatile yield is difficult to determine a priori. Moreover, the composition of volatiles is also dependent on the heating rate. In conventional models the reaction is stopped when a specified volatile yield is reached. The modelling of devolatilisation has been made more realistic by using simple devolatilisation models with two parallel reactions as proposed by Kobayashi. The two reactions have different kinetic parameters. The first reaction had a lower activation energy and a lower pre-exponential than the second. Hence when the heating rate was high, the second reaction started and more volatiles were released. As a result, the predicted volatile yield was higher. This approach did not predefine volatile yield but rather predicted it based on the two reaction models with particle temperature or heating rate calculated along the particle trajectory by the revised DPM model. In the revised model, the mass of unreacted coal was tracked and the devolatilisation reaction stopped when all the coal was reacted and converted to volatiles and char. The volatile composition included major combustion and gasification species as well as minor species such as H_2S , COS and HCl . The volatile composition was calculated within the devolatilisation sub-model and varied with the location coal, particle injection.

The chemical species that are needed to be included in the model have been reconsidered. The earlier models nine species were considered as the constituents of the coal volatiles. These were: O_2 , H_2 , N_2 , CO , CO_2 , H_2O , CH_4 , H_2S and HCl . However, syngas invariably contains a certain amount of COS either released as coal volatiles or formed by gas-phase reactions. Hence COS was also included. Furthermore, if CH_4 was the only hydrocarbon modelled, there would be some carbon remaining which could be combined with any other elements and unreacted carbon had to be assigned to char and the volatile yield had to be limited. For typical high volatile bituminous coals, there was always

Table 14 Predicted and measured syngas compositions (Ma and Zitney, 2012b)		
	CFD prediction, mol%, dry	Plant data, mol%, dry
A Single-stage gasifier		
CO	46.6	44.1
CO ₂	13.1	14.7
H ₂	37.6	37.9
CH ₄	0.05	0.05
B Two-stage gasifier		
CO	43.4	42.2–46.7
CO ₂	15.5	14.9–17.1
H ₂	36.1	32.3–34.4
CH ₄	2.06	1.04–2.29

not enough H to combine with remaining C to form CH₄. However, by including an aromatic hydrocarbon such as C₆H₆ any remaining C and H could form hydrocarbon species. The benzene represented a high molecular weight tar within the coal volatiles. The heterogeneous reactions between the char and the gas-phase species were modelled along the particle trajectories. Char reactions started only after devolatilisation was complete and all the coal had been converted to coal and volatiles. In reality, char combustion and gasification could start at a later stage of devolatilisation when the particle temperature was high enough and convective outflow of volatiles no longer prevented the gaseous reactants from entering the particle surface through film diffusion. The gas-phase turbulence was modelled by the standard k-ε model with standard wall functions. The mass fractions of the major gas-phase species were solved through species continuity equations. Minor species such as radicals were not modelled. The nine gas-phase reactions in the model included the oxidation of CH₄, CO and H₂, water-gas shift reaction, methane-steam reforming reactions and two reactions related to benzene. Reasonable boundary conditions were used to allow for the small heat loss from the gasifier. This approach ensured the tight convergence of the energy conservation and mass conservation of individual elements inside the CFD model. The predicted syngas compositions and exit gas temperatures were reasonable and comparable to reported data from commercial-scale gasifiers. The comparison for syngas composition is shown in Table 14. The detailed predictions related to velocity, temperature and mole fractions of individual species inside the gasifier also showed reasonable trends and provided insight into the physical and chemical processes involved. The predicted syngas compositions at the exits were not in equilibrium, indicating that the kinetics of both heterogeneous and homogeneous gas-phase reactions were important (Ma and Zitney, 2012a,b).

More modelling studies have been undertaken for entrained-flow gasifiers than for moving bed or fluidised bed gasifiers. Both 1-D and 3-D models have been developed but the majority are 3-D. These are frequently based on CFD using the commercial software FLUENT. In most cases the results of the modelling studies have given insight into the fundamental processes occurring in the gasifier. This has helped to improve gasifier designs. In some cases, the results have been compared with plant data and it has been possible to choose model inputs to give reasonable fit with the measured data. In a few cases modelling has been able to solve operational problems.

6 Conclusions

Power generators, oil refinery operators and producers of chemicals such as methanol and ammonia have turned in recent years to gasification to unlock the power of coal and other carbon-based fuels. Gasification involves reacting carbonaceous fuels with a combination of air, oxygen and steam to produce gaseous products which can be used as an energy source or as a feedstock for the synthesis of chemicals or other fuels. The fuel is combusted with insufficient oxygen to produce carbon dioxide and steam as in complete combustion but to produce a mixture such as carbon monoxide, hydrogen and light hydrocarbons. There are three main types of coal gasifiers namely moving (or fixed) bed, fluidised bed and entrained-flow. Gasifiers in commercial operation, especially for power generation, have incurred operational issues. A thorough understanding of their operation is essential for addressing existing challenges and improving future designs. Many complex processes take place in a coal gasifier and the development of computational models is an essential component for gaining this understanding.

Any coal gasification model must be capable of modelling the fundamental processes occurring in the gasifier. Firstly, volatile components in the coal such as light gases and tar are released by pyrolysis which is also known as devolatilisation. There are several approaches to modelling devolatilisation. A commonly used model is a single first-order reaction. A more realistic model incorporates a series of parallel independent reactions. A further refinement is utilising the FLASHCHAIN programme which predicts the complete product distribution and char characteristics given the proximate and ultimate analysis of the coal and the process operation conditions. The volatile components released undergo homogeneous reactions. These are more commonly modelled as global reactions rather than detailed reactions involving radicals. Following devolatilisation the char residue gasifies. This is commonly taken to occur by the following processes: gasification with oxygen, combustion with oxygen, gasification with carbon dioxide, gasification with steam and gasification with hydrogen. Two other reactions that are important are the water-gas shift reaction and the methanation reaction. The reactivity of the coal char is affected by several factors including particle temperature and pressure. At relatively low temperatures, the surface reaction is the slowest step but at higher temperatures, diffusion becomes rate-limiting. The processes taking place in the pores are commonly modelled by the random pore model or the shrinking core model.

Having considered the fundamental processes, the overall approach to modelling can incorporate different levels of complexity. First is the number of space dimensions; three levels are possible. Secondly, whether time is included. If it is, the model is dynamic. If not, the model is steady state. In zero-dimensional models, the output variables are evaluated in relation to the input variables without considering the details of processes occurring inside the control volume and these are not suitable for modelling gasifiers. One-dimensional models assume that all variables inside the equipment vary along one-space coordinate and these allow profiles of variables to be evaluated throughout the system. These have been successfully used to model all types of gasifiers. Two-dimensional models allow for changes in properties in the axial and radial directions. These may be adequate if the model has cylindrical symmetry. Three-dimensional modelling entails considerable mathematical and computational complexity but in many situations this is necessary for a realistic representation particularly of asymmetric geometries.

CFD models are a powerful tool for investigating many types of plant and in the last few decades such modelling has played an important role in improving the performance of pf plant. Using CFD models to describe coal gasification requires additional layers of complexity. Multiple phases are present as the gasifier contains solids and possibly liquids in addition to the gas phase. The phases in the reactor are complex and contain changing chemical mixtures. Both homogeneous and heterogeneous reactions must be considered. In addition to the continuity equation and the equation of motion, the energy equation and mass transfer equations must be solved as coupled equations. The existing CFD

models for gasifiers include MFIX, ANSYS-FLUENT, and BARRACUDA. For the future, gasifiers will require greater fuel flexibility, reliability, availability, maintainability and higher throughput and conversion. To achieve these aims, one requirement is better mathematical models for gasifiers. NETL have developed C3M to facilitate the use of multiphase CFD models by providing a tool that directly imports kinetic information into CFD models and providing a platform to perform virtual kinetic runs that elucidate the effect of operating conditions.

In a moving bed gasifier, the solid fuel is fed at the top of the reactor and slowly flows to the base where the residual solid is removed. Many processes take place such as drying, devolatilisation, gasification and combustion. Several models have been developed which are able to reproduce the processes taking place and make predictions under industrial-scale operating conditions. Many such models have been based on one-dimensional representations. The solid phase flow can be assumed to be plug-flow and the system can be assumed to be at steady state. This level of sophistication has been found to be adequate in many cases. Unlike entrained-flow and fluidised bed gasifiers, relatively few modelling studies have been performed on moving bed coal gasifiers. Recent work has tended to focus on biomass gasifiers. A recent simplified model of a fixed-bed countercurrent gasifier has been developed by Brundu and others. In this model, the four steps making up the gasification process, namely drying, pyrolysis, gasification and combustion are considered separately. The whole process has been modelled as six steps evolving one after another. The model adequately simulated the broad features of the variation of syngas components in a coal gasifier but the results were not compared with actual plant or rig data. The model has been extended to simulate transient behaviour. Grana and others have developed a general mathematical model of a fixed bed gasifier in which both transport phenomena and chemical kinetics were considered. The mathematical description included solid devolatilisation, gas phase reactions and gas-solid interactions. The model consisted of two models: one on the particle scale and the other on the reactor scale. The authors reported that the models required several hours of CPU time, due both to the stiff nature of the gas-phase kinetics and to the dynamic approach to the steady state solution. Kulkarni and Ganguli have developed a process simulation of a moving bed gasifier using Alaskan coal. All the processes occurring in a moving bed gasifier such as drying, devolatilisation, gasification and combustion were included. The system was assumed to be in steady state and plug flow was assumed. The model predictions were compared with available experimental results from the Lurgi gasification plant in Westfield, Scotland. The model results were in very good agreement for some components and not for others. The discrepancies were attributed to the fact that the model predicted a higher gasifier temperature than the experimental value. The sound operation of fixed bed gasifiers requires utilising coals with suitable ash properties, in particular, the ash fusion temperature must not be too low. Van Dyk and others have modelled mineral matter processes occurring in a Sasol-Lurgi gasifier using a FACTSAGE package. Several runs have demonstrated the applicability of FACTSAGE calculations for the prediction of AFT as well as blending strategies. Models have also been developed to address issues relating to alkali metals. Guhl and Meyer have developed a thermodynamic model of the BGL gasification process with particular consideration of alkali metals. The model enabled the partitioning of the volatile ash components into condensed and gaseous species in the raw gas and into slag to be assessed.

It is evident that the relatively few models developed recently to simulate moving bed gasifiers have tended to regard the system as consisting of several zones at steady state in which a particular process takes place. Many of the models utilise the Aspen Plus coding. The comparisons that have been made of model results with plant or rig data have indicated reasonable agreement.

Fluidised bed gasifiers can be considered to consist of two phases: a bubble and an emulsion phase. Bubbles entering the bed expand as they pass up through the bed, hence the bubble size increases with bed height. Each bubble can be assumed to consist of a bubble volume which is surrounded by a bubble cloud. Transport processes occur between the bubble phase, the cloud and the emulsion phase. Yan and others developed a 1-D isothermal model for FBG using the two-phase theory of fluidisation. This assumed that the emulsion phase remained fluidised whilst the excess gas flowed as bubbles through the bed. The model was later modified to incorporate an overall energy balance to improve

simulations. Yan then introduced the 'net flow' concept for modelling fluidised bed gasifiers. Net flow is different from the excess gas flow concept defined by two-phase theory and refers to the net generation of gas in the emulsion phase due to coal devolatilisation and homogeneous and heterogeneous reactions.

De Souza-Santos has developed a comprehensive mathematical model and computer programme (CSFB) to simulate the operation of bubbling and circulating bed boilers and gasifiers. The model is considered to be comprehensive as it includes the conservation equations for the emulsion phase and bubbles, empirical equations for hydrodynamics and a thorough mass balance which considers that both drying and volatilisation are not instantaneous. It was a one dimensional model and assumed that the system was at steady state. The system was represented by two main regions: bed and freeboard. The bed was divided into bubble and emulsion. The solid phase consisted of three components: fuel, inert and sulphur absorbent. The model did not assume an overall stirred-tank approach. Only the composition of the solid particulate phases in the bed was assumed to be well-mixed. The programme performed successive iterations and at each, boundary conditions for the three solid phases (carbonaceous, sulphur absorbent and inert) were obtained by solving differential energy balances for conduction, convection and radiative heat transfers between the distributor surface and the various phases. Though the model was one-dimensional, regardless of the apparent simplicity, the solution of the governing, non-linear and tightly coupled system of differential equations provided a complete and detailed representation of all significant processes occurring in the gasifier. The model results have been compared with operational results obtained from several pilot plants. These were reasonable. Overall, the comparison of model results with rig data could only be described as mixed. The model, however, was a useful tool for understanding the processes taking place in the gasifier and for predicting, in general terms, how changes in operational conditions might affect process parameters.

Chejne and collaborators have investigated several models for simulating coal gasification in fluidised beds. Initially a steady state, one-dimensional model and algorithm were developed. Devolatilisation and drying were considered to be instantaneous in the feed zone. The model was applied to solid particles submerged in a fluidiser of an atmospheric gasifier. The model results were compared with those from a pilot fluidised bed gasification plant and were found to be satisfactory. The model has been modified recently to model a pressurised fluidised bed gasifier. The results were compared with those from an experimental gasifier and the agreement was mixed. Gräbner and others have also reported a numerical simulation of a pressurised CFB gasifier. The applied gasification principle was the Power High-Temperature Winkler process. The model results showed that a core-annular flow regime developed up to at least half of the reactor's height. The main inaccuracies occurred in the gas modelling and instabilities of the two phase flow. However, the model was an effective tool for gasifier design evaluation and the prediction of operating performance for proposed design changes.

Nayak and Mewada extended an existing model for combustion of coal in a CFBC system by using four Aspen Plus reactor models and several subroutines. The different modules in Aspen Plus which were incorporated to model the overall gasification process were decomposition of feed, volatile reactions, char gasification and gas-solid separation. The model results were as expected and were used to determine the effect of parameters such as steam to coal ratio and oxygen flow rate on product gas composition. Singh and others have reviewed CFD modelling of fluidised bed combustion and gasification. They contend that reliable CFD models were essential for the optimisation of fluidised bed design and predicting many parameters such as inert material concentration in the bed, fuel mixing efficiency, temperature profiles of solid and gaseous species present in the bed, temperature profile of the furnace and heat flux. Simulation using CFD was one of the most appropriate approaches for predicting critical parameters needed to control efficient operation of gasifiers. These multidimensional models bridged the gap between sub-scale testing and the operation of fluidised beds by providing information about gasification processes that experimental data alone cannot provide.

A different approach has been adopted by Chavan and others for modelling the fluidised bed gasification process. They considered that gasification was a complex and non-linear process which was difficult to model by conventional ‘first principles’ models expressed in terms of mass, momentum and energy balance equations. The approach they suggested for modelling gasification utilised classical regression methods to formulate empirical models. These difficulties associated with regression based empirical modelling were overcome by using artificial intelligence (AI)-based modelling formalism known as Artificial Neural Networks (ANNs). Process data from India and elsewhere have been used to develop the models. The authors concluded that the model could be used to optimise gasifier design and choose the most suitable operating conditions for a particular type of coal.

Several new models for modelling fluidised bed gasifiers have been developed in the past decade. These have generally assumed steady state. A detailed CSFMB model which was produced by De Souza-Santos and others could model both moving bed and circulating bed gasifiers. CFD modelling has also been extensively used for modelling fluidised bed gasification. These have been applied to multi-dimensional systems. The results of the models have been compared with plant and rig data. The comparisons have generally been satisfactory. There is little indication that modelling results have been utilised to solve plant problems.

Entrained flow gasification technology is the most widely-used gasification technology but modelling this process is more complicated than modelling fluidised bed gasifiers due to the need to model ash slagging. Unlike FBG modelling for which the motion of the coal particles is generally described by an Eulerian approach, in entrained flow gasifiers which are more lightly loaded, the Lagrangian approach is more suitable. There have been some 1-D models to model entrained-flow gasifiers. Kasule and others have developed a 1-D, steady state model of a single-stage, downward-firing, oxygen-blown, slurry-fed, entrained-flow gasifier for use in context of IGCC process simulation. The model included a detailed energy balance model for the reacting phases and the gasifier wall, which incorporated the energy loss to the environment. The model was used to simulate the entrained-flow gasifier at the Tampa Electric Polk plant. A comparison of the syngas composition showed that the agreement was reasonable. Kasule and others have extended the steady state, 1-D model and developed a dynamic model of a downward-fired GE/Texaco entrained-flow gasifier. As in the steady state model, the dynamic model contained mass, momentum and energy balances for the gas and solid phases. The dynamic response of the gasifier to particular changes commonly undertaken during the practical operation of commercial gasifiers was investigated. The predicted transient response of the scaled exit gas temperature to a stepwise ramp turndown of gasifier slurry was consistent with the observed performance at the Coolwater plant. Tremel and Spliethoff have developed a one-dimensional plug flow model to simulate laboratory-scale Pressurised High Temperature Entrained Flow Reactor (PiTER). The model consisted of different submodels for fuel devolatilisation, intrinsic char gasification, surface area evolution, char thermal annealing, pore diffusion, boundary layer diffusion and particle size and density variation. The model results were compared with measurements from the PiTER gasifier. The comparison of simulation and experimental data for char conversion and overall conversion showed that the differences between the model and experimental data were small and the results demonstrate that the fuel conversion can be predicted by numerical calculation based on the different submodels.

Lee and others have developed a simple process for modelling a dry-feed entrained flow gasifier. The approach was different from a standard CFD analysis. A simplified flow pattern was adopted based on rough assumptions in a pseudo-2D model. The behaviour of the coal was described in terms of devolatilisation, heterogeneous reactions at the solid particle surface and homogeneous reactions of gaseous components. The kinetics of product formation were modelled by a set of first-order, parallel reactions. The authors acknowledged that as a simplified model, it contained uncertainties and the model results should be used to evaluate trends rather than to provide exact predictions. Gazzani and others have developed a reduced order model (ROM) as an alternative to comprehensive CFD to simulate a Shell-Prenflo entrained flow gasifier. ROM is computationally very efficient taking about

one minute in a typical desk-top or laptop computer. The ROM approach allowed a reasonably accurate prediction of the gasification process as part of a plant simulation model. Overall, the ROM predicted the syngas conditions at the scrubber outlet quite accurately.

The majority of models for entrained-flow gasifiers have been 3-D models. Bockelie and others have modelled these gasifiers over many years. They first developed a CFD modelling capability for entrained flow gasifiers as part of the US DOE Vision 21 project. The models were developed to address a broad range of issues related to reliability, availability and maintainability in particular to predict the impact on gasifier performance resulting from operational changes. The model was developed using GLACIER which was an in-house coal combustion and gasification modelling tool. The model simulated the slagging of hot mineral matter on the gasifier walls using the flowing slag wall modelling component of earlier studies undertaken as part of the US DOE Combustion 2000 programme. The model predictions were compared with those for the existing DOE funded study incorporating an ASPEN analysis and there was acceptable agreement between the predicted values of the two models. As CFD-based models require significant computational time to produce a steady state solution, Bockelie and others developed a simpler model that could be used for rapid calculations and to narrow the range of operating conditions for a CFD model. Model results were compared with three sets of measured data from three working gasifiers and there was satisfactory agreement between the predicted values for syngas composition and heating values. Bockelie and his co-workers have modelled slagging by incorporating an existing model for vaporisation and condensation, developed for PCC boilers. The ash vaporisation process was modelled by developing the necessary mathematical representation of the transformational pathways. More recent modelling has addressed syngas cooler plugging and fouling. The CFD modelling part of the project used the existing Fouling and Deposit Growth model. The model predicted the properties of the particles exiting the gasifier and indicated that most of the deposition occurred on uncooled surfaces upstream of the syngas cooler and on the tube sheet face of the cooler.

Silaen and Wang have developed models for entrained-flow gasifiers in order to help industry to resolve problems and improve gasifier operation. They were particularly interested to investigate the effects of operating conditions. They conducted numerical simulations of the coal gasification process in a generic two-stage entrained flow gasifier using the commercial CFD code FLUENT. The study focused on a two-stage entrained flow gasifier. Overall, the results indicated that fuel conversion efficiency could be considerably affected by the flow pattern and gasifier injection angle. Silaen and Wang undertook further investigations on the effects of different assumptions and parameters on predicted gasification performance including turbulence models, devolatilisation models, finite reaction rates and solid coal sizes. Silaen and Wang conducted additional investigations comparing three different gasification reaction models: instantaneous gasification, global equilibrium and finite-rate models. The overall result showed that the instantaneous gasification approach could provide an overall evaluation of relative changes of gasifier performance but did not adequately predict gasification processes at the local level in most parts of the gasifier as predicted by the finite rate model. Silanen and Wang undertook further modelling investigations in which the 3-D Navier-Stokes equations and eight species transport equations were solved with three heterogeneous global reactions, three homogeneous reactions and a two-step thermal cracking equation for volatile production. This model was used to investigate the effects of different operational parameters such as coal mixture (dry or slurry), oxidant (oxygen or air) and different coal distributions in a two-stage gasifier on the gasification process.

Chyou and others have adapted the instantaneous gasification model approach developed by Silaen and Wang to simulate the oxygen-blown coal gasification process within a cross-type, two-stage (E-Gas) gasifier with the commercial CFD solver ANSYS FLUENT. The authors concluded that the simplified instantaneous gasification model could be used as a tool for preliminary examination of the overall effect of thermal-flow and turbulence in a cross-type, two-stage gasifier. They developed their model to replace the instantaneous gasification model with the more realistic heterogeneous finite-rate reactions using the discrete phase model (DPM) to track each coal particle. This improved the

understanding of the gasifier thermal-flow behaviour and gasification process in the gasifier. Lee and others have assessed how well commercial codes developed for simulating overall IGCC systems model processes occurring in the gasifier. Aspen Plus is a widely used chemical process simulator, which is used to predict plant performance, based on mass and heat balance, phase and chemical equilibrium at steady state. The Aspen model consists of flow sheets of the important sections of the IGCC system. The authors concluded that though coal gasification models in commercial process analysis simulators were useful for interpreting the whole plant cycle, they could be improved. They suggested improvements to the treatment of devolatilisation, gas-gas and solid-gas reactions.

In the Advanced Process Engineering CoSimulator (APECS) sponsored by US Department of Energy's NETL, the widely used, steady state process simulator Aspen Plus has been run with various equipment models including CFD models based on FLUENT. In one case, the entrained-flow gasifier CFD model was coupled into an Aspen Plus steady state process simulation of a potential, coal-fired, IGCC and hydrogen production plant for the US DOE's FutureGen project. Very useful information relating to temperature contours, char conversion and concentration of chemical species was obtained. Due to the complexity of physical and chemical processes involved in gasification, it is very challenging to simulate all of them accurately in a comprehensive CFD model. Ma and Zitney have considered the existing Lagrangian discrete phase based CFD models and improved the accuracy of sub-models. The modelling for coal moisture release and devolatilisation has been improved. More chemical species have been included in the model. The predicted syngas compositions and exit gas temperatures were reasonable and comparable to reported data from commercial-scale gasifiers. The detailed predictions related to velocity, temperature and mole fractions of individual species inside the gasifier also showed reasonable trends and provided insight into the physical and chemical processes involved.

More modelling studies have been undertaken for entrained-flow gasifiers than for moving bed or fluidised bed gasifiers. Both 1-D and 3-D models have been developed but the majority are 3-D. These are frequently based on CFD using the commercial software FLUENT. In most cases the results of the modelling studies have given insight into the fundamental processes occurring in the gasifier. This has helped to improve gasifier designs. In some cases, the results have been compared with plant data and it has been possible to choose model inputs to give reasonable fit with the measured data. These remarks can be extended to apply to gasification modelling in general. There are many processes taking place in gasifiers and developing computational models of these processes is a complex task. These models are vital in understanding the processes taking place. The model inputs tend to be chosen to fit available data rather than 'a priori'. Insight gained by modelling has advanced the design of gasifiers and can improve gasifier performance. However, there are fewer examples where modelling has directly solved operational problems.

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