

EVALUATION OF DATA ON HIGHER HEATING VALUES AND ELEMENTAL ANALYSIS FOR REFUSE-DERIVED FUELS

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ABSTRACT

Elemental analyses and higher heating values taken from ASTM Round Robin Testing of RDF-3 have been evaluated. The data base was composed of five rounds of tests with eight to twelve laboratories performing four tests each. We found that established formulas can be used to calculate higher heating values on a moisture free basis (HHV2) from elemental analyses. A comparison is made between several methods of calculating HHV2. The Dulong formula and Institute of Gas Technology formula can predict HHV2 to within 3%.

NOMENCLATURE

(all values are on a dry basis)

- A = mass percent ash
- C = mass percent carbon
- Cl = mass percent chlorine
- H = mass percent hydrogen
- N = mass percent nitrogen
- O = mass percent oxygen
- S = mass percent sulfur
- Q = higher heating value

INTRODUCTION

The calorific or higher heating value and elemental composition (C, H, O, N, S, and Cl) are important parameters needed for the characterization of refuse-derived-fuels (RDF). The Subcommittee on Energy (E-38.01) of the American Society for Testing and Materials (ASTM) Committee E-38 on Resource Recovery carried out a testing program on RDF in 1978 and 1979 to develop standard test methods for the characterization of RDF. The particular RDF studied has been designated RDF-3¹. Higher heating value and elemental composition were among the properties determined by a variety of testing laboratories. We have evaluated the data on the higher heating values and elemental compositions of RDF-3, and applied these data to established formulas for fossil fuels which treat the higher heating values as a function of elemental composition.

Dulong postulated in the early 1800s that the higher heating value of a sample can be determined from its elemental composition. Around 1900, the Dulong formula began to be used to provide an estimate of the

¹ RDF-3 is defined as a shredded fuel derived from municipal solid waste (MSW) which has been processed for the removal of metal, glass, and other entrained inorganic materials. Generally, this material has a particle size such that 95 wt% passes through a 5-cm (2-in.) square mesh screen.

higher heating value of a coal sample from its elemental composition. According to Dulong's formula, the heat of combustion of a sample equals the heat of combustion of its elements regardless of whether it passes through one or more oxidation states [1]. Put in mathematical form:

$$Q \text{ (MJ/kg)}^2 = 0.336 C + 1.418 H + 0.094 S - 0.145 O \quad (1)$$

where Q is the higher heating value, and C, H, S, and O are mass percents of the elements in the sample on a dry basis. Formula 1 has been used to evaluate coal [2] and fossil fuels [1] and has been shown to give results with a probable error not exceeding 2% [3].

Formulas such as Dulong's have been used to confirm the correctness of the ultimate analysis. With recent developments in elemental analyzers, it may be more convenient to obtain the elemental composition of the sample than the higher heating value. In some instances, a lab is not equipped with a bomb calorimeter but can carry out an elemental analysis. In this case, the elemental analysis could be used to calculate the higher heating value of the sample. When doubt exists regarding the reliability of a higher heating value, there is no substitute for a bomb calorimetric determination.

While RDF-3 has a different ratio of the elements than fossil fuels, they both contain mainly C, H, O, and S. Therefore, the applicability of the Dulong Formula to RDF-3 appeared very likely.

Dulong's formula has a number of different forms and coefficients for the contribution of heat from the elements. The coefficients in Eq. (1) make certain assumptions about the heat released from each of the elements. Carbon is assumed to be amorphous (charcoal) rather than the standard state of graphite. Even though the elemental composition is reported on a dry basis, for computational purposes all the oxygen in the sample is assumed to be bound in the form of water. This is reflected in the coefficients which assume that a portion of the total hydrogen is bonded to the oxygen and is not available for combustion. The equation assumes all the oxygen in the fuel ends up as water and that the oxygen in the carbon dioxide comes solely from the combustion air.

In actual samples, such as coal, the oxygen is present in a mixture of ether, hydroxyl, or carbonyl forms.

The oxidation states of the sample and the amount of each state will change the apparent heat of combustion of the elements and lead to heating value formulas with different coefficients than those in Eq. (1).

The importance of higher heating values to fossil fuels such as coal, shale oils, and fuel oils has inspired many to fine-tune Dulong-type formulas to obtain better calculated higher heating values. Four other formulas besides Dulong's are examined here for their prediction capabilities. There is the formula by Tillman which only uses carbon to predict higher heating values of wood [4]:

$$Q \text{ (MJ/kg)} = 0.437 C - 1.67 \quad (2)$$

We also tried the Lloyd and Davenport formula derived for fossil fuels [5]:

$$Q \text{ (MJ/kg)} = 0.3578 C + 1.1357 H + 0.059 N + 0.1119 S - 0.0845 O \quad (3)$$

and the formula by Boie [6]:

$$Q \text{ (MJ/kg)} = 0.3515 C + 1.1617 H + 0.06276 N + 0.1046 S - 0.1109 O \quad (4)$$

which both include terms for fuel nitrogen. The Institute of Gas Technology (IGT) derived a formula for coal which also takes the ash content, A, of a sample into account [7]:

$$Q \text{ (MJ/kg)} = 0.3417 C + 1.3221 H + 0.1232 S - 0.1198 (O + N) - 0.0153 A \quad (5)$$

In all these formulas the symbols C, H, O, and S are defined the same as for the Dulong formula and A and N represent the mass percent of ash and nitrogen in a moisture free sample, respectively.

There are still other formulas which were not used in this study. In one, the oxygen coefficient has been modified depending on the geological history of a coal sample [8]. In another, the higher heating value is determined by the total oxidizing valencies of the elements in the sample [9]. None of the above formulas were designed for RDF-3 but were either derived for or fitted to other types of fuel data.

The experimental section describes an evaluation of the round robin RDF-3 data to obtain representative values for each round. In the section on results, the averaged results are examined for similarities and dif-

² 1 MJ/kg = 430.21 Btu_{th}/lb (thermochemical basis).

1 MJ/kg = 429.92 Btu_{IT}/lb (International Steam Tables basis).

ferences between the rounds. Next, the higher heating values obtained by experiment are compared with the values predicted by the formulas using the reported elemental compositions. Finally, in the section on error analysis, we explain how well one can expect to compute higher heating values and which elements have the greatest importance.

EXPERIMENTAL

Source of Data

Domalski and Abramowitz [10] completed an evaluation of some of the properties of RDF-3 which were determined as part of the ASTM Subcommittee E-38.01 Round Robin³ Testing Program. The evaluation dealt with selected RDF-3 properties: total moisture, residual moisture, ash, and higher heating values. In addition to determining these properties, each laboratory performed an elemental analysis on each of the samples. The elemental analyses were not thoroughly examined and therefore not published. Those elemental analyses have been combined with the reported higher heating values, moisture contents, and ash contents to create the data base used in this study. All participating laboratories tested the samples using the same ASTM standard analytical methods designated for coal samples.

Three round robins were performed over a period of a year (1978–1979) and analyzed by 8 to 12 laboratories, as shown in the first three columns of Table 1. The last two columns are explained in the next section. The fluff or RDF-3 for the first and second rounds were prepared by the National Center for Resource Recovery (NCRR), Washington, D.C., and sent to each of the participating laboratories. The fluff or RDF-3 for the third round was prepared by Americology (Division of American Can Co.), Milwaukee, Wisconsin. Size reduction of the fluff to 0.5 mm particle size was carried out by each of the participating laboratories.

Doubts about the interlaboratory homogeneity of the sample which was milled to 0.5 mm particle size was of concern. Improvement in precision was sought from an interlaboratory reference or comparison sample prepared only by one selected laboratory. Table 1 notes the interlaboratory set of tests for the second and third round robins. For the second round robin, the sample

TABLE 1 ASTM SUBCOMMITTEE E-38.01 ROUND ROBIN TESTING PROGRAM

Round robin test	Period of study	Number of labs	Tests	
			Done	Used
First round	June, July 1978	8	32	16
Second round Interlaboratory	Dec. 1978, Jan. 1979	11 11	44 44	30 36
Third round Interlaboratory	May, June 1979	12 12	48 48	32 35

of RDF-3 from NCRR was shipped to Wisconsin Electric Power Co., Milwaukee, Wisconsin, for milling to 0.5 mm particle size. The milled sample was then sent to each of the participating laboratories for analysis. Similar preparation was done for the third round except the sample prepared by Americology was shipped to Oak Ridge National Laboratory, Oak Ridge, Tennessee, for milling and distribution.

Each of three round robins can be viewed as a set of similar samples with the interlaboratory samples being sets identical to the corresponding round robin samples. Each participating laboratory made two sets of measurements on two different days for a total of four. Under ideal circumstances, all tests by the laboratories should have given exactly the same results. Assuming that the analysis errors were comparable to those found in coal analysis, that overall precisions for the analysis of refuse-derived-fuels were found to be much larger than the corresponding precisions for coal samples.

Data Consistency

The results from the round robin tests came from various laboratories with different degrees of experience and proficiency in preparing representative samples and making measurements. The small sample sizes used to determine the elemental composition of RDF-3 are particularly dependent on a laboratory's ability to prepare representative test samples. From time to time during the evaluation, questions arose regarding the consistency of the data. Fortunately, the method of determining the mass percent of the components requires the total mass percent to add up to exactly 100. By checking the total mass percent of a sample, called the mass accountability check, one has an independent test of the consistency of the data.

All but one of the elements, oxygen, were determined by laboratory test measurements. Oxygen was defined as the missing mass such that the sum of all components totalled 100% in the testing protocols.

³ A series of tests carried out by several laboratories to evaluate the accuracy, precision, and overall acceptability of a test procedure which determines a given property for a specific sample.

$$100 = A + C + H + O + N + S + Cl \quad (6)$$

Because of the definition of the amount of oxygen in the sample, failure of the data to satisfy Eq. (6) indicated some kind of inconsistency in the data. That is, the laboratories were not reporting values according to the testing protocol.

The mass accountability check was made using mass percents to two decimal places. The results of the check could be classified into five different cases. First, the sum of the elemental mass percents totalled 100. Second, transcription errors were indicated by a difference of one unit in one of the digits. Third, an excess amount of mass was present equal to the chlorine mass percent. This indicated the reported oxygen values neglected the chlorine. Fourth, small deviations (less than 1%) were present but of unknown origin. These errors were possible from rounding errors or minor errors in calculation. Lastly, large errors (usually near the value of the reported moisture content of the sample) were found.

The mass accountability check gave indications of which labs were at least doing their arithmetic correctly and those laboratories which were having problems. Some of the errors observed were correctable while others made the data unusable. Unusable data were eliminated.

Data Corrections and Elimination

Obvious transcriptional errors were corrected by examining the four measurements made of each component. The typographical errors were usually indicated by an outlier in one of the components. The number in error was changed to make the mass sum closer to 100. While this error was obvious for errors in the tens or units place, for the decimal places the error was usually considered acceptable (less than 1% error in total mass).

The neglect of chlorine error was accommodated by subtracting the chlorine mass percent from the reported oxygen value. Small errors (less than about 2%) were neglected and considered acceptable while the large errors were considered not acceptable and the corresponding test data were dropped from further analysis.

After the data sets were corrected or eliminated for errors found by mass accountability checks, a closer look was focused on outliers. Only the major components (HHV², carbon, hydrogen, and oxygen) were

checked separately in each of the round robin tests for outliers. Outliers were defined as values which did not lie within roughly plus or minus 2.5 standard deviations (98% confidence level) of the component's mean value. The 98% confidence interval eliminated the extreme results which would interfere with this study. Since the analyses were performed on subsamples of the same large sample, significant deviations from the mean value of the results were classified as outliers.

The last two columns of Table 1 show the number of tests done in the round and how many of the tests were used for computing the "true" composition of the round robin sample. In the first round of testing, half of the tests had to be discarded before a self-consistent set of representative values were found. For the second and third rounds over half of the tests were self-consistent. The interlaboratory results for the second and third rounds showed an improvement in the number of consistent results.

RESULTS

The data from each of the round robin tests were considered a distribution of measurements which represented the true values of the round. Being a distribution, the mean value can be taken as the true value of the sample and the standard deviation a measure of how well the true value is known. Table 2 lists the average value and 95% confidence intervals for each of the components for the various round robins.

Most of the average values for the various components agree, within experimental error, between the round robins. This is surprising since the RDF-3 was taken from different geographic locations at different times of the year. One exception is the moisture content where the interlaboratory results are smaller than the standard round robin results. This is explained by the drying of the interlaboratory samples before milling, so the low moisture contents represent the residual moisture in the samples. Another notable feature in the moisture data is the 14.0% error in round robin 3. This is caused primarily by four low moisture contents (less than 11%) reported by one laboratory. Since the moisture content of a sample is so dependent on its handling and storage, moisture was not used as a criteria for data consistency.

The ash content of the samples are identical for all round robins at the 95% confidence level except for round robin 2, which has an unusually low value. Since the ash content of a sample can also vary over a wide range, it was not used as a selection criteria for data consistency.

² Higher heating value on a dry basis.

TABLE 2 COMPARISON OF RDF-3 PROPERTIES BETWEEN ROUND ROBINS, AVERAGE VALUES, AND 95% CONFIDENCE INTERVALS

Component	Round Robin				
	1	2	2I	3	3I
HHV1 (MJ/kg) ^a	14.9 ± 1.3	15.2 ± 1.3	17.1 ± 0.4	12.6 ± 2.5	17.1 ± 0.5
HHV2 (MJ/kg)	17.4 ± 1.5	18.5 ± 0.7	17.7 ± 0.5	17.4 ± 1.1	17.1 ± 0.5
Moisture (%)	14.2 ± 1.1 ^b	17.9 ± 6.4 ^b	3.0 ± 1.1 ^c	27.9 ± 14.0 ^b	4.4 ± 1.0 ^c
Ash (%)	22.0 ± 3.5	14.6 ± 2.8	19.8 ± 1.8	21.4 ± 4.0	21.8 ± 3.4
C (%)	42.3 ± 0.9	44.6 ± 1.7	42.4 ± 0.7	42.3 ± 1.8	41.7 ± 1.7
H (%)	5.9 ± 0.5	5.9 ± 0.4	5.7 ± 0.3	5.8 ± 0.3	5.6 ± 0.4
O (%)	28.7 ± 3.5	33.9 ± 2.4	30.4 ± 2.5	29.0 ± 3.3	29.0 ± 3.0
N (%)	0.5 ± 0.1	0.4 ± 0.1	0.6 ± 0.2	0.8 ± 0.1	0.8 ± 0.1
S (%)	0.1 ± 0.1	0.1 ± 0.1	0.3 ± 0.1	0.5 ± 0.2	0.5 ± 0.2
Cl (%)	0.4 ± 0.2	0.4 ± 0.2	0.6 ± 0.2	0.6 ± 0.5	0.5 ± 0.3
Total mass ^d (%)	100.0 ± 0.7	99.8 ± 0.9	99.8 ± 2.0	100.4 ± 1.4	99.9 ± 1.9

a. 1 MJ/kg = 430.21 Btu_{th}/lb (thermochemical basis)

1 MJ/kg = 429.92 Btu_{IT}/lb (International Steam Tables basis)

b. The moisture is given on an as received basis and represents the total moisture in the initial sample.

c. The moisture represents the residual moisture of the milled sample received by each of the laboratories.

d. The sum of the components (ash, C, H, O, N, S, and Cl) for each test in a round.

The HHV1 (higher heating value on an as-received basis) values show a fair amount of scatter but can be explained by the variability of ash and moisture content of the samples. The somewhat larger HHV2 value for round robin 2 reinforces our observation that the low ash content seen in that round is real. However, the HHV2 values are the same for all round robins within experimental error. The similarities in HHV2 values may be a coincidence since the ash contents of all except the second round robin are so similar.

The elemental analyses of the samples show that the major components are carbon, hydrogen, and oxygen. All elemental mass percents agree within experimental error. The oxygen content has the highest error margin since it is dependent on all the other components. Nitrogen, chlorine, and sulfur are present in minor amounts and total to only one or two mass percent on a dry basis.

The total mass percent given in the last row of Table 2 shows confidence intervals range from 1% to 2% but averages are near 100%. Since the average does not

equal 100% exactly, it indicates some of the laboratories did not account for all the mass.

In order, carbon, oxygen, and hydrogen account for nearly all the combustible material on a mass basis. However, when we take the atomic weights of the elements into consideration, the order becomes hydrogen, carbon, and oxygen. If we take the ratio of the number of moles of the elements relative to carbon, then we determine the empirical formula of RDF-3 as shown in Table 3.

As seen in the elemental analyses, the empirical formulas of the RDF-3 samples are the same for all the round robins on a dry basis. The empirical formulas are identical on an ash free basis since the formula is defined as the ratio of the elements. For comparison, three other constituents which are surely present in RDF-3 are given at the end of the table along with their corresponding higher heating values. The empirical formula of RDF-3 is similar to that of cellulose except not as rich in oxygen. The higher heating value of RDF-3 is the same as that of cellulose, but this is

TABLE 3 COMPARISON OF C, H, AND O EMPIRICAL FORMULAS AND HIGHER HEATING VALUES

	Empirical Formula			Heating Value
	C	H	O	HHV2 (MJ/kg) ^a
Round Robin 1	1	1.65 ±0.14	0.51 ±0.07	17.4 ± 1.5
Round Robin 2	1	1.58 ±0.09	0.57 ±0.05	15.5 ± 0.7
Interlaboratory	1	1.59 ±0.07	0.54 ±0.04	17.7 ± 0.5
Round Robin 3	1	1.63 ±0.11	0.52 ±0.06	17.4 ± 1.1
Interlaboratory	1	1.60 ±0.08	0.52 ±0.05	17.1 ± 0.5
Cellulose	1	1.67	0.83	17.3
Lignin	1	1.20	0.42	24.7
Polyethylene	1	2	0	46.3

a. 1 MJ/kg = 430.21 Btu_{ch}/lb (thermochemical basis)
 1 MJ/kg = 429.92 Btu_{IT}/lb (International Steam Tables basis)

merely a coincidence since cellulose has no ash. If we use 80% of the cellulose higher heating value (to account for the 20% ash in RDF-3), then we see that the higher heating value of RDF-3 is higher than that possible from cellulose alone as the combustible material. Lignin (a major component of wood) and polyethylene (a common plastic) both have larger heating values and lower oxygen contents than our samples and are two of many RDF-3 constituents which might account for the observed values.

The observed higher heating values (HHV2) are compared with those calculated by five formulas and the results are given in Table 4. The upper half of the table contains the average calculated higher heating values while the bottom half shows the average errors defined as predicted minus experimental. The reported uncertainties are 95% confidence intervals determined from the distribution of the corresponding values.

For each of the formulas the mass percent of chlorine was added to the oxygen for computational purposes. This was done since chlorine was not a term in the formulas and if not measured separately, would have appeared as oxygen due to the definition of oxygen as missing mass.

The average errors in the bottom half of Table 4 show that all formulas predict the correct higher heating values to within a 12% error (2 MJ/kg) and in general are within 5%. The formula by Lloyd and Davenport always predicts a higher heating value which is too high. On the average, the Boie formula gives high values and the Tillman formula gives low values. The formulas by Dulong and IGT predict, on the average, values which are more evenly distributed

around the observed higher heating value and within 3% of the experimental value.

The Boie formula has been shown to give better results for fossil fuels than the Dulong formula[11]. This is not the case in our study of RDF-3. This may be due to the oxygen content of the samples. In general, fossil fuels have low oxygen contents (less than 10 mass percent) while RDF-3 has a much higher value (about 30 mass percent). The oxygen content may also explain the inability of the Lloyd and Davenport formula to predict higher heating values. This formula has a much smaller oxygen coefficient than the others.

The uncertainty of the errors (predicted - experimental) in Table 4 in general is smaller than expected. If the predicted and experimental values are uncorrelated the uncertainty of the observed error should be equal to the square root of the sum of the squares of the predicted and experimental uncertainties. While the calculated and observed uncertainties are close (less than 0.2 MJ/kg) for most of the rounds, it is not the case for round robin 3. Here the differences are greater than 0.5 MJ/kg and possibly due to correlation between the experimental and predicted values in the round.

ERROR ANALYSIS

The uncertainty associated with the HHV2 values determined by bomb calorimetry are mainly the errors of the calorimeter and the residual moisture. The formulas for predicting higher heating values involve more measurements (residual moisture, C, H, S, N and ash) so one may expect the calculated values to be more prone to error. By examining the calculated and observed uncertainties in the upper half of Table 4, we see that the confidence levels are comparable.

The source of the uncertainties in the calculated values is shown in Table 5. The two best formulas for predicting higher heating values, Dulong and IGT, were compared for the round robins which had the largest and smallest uncertainties. The error associated with oxygen is really due to errors in the other measurements since oxygen is defined to be the missing mass. Oxygen was removed as a variable by solving for it in terms of the other components and then substituting this into the two equations. The formulas were broken into contributions by each of the remaining components using differential error analysis. The coefficients obtained by the error analysis are given in Table 5. The chlorine coefficient is zero since it was added to oxygen in the results tabulated for Table 4. The

TABLE 4 COMPARISON OF EXPERIMENTAL AND PREDICTED HIGHER HEATING VALUES. ALL VALUES ARE AVERAGES GIVEN IN UNITS OF MJ/kg^a WITH 95% CONFIDENCE LEVELS

	Round Robin				
	1	2	2I	3	3I
Experimental					
HHV2	17.4 ± 1.5 ^b	18.5 ± 0.7	17.7 ± 0.5	17.4 ± 1.1	17.1 ± 0.5
Formula (predicted)					
Dulong	18.3 ± 1.0 ^c	18.4 ± 1.1	17.8 ± 0.6	18.2 ± 0.8	17.8 ± 1.0
Boie	18.5 ± 0.9	18.7 ± 1.0	18.1 ± 0.5	18.4 ± 0.8	18.0 ± 0.9
Lloyd	19.4 ± 0.8	19.8 ± 1.0	19.0 ± 0.5	19.3 ± 0.7	18.9 ± 0.9
Tillman	16.8 ± 0.4	17.8 ± 0.8	16.9 ± 0.3	16.8 ± 0.8	16.6 ± 0.7
IGT	18.3 ± 0.9	18.6 ± 1.0	17.9 ± 0.6	18.1 ± 0.8	17.7 ± 1.0
Errors (predicted - experimental)					
Dulong	0.9 ± 1.6 ^d	-0.1 ± 1.2	0.1 ± 0.9	0.7 ± 0.9	0.6 ± 1.0
Boie	1.1 ± 1.5	0.2 ± 1.0	0.4 ± 0.9	1.0 ± 0.8	0.9 ± 0.9
Lloyd	2.0 ± 1.5	1.3 ± 1.0	1.4 ± 0.9	1.9 ± 0.7	1.8 ± 0.9
Tillman	-0.6 ± 1.6	-0.7 ± 0.8	-0.8 ± 0.7	-0.6 ± 0.6	-0.5 ± 0.7
IGT	0.9 ± 1.5	0.1 ± 1.1	0.2 ± 0.9	0.7 ± 0.8	0.6 ± 0.9

a. 1 MJ/kg = 430.21 Btu_{th}/lb (thermochemical basis)

1 MJ/kg = 429.92 Btu_{IT}/lb (International Steam Tables basis)

b. The 95% confidence intervals are calculated from the distribution of the individual round robin test measurements.

c. The 95% confidence intervals are calculated from the distribution of the predicted values of individual tests in the round robin.

d. The 95% confidence intervals are calculated from the distribution of the computed errors of individual tests in the round robin.

same holds for nitrogen in the IGT formula. The individual errors add randomly so the total error is the square root of the sum of the squares.

The major contributor to the total error in the formula is hydrogen. The small mass contribution is multiplied by a very large heat coefficient giving substantial errors. This should not be surprising since we have

seen that hydrogen is the most abundant material in RDF-3 on a mole fraction basis. Ash and carbon contents are of similar importance in determining the uncertainties of calculated higher heating values. The minor components (N, S, and Cl) are of little significance and need not be measured to obtain precise higher heating values provided they are small.

**TABLE 5 ANALYSIS OF ABSOLUTE ERRORS
PREDICTED BY TWO FORMULAS**

(The Dulong and IGT formulas are used as examples showing the contribution of each component to the total error. Two rounds were selected for comparison, round robin 1 and 2 interlaboratory (2I), since they showed the largest and smallest calculated uncertainties, respectively. All values are in MJ/kg^a.)

Component	Dulong			IGT		
	Coeff.	Round Robin		Coeff.	Round Robin	
		1	2I		1	2I
Ash	0.145	0.51	0.26	0.104	0.37	0.19
C	0.481	0.42	0.34	0.462	0.41	0.32
H	1.563	0.78	0.48	1.442	0.72	0.44
O						
N	0.145	0.01	0.02	0.000	0.00	0.00
S	0.239	0.02	0.01	0.234	0.02	0.01
Cl	0.000	0.00	0.00	0.000	0.00	0.00
Total error		1.03	0.64		0.91	0.58

a. 1 MJ/kg = 430.21 Btu_{th}/lb (thermochemical basis)
1 MJ/kg = 429.92 Btu_{IT}/lb (International Steam Tables basis)

SUMMARY AND CONCLUSIONS

The round robin test data showed that a significant number of results were in poor agreement for RDF-3 samples indicating the difficulty some laboratories had in performing the analyses. This is evident by the number of laboratories tests which were eliminated because of poor mass accountability and identification as outliers. The omission of outliers improved agreement within a test round. The round robin tests which did appear to be representative of the rounds showed that they are statistically identical, that is, within the reported experimental uncertainties. The similarities between the round robin RDF-3 samples shows a remarkable consistency even though they were taken from different locations over the course of about a year.

The higher heating values of RDF-3 can be predicted reasonably well from elemental composition by using some of the formulas derived for other fuels. The Dulong and Institute of Gas Technology formulas gave the best agreement with the measured heating values and predicted HHV2 to within 3%. The uncertainty of the higher heating value calculated by formula is not much different than that measured by bomb calorimetry. Therefore, reliable data on the elemental composition should give accurate higher heating values. A commercial elemental analyzer has been shown

to give higher heating values from elemental composition in good agreement with bomb calorimetric values for fossil fuels[2]. The instrument used only 2–4 mg of sample but required 80–120 μm particle size to obtain reproducible results. With proper care in sample preparation, elemental composition of an RDF-3 sample can be converted to a meaningful higher heating value.

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