Calculation of heat generation and temperature change

Summary:

This article on the calculation of heat generation and temperature change focusses on the analytical functions use by the LDAT landfill waste degradation and transport model to calculate how the model parameter values change with temperature. The article contains temperature functions for the following parameters. Landfill gas and liquid density and viscosity; Solid waste dissolution solubility products; Monod bacteria growth and death rates; Henry's Law gas solubility coefficients; Chemical equilibrium coefficients. The procedure for calculating temperature changes in a landfill is outlined, and values for the following key parameters involved in the procedure are given: Landfill waste chemical compound enthalpies of formation; Landfill waste thermal conductivity; Landfill waste specific heats.

Temperature functions

The values of many of the parameters used in a landfill processes model change with temperature, and these changes can often be conveniently calculated using analytical functions of temperature. Temperature functions for density and viscosity are given in (White et al. 2014), where it is explained how these lead to temperature functions for liquid and gas permeability. See Table 1 in Annexe **Tables** at the end of this article.

Functions for bacteria growth rate, half saturation constant and death rate are given in Table 2, and are taken from (White and Beaven 2013). The function for Henry's coefficient is given in Table 3. Details of the relationship between the values of diffusion coefficients and temperature are given in the next column download article on 'Gas and liquid diffusion'. Bear in mind that the Knudsen diffusion coefficient is related to temperature indirectly through its functionality with permeability, density and viscosity. Temperature functions for the equilibrium coefficients, which feature in the sub-models of the processes of dissolution and chemical equilibrium and are discussed in (White et al. 2014), are widely available in the literature (Chapra 1997, Droste 1997, El-Fadel et al. 1996) or may be derived by using the appropriate values of the properties enthalpy and free energy of formation (Droste 1997). The equilibrium and dissolution coefficient temperature functions used in LDAT are given in Table 4.

Calculation of landfill temperature change

In LDAT, the temperature change in the waste contained in a model element e over a time period Δt is calculated by balancing the heat transferred by convection and conduction across the element interfaces m, the heat generated by the enthalpy of formation of the degradation compounds

within the element, and the change in specific heat assuming that all phases are locally at the same temperature at all times.

Thus,

$$\Delta T_e = \frac{q_e^\kappa + q_e^C + q_e^E}{\sum_P m_e^P C_p^P} \qquad (1)$$

The heat transferred into an element by conduction is,

$$q_e^\kappa = \sum_m \kappa_{em} A_{em} (T_m - T_e) \Delta t \qquad \frac{1}{\kappa_{em}} = \frac{0.5 l_e}{\kappa_e} + \frac{0.5 l_m}{\kappa_m} \qquad (2)$$

κ_e and κ_m are the heat conduction coefficients for element e and its neighbour element m. l_e is the length of element e in the direction m, and l_m is the corresponding length of its neighbour element m.

The heat transferred into an element by convection is,

$$q_e^C = \sum_P \sum_m C_p^P M_{em}^P (T_e - T') \qquad (3)$$

C_p^P is the phase specific heat capacity, M_{em}^P is the mass transferred across the element interface during Δt, and T' is the absolute temperature in the element from which the mass is transferred. m_e^P in equation (1) is the mass of the phase P in element e.

The heat generated is calculated by adding together the product of the change in mass of each compound n involved in the waste degradation chemistry and its enthalpy of formation E_n. Thus,

$$q_e^E = -\sum_P \sum_n \rho_{e,n}^P G_{deg,e,n}^P V_e E_n \Delta t \qquad (4)$$

The values of the enthalpies of formation of the degradation compounds, E_n, that are used by LDAT are given in Table 5. Apart from the values for protein, fat, and aqueous acid, which have been estimated by the authors, these have been sourced from the references cited with the Table. In theory enthalpies of formation are the heat released in the formation of complex compounds from simple compounds. Thus the reference values of simple components such as oxygen and hydrogen are by definition zero. In order to utilise the anaerobic degradation model in LDAT, which assumes that the reactions all take place in the liquid phase, the oxygen solubility has been raised to allow the oxygen in the gas phase to pass rapidly into the liquid phase, and thus become available to react

with the dissolved waste solids. Thus in Table 1 Henry's coefficient is given as 1.00 x 10⁻⁴ kPa⁻¹ instead of the normally quoted value of 4.24 x 10⁻⁷ kPa⁻¹.

Values that are assumed in the literature for the thermal conductivity κ of waste in landfills range from 0.15 to 1.0 W/m.K (Bente 2011, Hanson et al. 2013). The specific heats C_p^P of waste in landfills are based on the measured values for liquids (4.18 kJ/kg.K water), gas (1 kJ/kg.K air) and solids (0.8 kJ/kg.K), (Bente 2011).

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Chapra, S.C. (1997) Surface water-quality modelling. McGraw-Hill. ISBN 0070113645.
Droste, R.L. (1997) Theory and practice of water and wastewater treatment. John Wiley & Sons Ltd, 1997. ISBN 0471124443.
El-Fadel, M., Findikakis, A.N. and Leckie, J.O. (1996) Numerical modelling of generation and transport of gas and heat in landfills. Waste Management and Research 1996 14, 483-504.
Hanson, J.L., Yesiller, N., Onnen, M.T., Liu, W., Oettle, N.K. and Marinos. J, A. (2013) Development of a numerical model for predicting heat generation and temperatures in MSW landfills. Waste Management 33, 1993-2000.
White, J.K. and Beaven, R.P. (2013) Developments to a landfill processes model following its application to two landfill modelling challenges Waste Management 33(10), 1969-1981.
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Annexe **Tables**

Name	Notation	Formula	Units
Liquid viscosity	μ^L	$40\ln(175/T)$	kg/m/day
Gas viscosity	μ^G	$1.264 + 0.004(T-20)$	kg/m/day
Liquid density	ρ^L	$1000\exp(p^L/K_L)$	kg/m³
Gas density	ρ^G	$m(p^G + p_A)/R(T+273)$	kg/m³

p^L liquid pressure   kPa

p^G gas pressure   kPa

p_A atmospheric pressure   kPa

T temperature   ºC

m molecular weight   kg/mole

R gas constant   kN/(mole.ºK)

K_L liquid bulk modulus   kPa

Table 1 Density and viscosity as functions of temperature and pressure.

Dissolution	Rate of dissolution			0.5	day^{-1}
	Solubility product	Protein		5.0E-06	(M/l)^2
		Fat		6.4E-06	
		Carbohydrate		1.5E-05	
		Glucose		3.1E-05	
Monod	Growth rate	μ		0.075	day^{-1}
	Half saturation constant	K$_B$		0.5	kg/m^3
	Yield factor	Y		0.1	
	Death rate	k$_D$		0.0075	day^{-1}

Table 2 Solubility and Monod parameters at 20 °C

Note to Table 2. μ, K$_B$ and k$_D$ are multiplied by the function $e^{\alpha(T-T_0)/T}$ to allow for temperatures other than 20 °C. T and T_0 are in K and α is 23.4 for μ, and k$_D$ and -9.12 for K$_B$ T_0 = 293 °K, (El-Fadel, Findikakis et al. 1996)

Gas	Henry coefficient	α_H
	1/kPa	K
CO$_2$	1.61E-05	2400
CH$_4$	2.28E-07	1800
O$_2$	1.00E-04	1600
NH$_3$	5.00E-03	4200
N$_2$	1.74E-07	1300
H$_2$S	3.48E-05	2100
SO$_2$	9.15E-04	2900

Table 3 Henry's law coefficients at T_0 =298K, $\dfrac{H_n^T}{H_n^{T_0}} = e^{-\alpha_H\left(\frac{1}{T_0}-\frac{1}{T}\right)}$

Component	Equilibrium	a_0	a_1	a_2	a_3	a_4
Carbonate ion	$K = \dfrac{[H^+][CO_3^{2-}]}{[HCO_3^-]}$	10.63	-1.61E-02	1.74E-04	-7.63E-07	1.52E-09
Bicarbonate ion	$K = \dfrac{[H^+][HCO_3^-]}{[H_2CO_3]}$	6.58	-1.37E-02	2.01E-04	-9.39E-07	1.71E-09
Calcium carbonate	$K = [C_a^+][CO_3^-]$	8.05	9.11E-03	7.56E-05	-1.16E-07	0.0

$$pK = \sum_{n=0}^{4} a_n T^n \quad (T \text{ in } ^{\circ}\text{C})$$

Component	Equilibrium	a_{-1}	a_0
Water	$K = [H^+][OH^-]$	4.20	2920.43
Ammonia	$K = \dfrac{[H^+][NH_3]}{[NH_3^+]}$	0.09	2729.92
Aqueous and Acetic acid	$K = \dfrac{[H^+][H_3C_2O_2^-]}{[H_4C_2O_2]}$	4.85	-21.85
Protein	$K = [H^+][C_{46}H_{76}O_{17}N_{12}S^-]$	3.06	655.64
Fat	$K = [H^+][C_{55}H_{103}O_6^-]$	2.96	655.64
Carbohydrate	$K = [H^+][C_{12}H_{23}O_{12}^-]$	2.59	655.64
Glucose	$K = [H^+][C_6H_{11}O_6^-]$	2.28	655.64

$$pK = a_0 + a_{-1}/T \quad (T \text{ in K})$$

Table 4 Equilibrium and dissolution coefficient temperature functions

Compound	Enthalpy of formation	Source
Acetic acid	-8133	(1)
Ammonia	-4751	(1)
Ammonium ion	-7371	(1)
Aqueous acid	-8132	(3)
Biomass	-4425	(2)
Carbon dioxide	-8900	(1)
Carbonic acid	-11259	(1)
Hydrogen sulphide	-1152	(1)
Hydroxide ion	-13513	(1)
Methane	-4674	(1)
Nitrate	-3328	(1)
Nitrite	-2308	(1)
Sulphate	-9434	(1)
Waste as Protein	-1397	(3)
Waste as Fat	-1397	(3)
Waste as Carbohydrate	-6240	(3)
Waste as Glucose	-7078	(2)
Water	-15865	(1)

Table 5 Enthalpy of formation values in kJ/kg

(1) Droste (1997), (2) Bente(2011) (3) Authors' estimate.