Department of Chemical Engineering

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# MATHEMATICAL MODELLING OF
# ENTRAINED FLOW COAL GASIFICATION

A thesis submitted in partial fulfilment of the

requirements for the Doctor of Philosophy

by

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B.Eng. (Chem.) Hons.

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I hereby certify that the work embodied in this thesis is the results of original research and has not been submitted for a higher degree to any other University or Institution.

(Signed) _____

A. C. Beath

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# NEW TABLE OF CONTENTS

# ERRATA

**a) Typographical Errors.**

| Page | Location | Statement | Replacement |
|------|----------|-----------|-------------|
| xxi | Paragraph 2, Line 6 | *accuracy* | *accurate* |
| 1 | Paragraph 2, Line 4 | *theoretical* | *theoretically* |
| 4 | Paragraph 2, Line 10 | *initial* | *initially* |
| 22 | Paragraph 3, Line 10 | *of* | - |
| 66 | Paragraph 2, Line 7 | *gasifierss* | *gasifiers* |
| 93 | Table 4.2 | *Eq 39* | *Equation 2.8* |
| 181 | Paragraph 2, Line 7/8 | *The range of experimental results considered allows for* | - |

**b) The following text and equations should be included directly following page 102.**

algorithm was developed for the model and is described below. The expressions were obtained by 'inverting' the model and calculating the length of time per step of conversion, rather than the conversion per length of time. Due to the difficulties in calculations for this model a number of simplifications had to be made, namely to the kinetics and heat transfer models employed and in that only one particle size can be used. From results predicted with this model an adaptable algorithm for estimating the trend in conversion with time was construction, a version of which is given in equations 4.25 to 4.27 in terms of step time predictions and illustrated in figure 4.6. Two adjustable parameters are used in the algorithm with the first, $\Delta X_{i,specified}$, giving a suggested value for the size of the slice in terms of change in conversion and the second, $f(\text{Coal})$, is given in table 4.3 and allows for variation in size of slice dependent on the degree of conversion in the previous slice and the coal used. This requires input of a factor dependant on the coal used, $g(\text{Coal})$, which accounts for variations due to coal properties in the early stages of gasification, mostly affected by the quantity of volatile released from the coal, and generally ranges from 0.5 for a low volatile coal to 2.5 for a very high volatile coal.

$$\Delta t_i = \frac{\Delta t_{i-1}}{\Delta X_{i-1}} \cdot \Delta X_{i,specified} \cdot \frac{\alpha}{f(X,Coal)} \cdot \log_{10}(\beta X) \qquad \text{Equation (4.25)}$$

$$\alpha = 0.5208 . \log_{10}(6.232 \Delta X_{i,specified}) . \frac{P_{total}}{30} \qquad \text{Equation (4.26)}$$

$$\beta = 10^{\left( \frac{8.671}{\Delta X_{i,specified}^{0.8277}} - \frac{7.641}{\Delta X_{i,specified}^{0.5078}} \right)}$$

Equation (4.27)

**c) The following references should be included in section 10. REFERENCES.**

Bautista, J. R., Russel, W. B., Saville, D. A., 1986, "Time-Resolved Pyrolysis Product Distributions    Softening Coals", Ind. Eng. Chem. Fund., V25, pp536-544.

Gibbins, J. R., Kandiyoti, R., 1989, "The Effect Of Variations In Time-Temperature History On Product Distribution From Coal Pyrolysis", FUEL, V68, pp895-903.

Hastaoglu, M. A., Karmann, M., 1987, "Modelling Of Catalytic Carbon Gasification", Chem. Eng. Sci., V42, pp1121-1130

Reid, R. C., Prausnitz, J. M., Poling, B. E., 1987, "The Properties of Gases and Liquids", McGraw-Hill, New York.

Schoen, P., 1992, "Mathematical Model Of A Slagging Pulverised Coal Gasifier", Int. Power Eng. Conf., Hangzhou, China, May 17-21.

Sharma, D. K., Sulimma, A., van Heek, K. H., 1986, "Comparative Studies Of Pyrolysis Of Coal In Inert Gas, Steam And Hydrogen Under Pressure", Erdol Und Kohle - Erdgas – Petrochemie    Vereinigt Mit Brennstoff-Chemie, V39, pp173-176.

Strimbeck, G. R., Cordiner, J. B. Jr., Taylor, H. G., Plants, K. D., Schmidt, L. D., 1953, *See USBM  (1953)*.

Suuberg, E. M., 1977, *See Howard, J. B. in Chemistry of Coal Utilization, 2nd Suppl. Vol. (1981)*.

Wagner, R., Wanzl, W., van Heek, K. H., 1985, "Influence Of Transport Effects On Pyrolysis Reaction Of Coal At High Heating Rates", Fuel, V64, pp571-573.

# CLARIFICATIONS

| Page | Additional Comments |
|---|---|
| 3 | The higher efficiency referred to as occurring in gasifiers relative to pulverised coal boilers refers to the use of gasifiers in integrated gasification combined cycle (IGCC) power generation compared to conventional pulverised coal-fired boiler power plant.  This is due to the higher thermodynamic efficiency achieved in IGCC plant. |
| 21 | In relation to the use of equations (2.1) and (2.2) to prediction of devolatilisation rates at high pressures, it is necessary to input some measure of the expected ultimate volatile yields at the desired pressure, $V^*$ in equation (2.1) or $a_1$ and $a_2$ in equation (2.2).  These yields must either be experimentally obtained or estimated by another model, as equations (2.1) and (2.2) do not compensate for variations in pressure.   If the yields are input to either expression a devolatilisation rate can be estimated, although the accuracy of the estimate at pressures differing from atmospheric is unknown. |
| 29 | The identification of reaction steps in sequence from Step 1 to Step 17 should not suggest that the steps should progress in this order.  Therefore it is not necessary for oxygen gasification to precede carbon dioxide gasification, or carbon dioxide gasification to precede steam gasification, etcetera, during gasification. |
| 37 | The reaction order 'n' defined by equation (2.8) is for the oxygen gasification reaction and is used in the estimation of reaction rate according to equation (2.7). |
| 53 | In assuming that all nitrogen in the product gases from a gasifier is in the form of molecular nitrogen reference is made to *Strimbeck et al. (1953)*.  (This reference is listed in the references as *USBM (1953)*.)  The gasifier used in that study was a pilot scale entrained flow, high pressure and oxygen blown unit.  The dominance of production of molecular nitrogen compared to other nitrogen containing gases in gasifiers was also reported in Watkinson *et al.* (1991) for a range of gasifiers, including entrained flow, fluidised bed and fixed bed designs, using either oxygen or air and variously operating at high and atmospheric pressures.  This does not mean that other nitrogen containing species will not exist in gasifiers but suggests that they will be in only minor concentrations.  By |

| | |
|---|---|
| | neglecting these other nitrogen containing species it becomes possible to analytically solve some of the equations concerning gas phase equilibria and therefore this approximation is seen as justifiable for use in the model. |
| 86 | In the work of Neoh and Gannon (1984) a set of 13 coals of North American origin with rank ranging from lignite to anthracite was studied. The majority of these, nine of the 13, were in the range sub-bituminous to low volatile bituminous that would typically be considered applicable for use in entrained flow gasification. |
| 92 | The magnitudes of the reactivity correlation coefficients listed in Table 4.1 do not indicate the relative magnitudes of the different reactions but are solely used to represent the influence of coal rank (based on carbon content) on reaction rate for the individual gasification reactions. For example, from the figures in the table it is possible to state that rank appears to have greatest influence on the reaction rate of steam with carbon and the least influence on the reaction rate of hydrogen with carbon. The magnitude of the rates is estimated from the value of the pre-exponential rate constant calculated from the reactivity coefficient and other terms using Equation (4.8), as well as the activation energy for the reaction and other diffusional interferences that are independent of the calculated reactivity coefficient. |
| 96 | In the chemical reaction rate limited regime mass loss will occur both from the external particle surface and the internal pore surface, however as internal pore area is typically much greater than external particle area, reaction will effectively lead to increasing particle porosity with negligible particle shrinkage. For the pore diffusion hindered regime the rates of change in porosity and particle size will vary depending on the particle effectiveness factors for the heterogeneous reactions. At low effectiveness factor the particle will mostly shrink with reaction with little change in porosity, and at high effectiveness factor the particle porosity will increase with little reduction in particle size. |
| 101 | The gas properties of significance to modelling in an entrained flow coal gasifier are density, emissivity, diffusivity, specific heat and thermal conductivity. In general only the gases present in significant concentrations in the gasifier, carbon monoxide, carbon dioxide, steam, hydrogen, oxygen and nitrogen, are considered in the sub-models for gas properties. Density is calculated using the Ideal Gas Law, which involves the assumptions of non- |

interaction between gas molecules and therefore is subject to minor error at high pressures. The gas emissivity is assumed to be uniform for the entire spectrum of relevance to heat transfer, termed 'grey' gas modelling, and the calculation of emissivity is considered in section 2.6.2 (pp61-63), with inclusion of pressure dependent terms. Calculation of diffusivity for use in determination of boundary layer and pore diffusion effects is discussed in section 2.3.7.2 (pp48-52), with the expressions defined incorporating the effects of pressure on the calculated variables. Calculation of the specific heats and thermal conductivities of gas mixtures at high temperatures and pressures are not discussed in the thesis as relatively common methods were used. Specific heats were calculated from the average values for the individual gases (averaged on a molar basis), which in turn were estimated using quadratic polynomials of best fit to available experimental data with respect to changing temperature. The thermal conductivities of gas mixtures were estimated using the Brokaw Method (Reid, Prausnitz and Poling (1987)), with individual values estimated from linear regression of the available experimental data with respect to changing temperature. This method compensates for the anomalous influence of significant quantities of hydrogen on the overall thermal conductivity of the gas mixture. For both the estimation of specific heat and thermal conductivity of the gas mixtures no correction for high pressures was deemed necessary as the available experimental data indicated insignificant variation in property with pressure when compared to the uncertainties involved in the estimation of the property at atmospheric pressure.

# ORIGINAL TABLE OF CONTENTS

# ORIGINAL TABLE OF TABLES

# ORIGINAL TABLE OF FIGURES

**3. EVALUATION OF LITERATURE**

**4. DESCRIPTION OF MATHEMATICAL MODEL**

**5. SENSITIVITY ANALYSIS**

## 6. COMPARISON OF MODEL PREDICTIONS WITH AVAILABLE EXPERIMENTAL MEASUREMENTS

## 7. USE OF MODEL PREDICTIONS TO DETERMINE REACTION MECHANICS AND OPTIMUM GASIFIER FEED MIXTURES

**8. CONCLUSIONS**

**9. RECOMMENDATIONS FOR FURTHER WORK**

**10. REFERENCES**

**APPENDIX A: DETERMINATION OF INTRINSIC REACTIVITIES**

**APPENDIX B: SLAG LAYER MODEL**

# ABSTRACT

A mathematical model for entrained flow coal gasification was developed with the objective of predicting the influence of coal properties and gasification conditions on the performance of entrained flow gasifiers operating at pressures up to 21 atmospheres (2.1MPa). The model represents gasifiers as plug flow reactors and therefore neglects any mixing or turbulence effects. Coal properties were predicted through use of correlations from a variety of literature sources and others that were developed from experimental data in the literature. A sensitivity analysis of the model indicated that errors in the calculated values of coal volatile yield, carbon dioxide gasification reactivity and steam gasification may significantly affect the model predictions. Similarly errors in the input values for gasifier wall temperatures and gasifier diameter, when affected by slagging, can cause model prediction errors. Model predictions were compared with experimental gasification results for a range of atmospheric and high pressure gasifiers, the majority of the results being obtained by CSIRO at atmospheric pressure for a range of coals. Predictions were accurate for the majority of atmospheric pressure results over a large range of gas feed mixtures. Due to the limited range of experimental data available for high pressure gasification the capability of the model is somewhat uncertain, although the model provided accurate predictions for the majority of the available results. The model was also used to predict the trends in particle reactions with gasification and the influence of pressure, gasifier diameter and feed coal on gasifier performance. Further research on coal volatile yields, gasification reactivities and gas properties at high temperatures and pressures was recommended to improve the accuracy of model inputs. Additional predictions and model accuracy improvements could be made by extending the model to include fluid dynamics and slag layer modelling.

# ACKNOWLEDGMENTS

# SUMMARY

## 1. INTRODUCTION

The aim of this study is to develop a mathematical model of entrained flow coal gasification. Emphasis in the model will be on the ability to distinguish differences in gasification performance caused by changes in coal and gasification conditions, and for this reason accurate modelling of the coal gasification reactions is required rather than the fluid flow aspects. In order to allow general use of the model it is also desirable that coal related inputs can be estimated from basic coal analysis results, such as proximate and ultimate analyses.

Gasification of coal or other forms of carbon has been used for generation of combustible gases since the late 1700s. Important reactions identified in the gasification of coal are given in reactions 1 to 14. Reactions 1 to 5 are actually involved in gasifying the coal while reactions 6 to 14 are responsible for determining the gas composition.

**Devolatilisation**

$$Coal \rightarrow Char \ + \ Volatiles \qquad\qquad \text{Reaction (1)}$$

**Heterogeneous Gasification**

$$C + \tfrac{1}{Z}O_2 \rightarrow \left(2 - \tfrac{2}{Z}\right)CO + \left(\tfrac{2}{Z} - 1\right)CO_2 \qquad\qquad \text{Reaction (2)}$$

$$C + CO_2 \rightarrow 2CO \qquad\qquad \text{Reaction (3)}$$

$$C + H_2O \rightarrow H_2 + CO \qquad\qquad \text{Reaction (4)}$$

$$C + 2H_2 \rightarrow CH_4 \qquad\qquad \text{Reaction (5)}$$

**Homogeneous Combustion**

$$CO + \tfrac{1}{2}O_2 \longrightarrow CO_2 \qquad\qquad \text{Reaction (6)}$$

$$H_2 + \tfrac{1}{2}O_2 \longrightarrow H_2O \qquad\qquad \text{Reaction (7)}$$

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O \qquad\qquad \text{Reaction (8)}$$

$$H_2S + \tfrac{3}{2}O_2 \longrightarrow SO_2 + H_2O \qquad\qquad \text{Reaction (9)}$$

$$COS + \tfrac{3}{2}O_2 \longrightarrow CO_2 + SO_2 \qquad\qquad \text{Reaction (10)}$$

**Homogeneous Equilibrium**

$$H_2O + CO \longleftrightarrow H_2 + CO_2 \qquad\qquad \text{Reaction (11)}$$

$$CO + 3H_2 \longleftrightarrow CH_4 + H_2O \qquad\qquad \text{Reaction (12)}$$

$$SO_2 + 3H_2 \longleftrightarrow 2H_2O + H_2S \qquad\qquad \text{Reaction (13)}$$

$$COS + H_2O \longleftrightarrow CO_2 + H_2S \qquad\qquad \text{Reaction (14)}$$
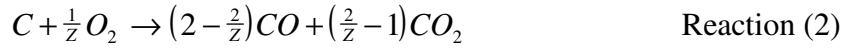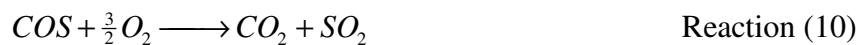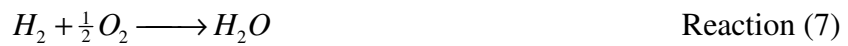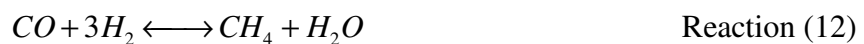
More recently the concept of coupling a gasifier with a gas turbine and steam generation plant to produce electricity has led to further development of gasification, these plants are termed integrated gasification combined cycle (IGCC). The form of gasifier used in IGCC can vary with the most common types being fixed bed, fluidised bed and entrained flow. In this study entrained flow gasification is considered and this involves the addition of pulverised coal with oxygen, or air, and steam into the gasifier. For IGCC use the gasifier will commonly be operated in the range of 20 to 30 atmospheres pressure.

## 2. LITERATURE REVIEW

The quantity of literature available for gasification is vast due to the large number of reactions involved, however only a small proportion of the literature is relevant to the high pressure and high temperatures experienced in large entrained flow gasifiers. Key areas of interest are the yield of volatiles from coal heated rapidly at both atmospheric and high pressures, rates of heterogeneous gasification reactions at high temperatures and pressures and the modelling of coal particle structure. Other topics of lesser significance are methods for modelling the homogeneous reactions and heat transfer during gasification.

## 3. EVALUATION OF LITERATURE

From detailed analysis of the available literature it was determined that sufficient information is available to produce a mathematical model of entrained flow gasification. The major limitation of the literature is the scant experimental experience with high pressure and high temperature heterogeneous gasification rates. This leads to difficulty in determining the best modelling method for these reactions and two alternate methods where identified, Langmuir-Hinshelwood and pressure order expressions.

## 4. DESCRIPTION OF MATHEMATICAL MODEL

A plug flow model for entrained flow coal gasification was developed from a combination of literature correlations, correlations developed from literature data and some experimental data. The model considers a number of discrete size fractions of coal particles flowing along the gasifier in parallel to the longitudinal axis of the gasifier. All reactions previously mentioned are considered to occur in the gasifier. The devolatilisation yield for a given coal is estimated from a published correlation that bases the yield on the

coal ultimate analysis, with another correlation changing this estimate depending on the pressure. This corresponds to literature results that indicate that volatile yield decreases with increasing pressure. Reactivities and coal particle structures are determined from general correlations obtained from the literature, although experimentally determined reactivities for a char that was formed under similar conditions are required. Heterogeneous reaction rates are calculated using a complex particle effectiveness factor dependant on particle pore structure, reactant gas diffusivity and coal reactivity. A comparison of model predictions using either Langmuir-Hinshelwood or pressure order expressions led to adopting the pressure order expressions as being more representative of gasification performance. The homogeneous combustion reactions listed previously are considered to occur instantaneously if oxygen is present and if it is not the homogeneous equilibrium reactions are assumed to be at equilibrium in the gasifier. Heat transfer in the gasifier is considered to occur by both convection and radiation, with convective transfer being approximated using established literature correlations and radiative transfer being modelled using the Long Furnace Model. This model assumes that no radiative transfer occurs along the gasifier and transfer is only within hypothetical thin slices of the gasifier. Coupled to this model is the assumption that the gas in the gasifier has significant emissivity and can be considered as a grey gas. The grey gas emissivity is calculated using a published algorithm. The model is not capable of calculating the temperature of the gasifier wall as generally insufficient data is available on the thermal properties of materials in the gasifier, so the temperature of the wall at different distances along the gasifier must be input from experimental data or estimated by other means. An empirical solution algorithm was produced to assist in the selection of step times in the model.

## 5. SENSITIVITY ANALYSIS

A study of the sensitivity of the developed mathematical model to changes in the values of inputs indicated significant sensitivity to a wide range of variables. Further analysis indicated that expected error ranges in the input values for coal volatile yield, carbon dioxide and steam reactivities, total coal surface area, gasifier wall temperatures and the internal diameter of the gasifier, if coated with slag, are sufficiently large to produce significant errors in the model predictions. These errors can be minimised by performing more accurate experimental measurements or developing more accurate correlations than are presently available.

## 6. COMPARISON OF MODEL PREDICTIONS WITH AVAILABLE EXPERIMENTAL MEASUREMENTS

Predictions were made using the mathematical model for comparison with experimental results from a selection of experimental gasifiers. The majority of the results considered were for the atmospheric pressure CSIRO gasifier, in which eight different coals were gasified using a wide range of conditions. Other atmospheric pressure results were for an United States Bureau of Mines gasifier with five different coals and a Brigham Young University gasifier with four different coals. At high pressures some results were available from an Institute of Gas Technology gasifier with four coals at pressures between 1.7 and 6.1 atmospheres and a different United States Bureau of Mines gasifier with one coal at pressures between 7.8 and 21.4 atmospheres.

In general, predictions made for the atmospheric pressure gasifiers were accurate, although less accuracy was evident for some particular coals. A general trend of increasing gasification performance with decreasing coal rank, as indicated by coal carbon content, was identified in experimental results and model predictions for all three atmospheric pressure gasifiers. The limited number of results available at high pressures led to inconclusive findings, with the majority of predictions being accuracy but those for some coals being extremely unreliable. More detailed analysis of the performance of some individual model components suggested that the volatile yield and reactivity estimates were more accurate than predicted in the sensitivity analysis.

## 7. USE OF MODEL PREDICTIONS TO DETERMINE REACTION MECHANICS AND OPTIMUM GASIFIER FEED MIXTURES

Additional model predictions were performed to predict trends in reaction behaviour and the variations in optimum feed mixtures with changing pressure, gasifier size and coal.

Detailed analysis of the progress of reactions at a single particle in the gasifier suggested a sequence of reactions commencing with devolatilisation then oxygen gasification, and continuing with simultaneous carbon dioxide and steam gasification. Some overlap between these reactions occurs but while the volatiles are being released it is predicted that it is not possible for reactant gases to diffuse to the particle. When devolatilisation has ceased the rate of oxygen gasification is much higher than the other reactions and dominates carbon conversion until the oxygen is depleted. Carbon dioxide

and steam gasification continue until the endothermic nature of the reactions lowers temperatures and the rates become insignificant.

In the study of optimum gas mixtures fed to the gasifier when pressure, gasifier diameter and coal are varied it was indicated that the optimum mixture can be affected by the changes. Predictions suggest that lower oxygen input is required at low gasification pressures than at high pressures. It is expected that this is due to the lower volatile yield at high pressures leaving more char to be consumed by heterogeneous reactions. Increasing gasifier diameter did not indicate changes in the optimum feed mixture but better gasifier performance was indicated at large gasifier diameters, excepting the largest diameter tested for which the predictions may have been affected by the use of some model components outside the limits of the correlations. The increase in gasifier performance with diameter is expected because of lower heat losses to the gasifier walls at higher diameters. The variations in gasification performance and optimum feed mixtures for different coals suggests that performance is linked to the reactivity and volatile yield of the coal and the optimum mixture is dependant on the moisture content and reactivity of the coal.

## 8. CONCLUSIONS

The mathematical model described and used in this study is the result of a combination of literature methods, correlations developed from literature data and experimental results. Errors associated with the methods used in the model were defined through a detailed sensitivity analysis. Key areas of possible inaccuracy are in the estimation of coal volatile yield, heterogeneous reactivities, particle structural properties, gasifier temperatures and gasifier diameter. Regardless of these possible inaccuracies the model predictions compared well with experimental results from atmospheric pressure gasifiers. Less conclusive comparison was possible for high pressure gasification, mostly due to the limited availability of high pressure experimental results. Predictions from the model suggested a sequencing of reactions occurring at a given particle commencing with devolatilisation then oxygen gasification followed by simultaneous carbon dioxide and steam gasification, with some overlap between the reactions. Optimum feed conditions and maximum gasifier performance were predicted to vary with changing gasifier pressure, gasifier diameter and feed coal. Various of the predictions suggested that errors in the model could arise at high pressures and large gasifier diameters due to extrapolation of gas physical property correlations outside the range of experimental data.

## 9. RECOMMENDATIONS FOR FURTHER WORK

It is suggested that further work be performed on the following topics to improve the accuracy of model predictions in future models.

(a) High Temperature and Pressure Heterogeneous Reaction Kinetics

(b) High Pressure Devolatilisation Yields

(c) Gas Physical Properties

(d) Slag Layer Modelling

(e) Fluid Dynamics Modelling

# GLOSSARY OF SPECIALISED TERMINOLOGY AND ABBREVIATIONS

| Term | Definition |
|---|---|
| ad | Coal analysis figures on an 'air dried' basis. |
| ar | Coal analysis figures on an 'as recieved' basis. |
| Atmosphere | Pressure measurement taken as equal to 101.325kPa in this study. |
| Boundary layer | Gas close to a particle which has composition or other properties that are significantly different from those of the bulk gas. |
| Carbon conversion | Gasified carbon relative to initial total coal carbon, usually expressed as a percentage. |
| Cold gas efficiency | Calcorific value of product gas at 25°C relative to calorific value of coal feed, usually expressed as a percentage. |
| daf | Coal analysis figures on a 'dry, ash free' basis. |
| Effectiveness factor | Ratio of actual heterogeneous reaction rate to that possible without diffusion resistances, usually approximated by an estimated proportion of total particle surface area available for reaction. |
| External reactivity | Reactivity calculated from experimental results on the basis that all reaction occurs on the external surface of the particle. |
| Fuel ratio | Ratio of volatile matter to fixed carbon in a coal used as an indicator of coal performance. |
| IGCC | Integrated gasification combined cycle electricity generation plant. |
| Intrinsic reactivity | Reactivity calculated from experimental results on the basis that reaction occurs at a proportion of the total particle surface area that is given by the particle effectiveness factor. |
| Vitrinite reflectance | Measure of coal rank based upon the degree of structure in vitrinite macerals of the coal. |

# NOMENCLATURE

| Symbol | Units | Definition |
|---|---|---|
| $\alpha$ | - | Proportion of volatile type. |
| $\alpha$ | - | Ratio of Knudsen to bulk diffusivities of reactant |
| $\alpha$ | - | Absorptivity of gas to radiation from source |
| $\sigma$ | - | Standard deviation in distribution. |
| $\sigma_a$ | $kg/m^3$ | Particle density |
| $\phi$ | - | Thiele Modulus |
| $\eta$ | - | Effectiveness factor |
| $\varepsilon$ | - | Particle porosity |
| $\varepsilon_{substance}$ | - | Emissivity of substance |
| $\rho_{gas}$ | $kg/m^3$ | Gas density |
| $\mu_{gas}$ | Pa.s | Gas viscosity |
| $\zeta$ | - | Ratio of steam to steam and carbon dioxide |
| a | - | Stoichiometry of reactant gas to carbon |
| $A_{external}$ | $m^2$ | External area of particle |
| $A_g$ | $m^2/kg$ | Internal area of particle |
| $A_{p,j}$ | $m^2$ | Transfer area of particle j |
| $A_{total}$ | $m^2$ | Total particle area |
| b | - | Stoichiometry of combined product gases to reactant |
| $C_{base}$ | % daf basis | Carbon content of base coal |
| $C_{p,gas}$ | J/kg/K | Specific heat of gas |
| d | m | Particle size |
| D | m | Gasifier internal diameter |
| $D_{eff,A}$ | $m^2/s$ | Effective diffusivity of compound A |
| $D_{A,K}$ | $m^2/s$ | Knudsen diffusivity of compound A |
| $D_{A,B}$ | $m^2/s$ | Binary diffusivity of compound A through compound B |
| $D_{A,mixture}$ | $m^2/s$ | Diffusivity of compound A through gas mixture |
| $d_{pore}$ | m | Pore diameter |
| E | MJ/kmol | Activation energy of reaction. |

| | | |
|---|---|---|
| h | $J/s/m^2$ | Convective heat transfer between substances |
| k | $s^{-1}$ | Frequency factor of reaction. |
| k | $kg/m^2/s/atm^n$ | Reaction rate |
| $k_0$ | $kg/m^2/s/atm^n$ | Pre-exponential term of reaction rate |
| $k_{0,base}$ | $kg/m^2/s/atm^n$ | $k_0$ for base coal |
| $K_{chemical}$ | $kg/m^2/s$ | Chemical rate |
| $K_{diff}$ | $kg/m^2/s/atm$ | Diffusion rate |
| $k_g$ | $J/K/m$ | Convective heat transfer coefficient |
| $k_{gas}$ | $J/m$ | Thermal conductivity of gas |
| $l_{pore}$ | m | Pore length |
| $m_C$ | kg | Mass of coal |
| $M_c$ | kg/kmol | Atomic mass of carbon |
| n | - | Pressure or Reaction order |
| $n_{pores}$ | - | Number of pores |
| Nu | - | Nusselt number |
| $P_{Compound}$ | atm | Partial pressure of Compound |
| Q | - | Ratio of volatile yield to Proximate Volatile Matter |
| q | $J/s/m^2$ | Radiative transfer between substances |
| R | MJ/kmol.K | Gas constant |
| $R_g$ | $m^3.atm/kmol/K$ | Gas constant |
| r | - | Reactivity coefficient |
| RF | - | Roughness factor |
| T | K | Temperature |
| $T_{gas\ or\ g}$ | K | Gas temperature |
| $T_{particle\ or\ p}$ | K | Particle temperature |
| $T_{wall\ or\ w}$ | K | Gasifier wall temperature |
| V | kg | Mass of volatiles released |
| V | % daf basis | Volatile yield at any time |
| $V^*$ | kg or %daf | Ultimate volatile yield |
| $V_{gas}$ | m/s | Gas Velocity |
| VM | kg | Proximate volatile yield |
| $VM_C$ | kg | Adjustment for volatile condensation |

| $V_{nr}{}^*$ | kg | Non-reactive volatiles (Yield at high pressure) |
|---|---|---|
| $V_P{}^*$ | % daf basis | Ultimate volatile yield at pressure P |
| $V_r{}^*$ | kg | Reactive volatiles (Yield at low pressure-$V_{nr}{}^*$) |
| $X_{Compound}$ | - | Mole fraction of Compound |
| z | - | Unadjusted ratio of combustion products |
| Z | - | Size corrected ratio of combustion products |