Chemical compounds

The purpose of this note is to identify the chemical compounds that are required to describe and quantify the behaviour of waste materials in landfills. These compounds are the building blocks that enable us to engage with the science of chemistry to connect together the processes that are taking place in landfills. We use these compounds as variables in the construction of the constitutive equations that describe many of the landfill waste bio-chemical and physical processes. The mathematics built in to the formula expressions that identify the compounds provides an additional numerical layer to the process constitutive equations that ensures they are chemically as well as physically consistent.

For example:

One of the chemical compounds contained in waste material is glucose. Glucose degrades into acetic acid, methane and carbon dioxide, and we can express this reaction in the form of the constitutive equation,

$C_6H_{12}O_6 = 2C_2H_4O_2 + CH_4 + CO_2$

In this equation the compound formula $C_6H_{12}O_6$ represents a mole of the glucose compound, $C_2H_4O_2$ is acetic acid, CH_4 is methane, and CO_2 is carbon dioxide. (Reference Post 17b re: mole.)

Note that in the reaction the total number of each type of element is conserved. So taking carbon as an example, we start off with 6 moles of carbon elements in the glucose compound on the left hand side, and produce 4 in the acetic acid and one each in the methane and carbon dioxide. See table below.

		Glucose	=	Acetic	+	Methane	+	Carbon dioxide
		C6H12O6		C2H4O2		CH4		CO2
Number of moles in equation		1		2		1		1
C	elements	6		2		1		1
	moles	6	=	4	+	1	+	1
H	elements	12		4		4		0
	moles	12	=	8	+	4	+	0
O	elements	6		2		0		2
	moles	6	=	4	+	0	+	2

We can usefully take this a step further by using the molecular weights of the elements in the compounds to calculate the molecular weights of each compound. For example the molecular weight of hydrogen is 1 gram/mol, carbon is 12 times heavier and oxygen 16. So the molecular weight of glucose is 6 x 12 + 12 x 1 + 6 x 16 = 180 g/mol. Substituting this information into our constitutive equation produces a mass balance as shown in the Table below. This also tells us that when 1 unit of mass of glucose in waste degrades it produces 66.7% by mass of acteic acid, 8.9% methane and 24.4% carbon dioxide.

		Glucose	=	Acetic	+	Methane	+	Carbon dioxide
		C6H12O6		C2H4O2		CH4		CO2
Molecular weight	g/mol	180		60		16		44
Number of moles		1		2		1		1
Mass balance	gram	180	=	120	+	16	+	44

The table below gives the molecular weights for the main chemical elements found in the compounds of interest in landfill processes. These compounds are also listed below, together with their molecular weights.

Name	Symbol	MW
		g/mol
Carbon	C	12.0
Hydrogen	H	1.0
Oxygen	O	16.0
Nitrogen	N	14.0
Sulphur	S	32.1
Iron	Fe	55.9
Calcium	Ca	40.7
Chlorine	Cl	35.5

Chemical elements and molecular weights to one decimal place

Group	Name	Symbol	MW
Solids and dissolved solids	Protein	C46H77O17N12S	1101.1
	Protein Ion	C46H76O17N12S_-	1100.1
	Fat	C55H104O6	860
	Fat Ion	C55H103O6_-	859
	Carbohydrate	C12H24O12	360
	Carbohydrate Ion	C12H23O12_-	359
	Glucose	C6H12O6	180
	Glucose ion	C6H11O6_-	179
	Calcium Carbonate	CaCO3	100.7
Bacteria populations	Biomass	C5H7NO2	113
Water and dissolved oxygen, nitrogen and hydrogen	Water	H2O	18
	Hydrogen ion	H_+	1
	Hydroxide ion	OH_-	17
	Dissolved Oxygen	O2	32
	Dissolved Hydrogen	H2	2
	Dissolved Nitrogen	N2	28

Acids	Aqueous Acid	C4H8O2	88
	Aqueous Acid ion	CH7COO_-	87
	Acetic Acid	C2H4O2	60
	Acetic Acid ion	CH3COO_-	59
Ammonia and nitrogen cycle ions	Dissolved Ammonia	NH3	17
	Ammonium ion	NH4_+	18
	Nitrite ion	NO2_-	46
	Nitrate ion	NO3_-	62
Sulphides	Dissolved Hydrogen Sulphide	H2S	34.1
	Sulphate ion	SO4_2-	96.1
Methane	Dissolved Methane	CH4	16
Dissolved carbon dioxide	Carbonic Acid	H2CO3	62
	Bicarbonate ion	HCO3_-	61
	Carbonate ion	CO3_2-	60

Dissolved solute ions and heavy metals	Calcium ion	Ca_2+	40.7
	Iron ion A	Fe_2+	55.9
	Iron ion B	Fe_3+	55.9

Gas phase	Oxygen Gas	O2	32
	Nitrogen Gas	N2	28
	Carbon Dioxide Gas	CO2	44
	HydrogenGas	H2	2
	Methane Gas	CH4	16
	Ammonia Gas	NH3	17
	Hydrogen Sulphide Gas	H2S	34.1
	Water Vapour	H2O	18