Initial and Boundary Condition parameter values for LDAT landfill models

Note that the example values are based on those used in the Ten Element Example – passive model. The values that are available in the LDAT model editor are not repeated here. To see these values the Ten Element Example – passive model should be selected from the Default Cases list on the LDAT Dashboard and cloned into the User Cases list. Then the Initial and Boundary Conditions parameter values may be seen by selecting the clone into the editor (for example by using Actions\Edit in the User Cases list or double clicking the Case name).

Some sets of the Initial and Boundary Conditions parameter values are not yet available for editing. Details of these built in values are given here. Most of these values are standard values that may be found in the literature. They are repeated here for convenience, and to serve as confirmation that LDAT uses values that are normally accepted. It is unlikely that a user would need to change these standard values – but it is intended to make these values available for user editing in due course.

The complete set of Initial and Boundary Condition parameter values for LDAT is shown in Table 1, together with a note marking those that are currently not available for editing. Additional Tables are then provided giving details of the built in values.

Editor Tab name	Application	Value group name	Note
Model	Model wide	Number of elements	
		Origin coordinates	
		Slice dimensions	
		van Genuchten values	
		Monod parameters	
		Waste converter EA	
		Waste converter Compounds	
		Dissolution parameters	Not editable
		Chemical pathways	Not editable
		Henry parameters	Not editable
		Binary and Fickian diffusion coeffs	Not editable
		Enthalpy data	Not editable
		Equilibrium and dissolution coefficient temperature functions	Not editable
Active elements	Element specific	Dry density and permeability	
		Heat Generation and Transfer	
		Effective density coefficients	
Waste type		Waste characteristics	
		Phase fractions and density	
		Initial liquid and gas compound concentrations vol/vol	
		Inhibition parameter values	
Boundary elements		BC Stresses	
		BC Permeability/Thermal conductivity	
		Liq/Gas mass v/v	
		Transient content control	
		Transient boundary conditions	
		BC Inert stock	
Calculation data	Model wide	Calculation options	
		Time Iteration Settings	
		Time Iteration Control	
		Inhibition/Temp options	
		van Genuchten options	

Dissolution parameters

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	

Chemical pathways

The products of waste degradation are estimated by starting with a simple specification of the solid waste in terms of the characteristic percentage content of: Green waste and wood; Food; Paper card and cartons; Textiles and carpets; and Inert material. This specification is then converted into the initial values for the Protein, Fat, Carbohydrates and Glucose chemical compounds. These compounds are classified further into fast, medium and slow degradable materials. The degradation can be anaerobic or aerobic when dissolved oxygen is available.

There are a large number of chemical degradation pathways available in LDAT. The core pathways are as follows.

The anaerobic chemical pathways are:

Protein as $C_{46}H_{77}O_{17}N_{12}S$ forms aqueous acid $C_4H_8O_2$ and acetic acid $C_2H_4O_2$ anaerobically
$C_{46}H_{76}O_{17}N_{12}S^- + 27.5H_2O = 7.39C_4H_8O_2 + 5.15C_2H_4O_2 + 6.14H_2CO_3 + 12NH_3 + H_2S + OH^-$
Fat represented as $C_{55}H_{104}O_6$ forms aqueous and acetic acid anaerobically
$C_{55}H_{103}O_6^- + 9.88H_2O + 6.56H_2CO_3 = 10.56C_4H_8O_2 + 6.72C_2H_4O_2 + 5.88CH_4 + OH^-$
Carbohydrate high order forms aqueous acid anaerobically
$C_{12}H_{23}O_{12}^- + 2H_2O = 2C_4H_8O_2 + CH_4 + 3H_2CO_3 + OH^-$
Glucose - Carbohydrate forms acetic acid anaerobically
$C_6H_{11}O_6^- + 2H_2O = 2C_2H_4O_2 + CH_4 + H_2CO_3 + OH^-$

There is a corresponding set of aerobic pathways:

Aerobic degradation of Protein ion
$C_{46}H_{76}O_{17}N_{12}S^- + 49.75O_2 + 26.5H_2O = 46H_2CO_3 + 12NH_3 + SO_4^- + OH^-$
Aerobic degradation of Fat ion
$C_{55}H_{103}O_6^- + 78O_2 + 4H_2O = 55H_2CO_3 + OH^-$
Aerobic degradation of Carbohydrate ion
$C_{12}H_{23}O_{12}^- + 12O_2 + H_2O = 12H_2CO_3 + OH^-$
Aerobic degradation of Glucose ion
$C_6H_{11}O_6^- + 6O_2 + H_2O = 6H_2CO_3 + OH^-$

The pathways for the breakdown of the products Aqueous and Acetic acids are:

Aqueous acid $CH_3(CH_2)_2COOH$, $C_4H_8O_2$ forms acetic acid anaerobically
$4C_4H_8O_2 + 6H_2O = 4C_2H_4O_2 + 6CH_4 + 2H_2CO_3$
Acetic acid forms methane
$C_2H_4O_2 + H_2O = CH_4 + H_2CO_3$

And those for Methane oxidation and Denitrification are:

Methane oxidation
$CH_4 + 2O_2 = H_2O + H_2CO_3$
Nitrification by nitrosomonas bacteria
$NH_4^+ + 1.5O_2 = NO_2^- + 2H^+ + H_2O$
Nitrification by nitrobactor bacteria
$NO_2^- + 0.5O_2 = NO_3^-$

The degradation of each pathway is facilitated by an associated bacteria compound, and in the cases of Protein, Fat, Carbohydrate and Glucose the bacteria growth reactions are:

Formation of biomass using protein $C_{46}H_{77}O_{17}N_{12}S$
$5C_{46}H_{76}O_{17}N_{12}S^- - 14NH_4^+ = 46C_5H_7NO_2 + 56H^+ - 27H_2O + 5SO_4^{2-}$
Formation of biomass using fat represented as $C_{55}H_{104}O_6$
$5C_{55}H_{103}O_6^- + 55NH_4^+ = 55C_5H_7NO_2 + 510H^+ - 80H_2O$
Formation of biomass using carbohydrate high order
$5C_{12}H_{23}O_{12}^- + 12NH_4^+ = 12C_5H_7NO_2 + 7H^+ + 36H_2O$
Formation of biomass using glucose (TUB)
$C_6H_{11}O_6^- + 1.2NH_4^+ = 1.2C_5H_7NO_2 + 0.2H^+ + 3.6H_2O$

All bacteria compounds are assumed to die off along the pathway:

Formation of glucose from biomass (TUB)
$6C_5H_7NO_2 + 19H_2O = 5C_6H_{11}O_6^- + 6NH_4^+ + OH^-$

The Glucose ion in the bacteria death pathway can be set in LDAT to become fully available to the Glucose degradation system, partially available, or simply act as a non-degradable compound.

<u>Henry parameters</u>

Gas	Henry coefficient	Transfer rate	α_H
	1/kPa	per day	K
CO_2	1.61E-05	3	2400
CH_4	2.28E-07	3	1800
O_2	4.24E-07	3	1600
NH_3	5.00E-03	3	4200
N_2	1.74E-07	3	1300
H_2S	3.48E-05	3	2100
SO_4^{2-}	9.15E-04	3	2900

Binary and Fickian diffusion coefficients

Compound pair		Binary diffusion coefficient m^2/day
N_2	O_2	1.80
N_2	CH_4	1.85
N_2	CH_4	1.42
O_2	CH_4	1.96
O_2	CO_2	1.41
CH_4	CO_2	1.47

Dissolved gas	Fickian diffusion coefficient m^2/day
CO2	1.66E-04
CH4	1.29E-04
H2	3.89E-04
H2S	1.22E-04
N2	1.62E-04
NH3	1.42E-04
O2	1.81E-04

Enthalpy data

Compound	Enthalpy of formation
Acetic acid	-8132
Ammonia	-4751
Ammonium ion	-7371
Aqueous acid	-8132
Bicarbonate ion	-11306
Biomass	-4400
Calcium ion	-9000
Carbonate ion	-11216
Carbon dioxide	-8900
Carbonic acid	-11259
Hydrogen sulphide	-1152
Hydroxidelon	-13524
Methane	-4674
Nitrate ion	-3328
Nitrite ion	-2308
Oxygen	-15000
Waste as Protein etc	-7000
Sulphate	-9434
Water	-15865

Equilibrium and dissolution coefficient temperature functions

Component	Equilibrium	a_0	a_1	a_2	a_3	a_4
Carbonate ion	$K=\frac{[H^+][CO_3^{2-}]}{[HCO_3^-]}$	10.63	-1.61E-02	1.74E-04	-7.63E-07	1.52E-09
Bicarbonate ion	$K=\frac{[H^+][HCO_3^-]}{[H_2CO_3]}$	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

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

Component	Equilibrium	a_{-1}	a_0
Water	$K=[H^+][OH^-]$	4.20	2920.43
Ammonia	$K=\frac{[H^+][NH_3]}{[NH_3^+]}$	0.09	2729.92
Aqueous and Acetic acid	$K=\frac{[H^+][H_3C_2O_2^-]}{[H_4C_2O_2]}$	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

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