

# ASSESSMENT OF CHAR MORPHOLOGY IN HIGH PRESSURE PYROLYSIS AND COMBUSTION



**Katharine Elaine Benfell, BSc, MSc (Hons), Auckland**

NOT FOR LOAN



*The* UNIVERSITY  
*of* NEWCASTLE  
AUSTRALIA

A Thesis Submitted to the Faculty of Science and Mathematics in Candidacy for the  
Degree of Doctor of Philosophy

*Department of Geology*

**- September 2001 -**

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

(Signed)

\_\_\_\_\_

## Acknowledgements

This thesis would never have been completed without the assistance of many people. I am indebted to my principal supervisor, Dr Judy Bailey, for her guidance, encouragement, support, depth of knowledge of all things coal and superior editing skills. I am delighted that our relationship has progressed from that between student and supervisor to friendship. I am also very grateful to my industrial co-supervisor Mr Jim Happ for promptly reviewing my chapters, helping me to see the industrial perspective of my work and being so enthusiastic about the study in general.

The financial and physical support of the Co-operative Research Centre for Black Coal Utilisation (Black Coal CRC), which is funded in part by the Co-operative Research Centres Program of the Commonwealth Government of Australia, was greatly appreciated. The Black Coal CRC funded a University of Newcastle Postgraduate Research Scholarship for the project and costs for trips to a number of conferences within Australia and overseas. I am equally grateful to the Department of Geology for providing me with a welcoming "home" for the duration of my study, and for supporting my trip to the 28<sup>th</sup> International Symposium on Combustion.

A number of staff were immensely helpful at various stages. Richard Bale, Esad Krupic, Sharon Francis, Kathy Allan, Judy Winwood-Smith, Elaine Swift and Carrol Doble of the Geology Department helped to keep everything running smoothly during the course of the project. Dr Gary Bryant, Dr Liza Elliott and Neil Gardner of the Department of Chemical Engineering assisted with the experimental work done in the Black Coal CRC laboratories.

I would also like to thank Dr Andrew Beath (formally of Pacific Power) and Mr. Peter Benyon from Pacific Power for providing the initial char samples used in this study, without which I would not have been able to proceed. Dr. Shan Ouyang from the Co-operative Research Centre for Clean Energy from Lignite conducted the pressurised drop tube furnace experiments that produced the chars used. I am grateful to Dr. Hongwei Wu for performing the atmospheric pressure drop tube furnace experiments for the lithotype suite. Thanks to Graham O'Brien and Barry Jenkins of CSIRO for the FMR analyses. Thanks also go to the suppliers of the coal samples studied.

At the outset of my project, the differences in training and background between myself as a geologist and my Black Coal CRC colleagues as chemical engineers was painfully apparent (at least to me). I am extremely grateful to all my colleagues for helping me get to grips with a chemical engineer's view of coal and its utilisation. In particular, Dr Guisu Liu, Dr Hongwei Wu, Dr Gary Bryant, Dr Liza Elliott, Dr Chris Bailey, Dr Raj Gupta and Professor Terry Wall helped me to bridge that gap whether my questions related specifically to my project or not.

Perhaps the greatest advantage of conducting this study within the environment of the CRC has been the opportunity to team up with others. Without this chance, I would not have collaborated with Dr Guisu Liu and Mr Daniel Roberts on our multidisciplinary joint paper for the 28<sup>th</sup> International Symposium on Combustion. I am grateful for the experience.

My Geology Department colleagues helped me to keep a sense of humour, especially during long hours of microscopy. Thank you Tania Wilson, Andrew Walker, Helen Beath, Gareth Chalmers, Dr Yan Yan Sun, Dr Jennifer Wadsworth, Kev Rumming, Mark Pawley, Dr Murray Little, Martine Graham and the tea-room jokers (you know who you are!) for making me laugh. Friday beers at the Staff House were definitely worthwhile.

People outside the work environment were also very significant in helping me. At a time when life was very tough, Bruce Furner made the difference between giving up and pushing on - thank you for being there. My parents, parents-in-law and sister have always held the greatest confidence in me and my ability to complete the thesis - thank you for believing in me. Thanks too, to my former MSc supervisors, Dr Basil Beamish and Associate Professor Kerry Rodgers, without them, I would never have chosen to study coal utilisation. More recently, members of the April 2000 Playgroup have provided much welcome support.

Finally, I would like to express my great love and appreciation for my husband, Steven, and son, Jason. Without your support, encouragement, tolerance, love and willingness to follow me on this path, I would never have reached this destination. Thank you.

# Table of Contents

ACKNOWLEDGEMENTS.....	II
TABLE OF CONTENTS.....	IV
GLOSSARY, ABBREVIATIONS AND SYMBOLS .....	XIII
ABSTRACT.....	XIX
<b>1 OVERVIEW, BACKGROUND AND PROJECT OBJECTIVES.....</b>	<b>1</b>
1.1 Introduction	1
1.2 Background	3
1.2.1 Principles of coal combustion	3
1.2.2 Principles of coal gasification	6
1.2.3 Differences between combustion and gasification environments	7
1.3 Coal and Char Composition, Structure and Reactivity	9
1.3.1 Coal rank, petrographic and mineral effects on intrinsic reactivity in combustion and gasification	9
1.3.1.1 Coal Rank and Petrographic Effects	9
1.3.1.2 Mineral Effects	11
1.3.2 Influence of coal structure on char formation and combustion or gasification rate	13
1.3.2.1 Effect of Active Sites, Porosity and Surface Area on Combustion and Gasification	13
1.3.2.2 Particle Size Effects on Coal and Char Reactivity	16
1.3.3 Influence of experimental procedure on coal and char in combustion and gasification	17
1.3.3.1 Heat Treatment Temperature Effects	18
1.3.3.2 Heating Rate Effects	19
1.3.3.3 Influence of Furnace Atmosphere	19
1.3.3.4 Pressure Effects	20
1.3.4 Char morphology and reactivity in combustion and gasification	21
1.4 Objectives and Approach	22
<b>2 EXPERIMENTAL .....</b>	<b>25</b>
2.1 Introduction	25
2.2 Coal selection	25
2.3 Sample Preparation	28
2.3.1 Feed coals	29
2.3.2 Particle size analysis	29
2.3.3 Sample setting for microscopic analysis	29
2.4 Combustion experiments	31
2.4.1 Laboratory-scale drop tube furnace (DTF)	31



3.7.2.2 Microlithotype Composition	73
3.8 Comparison of High Pressure Pyrolysis and Combustion Chars	74
3.9 Volatile Yield and Burnout	77
3.10 Review	78
<b>4 EFFECTS OF HIGH PRESSURE PYROLYSIS ON THE CHAR MORPHOLOGIES OF FOUR BITUMINOUS RANK COALS.....</b>	<b>80</b>
4.1 Introduction	80
4.2 Aims of Char Morphological Study	80
4.3 Parent Coal Characteristics	80
4.4 Char Preparation and Analysis	81
4.5 Evaluation of 1100 °C Series P3 and 1300 °C P4 High Pressure Pyrolysis Chars	81
4.5.1 Effect of coal rank	81
4.5.2 Effect of parent coal composition	82
4.5.2.1 Maceral Influences on Char Morphology	82
4.5.3 Effect of pressure	88
4.6 Effect of Temperature on Series P3 and P4 Chars	105
4.7 Review	105
4.7.1 Effect of pressure on Series P3 and P4 chars	105
4.7.2 Effect of temperature on Series P3 and P4 chars	106
<b>5 CHAR MORPHOLOGIES OF LITHOTYPE VARIANTS FROM DRAYTON COAL.....</b>	<b>107</b>
5.1 Introduction	107
5.2 Aims of Char Morphological Study	107
5.3 Parent Coal Characteristics	108
5.4 Char Preparation and Analysis	109
5.5 Evaluation of Pyrolysis Series P5 (PDTF) and P6 (DTF) Chars	109
5.5.1 Effect of parent coal composition	109
5.5.1.1 Maceral Influences on Char Morphology	109
5.5.1.2 Effect of maceral composition on mean diameter, porosity and sphericity of Lithotype Series P5 and P6 Chars	114
5.5.2 Effect of pressure	115
5.5.2.1 Morphology of Lithotype Series P5 and P6 Chars	115
5.5.2.2 Effect of pressure on mean diameter, porosity and sphericity of Lithotype Series P5 and P6 Chars	122
5.6 Volatile Yield	122
5.7 Review	124
<b>6 PREDICTION OF CHAR PROPERTIES USING THE FULL COAL REFLECTOGRAM .....</b>	<b>126</b>
6.1 Introduction	126

6.2 Aims of Reflectogram Study	127
6.3 Measurement of the Full Coal Reflectogram	128
6.4 Characteristics and Analysis of the Full Coal Reflectogram	129
6.5 Correlation of Full Coal Reflectogram with Char Properties	134
6.5.1 Evaluation of High Pressure Pyrolysis Chars Prepared at 1100 °C and 1300 °C (Series 2-5) and Combustion Chars Prepared at 1100 °C and 1 atm (Series 1)	135
6.5.1.1 Correlation of coal properties with char geometry	136
6.5.1.2 Correlation of coal properties with char group proportions	140
6.6 Predictability of Char Properties	143
6.7 Review	148
<b>7 DISCUSSION AND CONCLUSIONS .....</b>	<b>151</b>
7.1 Conclusions from Whole Coal Studies	151
7.1.1 Effect of coal rank and petrography	151
7.1.1.1 Coal rank and char morphology	151
7.1.1.2 Coal petrography and char morphology	151
7.1.2 Effect of furnace pressure	152
7.1.3 Effect of furnace temperature	153
7.2 Prediction of volatile yield and burnout	153
7.3 Conclusions from Lithotype Studies	153
7.3.1 Effect of coal petrography	153
7.3.2 Effect of furnace pressure	154
7.3.3 Prediction of volatile yield	155
7.4 Conclusions from Reflectogram Studies	155
7.4.1 Relationships to char properties	155
7.4.2 Predictability of char properties from the full coal reflectogram	155
7.5 Implications for Coal Reactivity Modelling	156
7.6 Recommendations for Future Work	157
<b>REFERENCES .....</b>	<b>159</b>
<b>APPENDIX I.....</b>	<b>172</b>
<b>APPENDIX II.....</b>	<b>175</b>
<b>APPENDIX III.....</b>	<b>179</b>
<b>APPENDIX IV .....</b>	<b>189</b>
THE LOW RANK CRC PRESSURISED DROP TUBE FURNACE	189
Furnace Operation	189
<b>APPENDIX V .....</b>	<b>191</b>
<b>APPENDIX VI .....</b>	<b>193</b>

Publications resulting from this project	193
Journal Articles	193
Conference Papers	193
Prior Publications	194
Journal Articles	194
Conference Papers	195

## Table of Figures

Figure 1.1 Schematic representation of the main chemical reactions and physical changes during entrained flow gasification .....	4
Figure 2.1 Map of Eastern Australia showing coal basins and sample locations .....	26
Figure 2.2 Dry feed coal (a), prepared polished coal blocks (b), high pressure pyrolysis char (c) and prepared polished char mount.....	30
Figure 2.3 Schematic diagram of the pressurised drop tube furnace at the Low Rank CRC.....	32
Figure 3.1 Percentage of Series P1 char subtypes formed for each coal.....	53
Figure 3.2 Percentage of Group I, II and III Series P1 chars for each coal.....	54
Figure 3.3 Drayton char pyrolysed at 1100°C and 8 atm .....	56
Figure 3.4 Drayton char pyrolysed at 1100°C and 8 atm .....	56
Figure 3.5 Drayton char pyrolysed at 1100°C and 15 atm .....	56
Figure 3.6 Drayton char pyrolysed at 1100°C and 15 atm .....	56
Figure 3.7 Percentage of char types for Series P1 chars prepared at 1, 5, 8 and 15 atm pressure.....	57
Figure 3.8 Percentage of Group I, II and III Series P2 chars for each coal.....	60
Figure 3.9 Percentage of Series P2 char subtypes formed for each coal.....	62
Figure 3.10 Series P2 char mean diameters, porosity and sphericity .....	63
Figure 3.11 Correlation between telovitrinite and vitrite+clarite .....	64
Figure 3.12 Correlation between inertinite and inertinite-rich microlithotypes.....	64
Figure 3.13 Correlation between minerals and mineral-rich microlithotypes .....	65
Figure 3.14 Correlation of vitrite, liptite and clarite with Group I chars.....	65
Figure 3.15 Correlation of vitrinertite-V, vitrinertite-I, vitrinertite V=I & trimacerals with Group II chars....	66
Figure 3.16 Correlation of inertite and durite with Group III chars .....	66
Figure 3.17 Percentage of char subtypes for 1, 5, 8 and 15 atm furnace pressure chars. ....	67
Figure 3.18 Percentage of char types for Series C1 chars .....	70
Figure 3.19 Percentage of char groups for Series C1 chars.....	72
Figure 3.20 Char mean diameter, porosity and sphericity for Series C1 chars.....	73
Figure 3.21 Correlation of (vitrite, liptite + clarite) with Group I combustion chars. ....	74
Figure 3.22 Correlation of vitrinertite-V, vitrinertite-I, vitrinertite V=I & trimacerals with Group II combustion chars .....	74
Figure 3.23 Correlation of (inertite + durite) with Group III combustion chars.....	74

Figure 4.1 Percentage of Group I, II and III Series P3 chars prepared at 5 atm and 1100 °C.....	85
Figure 4.2 Percentage of Group I, II and III Series P3 chars prepared at 10 atm and 1100 °C.....	85
Figure 4.3 Percentage of Group I, II and III Series P3 chars prepared at 15 atm and 1100 °C.....	86
Figure 4.4 Percentage of Groups I, II and III in Kogan Creek chars at 5,10 and 15 atm and 1100 °C. ....	88
Figure 4.5 Percentage of char subtypes prepared from Kogan Creek coal at 5,10 and 15 atm and 1100 °C ...	90
Figure 4.6 Percentage of Groups I, II and III in Fassifern chars prepared at 5,10 and 15 atm and 1100 °C....	90
Figure 4.7 Percentage of char subtypes prepared from Fassifern coal at 5,10 and 15 atm and 1100 °C.....	92
Figure 4.8 Percentage of Groups I, II and III in Lithgow chars prepared at 5,10 and 15 atm and 1100 °C.....	93
Figure 4.9 Percentage of char subtypes prepared from Lithgow coal at 5,10 and 15 atm and 1100 °C. ....	93
Figure 4.10 Percentage of Groups I, II and III in Jellinbah chars prepared at 5,10 and 15 atm and 1100 °C..	94
Figure 4.11 Percentage of char subtypes prepared from Jellinbah coal at 5,10 and 15 atm and 1100 °C.....	95
Figure 4.12 Percentage of Group I, II and III Series P4 chars prepared at 5 atm and 1300 °C.....	96
Figure 4.13 Percentage of Group I, II and III Series P4 chars prepared at 10 atm and 1300 °C.....	96
Figure 4.14 Percentage of Group I, II and III Series P4 chars prepared at 15 atm and 1300°C.....	97
Figure 4.15 Percentage of Groups I, II and III in Kogan Creek chars at 5,10 and 15 atm and 1300 °C .....	100
Figure 4.16 Percentage of char subtypes from Kogan Creek coal at 5,10 and 15 atm and 1300 °C .....	100
Figure 4.17 Percentage of Groups I, II and III in Fassifern chars at 5,10 and 15 atm and 1300 °C.....	101
Figure 4.18 Percentage of char subtypes prepared from Fassifern coal at 5,10 and 15 atm and 1300 °C.....	101
Figure 4.19 Percentage of Groups I, II and III in Lithgow chars prepared at 5,10 and 15 atm and 1300 °C.	102
Figure 4.20 Percentage of char subtypes prepared from Lithgow coal at 5,10 and 15 atm and 1300 °C. ....	103
Figure 4.21 Percentage of Groups I, II and III in Jellinbah chars at 5,10 and 15 atm and 1300 °C.....	104
Figure 4.22 Percentage of char subtypes prepared from Jellinbah coal at 5,10 and 15 atm and 1300 °C.....	104
Figure 5.1 Percentage of Group I, II and III Series P5 and P6 chars prepared at 1 atm and 1300 °C.....	110
Figure 5.2 Percentage of Group I, II and III Series P5 and P6 chars prepared at 5 atm and 1300 °C.....	110
Figure 5.3 Percentage of Group I, II and III Series P5 and P6 chars prepared at 10 atm and 1300 °C.....	112
Figure 5.4 Percentage of Group I, II and III Series P5 and P6 chars prepared at 15 atm and 1300 °C.....	112
Figure 5.5 Mean diameter, porosity and sphericity of Series P5 and P6 chars prepared at 1,5, 10 and 15 atm and 1300 °C versus vitrinite content.....	114
Figure 5.6 Percentage of Groups I, II and III in Dull lithotype chars at 1, 5, 10 and 15 atm and 1300 °C ....	116
Figure 5.7 Percentage of char subtypes from the Dull lithotype at 1, 5, 10 and 15 atm and 1300 °C.....	116
Figure 5.8 Percentage of Groups I, II and III in Dull-banded lithotype chars prepared at 1, 5, 10 and 15 atm and 1300 °C. ....	118
Figure 5.9 Percentage of char subtypes prepared from the Dull-banded lithotype at 1, 5, 10 and 15 atm and 1300 °C.....	118
Figure 5.10 Percentage of Groups I, II and III in Banded lithotype chars prepared at 1, 5, 10 and 15 atm and 1300 °C.....	119
Figure 5.11 Percentage of char subtypes prepared from the Banded lithotype at 1, 5, 10 and 15 atm and 1300 °C.....	119
Figure 5.12 Percentage of Groups I, II and III in Bright-banded lithotype chars prepared at 1, 5, 10 and 15 atm and 1300 °C. ....	120

Figure 5.13 Percentage of char subtypes prepared from the Bright-banded lithotype at 1, 5, 10 and 15 atm and 1300 °C.....	120
Figure 5.14 Percentage of Groups I, II and III in Bright lithotype chars prepared at 1, 5, 10 and 15 atm and 1300 °C.....	121
Figure 5.15 Percentage of char subtypes prepared from the Bright lithotype at 1, 5, 10 and 15 atm and 1300 °C.....	121
Figure 5.16 Mean diameter, porosity and sphericity of Series P5 and P6 chars prepared at 1, 5, 10 and 15 atm and 1300 °C versus char preparation pressure.....	122
Figure 5.17 Mean diameter, porosity and sphericity of Series P5 and P6 chars prepared at 1,5, 10 and 15 atm and 1300 °C versus volatile yield.....	123
Figure 5.18 Proportion of Group I, Group II and Group III Series P5 and P6 chars prepared at 1,5, 10 and 15 atm and 1300 °C versus volatile yield.....	123
Figure 6.1 Plot of maximum vitrinite reflectance, volatile yield and carbon content versus maximum reflectance for the three maceral groups.....	127
Figure 6.2 Manual full coal reflectogram of an Eastern Australian high volatile bituminous coal with approximately 60 % vitrinite content.....	129
Figure 6.3 Manual full coal reflectogram of a high vitrinite content Eastern Australian high volatile bituminous coal with approximately 80 % vitrinite content.....	130
Figure 6.4 Manual full coal reflectogram of a high inertinite Eastern Australian high volatile bituminous coal with approximately 30 % vitrinite content.....	131
Figure 6.5 Automated full coal reflectogram of an Eastern Australian high volatile bituminous coal plotted on the same reflectance scale as manual analyses and against cumulative frequency.....	133
Figure 6.6 Schematic illustration of the vitrinite reflectance distributions of coals.....	134
Figure 6.7 Mean diameter, porosity and sphericity of Series 2 and 3 pyrolysis and Series 1 combustion chars prepared at 1100 °C versus mean random telovitrinite reflectance.....	138
Figure 6.8 Mean diameter, porosity and sphericity of Series 2 and 3 pyrolysis and Series 1 combustion chars prepared at 1100 °C versus vitrinite content.....	138
Figure 6.9 Mean diameter, porosity and sphericity of Series 2 and 3 pyrolysis and Series 1 combustion chars prepared at 1100 °C versus full maceral reflectogram parameter.....	138
Figure 6.10 Mean diameter, porosity and sphericity of Series 4 and 5 chars prepared at 1300 °C versus mean random telovitrinite reflectance.....	139
Figure 6.11 Mean diameter, porosity and sphericity of Series 4 and 5 chars prepared at 1300 °C versus vitrinite content.....	139
Figure 6.12 Mean diameter, porosity and sphericity of Series 4 and 5 chars prepared at 1300 °C versus full maceral reflectogram parameter.....	139
Figure 6.13 Proportion of Group I, Group II & Group III Series 2 & 3 pyrolysis & Series 1 combustion chars prepared at 1100 °C vs. mean random telovitrinite reflectance.....	141
Figure 6.14 Proportion of Group I, Group II & Group III Series 2 & 3 pyrolysis & Series 1 combustion chars prepared at 1100 °C vs. vitrinite content.....	141

Figure 6.15 Proportion of Group I, Group II & Group III Series 2 & 3 pyrolysis & Series 1 combustion chars prepared at 1100 °C vs. full maceral reflectogram parameter.....	141
Figure 6.16 Proportion of Group I, Group II and Group III Series 4 and 5 chars prepared at 1300 °C versus mean random telovitrinite reflectance.....	142
Figure 6.17 Proportion of Group I, Group II and Group III Series 4 and 5 chars prepared at 1300 °C versus vitrinite content.....	142
Figure 6.18 Proportion of Group I, Group II and Group III Series 4 and 5 chars prepared at 1300 °C versus full maceral reflectogram parameter.....	142
Figure 6.19 Comparison between predicted and experimental proportions of Group I chars formed at 1, 5, 10 and 15 atm and 1300 °C.....	148

## Table of Tables

Table 1.1 Combustion and gasification process conditions .....	2
Table 1.2 Differences between combustion and gasification .....	8
Table 2.1 Coal samples and char preparation series .....	28
Table 3.1 Proximate, maceral, microlithotype and mean random telovitrinite reflectance data.....	38
Table 3.2 Char classification system.....	41
Table 3.3 Summary of various char morphology classification systems.....	43
Table 3.4 Char morphology and volatile yield for Series P1 chars .....	52
Table 3.5 Coefficients of determination, $r^2$ , for Series P1 chars .....	55
Table 3.6 Char morphology and volatile yield for Series P2 chars .....	58
Table 3.7 Coefficients of determination, $r^2$ , for Series P2 high pressure pyrolysis chars.....	61
Table 3.8 Coefficients of determination, $r^2$ , of macerals vs. microlithotypes.....	64
Table 3.9 Coefficients of determination, $r^2$ , for Series P2 chars .....	68
Table 3.10 Char morphology and burnout for Series C1 chars .....	69
Table 3.11 Coefficients of determination, $r^2$ , for Series C1 chars.....	71
Table 3.12 Summary of differences between combustion chars and their high pressure pyrolysis analogues .	76
Table 3.13 Coefficients of determination for correlation between burnout & pyrolysis char characteristics...	77
Table 4.1 Sample proximate, maceral, microlithotype and mean random telovitrinite reflectance data .....	81
Table 4.2 Char morphology for Series P3 chars. ....	84
Table 4.3 Coefficients of determination, $r^2$ , for Series P3 chars. ....	87
Table 4.4 Char morphology for Series P4 chars. ....	98
Table 4.5 Coefficient of determination, $r^2$ , for Series P4 chars .....	99
Table 5.1 Proximate analysis, mean feed diameter, maceral contents, and mean random telovitrinite reflectance for each lithotype.....	108
Table 5.2 Char morphology for Series P5 (PDTF) and P6 (DTF) chars.....	113
Table 5.3 Coefficients of determination for correlation between parent coal vitrinite content, full maceral reflectogram parameter, and the proportion of Group I chars.....	114

Table 5.4 Coefficients of determination for correlation between char volatile yield at each furnace pressure and properties of the parent coal.....	124
Table 6.1 Full maceral reflectogram parameter, vitrinite content and mean telovitrinite reflectance for Pyrolysis Series 2-5 samples and Combustion Series 1 samples .....	135
Table 6.2 Regression coefficients for mean telovitrinite reflectance, vitrinite content and FMRP for Pyrolysis Series 3-5 samples prepared at 5 atmospheres furnace pressure.....	143
Table 6.3 Regression coefficients for mean telovitrinite reflectance, vitrinite content and FMRP for Pyrolysis Series 3-5 samples prepared at 10 atmospheres furnace pressure.....	145
Table 6.4 Regression coefficients for mean telovitrinite reflectance, vitrinite content and FMRP for Pyrolysis Series 3-5 samples prepared at 15 atmospheres furnace pressure.....	146
Table 6.5 Equations for correlations of vitrinite content and FMRP with Group I % for Pyrolysis Series 3-5 samples prepared at 1300 °C and 5-15 atm furnace pressure .....	147
Table 6.6 Range of usefulness of various parameters for prediction of daughter char properties.....	150

## Glossary, Abbreviations and Symbols

ad or a.d.	Air-dried basis of analysis.
anisotropic	Coal or coke showing directional changes in optical reflectance due to rearrangement of carbon structural units by pressure or heating.
anthracite	Very high rank coal with a carbon content of circa 91 % in vitrite and a volatile matter content of less than 8 % (daf).
ash	The sum of the inorganic matter and the minerals in the coal as determined by proximate analysis (AS1038.3).
bituminous coal	A type of coal between subbituminous coal and semianthracite, including thermal and coking coals.
burnout	Degree of consumption of combustible material in the raw fuel, as a percentage. Percentage burnout is calculated using the ash tracer technique (Chapter 2.7).
Carboniferous	Period of the Geological Time Scale from about 360 million years before present to about 286 million years before present. Named for the rich coal deposits formed in many parts of the Northern Hemisphere during this time.
carbonisation	The heating of coal in the absence of oxygen to produce a carbon-rich solid (e.g. char) and liquid or gaseous products (e.g. coal gas, tars).
char	The completely or partially devolatilised product remaining after pyrolysis of pulverised coal.
clarain	A coal lithotype that has a semi-bright, shiny lustre, is finely laminated, with smooth or irregular fracture and has banding parallel to bedding (Allaby and Allaby, 1990).
coke	The solid formed by carbonisation of coal lumps above 900 °C and utilised in steel making.
combustion	Rapid reaction of coal with oxygen producing heat and light.

		Complete combustion yields CO <sub>2</sub> , H <sub>2</sub> O, N <sub>2</sub> , SO <sub>x</sub> and ash as the primary products. Incomplete combustion yields CO, hydrocarbons, tars and carbonaceous residues.
daf or d.a.f.		dry, ash free basis of analysis, without surface water or ash
db or d.b.		dry basis of analysis, without surface water
devolatilisation		Removal of volatile (gaseous and liquid) matter from coal by heating.
dmmf d.m.m.f.	or	dry, mineral matter free basis of analysis, without surface water or mineral matter
DTF		drop tube furnace
durain		A coal lithotype which is grey to brownish-black, banded, dull, with a granular and rough surface. Durain is harder than vitrain and more common (Allaby and Allaby, 1990).
EFR		entrained flow reactor
exinite		see "liptinite"
FC		proximate analysis fixed carbon
fixed carbon		The difference between the initial mass and the sum of the volatile matter, ash and moisture content as determined by proximate analysis.
fly ash		Fine inorganic and mixed organic/inorganic particles produced by solid fuel combustion and suspended in the flue gases.
FMRP		Full maceral reflectogram parameter
fuel ratio		Ratio of proximate analysis fixed carbon to volatile matter, used as a classification parameter.
fusain		A coal lithotype which is sooty black, with a silky lustre; it is fibrous and friable like charcoal (Allaby and Allaby, 1990).
fusibility		The capability of coal components to soften and reharden during heating. Fused chars may show vesicles due to degassing, rounding

	of angular edges and development of anisotropy.
gasification	Reaction of organic material with steam and air or oxygen to produce gaseous fuels (e.g. syngas).
Gondwana(n) coals	Coals found in rocks that were part of the Gondwana supercontinent (i.e. Australian, Indian, South African and Antarctic coals formed during the Permian period).
graphitisation	Development of a microstructure dominated by clusters of aromatic layers similar in structure to graphite.
heterogeneous combustion	Reaction of a solid (char, coke) with a gas (oxygen, steam, carbon dioxide) that causes oxidation of the carbon in the solid.
homogeneous combustion	Reaction of gases evolved from coal or char with oxidising gases.
IGCC	Integrated Gasification Combined Cycle.
inertinite	The name of the maceral group containing fusinite, inertodetrinite, macrinite, micrinite, sclerotinite and semifusinite. These macerals are relatively high in carbon due to partial oxidation during the coalification process.
isotropic	Material that shows no visible ordering of optical texture under reflected light.
lignite	Low rank coals characterised by high bed moisture (30-75 % ash free) and volatile matter (60-70 % d.a.f.) contents and calorific values less than $19.3 \text{ MJ.kg}^{-1}$ .
liptinite	The name of the maceral group containing alginite, cutinite, liptodetrinite, sporinite and sporinite. These macerals are relatively high in hydrogen and volatiles.
lithotype	The name of the coal type (at hand specimen scale), qualitatively assessed and dependent on the original plant structure and coalification path. Types are clarain, durain, fusain and vitrain.
M	proximate analysis moisture

macerals	The microscopically recognisable components of the coal, defined by shape, reflectance, colour, fluorescence, anisotropy, hardness and association. Macerals do not have constant chemical compositions.
microlithotype	The name of the association of different macerals within a minimum area of 50 $\mu\text{m}$ . In this thesis, microlithotypes are determined for whole particles since most particles are smaller than 50 $\mu\text{m}$ in diameter. Types are vitrite, inertite, liptite (monomaceral), clarite, durite, vitrinertite (bimaceral), and trimacerite (trimaceral) depending on the macerals present.
mineral matter	The inorganic fraction of the coal, appearing as included mineral grains within the macerals and excluded mineral grains along fractures and veins within the coal.
moisture content	The amount of water bound to the coal that is released by heating during proximate analysis.
$\text{NO}_x$	Oxides of nitrogen produced during coal combustion.
P	pressure
p.f.	Pulverised fuel - coal ground to pass through a 200 mesh/75 $\mu\text{m}$ sieve, mean particle diameter is about 50 $\mu\text{m}$ .
PDTF	high pressure drop tube furnace
Permian	Period of the Geological Time Scale from about 286 million years before present to about 248 million years before present. Often noted for the extensive glaciation of the southern hemisphere during this time.
petrography	The systematic description and interpretation of rock textures and composition under the microscope and as hand specimens.
proximate analysis	A chemical analytical technique in which a coal sample is treated at various temperatures and under different atmospheres to determine the moisture content, volatile matter, ash and fixed carbon contents.
pyrolysis	Devolatilisation (usually in an inert atmosphere) of moisture, gases

and tars from p.f. particles during the first tens of milliseconds of residence time in a furnace.

$R_{ort}$	Mean random telovitrinite reflectance in oil
rank	A measure of the degree of coalification experienced by a coal. Indicates coal maturity in terms of chemical and physical properties.
reflectance	The percentage of light, incident perpendicular to the flat polished surface of a maceral, which is reflected from that surface. Rank determinations using reflectance are carried out upon telovitrinite due to the homogeneity of its reflectance at a particular level of coalification.
reflectance, maximum	The highest reflectance measured when a polished sample is rotated about an axis parallel to the path of the incident plane polarised light. The mean of the total is usually reported.
reflectance, random	The reflectance of a polished sample measured in unpolarised light without sample rotation. The mean of the total is usually reported.
residence time	The length of time a particle takes to pass through the hot zone of a furnace.
semianthracite	Coal between bituminous coal and anthracite in rank. Characterised by low volatile matter contents (8-13.9 % d.a.f.) and high mean random telovitrinite reflectances (about 1.9-2.7 %).
soot	Very fine deposits (10-50 nm in diameter), consisting mainly of carbon from the hydrocarbons that surround the coal particle during heat treatment.
SO <sub>x</sub>	Oxides of sulphur produced during coal combustion.
subbituminous coal	Coal between lignite and bituminous coal in rank, with calorific values between approximately 19.3 and 30.1 MJ.kg <sup>-1</sup> . Subbituminous coals do not show any caking properties.
telovitrinite	The vitrinite maceral most often used for rank determinations. Characterised by structure showing preserved cell walls, infilled cell

	cavities and reflectances lower than those of associated inertinites.
turbostratic	Arrangement of layers composed of aromatic carbon rings in stacks. The aromatic stacks are linked by aliphatic chains and non-aromatic groups that hamper further linkage of the stacks.
ultimate analysis	A chemical analytical technique that determines the quantity of elemental carbon, hydrogen, nitrogen, sulphur and oxygen (by difference) in a coal sample.
VM	proximate analysis volatile yield
vesicle	A void within char or coke formed by the expansion of evolved steam or gases.
vitrain	A coal lithotype which is black, with a brilliant, glassy lustre, conchoidal fracture, and cubic cleavage. It is clean and structureless (Allaby and Allaby, 1990).
vitritinite	The name of the maceral group containing tellinite (has visible cell structure), collinite (structureless) and various submacerals. Vitritinite reflectance increases with coal rank and is commonly used as a rank indicator.
volatile matter	The material lost during proximate analysis at high temperatures and under reducing conditions after the moisture content has been removed.

## Abstract

Drives to reduce carbon dioxide emissions and improve efficiency make pressurised gasification an attractive option in future coal utilisation technologies. Process conditions in pressurised gasification differ from conventional entrained flow combustion in pressure, atmosphere, peak temperature and heating rate, yet there is sparse literature concerning coal behaviour under pressurised conditions. Previous work suggests that bituminous coals can show enhanced plasticity at high pressures and this phenomenon may not be predicted by standard tests of coking properties.

Previous modelling of char reactivity and burnout in combustion and gasification has failed to take account of the petrographic variability of coals. Current work to improve the predictive capacity of these models requires evaluation of the effects of different macerals and of char preparation pressure on char behaviour. Prior studies of whole coals subjected to high pressure and high temperature conditions have shown that daughter char morphology is influenced by particle heating rate, the size distribution of the feed coal, furnace pressure, feed rate, coal rank and the parent coal petrography.

Chars were produced by pyrolysis at 1100 or 1300 °C and 1, 5, 8, 10 and 15 atm furnace pressure, and by combustion at 1100 °C and 1 atm furnace pressure, from a suite of East Australian bituminous coals. The characteristics of the chars and their parent feed coals were quantified using semi-automated image analysis, as well as petrographic, particle size and chemical analyses. Relationships between the morphology of the chars and properties of the parent coal and furnace pressure were established.

Daughter char morphology and volatile yield was found to be related to the petrographic composition of the parent feed coals, their full reflectance profiles and the char preparation pressure. Chars derived from vitrinite-rich lithotypes and those prepared under high pressure conditions show larger mean diameters, porosities, sphericities and proportions of porous char types. Volatile yield is related to the vitrinite content of the lithotype. A parameter derived from full coal reflectograms proves to be effective for prediction of char morphology and trends in volatile yield. The Carbon Burnout Kinetic model is improved in its predictive value by including parent coal vitrinite content as an input parameter and could be further improved by utilising the full coal reflectogram parameter.