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Geological Society of London – Hydrogeological Group
Meeting on Landfill Hydrogeology
February 2008

**Modelling of liquid and gas transport in wastes –
optimising an aerobic treatment process**

Jim White and Richard Beaven, University of
Southampton, UK



Landfill Research at the University of Southampton

Science and strategies for the management and remediation of landfills.

The overall aim of the research is to provide the scientific basis from which new efficient, effective and economic post closure management strategies for landfills can be developed.

Research on:

- waste characterisation
- the use of tracers in landfills
- gas and leachate transport
- flushing characteristics of contaminants in wastes
- the development of improved predictive techniques to assess the long term performance of wastes in landfills

Funded by: Engineering and Physical Sciences Research Council (EPSRC)
Department for Environment, Food and Rural Affairs (defra)



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Presentation outline

Theoretical background to a leachate and gas flow model

Some of the uncertainties we are trying to address

Example of an anaerobic application and highlight some problems



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Acknowledgement

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Nick Walker	- Veolia Environmental Services



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Importance of the liquid phase

- Accommodates the chemical reactions that take place in a landfill, and that degrade and stabilise the waste material.
- Dissolves the solid phase into the liquid phase and makes solids available to take part in the chemical reactions.
- Is an important reactant in many of the stabilising chemical reactions.
- Provide the means by which a landfill can contaminate its immediate environment in the event of unplanned releases.
- Provide the opportunity to stabilise a landfill more rapidly by planned management of the liquid phase in flushing, treatment and leachate recirculation systems.
- Influences the production of gas in a landfill. Impacts on the transport of gas that shares the same pore spaces.



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Benefits of a better understanding of the movement of landfill gas and leachate

- assists the regulators and operators of landfills in carrying out their duties.
- improvement of estimates of stabilisation times for the biodegradation of waste.
- long term estimates of emissions of gas and liquids from caps and liners will become more accurate.
- interpreting gas pressure and flow data from gas wells in order to assess landfill gas generation rates will become a possibility.
- assessment of pressure heads on liners and at internal points in landfills to confirm slope stability will become more reliable.
- relationship between liquid flow, density changes, and waste settlement will become clearer.

4th ICLRS meeting at Gällivare in Sweden in June 2006



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Landfill Degradation and Transport model (LDAT)

Applications of LDAT:

To assess the consistency of landfill datasets and to extrapolate data

To expose areas where we need to improve our understanding of landfill systems

To understand how waste degrades in a landfill

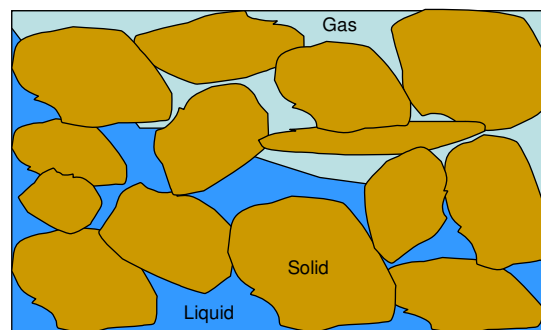
To understand how we can intervene to accelerate the bio-chemical stabilisation of waste in landfills



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Model components

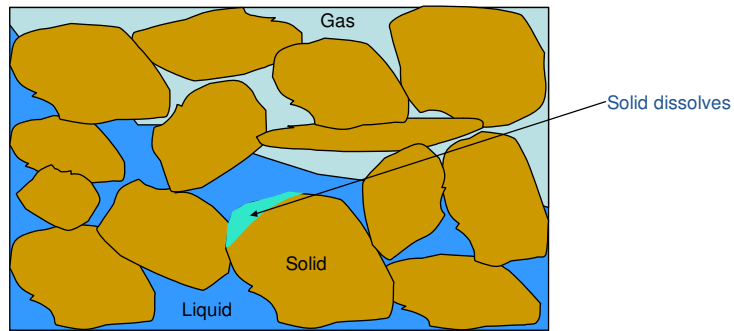
	Bio-chemical conversion	Transport
Solids	To liquid and gas	Settlement
Liquids	To gas	Seepage
Gas	In and out of solution	Venting and seepage



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Model components

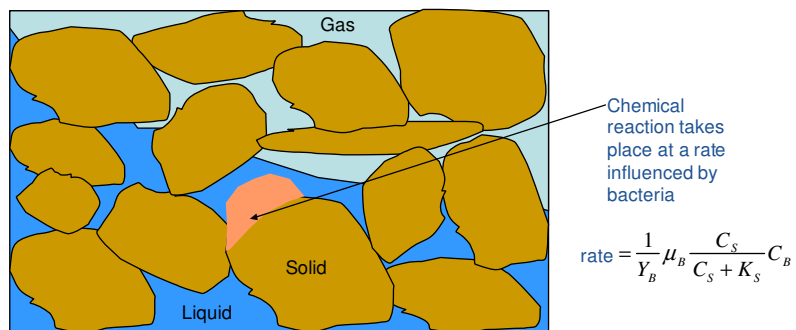
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Model components

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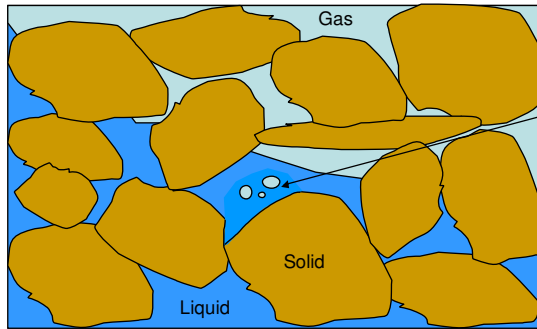
$$\text{rate} = \frac{1}{Y_B} \mu_B \frac{C_S}{C_S + K_S} C_B$$



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Model components

	Bio-chemical conversion	Transport
Solids	To liquid and gas	Settlement
Liquids	To gas	Seepage
Gas	In and out of solution	Venting and seepage



Chemical reaction changes phase concentrations and induces settlement and seepage

Chemistry of degradation

0, 1, 2	Protein as $C_4H_7O_2N_1S$ forms aqueous acid $C_2H_3O_2$ and acetic acid $C_2H_3O_2$ anaerobically $C_4H_7O_2N_1S + 20.38H_2O = 7.99C_2H_3O_2 + 5.15C_2H_3O_2 + 6.14CO_2 + 12NH_3 + H_2S$	22	Acetic acid forms methane $C_2H_3O_2 = CH_4 + CO_2$
3, 4, 5	Fat represented as $C_{27}H_{52}O_2$ forms aqueous and acetic acid anaerobically $C_{27}H_{52}O_2 + 15.54H_2O = 6.56CO_2 + 10.56C_2H_3O_2 + 6.72C_2H_3O_2 + 5.88CH_4$	23	Reduction of iron using acetic acid (TUB) $C_2H_3O_2 + 8Fe^{2+} + 2H_2O = 2CO_2 + 8Fe^{3+} + 8H^+$
6, 7, 8	Carbohydrate high order forms aqueous acid anaerobically $C_6H_{12}O_6 = 2C_2H_3O_2 + CH_4 + 3CO_2 + 2H_2O$	24	Formation of glucose from biomass (TUB) $6C_2H_3NO_2 + 18H_2O + 6H^+ = 5C_6H_{12}O_6 + 6NH_4^+$
9, 10, 11	Glucose - Carbohydrate forms acetic acid anaerobically $C_6H_{12}O_6 = 2C_2H_3O_2 + CH_4 + CO_2$	25, 26, 27	Formation of biomass using protein $C_4H_7O_2N_1S$ $5C_4H_7O_2N_1S - 14NH_3^+ = 46C_2H_3NO_2 + 61H^+ - 27H_2O + SO_4^{2-}$
12, 13, 14	Degradation of solid waste as $C_7H_{13}O_2N_1$ anaerobically $C_7H_{13}O_2N_1 + 6.23O_2 = 6CO_2 + 4.02H_2O + 0.32NH_3$	28, 29, 30	Formation of biomass using fat represented as $C_{27}H_{52}O_2$ $5C_2H_3O_2 + 55NH_3^+ = 55C_2H_3NO_2 + 515H^+ - 80H_2O$
15	Degradation of glucose aerobically (TUB) $C_6H_{12}O_6 + 6O_2 = 6CO_2 + 6H_2O$	31, 32, 33	Formation of biomass using carbohydrate high order $5C_2H_3O_2 + 12NH_3^+ = 12C_2H_3NO_2 + 12H^+ - 36H_2O$
16	Desulfurification using glucose (TUB) $C_6H_{12}O_6 + SO_4^{2-} + 2H^+ = 2C_2H_3O_2 + 2CO_2 + H_2S + 2H_2O$	34, 35, 36	Formation of biomass using glucose (TUB) $C_6H_{12}O_6 + 12NH_3^+ = 12C_2H_3NO_2 + 12H^+ + 36H_2O$
17	Denitrification by nitrosomonas bacteria $NH_4^+ + 1.5O_2 = NO_2^- + 2H^+ + H_2O$	37, 38, 39	Formation of biomass using $C_4H_7O_2N_1S$ $5C_4H_7O_2N_1S + 4.4NH_3^+ = 6C_2H_3NO_2 + 9H^+ + 5.8H_2O$
18	Denitrification by nitrobacter bacteria $NO_2^- + 0.5O_2 = NO_3^-$	40	Formation of biomass following denitrification by nitrosomonas bacteria $5C_2H_3O_2 + 6NH_3^+ = 6C_2H_3NO_2 + 18H_2O + 6H^+$
19	Denitrification using glucose (TUB) $C_6H_{12}O_6 + 1.6NO_2^- + 1.6H^+ = 2C_2H_3O_2 + 2CO_2 + 0.8N_2 + 2.8H_2O$	41	Formation of biomass following denitrification by nitrobacter bacteria $5C_2H_3O_2 + 6NO_2^- + 18H^+ + 6H^+ = 6C_2H_3NO_2 + 30H_2O$
20	Aqueous acid $CH_3(CH_2)_4COOH$ $C_6H_{12}O_6$ forms acetic acid anaerobically $4C_6H_{12}O_6 + 4H_2O = 4C_2H_3O_2 + 6CH_4 + 2CO_2$	42	Formation of biomass using aqueous acid as $CH_3(CH_2)_4COOH$ $C_6H_{12}O_6$ $5C_2H_3O_2 + 4NH_3^+ = 4C_2H_3NO_2 + 24H^+ + 2H_2O$
21	Desulfurification using acetic acid (TUB) $C_2H_3O_2 + 2SO_4^{2-} + 4H^+ + 4H_2 = 2H_2S + 2CO_2 + 6H_2O$	43	Formation of biomass using acetic acid (TUB) $C_2H_3O_2 + 0.4NH_3^+ = 0.4C_2H_3NO_2 + 1.2H_2O + 0.4H^+$

Pathways represented in LDAT

LDAT compounds z_i

0, 1, 2	Protein	$C_{48}H_{77}O_{12}N_{12}S$	23	Hydrogen ion	H^+
3, 4, 5	Fat	$C_{55}H_{104}O_6$	24	Hydroxide ion	OH^-
6, 7, 8	Carbohydrate	$C_{12}H_{24}O_{12}$	25	Hydrogen gas	H_2
9, 10, 11	Glucose	$C_6H_{12}O_6$	26	Water	H_2O
12, 13, 14	Solid Aerobic	$C_6H_8O_3.56N_0.32$	27	Hydrogen Sulphide	H_2S
15	Ammonium ion	NH_4^+	28	Nitrogen	N_2
16	Nitrite ion	NO_2^-	29	Ammonium gas	NH_3
17	Aqueous acid	$C_1H_2O_2$	30	Nitrate ion	NO_3^-
18	Acetic acid	$C_2H_4O_2$	31	Oxygen gas	O_2
19	Carbon Dioxide	CO_2	32	Sulphate	SO_4^{2-}
20	Methane	CH_4	33 - 51	Biomass	$C_1H_1NO_2$
21	Iron A	Fe^{2+}	52	Inert	
22	Iron B	Fe^{3+}			

Compounds represented in LDAT



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LDAT constitutive equation

To calculate the transient distribution of concentrations of components z use a mass balance equation to express,

Rate of change in component concentration $\frac{\partial z}{\partial t}$

is balanced by

Change in compression $\frac{\partial v_x}{\partial x}$ transport

Flow and diffusion

And any contribution from sources of the component G_i^p



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LDAT constitutive equation

To calculate the transient distribution of concentrations of components z use a mass balance equation to express,

Rate of change in component concentration	$\frac{\partial z}{\partial t}$
is balanced by	
Change in compression	$-zS \frac{\partial p}{\partial t}$
Flow and diffusion	$-z \frac{\partial v}{\partial x}$
And any contribution from sources of the component	G

$$\frac{\partial z}{\partial t} = -zS \frac{\partial p}{\partial t} - z \frac{\partial v}{\partial x} + G$$



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LDAT constitutive equation $\frac{\partial z}{\partial t} = -zS \frac{\partial p}{\partial t} - z \frac{\partial v}{\partial x} + G$

$$G = G^R + G^D + G^P$$

The source term is composed of three parts

G^R Recharge/abstraction

G^D Degradation

G^P Phase change through solid and gas solubility and water vapour generation



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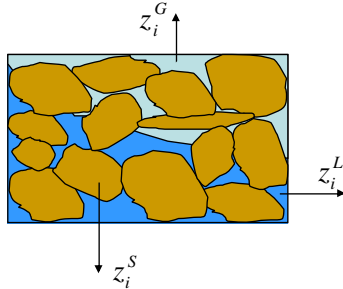
Waste component concentrations z_i^P

Concentration of component i in phase P z_i^P

Solid phase S

Liquid phase L

Gas phase G



$$z^L = \sum_i z_i^L = \theta$$

$$z^G = \sum_i z_i^G$$

$$z^L + z^G = \phi$$

$$z^S + z^L + z^G = 1$$

$$z^S = \sum_i z_i^S = 1 - \phi$$

$$\text{Degree of saturation } \zeta = \frac{z^L}{\phi}$$



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LDAT constitutive equation $\frac{\partial z}{\partial t} = -z^S \frac{\partial p}{\partial t} - z^L \frac{\partial v}{\partial x} + G$

If you add up all of the fluid phase component equations, and separately add the solid phase components you end up with two equations.

$$\text{Fluid} \quad z^L S^L \frac{\partial p^L}{\partial t} + z^G S^G \frac{\partial p^G}{\partial t} + \frac{\partial \phi}{\partial t} = z^L \frac{k^L}{\rho^L g} \frac{\partial^2 p^L}{\partial x^2} + z^G \frac{k^G}{\rho^G g} \frac{\partial^2 p^G}{\partial x^2} + \sum (G_i^L + G_i^G)$$

$$\text{Solid} \quad z_i^S S_i^S \frac{\partial p^S}{\partial t} - \frac{\partial \phi}{\partial t} = -z_i^S \frac{\partial v_i^S}{\partial x} + G_i^S$$

Note that $\frac{\partial \phi}{\partial t}$ is the term that decouples these equations.

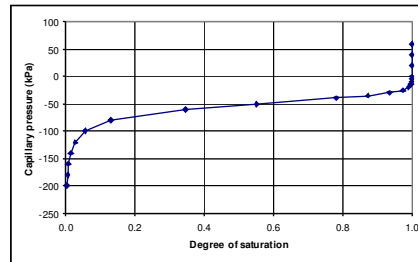


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LDAT constitutive equation $\frac{\partial z}{\partial t} = -z^L S \frac{\partial p}{\partial t} - z^L \frac{\partial v}{\partial x} + G$

Fluid $z^L S^L \frac{\partial p^L}{\partial t} + z^G S^G \frac{\partial p^G}{\partial t} + \frac{\partial \phi}{\partial t} = z^L \frac{k^L}{\rho^L g} \frac{\partial^2 p^L}{\partial x^2} + z^G \frac{k^G}{\rho^G g} \frac{\partial^2 p^G}{\partial x^2} + \sum (G_i^L + G_i^G)$

The fluid equation can be solved if you know how the gas pressure field is related to the liquid pressure field. This can be achieved by invoking a van Genuchten capillary pressure type of relationship. However relationships designed for the vadose zone may not be suitable for areas with medium to low gas concentrations in the body of the landfill waste.



After van Genuchten (1980)



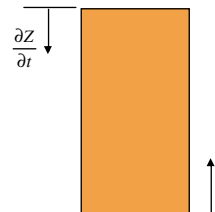
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LDAT constitutive equation

Solid $z_i^S S_i^S \frac{\partial p^S}{\partial t} - \frac{\partial \phi}{\partial t} = -z_i^S \frac{\partial v_i^S}{\partial x} + G_i^S$

And then the solid phase equation can be solved to give estimates of settlement to an elevation Z.

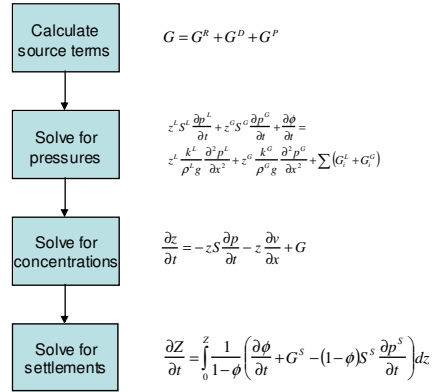
$$\frac{\partial Z}{\partial t} = \frac{1}{(1-\phi)} \int_0^Z \left((1-\phi) S^S \frac{\partial p^S}{\partial t} - \frac{\partial \phi}{\partial t} - \sum G_i^S \right) dz$$



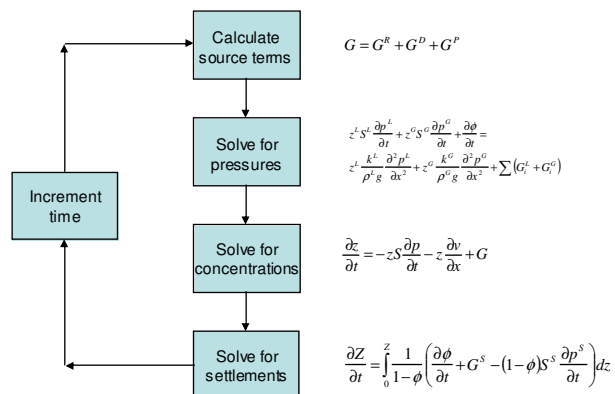
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LDAT constitutive equation

Thus the computational sequence is to calculate the source terms, solve for the pressure fields and back calculate the concentrations and settlement.



LDAT constitutive equation



LDAT constitutive equation $\frac{\partial z}{\partial t} = -zS \frac{\partial p}{\partial t} - z \frac{\partial v}{\partial x} + G$

Uncertainties

Compression - Bulk modulus and Gas Law

$$-zS \frac{\partial p}{\partial t}$$

For a liquid or solid component the bulk modulus can be used, and for a gas the Gas Law is used.

Bulk modulus

$$K \frac{\Delta V}{V} = -\Delta p \quad S = \frac{1}{K}$$

Gas Law

$$\rho = \frac{p + p_A}{RT} \quad S = \frac{1}{p + p_A}$$



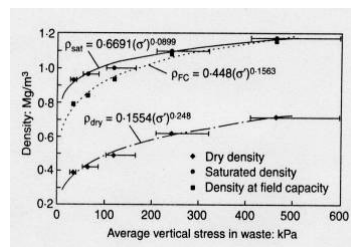
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LDAT constitutive equation $z^L S^L \frac{\partial p^L}{\partial t} + z^G S^G \frac{\partial p^G}{\partial t} + \frac{\partial \phi}{\partial t} = z^L \frac{k^L}{\rho^L g} \frac{\partial^2 p^L}{\partial x^2} + z^G \frac{k^G}{\rho^G g} \frac{\partial^2 p^G}{\partial x^2} + \sum (G_i^L + G_i^G)$

Uncertainties

Compression - Bulk modulus and Gas Law
Porosity/Dry density

$$\frac{\partial \phi}{\partial t} \quad \text{couples flow and settlement}$$



Powrie and Beaven (1999)

$$\rho'_s = A(\sigma - p)^n$$

$$\phi = 1 - \frac{\rho'_s}{\rho_s}$$

$$\frac{\partial \phi}{\partial t} = \frac{\rho'_s}{\rho_s} \frac{n}{(\sigma - p)} \frac{\partial p}{\partial t}$$

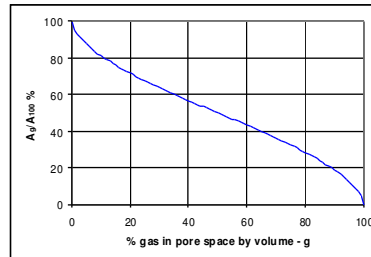
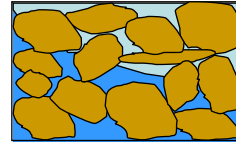


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LDAT constitutive equation

Uncertainties

- Compression - Bulk modulus and Gas Law
- Porosity/Dry density
- Flow and diffusion – Flow areas



Reduction in leachate flow area with increase in gas content



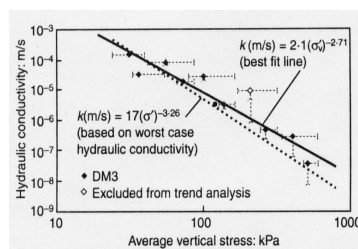
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LDAT constitutive equation $\frac{\partial z}{\partial t} = -zS \frac{\partial p}{\partial t} - z \frac{\partial v}{\partial x} + G$

Uncertainties

- Compression - Bulk modulus and Gas Law
- Porosity/Dry density
- Flow and diffusion – Flow areas
- Permeability

$$v = k \frac{\partial h}{\partial x}$$



Powrie and Beaven (1999)

$$k = C(\sigma - p)^m$$



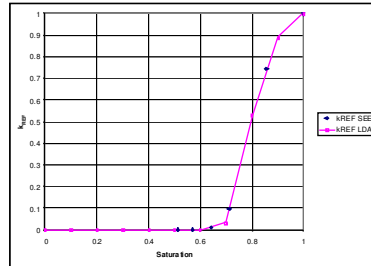
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LDAT constitutive equation

Uncertainties

- Compression - Bulk modulus and Gas Law
- Porosity/Dry density
- Flow and diffusion
 - Flow areas
 - Permeability
 - Relative permeability

$$v = k_{REF} k \frac{\partial h}{\partial x}$$



Relationship between relative permeability and saturation

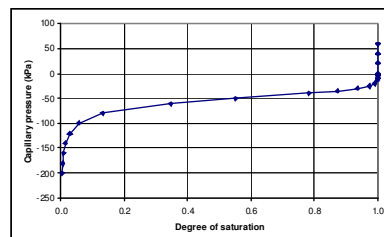


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LDAT constitutive equation

Uncertainties

- Compression - Bulk modulus and Gas Law
- Porosity/Dry density
- Flow and diffusion
 - Flow areas
 - Permeability
 - Relative permeability
 - Capillary pressure



Relationship between gas and liquid pressure fields - capillary pressure?



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LDAT constitutive equation $\frac{\partial z}{\partial t} = -zS \frac{\partial p}{\partial t} - z \frac{\partial v}{\partial x} + G$

Uncertainties

Compression - Bulk modulus and Gas Law

Porosity/Dry density

- Flow and diffusion
- Flow areas
 - Permeability
 - Relative permeability
 - Capillary pressure
 - Diffusion

$$v = k \frac{\partial h}{\partial x} + v_D$$

v_D is the diffusion velocity. We believe that diffusion can be accommodated this simple adjustment although we have not tested this approach.



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LDAT constitutive equation

Uncertainties

Compression - Bulk modulus and Gas Law

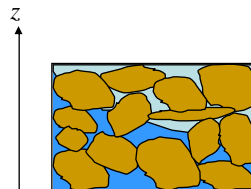
Porosity/Dry density

- Flow and diffusion
- Flow areas
 - Permeability
 - Relative permeability
 - Capillary pressure
 - Diffusion
 - Head gradients

$$v = k \frac{\partial h}{\partial x}$$

$$h = \frac{1}{\rho_{L/G} g} (p + \rho' g z)$$

$$\rho' = z_L \rho^L + z_G \rho^G$$



In the vertical direction the head gradient theoretically depends on concentrations



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Phase change G^P

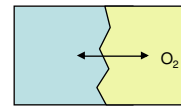
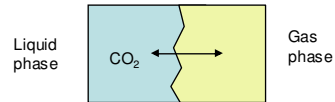
Uncertainties

Compression - Bulk modulus and Gas Law

Porosity/Dry density

- Flow and diffusion
- Flow areas
 - Permeability
 - Relative permeability
 - Capillary pressure
 - Diffusion
 - Head gradients

Gas phase change – Henry's constants and rates



Henry's Law

$$z^{Ln} = H_n z^{Gn} p^G \quad \frac{H_n^T}{H_n^{T_0}} = e^{-p_H \left(\frac{1}{T_0} - \frac{1}{T} \right)}$$

Gas	LDAT H at 25 °C
CH ₄	2.28E-07
O ₂	4.24E-07
N ₂	1.74E-07
CO ₂	1.61E-05
H ₂ S	3.48E-05
SO ₂	9.15E-04
NH ₃	1.04E-02

Gas	P _H
CH ₄	1800
O ₂	1600
N ₂	1300
CO ₂	2400
H ₂ S	2100
SO ₂	2900
NH ₃	4200

After Sander (1999)



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Water vapour G^P

Uncertainties

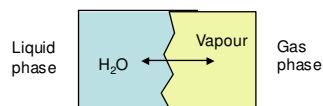
Compression - Bulk modulus and Gas Law

Porosity/Dry density

- Flow and diffusion
- Flow areas
 - Permeability
 - Relative permeability
 - Capillary pressure
 - Diffusion
 - Head gradients

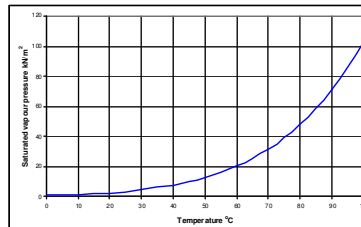
Gas phase change – Henry's constants and rates

Water vapour – Equation and rates



$$\Delta z_w^G = f_w (e_s(T) - z_w^G p^G) \Delta t$$

$$e_s(T) = 0.613 \exp\left(\frac{17.27}{237.3 + T}\right) + p_A$$



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AEROX project – aerobic degradation

Overall aim:

to contribute to the development of the scientific and technical understanding of the flow of air in waste materials using field data and numerical modelling

Specific objectives:

Develop the theory of air/ gas flow in drained waste materials

Incorporate the theoretical framework into LDAT

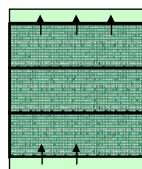
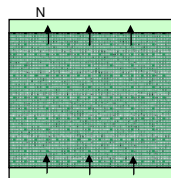
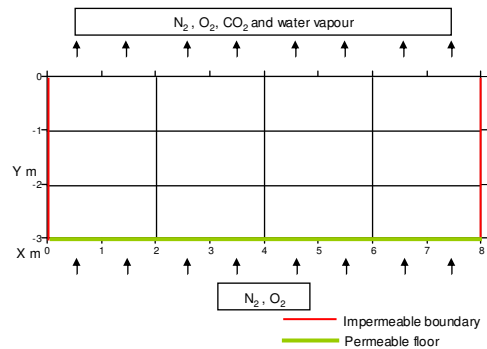
Manage a series of coordinated short-term field trials to generate key data

Use the LDAT model to analyse experimental data to gain a better understanding of controlled air distribution through municipal waste



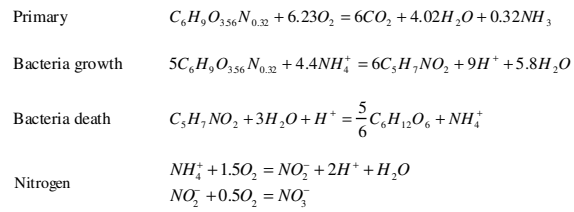
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LDAT configuration – aerobic degradation



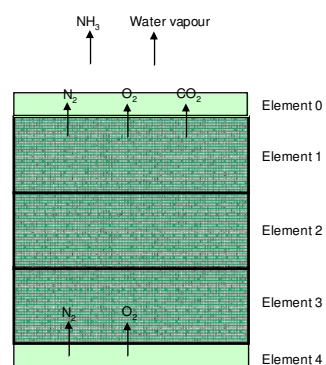
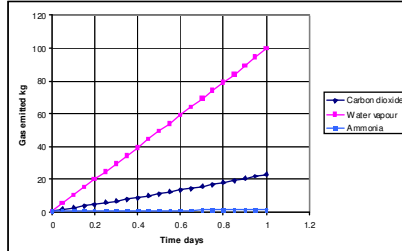
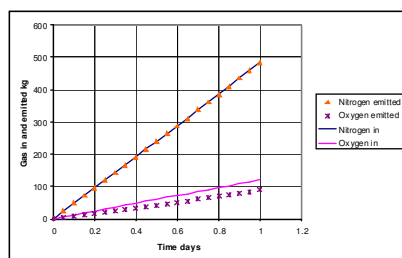
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Aerobic degradation - stoichiometry



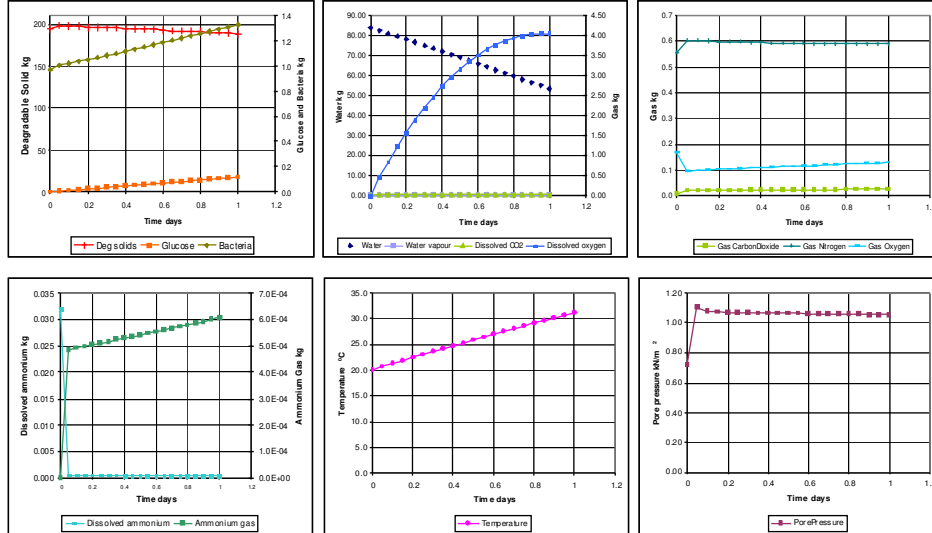
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Aerox model – inputs and outputs



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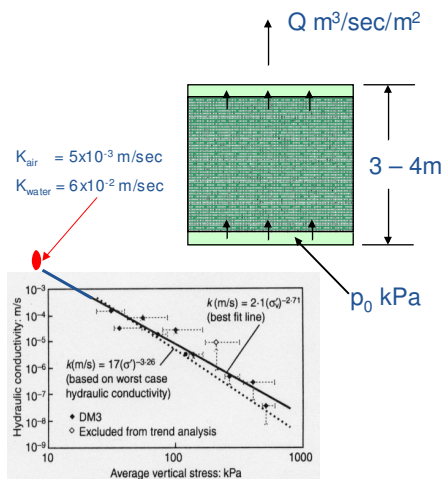
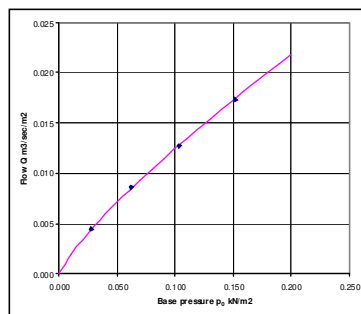
Aerox model – upper element



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Observations and conclusions

Aerox cell as a permeameter



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Observations and conclusions

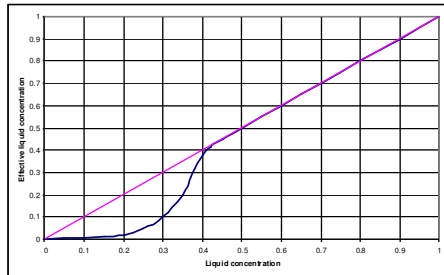
LDAT:

assumes each element is a well mixed reactor

$\rho' = 100 \text{ kg/m}^3$ whereas effective $\rho^G = 1.2 \text{ kg/m}^3$

requires much higher pressure gradients

we need capillary pressure and/or possibly work in terms of an effective z_L



$$h = \frac{1}{\rho^{L/G} g} (p + \rho' g z)$$

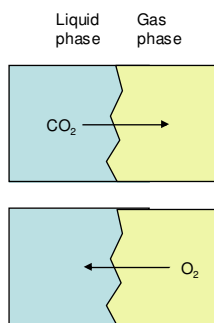
$$\rho' = z_L \rho^L + z_G \rho^G$$



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Observations and conclusions

Phase change parameters



Henry's Law

$$z^{Ln} = H_n z^{Gn} p^G$$

$$\frac{H_n^T}{H_n^{T_0}} = e^{-p_n \left(\frac{1}{T_0} - \frac{1}{T} \right)}$$

Gas	LDAT H at 25 °C
CH ₄	2.28E-07
O ₂	4.24E-07
N ₂	1.74E-07
CO ₂	1.61E-05
H ₂ S	3.48E-05
SO ₂	9.15E-04
NH ₃	1.04E-02

Gas	P _H
CH ₄	1800
O ₂	1600
N ₂	1300
CO ₂	2400
H ₂ S	2100
SO ₂	2900
NH ₃	4200

After Sander (1999)

LDAT model

Gas	H	i _i	Z _{ii}
	m ³ /kN	per day	"K
CO ₂	1.61 x 10 ⁵	0.5	2400
CH ₄	2.28 x 10 ⁷	0.5	1800
O ₂	1.00 x 10 ⁷	0.5	1600
NH ₃	1.04 x 10 ¹¹	0.5	4200



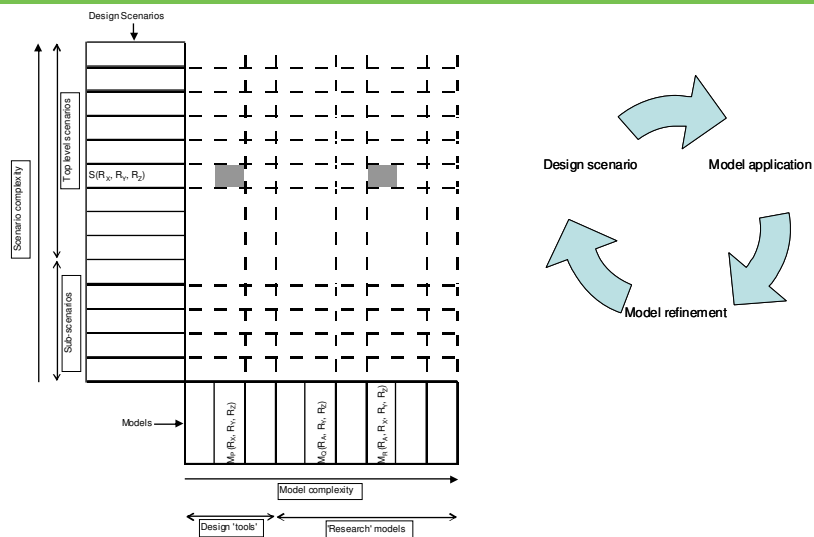
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Observations and conclusions

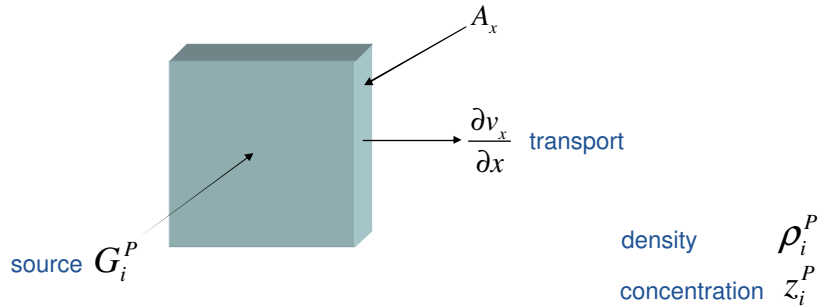
We still need to verify the relationships between component concentration and the parameters flow area, permeability, head and capillary pressure/effective density for waste materials.

We also need to verify the relationships for the solubility of gas and the production of water vapour in landfills.

Roles of numerical modelling



Representative elementary volume V_E



rate of change of mass

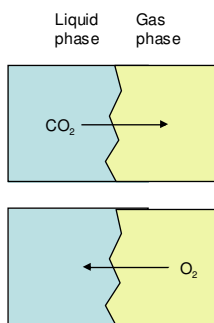
$$\frac{\partial(\rho_i^P z_i^P V_E)}{\partial t} = \rho_i^P G_i^P V_E - \sum_{X,Y,Z} \rho_i^P A_i^P \frac{V_E}{A_X} \frac{\partial(v_i^P)_x}{\partial x}$$



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Phase change G^P

Incorporation of gas phase change



Henry's Law

$$z^{Ln} = H_n z^{Gn} p^G \quad \frac{H_n^T}{H_n^{T_0}} = e^{-p_n \left(\frac{1}{T_0} - \frac{1}{T} \right)}$$

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