The role of the van Genuchten equations and effective density in LDAT

Summary:

Unsaturated flow models, which simulate the liquid and gas flow through porous materials, require the estimation of the values of the parameters 'gas relative permeability', 'liquid relative permeability' and 'capillary pressure'. The van Genuchten equations are widely used for this purpose.

The LDAT landfill waste and transport model is based on the concept that landfill waste is a complex porous material. It therefore relies on the van Genuchten equations to provide these parameter values for the LDAT landfill gas and liquid flow sub-model.

Gas and liquid relative permeabilities are the ratio between the phase (gas or liquid) permeability in unsaturated flow and the phase permeability in saturated flow. Capillary pressure is the difference between the gas pressure and the liquid pressure. All three values depend upon the effective degree of saturation of the pore space.

This article defines the van Genuchten equations which represent the analytical relationships between the phase relative permeabilities, capillary pressure and the effective degree of saturation. The article also explains the concept of 'effective density' in unsaturated flow, a concept that is unique to the LDAT model.

van Genuchten equations and effective density

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} , is derived by (van Genuchten 1980),

$$k_{REL}^{L} = \left(\boldsymbol{\varsigma}_{e}^{E}\right)^{\boldsymbol{\delta}^{L}} \left(1 - \left(1 - \left(\boldsymbol{\varsigma}_{e}^{E}\right)^{\frac{1}{\boldsymbol{\gamma}^{L}}}\right)^{\boldsymbol{\gamma}^{L}}\right)^{2}$$
(1)

The corresponding expression for relative permeability to gas is

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

$$\tag{2}$$

 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 (9). Examples of the functions represented by equations (1) and (2) are given in Figure 1.



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

Figure 1 Liquid and gas relative permeabilities equations (1) and (2)

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

gradient and the gravity induced head gradient in the vertical direction,

$$\left(\frac{\partial h^{P}}{\partial x}\right)_{em} = \frac{1}{\rho^{P}g} \left(\frac{\partial p^{P}}{\partial x}\right)_{em} + \frac{\rho_{E}^{P}}{\rho^{P}}f(em)$$
(3)

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,

$$\rho_E^L = \rho_E^G = \varsigma \rho^L + (1 - \varsigma) \rho^G \tag{4}$$

where ς 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 ς , 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,

$$\rho_E^G = \varepsilon^G \rho^L + \left(1 - \varepsilon^G\right) \rho^G \tag{5}$$

The corresponding mass in the liquid volume V^L , will become $ho^L V^L - arepsilon^G (
ho^L -
ho^G)$ and,

$$\rho_E^L = \rho^L - \varepsilon^G \left(\frac{V^G}{V^L} \right) \left(\rho^L - \rho^G \right) = \rho^L - \varepsilon^G \left(\rho^L - \rho^G \right) \frac{(1 - \varsigma)}{\varsigma}$$
(6)

Equations (5) and (6) 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 .

$$\varepsilon^{G} = 0 \qquad \qquad \zeta < \zeta_{REF} \tag{7}$$

$$\varepsilon^{G} = \left(\frac{\zeta - \zeta_{REF}}{1 - \zeta_{REF}}\right)^{\tau} \qquad \zeta_{REF} < \zeta < 1 \tag{8}$$

An illustration of the impact of this function on the liquid and gas densities is given in Figure 2 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 (4), 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 (3) change from the separated values to the fully mixed values as ζ varies from ζ_{REF} to 1.





The solution of the LDAT constitutive equation 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,

$$p_{C} = \frac{\rho_{L}g}{\alpha} \left(\left(\varsigma^{E} \right)^{-\frac{1}{\gamma}} - 1 \right)^{\frac{1}{\beta}}$$
(9)

In equation (9), 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 (9) $\gamma = 1 - \frac{1}{\beta}$ so that the function has essentially four parameters α , $\beta \zeta^{R}$ 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 ,

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



	LMC2 data	Example data
β	2	2.5
α	9.81	2.11

Figure 3 Capillary pressure, equation (9)

It is generally accepted that the shape of the relationship $p_C(\varsigma^E)$ 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.

van Genuchten, M.T. (1980) A closed form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Science Association of America. Journal 44, 892-898. Mualem, Y. (1976) A new model for predicting the hydraulic conductivity of unsaturated porous media. Water Resources Research 12, 513-522.