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ENERGY CONTENT OF BIOMASS: CALCULATION FROM ELEMENTAL COMPOSITION

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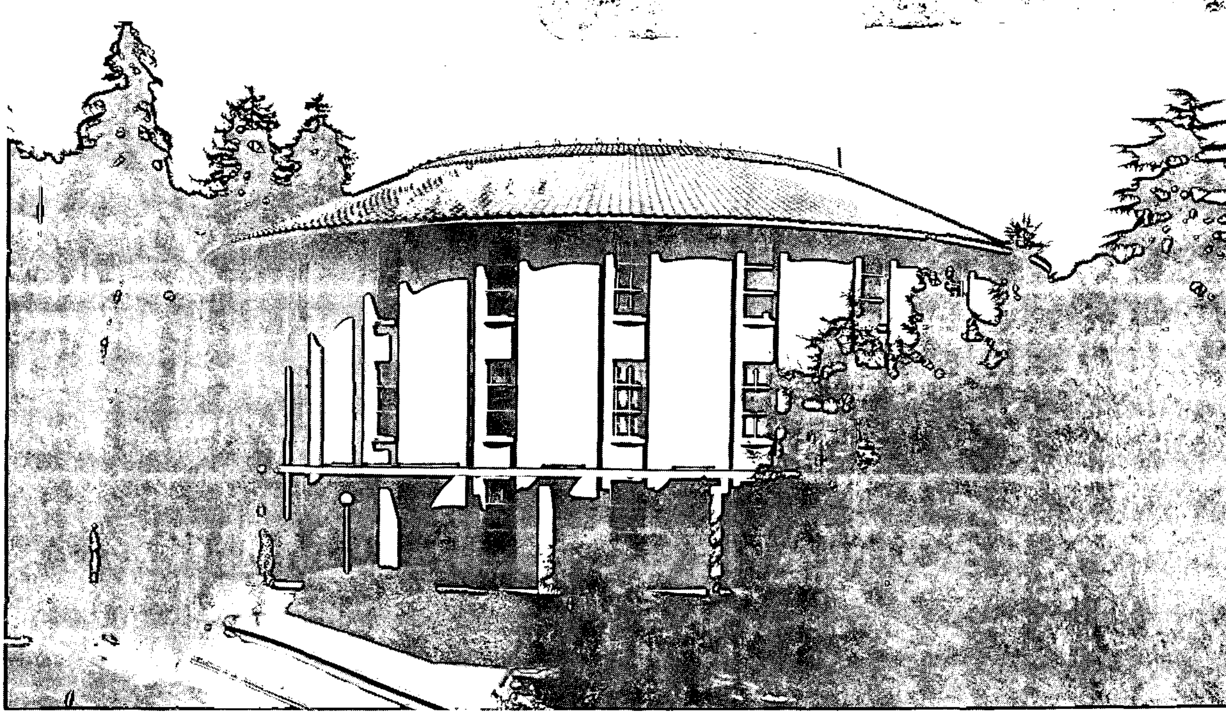

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ENERGY CONTENT OF BIOMASS:

CALCULATION FROM ELEMENTAL COMPOSITION

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Abstract

The heat of combustion, or energy content, of an organic compound or mixture can be estimated with reasonable accuracy from the elemental composition alone. The R-value of the fuel, which equals the number of grams of oxygen needed to burn a gram of fuel, times the factor 3.34 gives the specific heat of combustion in kilocalories per gram.

Introduction

In dealing with biomass as a renewable energy source it is useful o be able to estimate the "degree of reduction" of the total organic matter of plant material. This quantity, which we will call R, is proportional to the specific heat of combustion.[1] It is an expression of the energy content of the biomass and can be calculated from the elemental composition alone. Such an approximation is possible and so successful because the heats of combustion of organic compounds are large compared to the differences in value among isomers. Consequently, elemental composition is much more important than molecular structure. Also, since heats of combustion of mixtures are additive, the R-value can be used to estimate relative abundances of carbohydrate and lipid, whose R-values are quite different from one another.

R-Value and Heat of Combustion

The quantity, R, is defined as the number of grams of oxygen required to burn completely one gram of fuel material to CO_2, H_2O, and N_2. The required oxygen is calculated stoichiometrically from the amounts of carbon and hydrogen present less the amount of oxygen already in the fuel. The nitrogen present merely acts as a diluent since no oxygen is needed to convert it to N_2. Thus, the expression for R in terms of the elemental composition is given by

$$R = \frac{1}{100}\left[\frac{32}{2} \times \%C \frac{16}{2} \times \%H - \%O\right] \qquad (1)$$

where 32/12 is the weight of O required to convert 1 g of C to CO_2 while 16/2 is a like factor for the conversion of H to H_2O. Figure 1 shows a plot of specific heats of combustion (kcal per gram) of a series of 21 organic compounds versus R. (See also Table 1.) The range of values extends over a factor greater than 20, yet all the points can be well represented by a straight line through the origin. The slope of this line corresponds to a single value of 3.34 kcal evolved per gram of O_2 used for combustion. Thus, the heat of combustion, ΔH_c, of a mixture of organic compounds, or biomass, can be expressed as

$$\Delta H_c(\text{kcal/g}) = 3.34R \qquad (2)$$

Discussion

This constancy of the heat of combustion based on oxygen consumed rather than fuel consumed is remarkable and, at first, rather surprising when it is noted that elemental carbon and hydrogen have such different values for that quantity (kcal per gram of O_2 consumed): 2.95 and 4.27, respectively. However, even in a wide variety of organic compounds the %w of carbon in the CH portion of the molecule varies only between about 80% and 92%. Therefore, the kcal per gram of O_2 consumed varies only between 3.5 and 3.2 for the extreme H/C rations of 3/1 and 1/1. Most compounds of interest in biomass lie near the middle of that range, corresponding to the value of 3.34 mentioned above. Therefore, a calculation for the heat of combustion of an unknown from its R value [Equation (1)] should be good to within about 3%.

Just as N acts as a diluent in the combustion process so also does ash. Therefore the actual elemental composition of the whole sample must be used in Equation (1) and not the composition expressed on an ash-free basis. The presence of moisture in the sample causes no problem either. The additional amounts of H and O cancel each other in Equation (1) and water thus becomes another diluent. Ash and nitrogen must be determined, however, so that oxygen may be computed by difference.

Application to Mixtures of Biological Compound Types

Given the constancy of the heat of combustion based on oxygen consumed and also the near constancy of elemental composition of compound types such as protein, carbohydrate, and lipid, Spoehr and Milner[2] were able to determine the percentage of these three compound classes in Chlorella grown under different conditions from their R-values and nitrogen contents. From %N they obtained a protein value by assuming that all the nitrogen was in protein whose N content was 16%. Then, assuming additivity in R-value and average R-values for protein, carbohydrate, and lipid of 1.68, 1.12, and 1.70, respectively, they calculated carbohydrate and lipid content. Table 2, taken from their paper, gives an example of their results. They state: "The calculated percentages of lipid agreed closely with the values which were obtained by means of solvent extraction".

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References

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1. Spoehr, H.A., and Milner, H.W. The chemical composition of Chlorella; Effect of environmental conditions, (1949), Plant Physiol. 24, 120-149.

Table 1

R-Values and Specific Heats of Combustion of

Organic Compounds

Compound	Formula	R	Heat of Combustion (kcal/g)
Methane	CH_4	4.00	13.18
Ethane	C_2H_6	3.73	12.28
Propane	C_3H_8	3.64	11.96
n-Pentane	C_5H_{12}	3.56	11.58
n-Hexane	C_6H_{14}	3.53	11.51
n-Hexadecane	$C_{16}H_{34}$	3.47	11.32
Cetyl Palmitate	$C_{32}H_{64}O_2$	3.13	10.50
Benzene	C_6H_6	3.08	10.03
Anthracene	$C_{14}H_{10}$	2.97	9.55
Aniline	C_6H_7N	2.67	8.73
Acetone	C_3H_6O	2.21	7.36
Acetonitrile	C_2H_3N	2.15	7.38
Ethylenediamine	$C_2H_8N_2$	2.13	7.54
Ethanol	C_2H_6O	2.09	7.10
Dimethyl ether	C_2H_6O	2.09	7.56
Acetaldehyde	C_2H_4O	1.82	6.34
Ethyl acetate	$C_4H_8O_2$	1.82	6.10
Sucrose	$C_{12}H_{22}O_{11}$	1.12	3.95
Acetic acid	$C_2H_4O_2$	1.07	3.49
Formic acid	CH_2O_2	.35	1.37
Oxalic acid	$C_2H_2O_4$	.18	.67

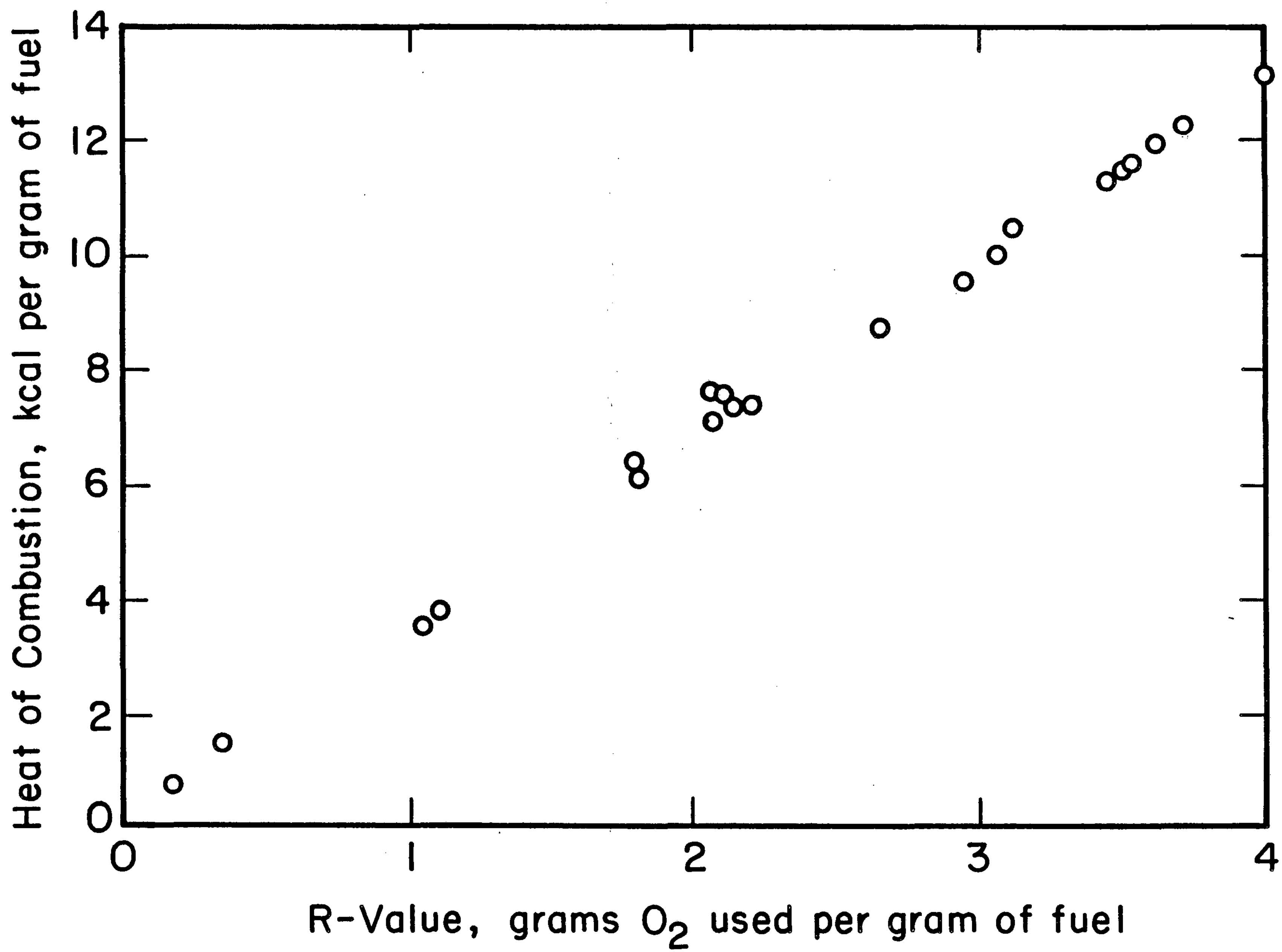
Table 2

Constituents of Chlorella Calculated From R-Value[2]

R-Value	Protein %	Carbohydrate %	Lipid %
1.52	58.0	37.5	4.5
1.68	50.0	32.2	17.7
2.00	28.3	26.2	45.5
2.24	15.7	19.0	65.3
2.52	8.7	5.7	85.6

Figure Caption

Figure 1 -- Specific heats of combustion of organic compounds


Heat of Combustion, kcal per gram of fuel
14
12
10
8
6
4
2
0
0
1
2
3
4
R-Value, grams O2 used per gram of fuel

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