

The liquid and gas flow algorithm used in LDAT

Summary:

The LDAT landfill degradation and transport model contains a liquid and gas flow sub-model. The following is a description of the LDAT liquid and gas flow algorithm, which is the calculation procedure that LDAT uses to solve the landfill process analytical constitutive equations. This is a finite difference algorithm that operates upon a framework of rectangular representative elementary landfill waste volumes.

Multi-phase multi-component landfill processes models are used to support the design of landfill management and engineering systems that implement leachate flushing /recirculation, aeration, and gas extraction and collection. These models have the capability to represent the multi-component two phase flow of liquid and gas through the pore space of the solid phase of the waste material.

The constitutive equation is the implementation of Darcy's Law which relates flow of liquid and gas to pressure gradients and permeability in unsaturated porous materials. The permeability to liquid and gas in saturated waste are obtained using the Powrie and Beaven permeability model that relates them to effective stress. The relative permeability of unsaturated material is obtained using the van Genuchten equation that relates relative permeability to the effective degree of saturation.

The solution of the constitutive equation requires the estimation of the pore space capillary pressure which connects the liquid and gas pressure fields. This is achieved by using the van Genuchten equation that relates capillary pressure to the effective degree of saturation.

The solution also requires a connection to be made between the solid phase of the waste and the liquid and gas phases. This is achieved using the Powrie and Beaven dry density (porosity) model that relates them to the effective stress.

Full details of the Darcy, Powrie and Beaven and van Genuchten equations are provided, together with the derivation of the LDAT numerical solution algorithm.

1. Introduction

Multi-phase multi-component landfill processes models have a role in supporting the design of landfill management and engineering systems that implement leachate flushing /recirculation, aeration, and gas extraction and collection. There is a requirement for such models to have the capability to represent the multi-component two phase flow of liquid and gas through the pore space of the solid phase of the waste material.

This following describes the liquid and gas flow algorithm of the landfill degradation and transport model LDAT. The algorithm has been significantly refined since it was first published, (White et al. 2004), and now accommodates unsaturated flow which includes a multi-component gas flow phase.

LDAT is a general model of landfill processes consisting of a set of linked process sub-models. Each process sub-model references the same set of Primary Variables, which are sufficient to specify the state of the waste at any point in time and space. All other variables, the Secondary Variables, required by a sub-model are derived from the Primary Variables using a set of common constants and empirical relationships. Examples of Secondary Variables include density and permeability.

In the case of LDAT the Primary Variables are the mass of each chemical compound in each of the solid, liquid and gas phases m_n^P , together with the stresses applied to those phases. The stresses are the total stress applied to the solid phase, σ , the liquid and gas pressures, p^L and p^G , and temperature T . (White and Beaven 2013).

The sub-models together effectively solve the constitutive equations of landfill waste degradation and transport within the framework of a finite difference grid that represents the landfill spatially.

The source term of the constitutive equation is arranged to accommodate degradation, gas solubility, gas diffusion, and the impact of temperature changes due to heat generation and transfer. The remainder of the equation is decoupled from the solid phase terms which form the basis of the settlement sub-model, with liquid/gas phase transport calculated in a sub-model as described in Sections 2 and 3.

Following the description of the LDAT degradation algorithm given in (White and Beaven 2013), the aim of this paper is to provide details of the LDAT flow algorithm.

Notation

<i>C</i>	Subscript denoting capillary pressure see equation (16)	
<i>E</i>	Subscript denoting ‘effective’	
<i>e</i>	Subscript indexing finite difference element see Figure 1 and Note 1 below.	
<i>m</i>	Subscript indexing elements neighbouring <i>e</i> , see Figure 1 and Note 1 below	
<i>n</i>	Subscript indexing component	
<i>REF</i>	Subscript denoting reference value	
<i>REL</i>	Subscript denoting relative value	
<i>vh</i>	Subscript denoting vertical to horizontal ratio	
<i>D</i>	Superscript denoting dry density see equation (17)	
<i>G</i>	Superscript denoting gas phase	
<i>L</i>	Superscript denoting liquid phase	
<i>MAX</i>	Superscript denoting maximum value	
<i>MIN</i>	Superscript denoting maximum value	
<i>P</i>	Superscript denoting phase. Liquid phase $P = L$, Gas phase $P = L$, Solid phase $P = S$	
<i>R</i>	Superscript denoting residual value	
<i>S</i>	Superscript denoting solid phase	
<i>A</i>	Area	m^2
<i>a</i>	See equation (27)	m^3/kPa
<i>B</i>	Right hand side of solution matrix, see equation(34)	m^3
<i>b</i>	See equations (28) and (29)	m^3
<i>C</i>	Left hand side of solution matrix, see equation(35)	m^3/kPa
<i>c</i>	See equation(31)	m^3
<i>d</i>	Element dimension	m
<i>G</i>	Source flow concentration	$m^3/(day.m^3)$

g	Acceleration due to gravity	kN/kg
h	Pressure head	m
i	Column index in solution matrix	
J	Mass transmissivity, see equation (20)	kg/(day.m)
k, K	Permeability	m/day
l	absolute value of distance between element centres	m
M	Mass transfer	kg
m	Mass	kg
p	Pressure	kPa
Q	Volume transfer	m ³
S	Storage coefficient	1/kPa
S'	Volumetric storage coefficient, see equation (31)	m ³ /kPa
T	Temperature	°C, °K
t	Time	day
V	Volume	m ³
v	Component flow velocity	m/day
x	Coordinate	m
z	Concentration	
α	See equation (16)	m ³ /m ³
β	See equation (16)	m ⁻¹
δ	See equations (8) and (9)	
ε	See equations (14) and (15)	
ϕ	Porosity	
γ	See equations (8), (9) and (16)	
η	See equation (5)	
λ	See equation (17)	

μ	Viscosity	kPa.day
θ	Moisture content	
ρ	Density	kg/m ³
σ	Total stress	kPa
σ_0	Surface stress	kPa
σ'	Effective stress	kPa
ζ	Degree of saturation	
τ	See equation(15)	
ω	See equation(22)	m ²

2. The LDAT liquid and gas flow constitutive equations

The bio-chemical and physical processes that take place in a waste landfill may be represented analytically by a set of algebraic constitutive equations. The solution of these equations may be obtained numerically by re-casting them as a calculation procedure, or algorithm. This section describes the constitutive equations and algorithm that may be used to represent the flow of the liquid and gas phases in the waste material. These are based on those used in the landfill degradation and transport model LDAT (White et al. 2004, White and Beaven 2013) which in turn have been derived from a range of sources including (Darcy 1856, Bear 1979, Bear and Verruijt 1992, Ghabaee and Rodwell 1989, Das 1983, Droste 1997, Moody et al. 1992, Hydrogeologic 1996, McDonald and Harbaugh 1988, Bente 2011).

LDAT solves the landfill process constitutive equations using a finite difference algorithm within a framework of rectangular representative elementary volumes. The framework for the finite difference algorithm is a three dimensional rectangular element e as shown in Figure 1.

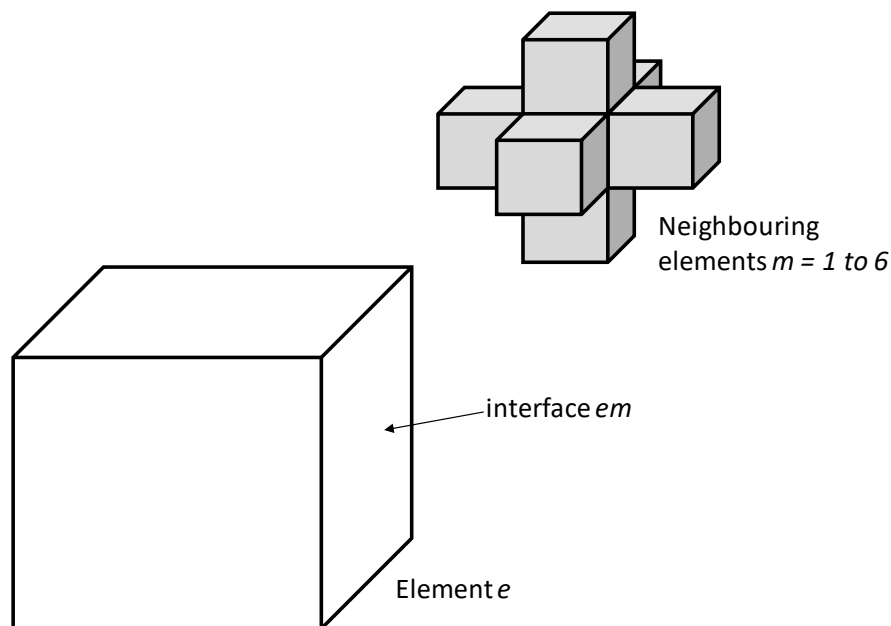


Figure 1 Finite difference three dimensional rectangular element.

Note: Each element has a number, in this case e . There are six interfaces with neighbouring elements. The interfaces are designated by the integer $m = 1$ to 6 . The number of a neighbouring element i is obtained from an array mapping function $i = array_map(e, m)$.

The space occupied by the waste material in the landfill is represented by a three dimensional array of these elements. Each element is surrounded by six neighbouring elements some of which may be

boundary elements. The array of six neighbouring elements is indexed by $m = 1$ to 6, Figure 1. The suffix em attached to a variable denotes that the variable is evaluated at the interface between the element and its neighbour m . In the case of vectors it also denotes direction, which is positive in the outward direction normal to the interface. A single suffix e attached to a variable denotes that the variable is evaluated at the centroid of element e .

The waste material is represented as the assembly of a number of component chemical compounds and species (chemical elements), each of which can exist in one or all of the three phases solid, liquid, and gas. The conservation of the mass $m_{e,n}^P = \rho_{e,n}^P z_{e,n}^P V_e$ of the n^{th} component of the waste in phase P (solid, liquid or gas) in the context of a representative elementary volume, V_e , may be expressed by the following equation,

$$\frac{\partial m_{e,n}^P}{\partial t} = \rho_{e,n}^P G_{e,n}^P V_e - \sum_m \rho_{em,n}^P A_{em,n}^P v_{em,n}^P \quad (1)$$

For the gas and liquid phases $v_{em,n}^P$ is the interstitial flow velocity (m/day) of component n . For the solid phase it represents the solid particle displacement velocity. $G_{e,n}^P$ is the source term ($\text{m}^3/\text{day}/\text{m}^3$) associated with component n in phase P . $\rho_{em,n}^P$ is the component density and $A_{em,n}^P$ is the area associated with the flow or displacement velocity $v_{em,n}^P$. The mass of component n in phase P can be expressed as $m_{e,n}^P = \rho_{e,n}^P z_{e,n}^P V_e$ where $z_{e,n}^P$ is the component volumetric concentration or volume fraction (m^3/m^3).

The mass of a component $m_{e,n}^P$ is the key parameter that LDAT calculates and tracks through time and space.

In the process of solving equation (1), which ensures that mass is balanced, the condition $\sum_n z_{e,n}^P = 1$ is applied to preserve volumetric consistency. Therefore, in order to be able to apply this condition, $m_{e,n}^P$ in equation (1) is replaced by $\rho_{e,n}^P z_{e,n}^P V_e$ to obtain,

$$\frac{z_{e,n}^P}{\rho_{e,n}^P} \frac{\partial \rho_{e,n}^P}{\partial t} V_e + \frac{\partial z_{e,n}^P}{\partial t} V_e = G_{e,n}^P V_e - \frac{1}{\rho_{e,n}^P} \sum_m \rho_{em,n}^P A_{em,n}^P v_{em,n}^P \quad (2)$$

Since changes in density are due to compression or expansion accompanying changes in pressure, the

term $\frac{z_{e,n}^P}{\rho_{e,n}^P} \frac{\partial \rho_{e,n}^P}{\partial t}$ may be replaced without loss of generality by $z_{e,n}^P S_{e,n}^P \frac{\partial p_e^P}{\partial t}$ where p_e^P is the phase pressure and $S_{e,n}^P$ is a storage coefficient with units 1/kPa. For the liquid and solid phases the storage

coefficient is equal to the reciprocal of the respective bulk moduli and, for the gas phase, $S_{e,n}^G$ is obtained from the gas law.

The individual concentrations of the compounds $z_{e,n}^P$ are related to the overall concentrations of the solid, liquid and gas phases z_e^S , z_e^L and z_e^G , and to the porosity of the solid phase ϕ_e by the relationships,

$$z_e^P = \sum_n z_{e,n}^P \quad \text{and} \quad \sum_P z_e^P = 1$$

$$\phi_e = z_e^L + z_e^G, \quad 1 - \phi_e = z_e^S$$

Note also that z_e^L is the volumetric moisture content θ_e and that the degree of saturation is $\zeta_e = \frac{z_e^L}{\phi_e}$.

The source terms $G_{e,n}^P$ are each composed of four parts, a recharge/abstraction term, a degradation term, a phase change term, and a diffusion/dispersion term. The way in which LDAT evaluates the degradation term is described in (White and Beaven 2013). Since the effects of diffusion and dispersion are dealt with in the source terms, the assumption may be made in the flow algorithm that, for each phase, the velocity in a particular direction of each of the components in that phase is the same.

For the liquid and gas phases the interstitial velocity v_{em}^P can be estimated using Darcy's equation,

$$z_{em}^P v_{em}^P = -k_{em}^P \left(\frac{\partial h^P}{\partial x} \right)_{em} \quad (3)$$

$\left(\frac{\partial h^P}{\partial x} \right)_{em}$ are the head gradients and k_{em}^P are the permeabilities of the waste in the em direction, for

the relevant liquid or gas components. The permeabilities may be expressed as,

$$k_{em}^P = k_{REL}^P (\zeta_e^E) K_{em}^P \quad \zeta_e^E = \frac{\zeta_e - \zeta_e^R}{\zeta_e^{MAX} - \zeta_e^R} \quad (4)$$

ζ_e^E is the effective degree of saturation which falls to zero when the actual degree of saturation, ζ_e , reaches the residual degree of saturation, ζ_e^R , for the material. ζ_e^{MAX} is the maximum degree of saturation that the material can reach, $1 - \zeta_e^{MAX}$ being related to the residual amount of trapped gas that will be retained by the material.

K_{em}^P are the fully saturated hydraulic conductivity, and the permeability to gas in the absence of liquid, respectively. $k_{REL}^P(\zeta_e^E)$ are functions of effective leachate saturation, ζ_e^E , with values that lie between 0 and 1, and thus modify the values of K_{em}^P to allow for the impact on permeability of partially saturated conditions.

The hydraulic conductivity of the waste in a saturated condition may be estimated using the empirical relationship between hydraulic conductivity and effective stress σ' (kN/m²) proposed by (Powrie and Beaven 1999).

$$K_{em}^L = k_{vh} K_{REF}^L \left(\frac{\sigma'}{\sigma'_{REF}} \right)^\eta \quad (5)$$

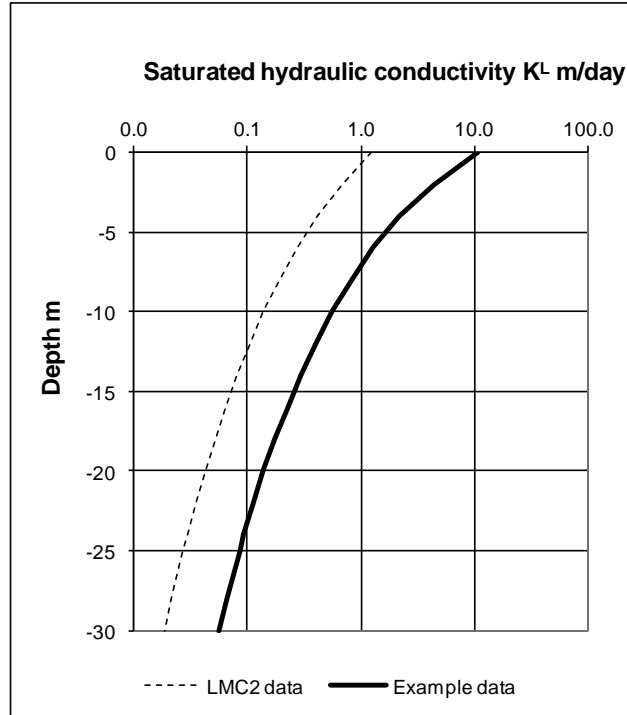
K_{REF}^L , σ'_{REF} and η are empirical coefficients which will be sensitive to the condition and nature of the particular waste being modelled. Examples of evaluations of equation (5) are shown in Figure 2.

k_{vh} is the ratio of vertical to horizontal permeability.

In LDAT the effective stress, σ' (kPa), is calculated using,

$$\sigma' = \sigma - \varphi^L - (1 - \zeta) p^G$$

where σ is the total stress applied by the load due to overburden and any applied surface load per unit area, σ_0 , or surface stress (kPa).



Parameter		Notation	Units	LMC2 data ¹	Example data ²
Hydraulic conductivity	Reference permeability	K_{REF}^L	m/day	8.25	20
	Reference effective stress	σ'_{REF}	kPa	40	40
	Power law index	η		-2.71	-2.71
	Surface stress	σ_0	kPa	80	50

1. Values used in (White and Beaven, 2013)
2. Values used for the modelling example described in Section 3

Figure 2 Parameters for saturated hydraulic conductivity, equation (5).

The value of K_{em}^L may be adjusted for temperature through viscosity and density using the following approach, (Das 1983). If ρ_{REF,T_0}^L and μ_{REF,T_0}^L are the reference density and viscosity at the temperature T_0 at which the reference permeability K_{REF,T_0}^L in equation (5) has been measured, then the permeability to a liquid with density ρ_T^L and viscosity μ_T^L is given by replacing K_{REF}^L in equation (5) by,

$$K_{REF,T}^L = K_{REF,T_0}^L \frac{\mu_{REF,T_0}^L \rho_T^L}{\rho_{REF,T_0}^L \mu_T^L} \quad (6)$$

Equation (6) may also be used to estimate the gas permeability under conditions of gas saturation thus,

$$K_{em}^G = K_{em}^L \frac{\mu^L}{\rho^L} \frac{\rho^G}{\mu^G} \quad (7)$$

Examples of functional relationships between density and viscosity, and temperature and pressure are given in Table 1.

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/m ³
Gas density	ρ^G	$m(p^G + p_A)/R(T + 273)$	kg/m ³

p^L	liquid pressure	kPa
p^G	gas pressure	kPa
p_A	atmospheric pressure	kPa
T	temperature	°C
m	molecular weight	kg/mole
R	gas constant	kN/(mole.°K)
K_L	liquid bulk modulus	kPa

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

When there is two phase flow and the material is partially saturated, the area of liquid flow reduces because of the presence of gas, and the permeability reduces because of capillarity effects.

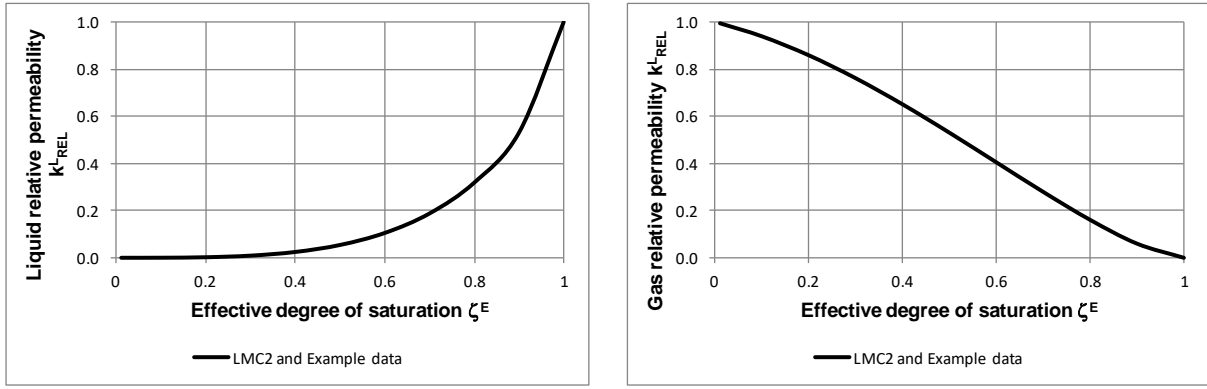
An analytical expression that covers both of these effects by evaluating the liquid phase relative permeability value, k_{REL}^L in equation (4), is derived by (van Genuchten 1980),

$$k_{REL}^L = (\zeta_e^E)^{\delta^L} \left(1 - \left(1 - (\zeta_e^E)^{\frac{1}{\gamma^L}} \right)^{\gamma^L} \right)^2 \quad (8)$$

The corresponding expression for relative permeability to gas is

$$k_{REL}^G = (1 - \zeta_e^E)^{\delta^G} \left(1 - (\zeta_e^E)^{\frac{1}{\gamma^G}} \right)^{2\gamma^G} \quad (9)$$

δ^L and δ^G are pore space geometry correlation coefficients proposed by (Mualem 1976). γ^L and γ^G are related to the parameter γ in the capillary pressure function proposed by van Genuchten, equation (16). Examples of the functions represented by equations (8) and (9) are given in Figure 3.



Relative permeability	Liquid correlation	δ^L	0.5
	Liquid gamma	γ^L	0.7
	Gas correlation	δ^G	0.5
	Gas gamma	γ^G	0.5

Figure 3 Liquid and gas relative permeabilities equations (8) and (9)

$\left(\frac{\partial h^P}{\partial x}\right)_{em}$, the head gradient, in Darcy's equation (3) has two components, the phase pressure head gradient and the gravity induced head gradient in the vertical direction,

$$\left(\frac{\partial h^P}{\partial x}\right)_{em} = \frac{1}{\rho^P} g \left(\frac{\partial p^P}{\partial x}\right)_{em} + \frac{\rho_E^P}{\rho^P} f(em) \quad (10)$$

where, $f(em)=1$, em : pair of elements connected vertically, otherwise $f(em)=0$.

ρ_E^P is the phase effective liquid/gas density. If the gas and liquid phases are assumed to be fully mixed, the effective density for both phases will be,

$$\rho_E^L = \rho_E^G = \zeta \rho^L + (1-\zeta) \rho^G \quad (11)$$

where ζ is the degree of saturation.

However it is conceivable that the phases will not fully mix but will remain separate to a certain degree. Suppose that when the degree of saturation is ζ , the degree of saturation of the gas is actually ε^G . This means that if the volume of gas present is V^G , $\varepsilon^G V^G$ of the gas is replaced by liquid and the mass in the gas phase becomes $\rho^G V^G + \varepsilon^G V^G (\rho^L - \rho^G)$

Thus the effective density of the fluid (liquid and/or gas) fraction controlled by the gas phase pressure is given by,

$$\rho_E^G = \varepsilon^G \rho^L + (1-\varepsilon^G) \rho^G \quad (12)$$

The corresponding mass in the liquid volume V^L , will become $\rho^L V^L - \varepsilon^G V^G (\rho^L - \rho^G)$ and,

$$\rho_E^L = \rho^L - \varepsilon^G \left(\frac{V^G}{V^L} \right) (\rho^L - \rho^G) = \rho^L - \varepsilon^G (\rho^L - \rho^G) \frac{(1-\zeta)}{\zeta} \quad (13)$$

Equations (12) and (13) give a range of gas and liquid effective densities from conditions where the phases are completely separated to fully mixed, as ε^G varies from 0 to ζ .

This concept of effective density may be used in a modelling context by devising a simple algebraic functional relationship between ε^G and ζ . The relationship given by equations (14) and (15) is employed in LDAT. The characteristic shape of this relationship can be varied by choosing appropriate values for the parameters ζ_{REF} and τ .

$$\varepsilon^G = 0 \quad \zeta < \zeta_{REF} \quad (14)$$

$$\varepsilon^G = \left(\frac{\zeta - \zeta_{REF}}{1 - \zeta_{REF}} \right)^\tau \quad \zeta_{REF} < \zeta < 1 \quad (15)$$

An illustration of the impact of this function on the liquid and gas densities is given in Figure 4 for $\zeta_{REF} = 0.2$ and $\tau = 5$. The effect of this refinement analytically is that the two phases are treated as separate as far as density is concerned over the lower range of saturation but tend towards the fully mixed density values over the higher range of saturation. Fully mixed conditions, equation (11), are modelled throughout when $\zeta_{REF} = 0$ and $\tau = 1$. Since no mixing takes place when $\zeta < \zeta_{REF}$, fully separated conditions are modelled throughout when ζ_{REF} is set equal to 1. For intermediate values of ζ_{REF} the effective liquid and gas densities used to evaluate the vertical head gradients for each phase using equation (10) change from the separated values to the fully mixed values as ζ varies from ζ_{REF} to 1.

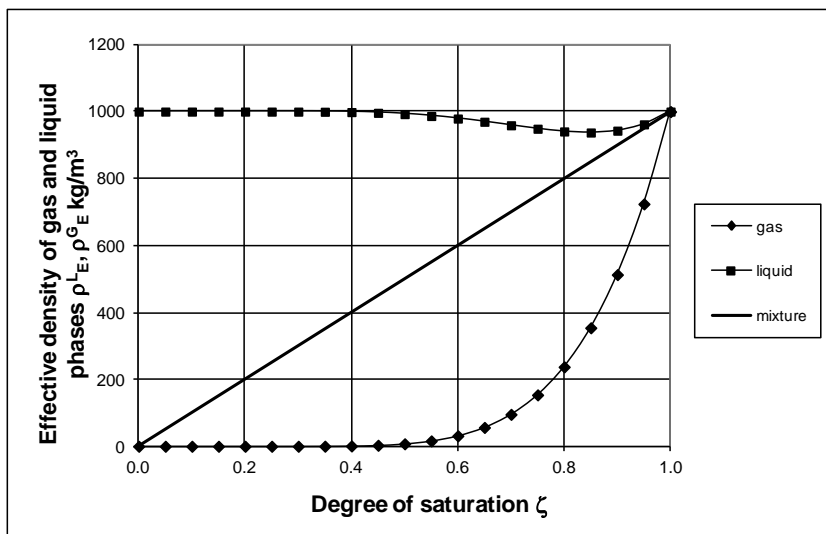


Figure 4 Effective liquid and gas densities

As will be seen in Section 3 the solution of equation (2) requires there to be a relationship between the liquid and gas pressure fields, p^L and p^G . This is obtained from the capillary pressure

$p_C = p^G - p^L$ which may be obtained by using the (van Genuchten 1980) expression relating p_C to the effective degree of saturation,

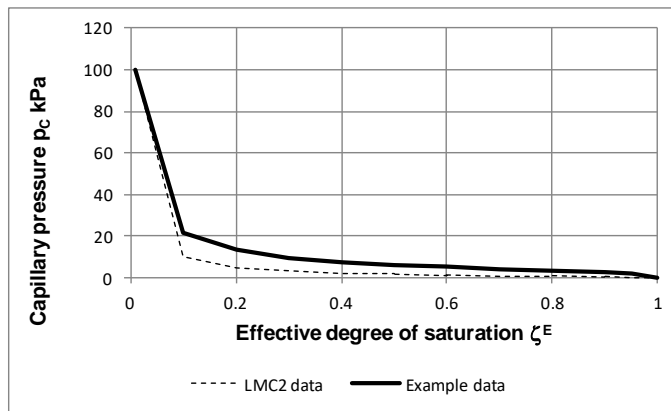
$$p_C = \frac{\rho_L g}{\alpha} \left((\zeta^E)^{\frac{1}{\gamma}} - 1 \right)^{\frac{1}{\beta}} \quad (16)$$

In equation (16), as the value of ζ approaches the residual degree of saturation, and ζ^E tends to zero, the capillary pressure becomes infinitely large. In LDAT to prevent the value of p_C becoming unrealistically large it is capped at 100 kPa at a small value of ζ^E , $\zeta^{E,MIN} = 0.01$. In equation (16)

$\gamma = 1 - \frac{1}{\beta}$ so that the function has essentially four parameters α , β , ζ^R and ζ^{MAX} . If the function is

also constrained to cap the value of p_C to p_C^{MAX} at $\zeta^E = \zeta^{E,MIN}$, then α is also a function of β ,

$$\alpha = \frac{\rho^L g}{p_C^{MAX}} \left(\zeta^{E,MIN} - \frac{1}{\gamma} - 1 \right)^{\frac{1}{\beta}} \approx \frac{\rho^L g}{p_C^{MAX}} \left(\zeta^{E,MIN} \right)^{-\frac{1}{\beta-1}}$$



	LMC2 data	Example data
β	2	2.5
α	9.81	2.11

Figure 5 Capillary pressure, equation (16)

It is generally accepted that the shape of the relationship $p_C(\zeta^E)$ will change depending on whether or not the material is in the process of increasing or decreasing in saturation (imbibing or draining).

This hysteresis effect is very complicated and is not presently modelled in LDAT.

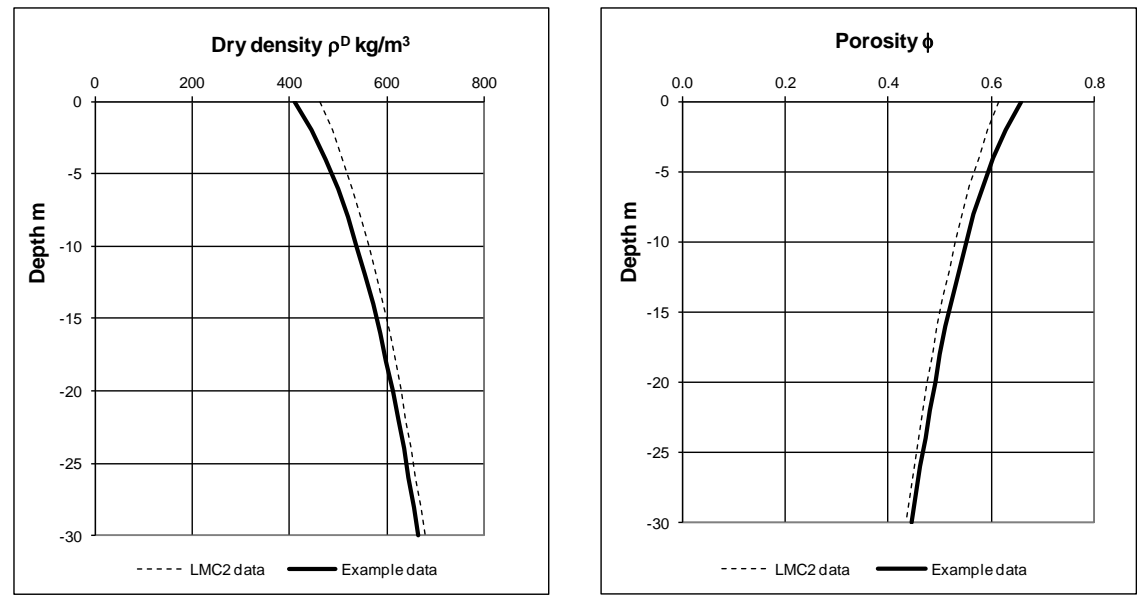
When equation (2) is written separately for the liquid and gas phases, and the resulting equations are added together to solve for the liquid and gas pressure fields, the term $\frac{\partial z_e^L}{\partial t} + \frac{\partial z_e^G}{\partial t} = \frac{\partial \phi_e}{\partial t}$ emerges.

$\frac{\partial \phi_e}{\partial t}$ is in fact the term that couples the liquid and gas phase equations to the solid phase and may be calculated using the Powrie and Beaven (1999) relationship for dry density ρ_e^D , Figure 6.

$$\rho_e^D = \rho_{REF} \left(\frac{\sigma'_e}{\sigma'_{REF}} \right)^\lambda \quad (17)$$

Since $\phi_e = 1 - \frac{\rho_e^D}{\rho^S}$, where ρ^S is the solid phase material density,

$$\frac{\partial \phi_e}{\partial t} \approx \frac{\rho_e^D}{\rho^S} \frac{\lambda}{\sigma'} \frac{\partial p_e^G}{\partial t} \approx z_e^S S_e^\phi \frac{\partial p_e^G}{\partial t} \quad (18)$$



Parameter		Notation	Units	LMC2 data	Example data
Dry density	Reference dry density	ρ_{REF}	kg/m ³	388	388
	Reference effective stress	σ'_{REF}	kPa	40	40
	Power law index	λ		0.248	0.248
	Overburden	σ_0	kPa	80	50
Porosity	Material density	ρ^S	kg/m ³	1200	1200

Figure 6 Dry density and porosity profiles

3. Finite difference algorithm for the liquid and gas flow sub-model

The constitutive equations described in Section 2 are solved in LDAT within the framework of a two dimensional rectangular grid of constant volume elements that discretise the space occupied by the waste. Boundary conditions and initial conditions are prescribed for the concentrations of all of the compounds present, and the equations are solved numerically in time and space using the finite difference method.

In each time step the sub-models which affect the source term, such as the bio-degradation and phase change algorithms, are run first to evaluate $G_{e,n}^P$ in equation (2). These calculations are based on the conditions at the beginning of each time step whilst they should be based on conditions that are averaged over the time step. The error caused by this emerges as a volumetric error in that at the end of the time step, whilst the model mass balance is conserved, the volume of the contents of an element, V_e' , will be calculated to be different from the physical volume of the element, V_e . This may be remedied by repeating the calculation in an iterative loop, or by adjusting the source term with a volume numerical correction term $\Delta V_e = V_e' - V_e$ during the next time step, see equation (31). The latter approach is used in LDAT to avoid the excessive computation times caused by the iterative approach.

To develop the finite difference algorithm for the liquid and gas flow sub-model, equations (3) and (10) are first substituted into equation (2). Equation (2) is a set of three groups of equations, one group for each phase, with each group containing the individual equations for each component n . By adding together the equations in the liquid and gas phase groups, and using equation (16), an overall flow equation for the gas pressure, p^G , may be obtained and solved numerically to give the transient gas pressure field.

Once this has been done, the process is reversed to back calculate the liquid pressure field from equation (16) and the overall mass transfers in the system from equations (3) and (10). The individual compound concentrations and masses can then be obtained from a further back calculation using the equations represented by equations (1) and (2). The details of this derivation of the flow algorithm are as follows.

The summation in the last term in equation (2) is first written in the following finite difference form,

$$\begin{aligned} \sum_m \rho_{em,n}^P A_{em,n} v_{em}^P &= \sum_m -\rho_{em,n}^P A_{em,n} \frac{k_{em}^P}{z_{em}^P} \left(\frac{\Delta h^P}{\Delta x} \right)_{em} \\ &= \sum_m \rho_{em,n}^P \frac{z_{em,n}^P}{z_{em}^P} \frac{A_{em} k_{em}^P}{l_{em}} (h_e^P - h_m^P) = \sum_m J_{em,n}^P (h_e^P - h_m^P) = \sum_m J_{em,n}^P \Delta h_{em}^P \quad (19) \end{aligned}$$

Where,

$$J_{em,n}^P = \rho_{em,n}^P \frac{z_{em,n}^P}{z_{em}^P} \frac{A_{em} k_{em}^P}{l_{em}} \quad (20)$$

and is calculated according to the fluid phase and the direction of flow; that is, if $h_e^P > h_m^P$ then $k_{em}^P = k_e^P$ otherwise $k_{em}^P = k_m^P \cdot \rho_{em,n}^P$, $z_{em,n}^P$ and z_{em}^P are treated similarly. h_e^P is the fluid phase head at the centre of element e .

It is assumed that $A_{em,n} = z_{em,n}^P A_{em}$.

A_{em} is the area of the interface between elements e and m .

l_{em} is the absolute value of the distance between the centres of elements e and m .

Using equation (10) gives,

$$\Delta h_{em}^P = h_e^P - h_m^P = \frac{1}{\rho_{em}^P g} (p_e^P - p_m^P) + \frac{\rho_{em}^{EP}}{\rho_{em}^P} (x_e - x_m) = \frac{1}{\rho_{em}^P g} \Delta p_{em}^P + \frac{\rho_{em}^{EP}}{\rho_{em}^P} \Delta x_{em}$$

Thus in equation (19),

$$\begin{aligned} \sum_m J_{em,n}^P \Delta h_{em}^P &= \sum_m \left(\frac{1}{\rho_{em}^P g} J_{em,n}^P \Delta p_{em}^P + \frac{\rho_{em}^{EP}}{\rho_{em}^P} J_{em,n}^P \Delta x_{em} \right) \\ &= - \sum_m \left(\frac{1}{\rho_{em}^P g} J_{em,n}^P p_m^P \right) + p_e^P \sum_m \frac{1}{\rho_{em}^P g} J_{em,n}^P + \sum_m \frac{\rho_{em}^{EP}}{\rho_{em}^P} J_{em,n}^P \Delta x_{em} \end{aligned}$$

$\Delta x_{em} = x_e - x_m$ is the distance between the centres of elements e and m and is calculated taking into account sign and expressed as a positive or negative quantity. Note that $\Delta x_{em} = 0$ when the elements e and m are not connected vertically.

The densities ρ_{em}^P and ρ_{em}^{EP} are weighted values across the em interface thus,

$$\rho_{em}^P = \frac{\rho_e^P d_e + \rho_m^P d_m}{2l_{em}} \quad \text{and} \quad \rho_{em}^{EP} = \frac{\rho_e^{EP} d_e + \rho_m^{EP} d_m}{2l_{em}}$$

d_e and d_m are the lengths of elements e and m in the em direction. ρ_e^P and ρ_e^{EP} are the overall phase densities and overall effective phase densities in element e .

Dealing with all of the terms in equation (2) we have,

$$z_n^P S_n^P V_E \frac{\Delta p_e^P}{\Delta t} + V_E \frac{\Delta z_n^P}{\Delta t} = G_n^P V_E + \frac{1}{\rho_{e,n}^P} \sum_m \left(\frac{1}{\rho_{em}^P g} J_{em,n}^P p_m^P \right) - p_e^P \frac{1}{\rho_{e,n}^P} \sum_m \frac{1}{\rho_{em}^P g} J_{em,n}^P - \frac{1}{\rho_{e,n}^P} \sum_m \frac{\rho_{em}^{EP}}{\rho_{em}^P} J_{em,n}^P \Delta x_{em} \quad (21)$$

Writing,

$$\omega_{em}^P = \sum_n \Delta t \frac{J_{em,n}^P}{\rho_{e,n}^P} \quad (22)$$

and summing equation (21) over the components in each phase, we can obtain the aggregated two fluid phase equations.

Thus for the gas phase,

$$z_e^G S^G V_e \Delta p_e^G + \Delta z_e^G V_e = V_e \Delta t G_e^G + \sum_m \left(\frac{\omega_{em}^G}{\rho_{em}^G g} p_m^G \right) - p_e^G \sum_m \frac{\omega_{em}^G}{\rho_{em}^G g} - \sum_m \omega_{em}^G \frac{\rho_{em}^{EG}}{\rho_{em}^G} \Delta x_{em} \quad (23)$$

For the liquid phase,

$$z_e^L S^L V_e \Delta p_e^L + \Delta z_e^L V_e = V_e \Delta t G_e^L + \sum_m \left(\frac{\omega_{em}^L}{\rho_{em}^L g} p_m^L \right) - p_e^L \sum_m \frac{\omega_{em}^L}{\rho_{em}^L g} - \sum_m \omega_{em}^L \frac{\rho_{em}^{EL}}{\rho_{em}^L} \Delta x_{em}$$

Or using equation (16), $p_c = p^G - p^L$, and assuming that p_c is constant during the time increment,

$$\begin{aligned} z_e^L S^L V_e \Delta p_e^L + \Delta z_e^L V_e &= V_e \Delta t G_e^L + \sum_m \left(\frac{\omega_{em}^L}{\rho_{em}^L g} p_m^G \right) - p_e^G \sum_m \frac{\omega_{em}^L}{\rho_{em}^L g} \\ &+ \sum_m \frac{\omega_{em}^L}{\rho_{em}^L g} \Delta p_{em}^C - \sum_m \omega_{em}^L \frac{\rho_{em}^{EL}}{\rho_{em}^L} \Delta x_{em} \end{aligned} \quad (24)$$

Introducing for convenience the additional variables a and b equation (23) and (24) become,

$$z_e^G S^G V_e \Delta p_e^G + \Delta z_e^G V_e = V_e \Delta t G_e^G + \sum_m a_{em}^G p_m^G - p_e^G \sum_m a_{em}^G - \sum_m b_{em}^G \quad (25)$$

$$z_e^L S^L V_e \Delta p_e^L + \Delta z_e^L V_e = V_e \Delta t G_e^L + \sum_m a_{em}^L p_m^G - p_e^G \sum_m a_{em}^L - \sum_m b_{em}^L + \sum_m b_{em}^C \quad (26)$$

$$a_{em}^P = \frac{\omega_{em}^P}{\rho_{em}^P g} \quad (27)$$

$$b_{em}^C = \frac{\omega_{em}^P}{\rho_{em}^P g} \Delta p_{em}^C = a_{em}^P \Delta p_{em}^C \quad (28)$$

$$b_{em}^P = \omega_{em}^P \frac{\rho_{em}^{EP}}{\rho_{em}^P} \Delta x_{em} = a_{em}^P \rho_{em}^{EP} g \Delta x_{em} \quad (29)$$

These two phase equations are now combined, with use being made of the fact that

$$\Delta z_e^G + \Delta z_e^L = \Delta \phi_e$$

and the notation,

$$a_{em}^{L/G} = a_{em}^L + a_{em}^G$$

$$b_{em}^{L/G} = b_{em}^L + b_{em}^G$$

$$G_e^{L/G} = G_e^L + G_e^G$$

Also note that $\Delta p_e^L = \Delta p_e^G = \Delta p_e$. Again for convenience we will now write $p_e = p_e^G$ to obtain by adding equations (25) and (26),

$$z_e^G S^G V_e \Delta p_e + z_e^L S^L V_e \Delta p_e + \Delta \phi_e V_e = V_e \Delta t G_e^{L/G} + \sum_m a_{em}^{L/G} p_m - p_e \sum_m a_{em}^{L/G} - \sum_m b_{em}^{L/G} + \sum_m b_{em}^C \quad (30)$$

The change in porosity term, $\Delta \phi_e V_e$ is the term that decouples the flow equation from the solid phase equations that are used in the settlement sub-model of LDAT to calculate the transfers of the solid phase components in and out of a finite difference element. $\Delta \phi_e V_e$ may be estimated using equation (18), $\Delta \phi_e = z_e^S S^\phi \Delta p_e$. This approximation can result in a difference between the dry density calculated by the algorithm, ρ'^D , and that calculated by equation (17) ρ^D . This can be corrected by adjusting the source term with a density numerical correction term $\Delta V_e^{\rho^D} = 0.5(\rho'^D - \rho^D) V_e / \rho^S$, see equation (31).

Introducing

$$S'_e = (z_e^G S^G + z_e^L S^L + z_e^S S^\phi) V_e$$

$$b_e = -\sum_m b_{em}^{L/G} + \sum_m b_{em}^C$$

$$c_e = V_e \Delta t G_e^{L/G} + \Delta V_e' + \Delta V_e^{\rho^D} \quad (31)$$

equation (30) becomes,

$$S'_e \Delta p_e = b_e + c_e + \sum_m a_{em}^{L/G} p_m - p_e \sum_m a_{em}^{L/G} \quad (32)$$

This is a set of linear equations, one for each element in the array, which over the time increment from t to $t + \Delta t$ may be solved for $p_e^{t+\Delta t}$ given p_e^t , when appropriate boundary and initial conditions are specified. Substituting,

$$\Delta p_e = p_e^{t+\Delta t} - p_e^t \text{ and } p_e = \frac{p_e^{t+\Delta t} + p_e^t}{2}$$

into equation (32) gives,

$$S'_e(p_e^{t+\Delta t} - p_e^t) = b_e + c_e + \sum_m \frac{1}{2} a_{em}^{L/G} (p_m^{t+\Delta t} + p_m^t) - (p_e^{t+\Delta t} + p_e^t) \sum_m \frac{1}{2} a_{em}^{L/G}$$

or,

$$\sum_m \frac{1}{2} a_{em}^{L/G} p_m^{t+\Delta t} - \left(\sum_m \frac{1}{2} a_{em}^{L/G} + S'_e \right) p_e^{t+\Delta t} = p_e^t \sum_m \frac{1}{2} a_{em}^{L/G} - S'_e p_e^t - \sum_m \frac{1}{2} a_{em}^{L/G} p_m^t - b_e - c_e \quad (33)$$

Equation (33) is a set of N_e equations corresponding to the number of active equations which may be written in matrix form where e becomes the row number and i is the column number being the element number corresponding to interface m and obtained from an array mapping function $i = \text{array_map}(e, m)$, see Figure 1.

$$[C][p_e^{t+\Delta t}] = [B] \quad (34)$$

$$C_{ei} = \frac{1}{2} a_{em}^{L/G}$$

$$C_{ee} = - \left(\sum_m \frac{1}{2} a_{em}^{L/G} + S'_e \right)$$

$$B_e = p_e^t \sum_m \frac{1}{2} a_{em}^{L/G} - S'_e p_e^t - \sum_m \frac{1}{2} a_{em}^{L/G} p_m^t - b_e - c_e$$

Note that the total volumetric phase transfer across an interface em in time Δt is (positive outwards)

$$\Delta Q_{em}^P = a_{em}^P \Delta p_{em}^P + b_{em}^P$$

This is related to the mass transfer of phase component n by,

$$\Delta M_{em,n}^P = \Delta t J_{em,n}^P \frac{\Delta Q_{em}^P}{\omega_{em}^P}$$

Again positive outwards.

The volume of the component n transferred in time Δt across the interface em depends on the density in element e or element m :

$$\Delta Q_{em,n}^P = \frac{1}{\rho_{e,n}^P} \Delta M_{em,n}^P \text{ for element } e$$

And

$$\Delta Q_{em,n}^P = \frac{1}{\rho_{m,n}^P} \Delta M_{em,n}^P \text{ for element } m$$

These volume transfer equations are used in LDAT to regulate the value of Δt so that the changes in the overall phase volume in an element, and the volume numerical correction in equation (31), are limited to around 5% in any time step. This level has been found to produce stable calculations that balance the mass throughout the model and provide volumetric consistency.

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