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A versatile entrainment function for dense-gas dispersion

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1. INTRODUCTION

Dense gas dispersion for risk assessment is usually modelled by simple box models or shallow-water type models, in which vertical distributions are parameterised by similarity profiles. The dilution by ambient air will depend on cloud density and the available turbulent kinetic energy generated by shear production and convective heat flux driven by the temperature differences between the ground and a cloud released with negative enthalpy. The vertical integral of excess buoyancy is gradually moderated, as the cloud accumulates heat from the ground and spreads in the crosswind direction and eventually the mixing will approach passive dispersion. Thus, a dense-gas entrainment function must be quite general. There are very few field measurements of dense-gas turbulence, so instead we match the formula with generic reference cases such as free convection, forced convection, stratified shear flow and passive dispersion.

2. LITERATURE REVIEW

In box models for dense-gas dispersion mixing is simplified to an air flux across a virtual interface surrounding a well-mixed volume. The mixing rate is referred to as the entrainment velocity u_e $[\mathrm{ms}^{-1}]$ and a typical parameterisation (Britter 1988) for this is

$$\frac{u_e}{\sqrt{e}} = \frac{2.85}{6.95 + Ri} \qquad e = u_*^2 \tag{1}$$

The Richardson number $Ri \equiv \Delta\rho gh/\rho e$ is a measure of cloud stability defined by a characteristic density difference $\Delta\rho$, gravity g, a characteristic layer height h, and a measure of turbulent kinetic energy e. For practical reasons Britter (1988) applied the ambient friction velocity $e = u_*^2$, whereas other developers apply the friction velocity within the gas layer. The product of the characteristic layer height and box-model concentration is usually set equal to the depth integral of the true distribution. Britter (1988) applied the surface concentration as reference and operated with a relatively low layer height, whereas van Ulden (1983) defined the layer height as twice the centre of gravity, giving a relatively low box-model concentration. It is worth noting that calibration coefficients of entrainment functions similar to Equation (1) depend on such model definitions.

Dense gas clouds of practical interest are usually cold with heat convection from the ground as an additional source of turbulent kinetic energy. The velocity scale for this process is defined by:

$$w_*^3 = \frac{\varphi gh}{\rho c_p T} \tag{2}$$

where φ [W m^{-2}] is the heat flux, c_p [J (kgK)$^{-1}$] is heat capacity and T [K] is the absolute cloud temperature. Eidsvik (1980) proposed an entrainment model (F2 in Table 1) based on a combined turbulence scale

$$\frac{u_e}{\sqrt{e}} = \frac{2.5}{8.7 + Ri} \qquad e = 1.7u_*^2 + 0.5w_*^2 \tag{3}$$

where u_* is the friction velocity estimated inside the plume.

The DEGADIS entrainment function, labelled F3 in Table 1, has yet another definition of the turbulence scale (Spicer and Havens, 1986). The Richardson-number dependence seems very different, but actually it is just a slight modification. The limit of weak cloud stability $Ri \to 0$ depends on ambient stability as reflected by the coefficient α of the power-law approximation to the wind profile.

In an early version of the SLAB entrainment function, labelled F4 in Table 1, the turbulence parameterisation includes the front velocity of the spreading plume $u_f \cong \sqrt{g'h}$ and the velocity slip between plume and ambient air and δu (Morgan et al., 1983). Later on (Ermak 1990) modified the SLAB model for inclusion of ambient stability similar to Spicer and Havens (1986). The remaining models labelled F5 and F6 are discussed below.

3. REFERENCE CASES

Table 2 lists a set of reference cases. The first case is passive dispersion of a neutrally buoyant surface plume with a growth rate proportional to the turbulent friction velocity u_*. The proportionality factor λ_1 depends on the definition of the box-model height h and the quoted value is calculated from Sutton's (1953) analytical solution using van Ulden's (1983) interface definition, which set the height h to twice the centre of gravity.

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Table 1 Selected entrainment functions.

ID	Entrainment function	Special definitions	Asymptotes for ref. cases λ_1	λ_2	λ_3	λ_4
F1	$\frac{u_e}{\sqrt{e}} = \frac{2.85}{6.95+Ri}$ (Britter, 1988)	$e = u_*^2; h = \frac{q}{c_0 u}$	0.41	2.85	0	0
F2	$\frac{u_e}{\sqrt{e}} = \frac{2.5}{8.7+Ri}$ (Eidsvik, 1980)	$e = 1.69u_*^2 + 0.47w_*^2$	0.39	7.7	0.21	1.2
F3	$\frac{u_e}{\sqrt{e}} = \frac{0.35(1+\alpha)}{0.88+0.099Ri^{1.04}+1.4\cdot 10^{-25}Ri^{5.7}}$ DEGADIS (Spicer and Havens, 1986)	$e = u_*^2 + 0.25w_*^2$ $h = \Gamma\left(\frac{1}{1+\alpha}\right)\frac{\sigma_z}{1+\alpha}; u \approx u_1\left(\frac{z}{z_1}\right)^\alpha$	0.46	3.7	0.23	0.46
F4	$\frac{u_e}{\sqrt{e}} = \frac{0.4}{1+0.28Ri}$ Early SLAB (Morgan et al., 1983)	$e = u_*^2 + 0.02\delta u^2 + 0.27w_*^2$	0.4	1.4	0.21	0.2
F5	$\frac{u_e}{\sqrt{e}} = \frac{2.25u_*^3/e^{3/2}+0.25}{2.5+Ri}$ (Jensen and Mikkelsen, 1984)	$e = u_*^2 + w_*^2$	1	2.5	0.1	0.25
F6	$\frac{u_e}{\sqrt{e}} = \frac{0.25}{3.3+Ri}$ (Nielsen, 1998)	$e = \left(u_*^3 + 0.1w_*^3\right)^{2/3}$	0.75	2.5	0.34	0.25

With this definition the layer always have the right potential energy. The more common choice of h equal to the centre of gravity leads to $\lambda_1 \approx 0.35$.

The entrainment rate in the limit of strongly stratified shear flow was determined in the laboratory experiment by Kato and Phillips (1969). The setup was an annular tank with stratified water and constant shear stress induced by a moving screen at the surface. This produced a turbulent well-mixed upper layer, which gradually entrained the quiescent stratified fluid below.

The entrainment rate in the limit of weak free convection is Bo Pedersen's (1980) interpretation of Farmer's (1975) measurements of the thermal development in an ice-covered lake in the spring season. The thermal expansion coefficient of water is negative near the freezing point and solar heating at the surface produced a convective layer. The mixing rate was deduced from the vertical phase propagation of the diurnal component of the temperature signals.

Table 2 Empirical mixing rates at reference cases defined by $Ri_{u_*} \equiv \Delta\rho g h / \rho u_*^2$ and $Ri_{w_*} \equiv \Delta\rho g h / \rho w_*^2$

Situation	Rate	Condition	Parameters
Passive dispersion	$\frac{u_e}{u_*} \approx \lambda_1$	$Ri_{u_*} \to 0$ $w_* = 0$	λ_1=0.75 (Nielsen, 1998)
Stratified shear flow	$\frac{u_e}{u_*} \approx \frac{\lambda_2}{Ri_{u_*}}$	$Ri_{u_*} \gg 0$ $w_* = 0$	λ_2=2.5 (Kato & Phillips, 1969)
Weak free convection	$\frac{u_e}{w_*} \approx \lambda_3$	$Ri_{w_*} \to 0$ $u_* = 0$	λ_3=0.37 (Bo Pedersen, 1980)
Strong free convection	$\frac{u_e}{w_*} \approx \frac{\lambda_4}{Ri_{w_*}}$	$Ri_{w_*} \gg 0$ $u_* = 0$	λ_4=0.25 (Deardorff et al., 1980)

The entrainment rate in the limit of strong free convection was measured in the laboratory experiment of Deardorff et al. (1980) in which initially stratified water was heated from the bottom.

For comparison we include the limit values of the entrainment functions in Table 1. Some differences are a result of varying definitions of the layer height and box-model concentration.

4. MATCHING REFERENCE CASES

Jensen (1981) simplified the turbulent kinetic energy equation to:

$$\overbrace{\frac{\partial \bar{e}}{\partial t}}^{t_1} + \overbrace{\frac{\partial \bar{u}_j \bar{e}}{\partial x_j}}^{t_2} = \overbrace{u_*^2 \frac{\partial \bar{u}_i}{\partial x_j}}^{t_3} + \overbrace{\frac{\overline{\rho' u_j'} g_j}{\bar{\rho}}}^{t_4} - \overbrace{\frac{\partial \overline{u_j' u_i' u_i'}}{\partial x_j}}^{t_5} - \overbrace{\frac{\overline{\rho' u_j'}}{\bar{\rho}}}^{t_6} - \overbrace{\varepsilon}^{t_7} \tag{4}$$

where the indices refer to direction. The terms in the equation are the temporal change t_1; advection t_2; work by friction t_3; work by gravity t_4; turbulent diffusion t_5; work by pressure perturbations t_6; and the energy dissipation rate $t_7 = \varepsilon$ [m^{2}s^{-3}]. A scale analysis of this equation leads to:

$$\overbrace{c_1 \frac{e-e_0}{h} u_e}^{t_1+t_2} \approx \overbrace{c_2 \frac{u_*^3}{h}}^{t_3} + \overbrace{c_6 \frac{w_*^3}{h} - \frac{\Delta\rho g u_e}{\rho}}^{t_4} + \overbrace{c_3 \frac{e^{3/2}}{h}}^{t_5+t_6} - \overbrace{c_4 \frac{e^{3/2}}{h}}^{t_7} \tag{5}$$

where the turbulence scale is defined by $e = u_*^2 + c_5^2 w_*^2$.

The buoyancy term is split into two parts - energy production by heat convection t_{4a} and energy consumption by entrainment t_{4b}. The last three terms are all proportional to the cube of a velocity scale divided by a length scale. Rearranging (5) leads to the following entrainment function:

$$\frac{u_e}{\sqrt{e}} = \frac{c_2\left(u_*/\sqrt{e}\right)^3 + c_6\left(w_*/\sqrt{e}\right)^3 + c_3 - c_4}{c_1\left(1-e_0/e\right) + Ri} \tag{6}$$

Jensen (1981) originally set $c_5 = 1$ and neglected the buoyancy production by convection $c_6 = 0$. Furthermore, Jensen and Mikkelsen (1984) found it necessary to set $e_0 = 0$ in order to avoid a singularity for the limit of passive dispersion. This may appear like a bold assumption of an ever-quiescent ambient fluid, but the motivation was simply to match the limit of passive dispersion. Such pragmatism is permitted, since in this case the energy budget degrades to a balance between production and dissipation with insignificant energy feedback by entrainment.

In search of a solution including turbulence production by heat convection, we need additional boundary conditions. The first assumption is that energy diffusion and pressure transport cancel each other (c_3=0). The second assumption is that the ratio between energy dissipation t_7 and turbulence production $t_3 + t_{4a}$ is fixed:

$$\frac{c_4\left(u_*^3 + c_5^3 w_*^3\right)}{c_2 u_*^3 + c_6 w_*^3} = 1 - R_f^T \tag{7}$$

This approach is based on the bulk flux Richardson number R_f^T, which is defined as the ratio of energy recovery due to entrainment and the energy production. It is empirically known to be $R_f^T \approx 0.045$ for subcritical flows and $R_f^T \approx 0.18$ for supercritical ones (Bo Pedersen, 1980). Dense-gas dispersion usually falls in the latter category. A solution is only possible with a slightly modified velocity scale $e = \left(u_*^3 + c_5^3 w_*^3\right)^{2/3}$ and when the following relation is obeyed:

$$\lambda_2 \lambda_3^3 = \lambda_4 \lambda_1^3 \tag{8}$$

It happens that this is almost true, e.g. if the weak convection limit is altered from λ_3≈0.37 to λ_3≈0.34. The general solution (Nielsen, 1998) is

$$\frac{u_e}{\sqrt{e}} = \frac{\lambda_2}{\lambda_2/\lambda_1 + Ri} \quad e = \left(u_*^3 + \lambda_4/\lambda_2\, w_*^3\right)^{2/3} \tag{9}$$

and by insertion of $R_f^T = 0.18$ and the values in Table 2 we obtain:

$$\frac{u_e}{\sqrt{e}} = \frac{2.5}{3.3 + Ri} \quad e = \left(u_*^3 + 0.1 w_*^3\right)^{2/3} \tag{10}$$

This function is easy to match with alternative data and the limit of passive dispersion λ_1 could be parameterised by the ambient stability.

5. ESTIMATES OF IN-PLUME TURBULENCE

The heat transfer from the ground to a cold dense gas cloud varies from free to forced convection depending on the velocity and temperature difference between cloud and surface. Jensen (1981) proposed an analogy with the atmospheric surface layer and applied local Monin-Obukhov scaling within the gas layer and wrote

$$\begin{aligned} u(z) &= u_*/\kappa\left[\ln z/z_0 - \psi_m(z/L)\right] \\ \Delta T(z) &= \theta_*/\kappa\left[\ln z/z_0 - \psi_h(z/L)\right] \end{aligned} \tag{11}$$

where κ is the von Karman constant, z_0 is the surface roughness, and the diabatic correction functions ψ_m and ψ_h (e.g. Paulson 1970) depend on the stability parameter z/L. The heat flux

$$\varphi = \rho c_p c_h u \Delta T \tag{12}$$

is parameterised by the exchange coefficient (Brutsaert, 1982)

$$c_h = \frac{\kappa^2}{\left[\ln z/z_0 - \psi_m(z/L)\right]\left[\ln z/z_0 - \psi_h(z/L)\right]} \tag{13}$$

Elimination of u_* and θ_* from the definition of Monin-Obukhov length L yields an equation for the stability parameter

$$\frac{z}{L} = \mathrm{Ri}_{\Delta T} \frac{\left[\ln z/z_0 - \psi_m(z/L)\right]^2}{\left[\ln z/z_0 - \psi_h(z/L)\right]} \tag{14}$$

where the convection Richardson is defined by

$$\mathrm{Ri}_{\Delta T} = \frac{T(z) - T(z_0)}{T} \frac{gh}{u(z)^2} \tag{15}$$

Jensen (1981) evaluated the heat convection Richardson number for the characteristic layer height $z \approx h$, solved (14) for the stability parameter z/L and found the in-plume turbulence scales (u_*, w_*) by Equations (2,12,13). This approach will fail for the combination of a high convection Richardson number and a low ratio between layer height and surface roughness. In these extreme situations we may have to use the parametrisation of Zeman (1982) who proposed

$$\begin{aligned} u_* &= c_d \bar{u} \\ u_* \theta_* &= \Delta T \left[c_d \left| u_* \right| + 0.21 \left(\alpha g \Delta T / T \right)^{1/3} \right] \end{aligned} \tag{16}$$

where α is the thermal molecular diffusivity [$m^2 s^{-1}$] and c_d is a friction coefficient set to 0.08.

6. CONCLUSION

We present a simple entrainment function $u_e / \sqrt{e} = 0.25 \left(3.3 + Ri\right)^{-1}$ using $e = \left(u_*^3 + 0.1 w_*^3\right)^{2/3}$. This is calibrated by reference data for the cases of free convection, forced convection, stratified shear flow and passive dispersion. The remaining task is to predict the turbulence conditions inside the gas plume. In the lack of accurate field date we suggest an analogy with the atmospheric surface layer using a local Monin-Obukhov scaling for the gas layer.

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