Supplementary Information (3 pages)

Additional information on the data calculated for use in the study.

The following information is provided to the article in Environmental Science and Technology on

Determination of the Internal Chemical Energy of Wastewater

by

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This document was prepared on 15th November 2010

TABLE S-1: List of common organic compounds and their derived energy per gCOD values

Compound	Formula	ΔH/gCOD
Benzene	C_6H_6	10.2
Linoleic acid	$C_{18}H_{32}O_2$	13.4
Benzoic acid	C_6H_5COOH	13.4
Myristic acid	$CH_3(CH_2)_{12}CO_2H$	13.6
Lauric acid	$CH_3(CH_2)_{10}CO_2H$	13.6
Acetic acid	CH_3COOH	13.6
Phenol	C_6H_5OH	13.6
Palmitic Acid	$CH_3(CH_2)_{14}CO_2H$	13.6
Oleic acid	$CH_3(CH_2)_7CH{=}CH(CH_2)_7CO_2H$	13.7
Methane	CH_4	13.9
Ethane	C_2H_6	13.9
Lactic acid	$CH_3CH(OH)COOH$	14.0
Ethanol	C_2H_5OH	14.3
Glucose	$C_6H_{12}O_6$	14.3
Propene	C_3H_6	14.3
Cyclopropane	C_3H_3	14.5
Ethanal	CH_3CHO	14.6
Ethene	C_2H_4	14.7
Sucrose	$C_{12}H_{22}O_{11}$	14.7
Methanol	CH_3OH	15.1
Chloroethylene	C_2H_3Cl	15.7
Oxalic acid	$(COOH)_2$	15.9
Formic acid	$HCOOH$	15.9
Ethyne	C_2H_2	16.3
Hexachlorobenzene	C_6Cl_6	16.5
Dichloroethylene (1,1)	$C_2H_2Cl_2$	17.1
Dichloroethylene (1,2)	$C_2H_2Cl_2$	17.2
Methanal	$HCHO$	17.8
Trichloroethylene	C_2HCl_3	20.0
Teterachloroethylene	C_2Cl_4	26.0
Chloroform	$CHCl_3$	29.1
Trichloroacetic acid	CCl_3COOH	30.4

S-2 Energy Calculations made from Shizas and Bagley's (3) data compared to those made in this paper.

Shizas and Bagley (3) use a sample of municipal wastewater which prior to drying contains 431 mg/L COD. This sample is then oven dried to give a total solids measurement of 1980 mg/L. The dried sample is used in a bomb calorimeter giving 3.2 kJ/g dried weight.

Calculations derived from this data cited in various papers (5, 7-9, 14):

$$3.2\ \text{kJ/g} \times 1.98\ \text{g/L} = 6.3\ \text{kJ/L wastewater}$$

$$6.3\ \text{kJ/L} \times \frac{1}{0.431\ \text{gCOD/L}} = 14.7\ \text{kJ/gCOD}$$

If the exercise is repeated on the data from the present paper using the oven dried samples and the measurement taken for COD prior to drying the results would have been:

Cramlington

$$8.3\ \text{kJ/L} \times \frac{1}{0.718\ \text{gCOD/L}} = 11.6\ \text{kJ/gCOD}$$

Hendon

$$5.6\ \text{kJ/L} \times \frac{1}{0.576\ \text{gCOD/L}} = 9.9\ \text{kJ/gCOD}$$

This is an underestimation of 60% and 45% respectively.