CCSD Communiqué

FACTSHEET – Coal Matter Reactions in Gasification

Specification of a Gasification Test Procedure & Identification of Test Parameters and Assessment Tools

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One of the aims of the CCSD gasification research program is to identify key performance parameters and develop procedures allowing coals to be tested and assessed for their suitability for use in entrained-flow gasification. The mineral matter/slag aspect of such a test is reasonably advanced: coals can be tested for their 'slag viscosity' and, if deemed unsuitable, strategies can be developed to improve the coal's suitability [1, 2]. No such tests exist, however, for the carbon conversion aspect of coal gasification. This has been due to limited knowledge and data on which aspects of coal conversion are fundamentally and practically important, and a lack of accepted procedures, performance criteria, facilities and know-how to measure these parameters and relate them to gasification technology operations.

Test Parameters

CCSD research activities have determined that there are two key parameters than can be used to characterise coal conversion behaviour in entrained flow gasification: the **volatile yield** (which can be estimated from rapid pyrolysis measurements in the wire mesh reactor), and the **reactivity of the char** produced (which can be determined using high pressure intrinsic reactivity measurements using a TGA). Together, these data provide an indication of how a coal will perform relative to other coals for which similar data exist.

Interpreting these bench-scale data using measurements of **burnout levels, gas quality and char structural characteristics** obtained under more realistic high temperature conditions is also required. These measurements, made in the PEFR facility, allow more quantitative and comprehensive assessments of gasification performance to be made (see, for example, the PEFR data shown in **Figure 1**).

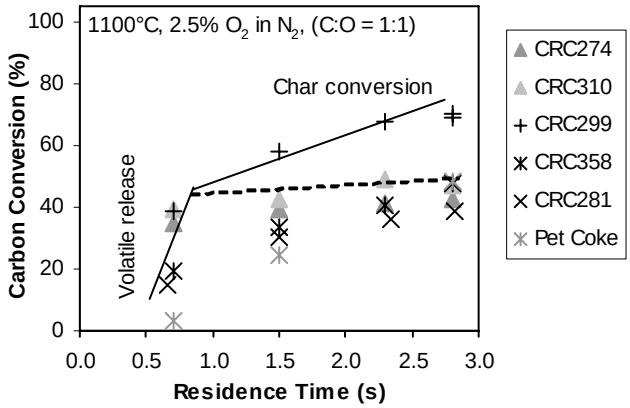

Figure 1: A selection of PEFR data depicting the relative roles of coal pyrolysis yields and char reaction rates in the overall process of coal conversion.

Coal Test Procedure

Based on determining the above coal performance properties, the current version of the test procedure comprises the following:

- Measurement of true volatile yields from pyrolysis at 1100°C, with a heating rate of 1000°C/s and a pressure of 20 bar, using the wire mesh reactor.
- Measurement of reaction rate of the char produced from the above WMR test with CO_2 and H_2O at 900°C and 800°C respectively, at pressures of 20 bar using the TGA. (Where possible, analysis of these data should be complemented with structural characterisation of the char.)
- Measurement of coal conversion behaviour and gas quality in the pressurised entrained flow reactor (PEFR) at 1400°C. Measurements would be made in a gas mix of $N_2/O_2/H_2O$ with a range of O:C stoichiometries and residence times. Depending on conversion levels achieved in the tests, molar O:C stoichiometries in the range 0.5-2.0 cover the relevant range for practical gasification applications. The maximum residence time available in the PEFR facility, whilst maintaining appropriate entrained flow conditions, is approximately 3 seconds. Therefore, it is not possible (or required) to achieve complete conversion for all coals under the full range of experimental conditions.

Results from these tests will give a ranking of coals in each of these key performance areas, which can be quantitatively assessed in reference to existing CCSD data.

At this stage, these data provide a relative indication of a coals likely gasification 'quality' rather than a quantitative index which can be used to definitively assess coals. To extend the current work to achieve such an outcome will require 'calibration' of this laboratory based work with industrial gasification performance data so that impacts of the coal performance

parameters on operation and performance of larger-scale, more realistic gasification systems can be assessed. An important stage in the further development of coal test procedures and definition of appropriate performance criteria, therefore, is to obtain reference data from pilot and, ultimately, full-scale gasification facilities.

An example of the relative rankings of the CCSD coals on the basis of conversion under reference PEFR conditions (1100°C and 1400°C) is shown in Table 1.

			Carbon Conversion in PEFR Test (%)			
Coal	Proximate VM (%daf)	VY (%daf) from WMR	1100°C	1400°C	1100°C + Steam	1400°C + Steam
CRC281	10.5	1.2	41.9	46.9	18.6	
CRC358	24.4	19.9	44.0	56.1		
CRC310	30.2	27.3	54.6			
CRC284	32.2	30.1	41.9			
CRC274	32.6	26.2	55.7	66.0	29.6	48.7
CRC298	34.8	32.4	51.8	61.2		
CRC240	35.5	33.5	52.4			
CRC263	35.7	34.1	50.8	70.7	24.8	
CRC296	35.9	34.7	48.6	95.7		
CRC283	36.7	36.3	48.5			
CRC299	38.0	32.3	72.8	100	32.9	78.9
CRC272	40.6	40.3	49.8			
CRC252	49.9	50.7	65.1	100	37.3	73.4

Table 1: Volatile Yield (VY) from high heating rate wire mesh reactor measurements (15 bar 1000°C/s, 1100°C) and carbon conversion (%) of CCSD coals in the PEFR at 20 bar, close to 100% stoichiometry (~1:1 O:C) and with a residence time of ~2.7 s.

Assessment Tools

A model of the gasification process, combined with a system or process model of an IGCC plant, will allow the above data to be used to assess coal performance in gasification systems.

These models are the subject of current CCSD research. For predictive models to be developed and ultimately validated, and for such tools to have a troubleshooting/problem solving ability, detailed reaction rate data for each of the key gasification reactions will be required. This is the subject of the current program associated with the PEFR and bench-scale facilities that will take this work beyond the comparative base established in the initial investigations.

Requirements for Future Work: Validation and Application

When bench-scale volatile yield and rate data are considered in conjunction with conversion and gas composition data obtained from the PEFR measurements, they provide a means by which the relative performance of a specific coal can be estimated in terms of burnout efficiency and gas quality [3]. Whilst it is clear from this work which aspects of coal conversion under gasification conditions are important, the impact of these parameters on the overall performance of a gasification system is not yet quantifiable. In order to apply these findings to more quantitative assessments of coal gasification behaviour, data obtained under true gasification conditions are required.

An important stage in the further development of coal test procedures and definition of appropriate performance criteria, therefore, is to obtain reference data from pilot and, preferably, full-scale gasification facilities. A proposal to conduct the first pilot scale evaluation of a suite of Australian coals using an existing (international) pilot scale gasification facility has been developed. This program seeks to provide key reference data for definition of appropriate coal test parameters and for the development and validation of coal gasification performance models. Such data will provide the means to identify important links between current CCSD research and the application of the outcomes to real gasifier performance assessment requirements.

References

1. J H Patterson. *Evaluation of the slag flow characteristics of Australian bituminous coals in slagging gasifiers,* Final Report for ACARP Project C7052 (2000).
2. J H Patterson and T Do. *Survey of the Suitability of Export Thermal Coals for IGCC Use,* Final Report for ACARP Project C12056 (2004).
3. D J Harris, D G Roberts and D G Henderson. *Gasification Behaviour of Australian Coals at High Temperature and Pressure,* 21st Annual International Pittsburgh Coal Conference, Osaka, Japan (2004).

Further Reading and Information

Listed here are relevant publications (CCSD reports, journal articles, conference papers etc) which describe in some detail the work performed as the basis of this 'fact sheet'.

Development of bench-scale techniques (WMR, TGA etc):

D J Harris, D G Roberts, C J Mill, M D Kelly, Y Otake and T F Wall (1999). *Development of Bench-Scale Techniques for Coal Reactivity Characterisation at Elevated Pressure,* Final Report for ACARP Project C6052, CRC for Black Coal Utilisation.

D J Harris, D G Roberts, C J Mill and J F Stubington (1999). *High Intensity Gasification: Investigating Coal Reactivity Using Bench Scale Techniques*, CHEMECA '99: Coal Special Session, Newcastle.

Fundamental investigations of pyrolysis, char reactions, etc:

C J Mill, D J Harris and J F Stubington (1998). *Pyrolysis of Fine Coal Particles at High Heating Rates and High Pressure*, 8th Australian Coal Science Conference, Sydney.

D G Roberts and D J Harris (2000). *Char Gasification with O_2, CO_2 and H_2O: Effects of Pressure on Intrinsic Reaction Kinetics*, Energy & Fuels 14(2), 483-489.

D G Roberts, D J Harris and T F Wall (2000). *Total Pressure Effects on Chemical Reaction Rates of Chars in O_2, CO_2 and H_2O*, Fuel 79(15), 1997-1998.

D G Roberts, D J Harris and T F Wall (2003). *On the Effects of High Pressure and Heating Rate during Coal Pyrolysis on Char Gasification Reactivity*, Energy & Fuels 17(4), 887-895.

Measurement of gasification parameters of coals (bench scale):

D J Harris, M D Kelly and D G Roberts (2002). *Reactivity Characterisation of Australian Coals for use in Advanced Technologies*, CRC for Black Coal Utilisation Research Report 35.

D G Roberts and D J Harris (2004). *Bench-Scale Assessment of International Coals for use in Gasification,* CCSD Project 3.1 Task 2 Milestone Report (CSIRO Report Number ET/IR685).

Measurements of gasification behaviour of coals (PEFR scale):

D J Harris, D G Roberts and D G Henderson (2003). *Gasification Behaviour of Australian Coals,* Final Report for ACARP Project C9066.

D J Harris, D G Roberts and D G Henderson (2003). *Gasification Behaviour of Australian Coals*, 12th International Conference on Coal Science, Cairns, Queensland, Australia.

D J Harris, D G Roberts and D G Henderson (2004). *Gasification Behaviour of Australian Coals at High Temperature and Pressure*, 21st Annual International Pittsburgh Coal Conference, Osaka, Japan.