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Setting threshold values of particle sizes for determination of the appropriate dispersion/deposition model during various atmospheric stability conditions

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HIGHLIGHTS

- Cutoff diameters between gravitational and diffusional settling are suggested.
- The cutoff diameter largely depends on the meteorological stability.
- The commonly accepted cutoff value has been shown to be conservative.
- The methodology can assist risk assessment of solid or liquid-particle emissions.

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ABSTRACT

An approach is suggested for the estimation of air borne critical particle diameter that determines the dominant removal mechanism from atmospheric dispersion of plumes for six main Pasquill–Gifford meteorological stability conditions. A methodology was developed to apply in rural regions since relevant meteorological input data have been developed mainly for such areas. Our *critical diameter* methodology refines the commonly accepted “50 micron diameter”, considered as a border value above which gravitational settling is dominant and below which, turbulent dispersion is expected to prevail. The interrelationships of particle release heights and downwind deposition distances (for various stability conditions) as well as particle sizes and densities are implemented in the turbulent dispersion and gravitational settling estimations, in order to determine the dominant mechanism for particles reaching the ground following their releases from various heights.

1. Introduction

The fall velocity and deposition of particles on the earth's surface has been widely modeled and discussed in the literature (e.g. Hanna et al., 1982; Slade, 1968; Van der Hoven, 1968). Although no specific particle diameter was shown to clearly indicate the particle size above which the dominance of gravitational settling over dry deposition from diffusion becomes obvious, it is commonly assumed that particles or aerosols with diameters greater than 50 μm are usually removed from the plume by gravitational settling (Anderson, 1961; CCPS, 2000).

Suggestions for using one removal mechanism over the other are not widely reported. Hanna et al. (1982) indicate the approximate particle diameter of 200 μm as the cutoff above which diffusion is no longer important (because the particles fall through the turbulence so fast) and below which the particles are assumed to be dispersed by turbulence in the same way as particles having no inertia. The latter are removed from the atmosphere by the so-called dry deposition process, where the deposition velocity is defined as the *ratio* of the (measured) flux to the concentration of the aerosols close to ground level. The deposition velocity has been extensively researched (e.g. Donateo and Contini, 2014; Nho-Kim et al., 2004). This deposition velocity does not consider the dominant mechanism that brings the aerosols/particles to the vicinity of the ground level from their release height, which is the main concern of the present study.

The purpose of this paper is to determine, for a given downwind distance and atmospheric stability, the critical particle diameter (in

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terms of aerodynamic diameter) above which gravitational settling of non-neutrally buoyant particles released from a certain source above the ground should be considered over atmospheric diffusion. It turns out that the cutoff diameter between gravitational and diffusion-governed settling depends largely, *inter alia*, on the meteorological stability condition prevailing during the dispersion process.

Evidently, as further discussed in chapter 4, the critical particle size greatly influences not only the distance up to which gravitational settling is dominant, but also the human exposure pathways via which hazardous particles can enter the body via inhalation or percutaneous/dermal or both (Harley et al., 2012; Hoffmann, 2011; Marquart et al., 2003). Moreover, the doses incurred by inhalation depend largely on particle size within the respirable range, thus making this analysis a significant decision making tool for risk assessment of hazardous materials being released into the environment during both routine operation and accidental occurrences, as well as for risk management and emergency planning purposes.

2. Methodology

2.1. Gravitational settling of non-neutrally buoyant particles

The trajectory of the falling non-neutrally buoyant particles depends on the gravitational settling velocity and the horizontal wind velocity. The latter is affected by the height and the atmospheric stability.

Let x be the distance (in meters) from an elevated source in the downwind direction (x-axis) and h be the height (in meters) of the releasing source. The fallout distance of non-neutrally buoyant particles depends on both the fall velocity v_g and the horizontal wind speed at a certain height $u(h)$, and can be generally described by the following differential equations (1) and (2).

$$dx = u(h)dt \tag{1}$$

$$dh = v_g dt \tag{2}$$

where $u(h)$ is the wind speed at height h meters above ground (in m/s) as calculated in equation (3) for release heights smaller than 200 m (Hanna et al., 1982) and v_g is the fall velocity (in m/s) of the (sphere-shaped) particle of certain density ρ_p moving through a fluid (in our case – the air) of density ρ_f and viscosity μ_f.

$$u(h \le 200\ m) = u_0 \left(\frac{h}{h_0}\right)^n \tag{3}$$

where u_0 is the reference wind speed [m/s], h_0 is a reference height above ground [m] (usually considered as 10 m) and n is the "Hellman exponent" (friction coefficient) that depends on both stability conditions and surface roughness [dimensionless], as shown below in Table 1. For h > 200 m, the wind velocity is assumed to have to the value of u at 200 m (i.e. $u = u_{200}$).

The consequence of acting forces on a particle results in the fall velocity — the speed at which a particle fall gravitationally. The fall velocity (also known as the terminal velocity) is a function of shape, density and size of the particle (Zannetti, 1990). A constant value of velocity is reached when all forces (gravity, drag, buoyancy, etc.) acting on the particle are balanced — that is, when the sum of all the forces is equal to zero (no acceleration). For a smooth spherical particle, neglecting the effect of slip flow, this balance may be expressed as shown in equation (4) (Slade, 1968):

$$v_g = \sqrt{\frac{4D_p g\left(\rho_p - \rho_f\right)}{3C_D \rho_f}} \tag{4}$$

where v_g is the fall velocity [m/s], D_p is the particle diameter [m], g is the gravitational constant [m/s^2], ρ_p is the particle density [kg/m^3], ρ_f is the fluid density [kg/m^3] and C_D is the drag coefficient [dimensionless].

Table 1
Friction coefficient (n) as a function of atmospheric stability condition (CCPS, 2000; Hanna et al., 1982; Irwin, 1979).

Stability condition	A	B	C	D	E	F
Standard terrain	0.07	0.07	0.10	0.15	0.35	0.55
Urban terrain	0.15	0.15	0.20	0.25	0.40	0.60

Assuming the particle diameter is constant (i.e. does not change with the downwind distance due to evaporation or condensation), equations (1) and (2) can be integrated with respect to the change of height to result in the fallout distance x:

$$x(for\ h \le 200\ m) = \int_0^h \frac{u(h)}{v_g} dh = \int_0^h \frac{u_0\left(\frac{h}{h_0}\right)^n}{v_g} dh = \frac{u_0}{v_g}\int_0^h \left(\frac{h}{h_0}\right)^n dh \tag{5a}$$

Following integration, the fallout distance x for heights smaller or equal to 200 m can be estimated based on equation (5b):

$$x(for\ h \le 200\ m) = \frac{u_0 h^{n+1}}{v_g h_0^n (n+1)} \tag{5b}$$

where x is the downwind distance [m], v_g is the fall velocity [m/s], u_0 is the wind speed at a reference height h_0 [m/s], h is the height from which particles are released [m], h_0 is the reference height [m] and n is the friction coefficient [dimensionless].

For release heights greater than 200 m, one should calculate the downwind location where x (h = 200 m), where equation (5b) is valid and add the additional segment not affected by the change of wind speed with height, as shown below in equation (6a).

$$x(for\ h > 200\ m) = x(h = 200\ m) + \int_{200}^h \frac{u_{200}}{v_g} dh \tag{6a}$$

Following integration and rearrangement of terms yields equation (6b):

$$x(for\ h > 200\ m) = \frac{200u_{200}}{v_g}\left[\frac{h}{200} - \frac{n}{n+1}\right] \tag{6b}$$

where u_{200} is the wind speed at 200 m above ground [m/s].

The applicable model for obtaining the particle fall velocity is flow regime dependent. The flow regime can be calculated using the following equation (7) (Spellman and Whiting, 2004):

$$K = D_p\left(\frac{g\rho_p\rho_f}{\mu_f^2}\right)^{\frac{1}{3}} \tag{7}$$

where K is a dimensionless constant that determines the range of the fluid-particle dynamic laws [dimensionless] and μ_f is the dynamic fluid viscosity [kg/ms].

The K value determines the appropriate range of the fluid-particle dynamic laws that apply. If K < 3.3, then Stokes law