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# DERIVATION OF THE SPECIFIC ENERGY OF VICTORIAN BROWN COAL FROM PROXIMATE AND ULTIMATE ANALYSES

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## ABSTRACT

Relationships between specific energy and proximate and ultimate analyses are derived for brown coal. The equation based on the ultimate analysis data provides the closest correspondence between the calculated specific energy and that measured directly by bomb calorimetry.

## INTRODUCTION

Specific energy is one of the most important properties of coal. It can be measured accurately by bomb calorimetry, but this method is time consuming. Many attempts have been made to relate the specific energy to the corresponding proximate and ultimate analysis data [1–4]. Equations exist for the calculation of coal specific energy [1–4], but few of these are relevant to brown coal. Due to its high volatile matter and moisture content, brown coal has a more complex matrix than higher rank coals. The properties of brown coal from different locations are quite different, and a specific energy equation needs to take these factors into account.

Ferguson and Rowe [2] have derived an equation relating the specific energy and proximate analyses for 23 samples of American lignites

$$Q_g = -2.26 \times 10^5/M + 108A + 297VM + 281FC \tag{1}$$

where $Q_g$ is the specific energy in Btu $\text{lb}^{-1}$, dry and ash-free basis, $M$ is the moisture content (%a.d.) *, $A$ is the ash content (%d.b.) *, $VM$ is the volatile matter content (%d.b.) and $FC$ is the fixed carbon content (%d.b.). This equation gave a standard deviation of ±1.2% from the corresponding bomb calorimetry measurements of the specific energy of these 23 lignite samples.

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* a.d., Air dried; d.b., dry basis.

King and Attwood [3] have derived an equation relating specific energy and ultimate analysis data specifically for brown coal

$$Q_{g,dry}(\mathrm{MJ\ Kg^{-1}}) = 0.3530[\mathrm{C}] + 0.8712[\mathrm{H}] + 0.0696[\mathrm{S}] - 0.0732[\mathrm{O}] \qquad (2)$$

where [C], [H], [S] and [O] are carbon, hydrogen, sulphur and oxygen content data. A set of 100 samples was tested with an average deviation $\%E_{av} = 0.80$ and maximum deviation $\%E_m = 2.92$.

In this report, eqns. (1) and (2) were used for the calculation of specific energy of Victorian brown coal. Also the relationships of specific energy with proximate and ultimate analyses data have been derived using a progressive linear regression program in FORTRAN. This program is based on a multi-variable least-squares fitting principle and has the ability to select the effective variables and ignore those variables of insignificant consequence. A set of 151 brown coal samples was investigated. Computing was carried out on a VAX 11/780 computer.

## RESULTS AND DISCUSSION

### *Specific energy from proximate analysis data*

Using eqn. (1), the specific energy of three Victorian brown coal samples was calculated and the results are listed in Table 1. It is apparent that eqn. (1) cannot be used in general for Victorian brown coal, as at least one negative $Q_{calc.}$ was obtained.

An equation relating specific energy to proximate analysis data derived by computer in the present work is

$$Q_{g,dry}(\mathrm{MJ\ Kg^{-1}}) = 443.9/M - 0.176A + 0.075VM + 20.33 \qquad (3)$$

where $Q_{g,dry}$ is the gross specific energy in (MJ $\mathrm{Kg^{-1}}$). For the samples of brown coal investigated, this equation yielded an average deviation

TABLE 1

Application of the Ferguson and Rowe equation [2] to the calculation of the specific energy of 3 samples of brown coal

| Sample | Proximate analysis | | | | $Q_{g,dry}$ (MJ $\mathrm{Kg^{-1}}$) | $Q_{calc.}$ (MJ $\mathrm{Kg^{-1}}$) | $\Delta Q$ | $\%E$ |
|---|---|---|---|---|---|---|---|---|
| | $M$ (%a.d.)[a] | $A$ (%d.b.)[b] | $VM$ (%d.b.)[b] | $FC$ (%d.b.)[b] | | | | |
| Morwell coal | 12.7 | 3.8 | 47.7 | 48.5 | 26.21 | 24.18 | −2.03 | 7.76 |
| Gelliondale coal | 7.3 | 5.4 | 49.9 | 44.7 | 25.99 | −6.95 | −32.94 | 126.7 |
| Loy Yang coal | 15.6 | 1.1 | 51.7 | 47.2 | 26.16 | 33.09 | +6.93 | 26.4 |

[a] Air dried.

[b] Dry basis.

TABLE 2

Specific energy from proximate analysis by eqn. (3)

| No. | Proximate analysis | | | $Q_{g,act.}$ (MJ $Kg^{-1}$) | $Q_{g,calc.}$ (MJ $Kg^{-1}$) | Deviation $E$ (MJ $Kg^{-1}$) | Relative $\%E$ |
|---|---|---|---|---|---|---|---|
| | Moisture (%d.b.) | Ash (%d.b.) | *VM* (%dmif) [a] | | | | |
| 1 | 164.6 | 0.9 | 48.1 | 26.28 | 26.46 | −0.18 | −0.70 |
| 2 | 180.1 | 1.0 | 51.6 | 25.95 | 26.48 | −0.53 | −2.02 |
| 3 | 171.7 | 1.0 | 51.3 | 25.72 | 26.57 | −0.85 | −3.32 |
| 4 | 153.8 | 4.4 | 46.6 | 25.95 | 25.92 | 0.03 | 0.11 |
| 5 | 137.5 | 3.7 | 53.1 | 27.42 | 26.87 | 0.55 | 1.99 |
| 6 | 130.4 | 3.2 | 47.2 | 27.49 | 26.70 | 0.79 | 2.88 |
| 7 | 170.3 | 2.3 | 50.4 | 26.28 | 26.30 | −0.02 | 0.07 |
| 8 | 166.0 | 2.3 | 50.6 | 26.55 | 26.38 | 0.17 | 0.64 |
| 9 | 167.4 | 2.0 | 48.5 | 27.20 | 26.25 | 0.95 | 3.48 |
| 10 | 153.8 | 2.2 | 52.4 | 26.02 | 26.75 | −0.73 | −2.79 |
| 11 | 121.7 | 1.1 | 56.9 | 26.81 | 28.04 | −1.23 | −4.57 |
| 12 | 122.2 | 4.0 | 47.7 | 28.24 | 26.82 | 1.42 | 5.02 |
| 13 | 104.9 | 3.5 | 48.1 | 25.56 | 27.54 | 1.98 | −7.72 |
| 14 | 222.6 | 1.4 | 48.0 | 26.19 | 25.67 | 0.53 | 2.01 |
| 15 | 204.9 | 1.4 | 47.3 | 26.53 | 25.79 | 0.75 | 2.81 |
| 16 | 179.3 | 1.1 | 54.1 | 26.42 | 26.66 | −0.24 | −0.89 |
| 17 | 177.8 | 1.6 | 50.1 | 26.52 | 26.29 | 0.23 | 0.87 |
| 18 | 157.1 | 1.1 | 52.4 | 26.32 | 26.88 | −0.56 | −2.12 |
| 19 | 244.8 | 1.3 | 49.5 | 25.86 | 25.61 | 0.25 | 0.95 |
| 20 | 111.9 | 4.3 | 48.2 | 29.31 | 27.14 | 2.17 | 7.40 |

[a] Mineral inorganic free.

$\%E_{av} = \pm 2.59$ and a maximum deviation $\%E_m = 8.27$. Some of the calculated results are listed in Table 2.

Proximate analysis can be easily and rapidly obtained either by the traditional method [5] or by the thermogravimetric method [6], and hence eqn. (3) provides a rapid route to specific energy. However, the accuracy of the calculation is not high because, for coal samples with similar proximate analysis data, the actual corresponding specific energy data are quite different.

## *Specific energy from ultimate analysis data*

The calculation of specific energy for the set of 151 samples investigated using King and Attwood's equation (eqn. (2)) gave an average deviation $\%E_{av} = \pm 0.926$ and a maximum deviation $\%E_m = 2.92$.

An equation obtained by computer in the present work which relates specific energy to ultimate analysis data is

$$Q_{g,dry} = 0.160[C] + 0.992[H] - 0.208[O] + 16.055 \qquad (4)$$

TABLE 3

Specific energy from ultimate analysis by eqn. (4)

| No. | Ultimate analysis (%dmif) | | | | | $Q_{g,act.}$ (MJ Kg$^{-1}$) | $Q_{g,calc.}$ (MJ Kg$^{-1}$) | Deviation $E$ (MJ Kg$^{-1}$) | Relative %$E$ |
|---|---|---|---|---|---|---|---|---|---|
| | C | H | N | S | O | | | | |
| 1 | 68.0 | 4.7 | 0.52 | 0.28 | 26.4 | 26.28 | 26.08 | 0.20 | 0.75 |
| 2 | 65.9 | 4.8 | 0.51 | 0.23 | 28.6 | 25.95 | 25.39 | 0.56 | 2.17 |
| 3 | 66.8 | 4.7 | 0.44 | 0.23 | 27.8 | 25.72 | 25.60 | 0.12 | 0.47 |
| 4 | 67.8 | 4.6 | 0.66 | 1.04 | 25.9 | 25.95 | 26.06 | −0.11 | −0.40 |
| 5 | 69.4 | 5.2 | 0.61 | 0.34 | 24.5 | 27.42 | 27.20 | 0.22 | 0.81 |
| 6 | 70.1 | 4.9 | 0.53 | 0.25 | 24.2 | 27.49 | 27.07 | 0.42 | 1.51 |
| 7 | 68.5 | 4.8 | 0.46 | 0.23 | 26.0 | 26.28 | 26.34 | −0.06 | −0.24 |
| 8 | 68.8 | 4.8 | 0.50 | 0.21 | 25.7 | 26.55 | 26.46 | 0.90 | 0.36 |
| 9 | 70.1 | 5.1 | 0.50 | 0.18 | 24.1 | 27.20 | 27.29 | −0.09 | −0.34 |
| 10 | 67.7 | 4.8 | 0.49 | 0.29 | 26.6 | 26.02 | 26.07 | −0.05 | −0.19 |
| 11 | 68.6 | 5.2 | 0.42 | 0.93 | 24.9 | 26.81 | 26.99 | −0.18 | −0.66 |
| 12 | 70.6 | 5.0 | 0.53 | 4.60 | 19.3 | 28.24 | 28.27 | −0.03 | −0.12 |
| 13 | 67.5 | 4.6 | 0.67 | 0.22 | 27.0 | 25.56 | 25.78 | −0.22 | −0.85 |
| 14 | 67.9 | 4.5 | 0.46 | 0.35 | 26.8 | 26.19 | 25.78 | 0.41 | 1.55 |
| 15 | 68.7 | 4.6 | 0.51 | 0.58 | 25.6 | 26.53 | 26.26 | 0.27 | 0.27 |
| 16 | 68.4 | 5.2 | 0.52 | 0.27 | 25.6 | 26.42 | 26.81 | −0.39 | −1.47 |
| 17 | 69.1 | 5.0 | 0.46 | 0.30 | 25.1 | 26.52 | 26.82 | −0.31 | −1.52 |
| 18 | 68.6 | 4.8 | 0.52 | 0.26 | 25.8 | 26.32 | 26.40 | −0.08 | −0.31 |
| 19 | 66.7 | 4.9 | 0.57 | 0.24 | 27.6 | 25.86 | 25.82 | 0.04 | 0.15 |
| 20 | 72.3 | 5.3 | 0.50 | 4.33 | 17.6 | 29.31 | 29.20 | 0.11 | 0.38 |

where [C], [H] and [O] are carbon, hydrogen and oxygen content data derived from the ultimate analysis (%dmif). The sulphur [S] and nitrogen [N] contents in ultimate analysis are negligible in this context. This equation gives $\%E_{av} = \pm 0.881$ and $\%E_m = -2.87$.

Some calculated specific energies as obtained from ultimate analysis data are shown in Table 3. The results as calculated from ultimate analysis data are much more accurate than those obtained from corresponding proximate analysis data. The average deviation is essentially three times less in the latter case.

The accuracy of eqn. (4) is similar to that of eqn. (2). However, the specific energy results derived from both of these equations cannot satisfy the Australian Standard AS1038, which is concerned with the methods for the analysis and testing of coal and coke. In Part 5.1—Gross Specific Energy of Coal and Coke—Adiabatic Calorimeters [7], the repeatability is defined as 0.10 MJ $\text{Kg}^{-1}$. In this context, the repeatability is defined as the maximum acceptable difference between duplicate determinations carried out in the same laboratory on the same sample and by the same operator. Hence the calculation of specific energy from proximate and ultimate analyses cannot replace the experimental determination of this parameter. However, these equations are useful for preliminary estimates of specific energy of coal samples.

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