



Air Dispersion Modeling

Foundations and Applications

Alex De Visscher



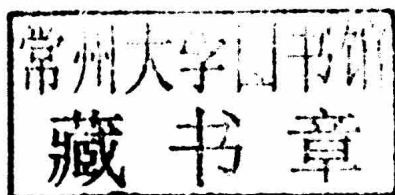
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ALEX DE VISSCHER

University of Calgary



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To Julie

LIST OF SYMBOLS

a	acceleration (m s^{-2})
	activity (—)
A	droplet surface area per unit air volume ($\text{m}^2 \text{m}^{-3} = \text{m}^{-1}$)
	frequency factor [s^{-1} (first order); $\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$ (second order)]
	absorbance (—)
A_f	frontal area (m^2)
A_p	plan area (m^2)
A_T	total area (m^2)
A_s	stack cross-sectional area (m^2)
B	Bowen ratio (—)
b_a	empirical constant ($\text{m}^2 \mu\text{g}^{-1}$)
c	speed of light in vacuum (m s^{-1})
	amount concentration or mass concentration (mol m^{-3} or g m^{-3})
C	Cunningham slip correction factor (—)
	number concentration (molecules cm^{-3})
c_0	gas-phase concentration in equilibrium with the surface ($\mu\text{g m}^{-3}$)
C_0	Lagrangian structure function constant (—)
c_{air}	air-phase pollutant concentration ($\mu\text{g m}^{-3}$)
C_D	drag coefficient (—)
C_G	net radiation fraction going into the ground (—)
$c_{i,\text{air}}$	air-phase concentration of pollutant at interface ($\mu\text{g m}^{-3}$)
$c_{i,\text{water}}$	water-phase concentration of pollutant at interface ($\mu\text{g m}^{-3}$)
c_m	mass concentration (g m^{-3})
c_{odor}	odor concentration (ou m^{-3})
c_p	specific heat ($\text{J kg}^{-1} \text{K}^{-1}$)
$c_{p,\text{air}}$	specific heat of air ($\text{J kg}^{-1} \text{K}^{-1}$)
C_{vis}	visual contrast (—)
$C_{\text{vis},x=0}$	visual contrast at zero distance (—)
c_w	droplet-phase pollutant concentration ($\mu\text{g m}^{-3}$)
c_{water}	water-phase pollutant concentration ($\mu\text{g m}^{-3}$)
C_x	yz plane integrated plume concentration (g m^{-1})
$\text{cov}()$	covariance (product of units of correlating functions)
d	displacement height (m)
	day of the year (d)
d_p	particle diameter (m)
D	molecular diffusivity (gas phase) ($\text{m}^2 \text{s}^{-1}$)
D_{ij}	binary diffusion coefficient of compound i in compound j ($\text{m}^2 \text{s}^{-1}$)
D_w	molecular diffusivity (water phase) ($\text{m}^2 \text{s}^{-1}$)
$\bar{\epsilon}$	turbulent kinetic energy ($\text{m}^2 \text{s}^{-2}$)
E	activation energy (J mol^{-1})
	irradiance (W m^{-2} or W cm^{-2})
e_p	photon energy (J photon^{-1} or simply J)

E_p	photon irradiance (photons $\text{cm}^{-2} \text{s}^{-1}$ or simply $\text{cm}^{-2} \text{s}^{-1}$)
$E_{p,\lambda}$	spectral photon irradiance (photons $\text{cm}^{-2} \text{s}^{-1} \text{nm}^{-1}$ or simply $\text{cm}^{-2} \text{s}^{-1} \text{nm}^{-1}$)
E_λ	spectral irradiance ($\text{W m}^{-2} \text{nm}^{-1}$ or $\text{W cm}^{-2} \text{nm}^{-1}$)
f	Coriolis parameter (s^{-1})
F	deposition flux ($\mu\text{g m}^{-2} \text{s}^{-1}$)
	broadening factor in falloff kinetics (—)
f_0	reactivity factor (—)
F_b	buoyancy flux parameter ($\text{m}^4 \text{s}^{-3}$)
F_c	“complementary” (stochastic) force (N)
	falloff parameter (—)
F_d	pollutant flux at droplet surface ($\mu\text{g m}^{-2} \text{s}^{-1}$)
	drag force (N)
F_m	momentum flux parameter ($\text{m}^4 \text{s}^{-2}$)
f_y	dispersion factor in the y direction (—)
f_z	dispersion factor in the z direction (—)
Fr_H	Froude number for hill height (—)
Fr_W	Froude number for hill width (—)
g	acceleration of gravity (m s^{-2})
h	Planck constant (J s)
	effective source height (m)
	hour angle (rad or $^\circ$)
	vertical thickness scale (m)
	denser-than-air plume height (m)
H	enthalpy (J)
	height of a hill (m)
	height of a building (m)
	dimensionless Henry constant (—)
h_a	average plume height (m)
H_c	height of the cavity (depends on location) (m)
H_{cp}	Henry constant on a concentration/pressure basis ($\text{mol m}^{-3} \text{Pa}^{-1}$)
h_d	dividing streamline height (m)
h_m	horizontal flame extent (m)
h_{fv}	vertical flame height (m)
h_{mix}	mixing layer height (m)
H_r	height of obstacles defining roughness (m)
H_R	height of the cavity at its maximum (m)
h_s	source height (m)
h_t	altitude of terrain (m)
H_W	height of the far wake (m)
h_*	vertical height scale (m)
I	actinic flux (photons $\text{cm}^{-2} \text{s}^{-1} \text{nm}^{-1}$ or simply $\text{cm}^{-2} \text{s}^{-1} \text{nm}^{-1}$)
	ionic strength (mol kg^{-1})
$i_{\text{background}}$	light intensity of background
iF	intake fraction (—)
i_{object}	light intensity of object
i_u	turbulent intensity in the x direction (m)
i_v	turbulent intensity in the y direction (m)
i_w	turbulent intensity in the z direction (m)
J	mass flux (moving frame of reference) ($\text{g m}^{-2} \text{s}^{-1}$)

j_i	photochemical rate constant of reaction i (s^{-1})
k	von Kármán constant (–)
	Boltzmann constant ($J \text{ molecule}^{-1} K^{-1}$ or $J K^{-1}$)
K	equilibrium constant (–)
k_0	apparent second-order rate constant in low-pressure limit ($cm^3 \text{ molecule}^{-1} s^{-1}$)
k_G	air-phase mass transfer coefficient ($m s^{-1}$)
K_h	turbulent heat diffusivity ($m^2 s^{-1}$)
k_i	rate constant of reaction i [s^{-1} (first order); $cm^3 \text{ molecule}^{-1} s^{-1}$ (second order)]
k_L	water-phase mass transfer coefficient ($m s^{-1}$)
K_m	turbulent momentum diffusivity ($m^2 s^{-1}$)
K_s	solubility constant (–)
K_x	turbulent mass diffusivity in the x direction ($m^2 s^{-1}$)
K_y	turbulent mass diffusivity in the y direction ($m^2 s^{-1}$)
K_z	turbulent mass diffusivity in the z direction ($m^2 s^{-1}$)
k_{∞}	rate constant at high pressure limit ($cm^3 \text{ molecule}^{-1} s^{-1}$)
L	Obukhov length (m)
	length of a building, projected along the wind direction (m)
l	path length (m or cm)
L_f	flame length (m)
L_l	integral length scale (m)
L_R	length of the cavity (m)
LAI	leaf area index (–)
m	mass (kg)
m_a	mass of ambient air (kg)
m_w	mass of water vapor (kg)
M	molar mass ($g \text{ mol}^{-1}$ or $kg \text{ mol}^{-1}$)
M	variance–covariance matrix of velocity fluctuation matrix ($m^2 s^{-2}$)
	material balance matrix (s^{-1})
M_{air}	molar mass of air ($g \text{ mol}^{-1}$ or $kg \text{ mol}^{-1}$)
M_c	pollutant molar mass ($kg \text{ mol}^{-1}$)
M_u	mass exchange rate constant between layers (s^{-1})
n	amount of substance (i.e., number of moles) (mol)
	fractional cloud cover (–)
	integrated stochastic perturbation function ($m s^{-1}$)
N	mass flux (fixed frame of reference) ($g m^{-2} s^{-1}$)
N_A	Avogadro constant ($molecules \text{ mol}^{-1}$ or mol^{-1})
N_{BV}	Brunt–Väisälä frequency (s^{-1})
N_i	flux of i in a fixed frame of reference ($mol m^{-2} s^{-1}$)
n_{iA}	order of reaction i with respect to compound A (–)
ou	odor unit
p	pressure ($Pa = kg m^{-1} s^{-2}$)
	probability density function of location and velocity ($s m^{-2}$)
P	probability density function (inverse of units of the distributed variable)
p_0	pressure at the surface (Pa)
p_c	critical pressure (Pa)
p^*	nondimensionalized pressure (–)
PM _{2.5}	mass concentration of particulate matter smaller than 2.5 μm diameter ($\mu g m^{-3}$)
q	heat ($J = kg m^2 s^{-2}$)
	sensible heat flux ($J m^{-2} s^{-1}$)

	water/air mass ratio (–)
	pollutant mass fraction (–)
Q	emission rate (g s^{-1})
q_A	anthropogenic heat flux ($\text{J m}^{-2} \text{s}^{-1}$)
Q_c	heating value (kW)
q_G	heat flux into the ground ($\text{J m}^{-2} \text{s}^{-1}$)
q_i	mass fraction of compound i (–)
q_{tL}	latent heat flux ($\text{J m}^{-2} \text{s}^{-1}$)
$\underline{Q}_{\text{mdf}}$	downward mass flux between two layers ($\text{kg m}^{-2} \text{s}^{-1}$)
$\underline{Q}_{\text{mi}}$	exchanged mass flux between two layers ($\text{kg m}^{-2} \text{s}^{-1}$)
Q_{miu}	upward mass flux between two layers ($\text{kg m}^{-2} \text{s}^{-1}$)
Q_s	sensible heat emission (kW)
r	albedo (–)
r_a	aerodynamic resistance (s m^{-1})
r_{ac}	surface canopy resistance (s m^{-1})
r_b	quasi-laminar resistance (s m^{-1})
r_c	surface resistance (s m^{-1})
r_{cf}	foliar resistance (s m^{-1})
r_{cg}	ground resistance (s m^{-1})
r_{cl}	resistance of leaves, twigs, bark, ... (s m^{-1})
r_{cut}	cuticle resistance (s m^{-1})
$r_{\text{cut,d}}$	dry cuticle resistance (s m^{-1})
$r_{\text{cut,w}}$	wet cuticle resistance (s m^{-1})
r_{cw}	water resistance (s m^{-1})
r_{dc}	canopy resistance
r_{fg}	correlation coefficient between f and g (–)
r_{gd}	dry ground resistance (s m^{-1})
r_{gw}	wet ground resistance (s m^{-1})
r_{gs}	ground resistance below surface canopy (s m^{-1})
r_i	resistance parameter (s m^{-1})
r_{lu}	cuticle resistance parameter (s m^{-1})
r_m	mesophyll resistance (s m^{-1})
r_{st}	stomatal resistance (s m^{-1})
R	ideal gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)
	solar radiation energy flux ($\text{J m}^{-2} \text{s}^{-1}$)
	spread parameter in bi-Gaussian convective cycling model (–)
	building length scale (m)
	precipitation rate (mm h^{-1})
	atmospheric resistance (s m^{-1})
	reflection probability (–)
R_A	reaction rate of compound A ($\text{molecules cm}^{-3} \text{s}^{-1}$)
R_i	reaction rate of reaction i ($\text{molecules cm}^{-3} \text{s}^{-1}$)
R_L	Lagrangian autocorrelation coefficient (–)
R_N	net radiation energy flux ($\text{J m}^{-2} \text{s}^{-1}$)
r_s	stack radius (m)
r_t	total resistance to deposition (s m^{-1})
$R_{vv'}$	autocorrelation coefficient (–)
$R'_{vv'}$	autocorrelation function ($\text{m}^2 \text{s}^{-2}$)
Re	Reynolds number ($= \text{dup}/\mu = du/v$) (–)

Re_*	Reynolds number based on friction velocity ($=z_0 u_* \rho / \mu = z_0 u_* / \nu$) (—)
RH	relative humidity (%)
s	stability parameter (s^{-2})
	distance traveled by plume center (m)
S	skewness of vertical wind speed distribution ($m^3 s^{-3}$)
S^o	standard entropy ($J mol^{-1} K^{-1}$)
S_r	spacing of obstacles defining roughness (m)
S'_{uu}	spectrum function of wind speed variance ($m^2 s^{-1}$ if function of v)
S_{uu}	normalized spectrum function of wind speed variance (s if function of v or ω ; m if function of κ)
S_w	saturation (—)
Sc	Schmidt number ($=\nu/D$)
t	time (s or h)
t_0	time of the solar noon (h)
$t_{1/2}$	half life (s)
T	temperature (K)
t_a	apparent time (s)
T_a	ambient temperature (K)
T_c	critical temperature (K)
T_i	integral time scale (s)
$T_{i,L}$	Lagrangian integral time scale (s)
T_s	stack gas temperature (K)
	surface air temperature (K)
T_v	virtual temperature (K)
u	wind speed in the x direction ($m s^{-1}$)
U	wind speed in the X direction, Lagrangian frame of reference ($m s^{-1}$)
	internal energy (J)
\bar{u}	average wind speed ($m s^{-1}$)
u'	wind speed fluctuation ($m s^{-1}$)
u_0	wind speed variable in nocturnal atmosphere stability calculations ($m s^{-1}$)
u_1	wind speed in the x_1 (i.e., x) direction ($m s^{-1}$)
u_2	wind speed in the x_2 (i.e., y) direction ($m s^{-1}$)
u_3	wind speed in the x_3 (i.e., z) direction ($m s^{-1}$)
U_a	ambient wind speed ($m s^{-1}$)
U_{atm}	wind speed ($m s^{-1}$)
u_c	characteristic velocity ($m s^{-1}$)
U_c	wind speed in a cavity ($m s^{-1}$)
u_{H_r}	wind speed at height H_r ($m s^{-1}$)
U_{sc}	velocity of plume centerline ($m s^{-1}$)
U_w	wind speed in a far wake ($m s^{-1}$)
u_*	friction velocity ($m s^{-1}$)
u_{*w}	water-side friction velocity ($m s^{-1}$)
u_τ	local friction velocity (between obstacles) ($m s^{-1}$)
v	wind speed in the y direction ($m s^{-1}$)
V	wind speed in the Y direction, Lagrangian frame of reference ($m s^{-1}$)
\mathbf{V}	velocity fluctuation matrix ($m s^{-1}$)
\bar{V}	total wind speed ($m s^{-1}$)
v_d	deposition velocity ($m s^{-1}$)
v_s	settling velocity ($m s^{-1}$)

v_t	transfer velocity (m s^{-1})
w	wind speed in the z direction (m s^{-1})
	work (J)
W	wind speed in the Z direction, Lagrangian frame of reference (m s^{-1})
	width of a hill (m)
	width of a building, projected across the wind flow (m)
	Wiener process
w_*	convective velocity (m s^{-1})
w_1	average vertical wind speed of updrafts (m s^{-1})
w_2	average vertical wind speed of downdrafts (m s^{-1})
w_b	emission velocity at the surface (m s^{-1})
W_c	half-width of the cavity (m)
	wet fraction of the cuticle (–)
w_e	entrainment velocity (m s^{-1})
W_g	wet fraction of the ground (–)
w_s	stack gas velocity in the vertical direction (m s^{-1})
W_{st}	wet fraction of the stomata (–)
w_w	water weight fraction of air (–)
W_w	width of the far wake (m)
w'_w	water–air weight ratio (–)
x	downwind distance from the source (m)
	coordinate in the west–east direction (Eulerian models) (m)
	distance from the upwind side of a building (m)
X	downwind distance coordinate, Lagrangian frame of reference (m)
x_1	coordinate in the west–east direction (Eulerian models) (m)
x_2	coordinate in the south–north direction (m)
x_3	vertical distance (m)
x_f	downwind distance to the source of final plume rise (m)
x_v	distance to virtual source (m)
x_{vis}	visibility (m)
y	crosswind distance from the plume axis (m)
	coordinate in the south–north direction (m)
Y	crosswind distance coordinate, Lagrangian frame of reference (m)
y_i	mole fraction of i in the gas phase (–)
z	vertical distance from the surface (terrain following coordinates) (m)
	vertical distance from the surface at the source (Cartesian coordinates) (m)
Z	vertical distance coordinate, Lagrangian frame of reference (m)
	vertical distance coordinate, terrain following coordinates (m)
z_0	roughness length (m)
z_j	junction height (m)

Greek letters

α	along-plume entrainment rate parameter (–)
	quasi-laminar layer thickness parameter (–)
	mass transfer enhancement factor (–)
α_a	absorption coefficient (m^{-1})
α_c	sea roughness parameter (–)
α_{ext}	extinction coefficient (m^{-1})

α_k	Kolmogorov constant (—)
α_s	scattering coefficient (m^{-1})
$\alpha_{s,\text{air}}$	scattering coefficient for air molecules (m^{-1})
$\alpha_{s,\text{PM}}$	scattering coefficient for PM (m^{-1})
β	ratio of Lagrangian to Eulerian integral time scales (—)
	across-plume entrainment rate parameter (—)
	parameter describing height dependence of density in denser-than-air plumes (—)
γ	vertical slope of potential temperature above the planetary boundary layer (K m^{-1})
	wavelength (m)
	activity coefficient
Γ	dry adiabatic lapse rate (K m^{-1})
Γ_s	moist adiabatic lapse rate (K m^{-1})
δ	solar declination (rad or $^\circ$)
$\Delta_f H^\circ$	standard enthalpy of formation (kJ mol^{-1})
Δh	plume rise (final) (m)
Δh_{sd}	stack downwash (m)
$\Delta_r G^\circ$	standard Gibbs free energy of reaction (kJ mol^{-1})
$\Delta_r H^\circ$	standard enthalpy of reaction (kJ mol^{-1})
$\Delta_r S^\circ$	standard entropy of reaction ($\text{J mol}^{-1} \text{K}^{-1}$)
ΔU	velocity deficit (m s^{-1})
$\Delta_{\text{vap}} H$	enthalpy of vaporization (J kg^{-1})
Δz	plume rise (transitional) (m)
$\Delta \theta$	temperature jump at capping inversion (K)
ε	height of obstacles defining surface roughness (m)
	energy dissipation rate ($\text{m}^2 \text{s}^{-3}$)
	emissivity (—)
	molar decadic absorption coefficient ($\text{cm}^2 \text{molecule}^{-1}$ or simply cm^{-2})
ζ	dimensionless height variable in Monin–Obukhov theory (—)
η	Kolmogorov length microscale (m)
θ	potential temperature (K)
	dimensionless temperature variable (—)
	terrain slope (rad)
θ_c	temperature ($^\circ\text{C}$)
θ_f	temperature ($^\circ\text{F}$)
θ_m	vertical average potential temperature in mixing layer (K)
θ_v	virtual potential temperature (K)
θ_*	friction temperature (K)
κ	thermal diffusivity ($\text{m}^2 \text{s}^{-1}$)
	wave number (rad m^{-1} or simply m^{-1})
λ	height scale for Coriolis effects (m)
	thermal conductivity ($\text{J m}^{-1} \text{K}^{-1}$)
	latitude (rad or $^\circ$)
	molecule mean free path (m)
	scavenging coefficient (s^{-1})
	wavelength (m or nm)
λ_1	area fraction of updraft (—)
λ_2	area fraction of downdraft (—)
λ_f	frontal area parameter (—)
λ_l	spatial Taylor microscale (m)

Λ_L	Lagrangian integral length scale (m)
λ_p	plan area parameter (—)
Λ	temperature lapse rate (K m ⁻¹)
	scavenging ratio (s ⁻¹)
μ	dynamic viscosity (Pa s)
ν	kinematic viscosity (m ² s ⁻¹)
	frequency (s ⁻¹)
ρ	density (kg m ⁻³)
ρ_a	ambient air density (kg m ⁻³)
ρ_p	particle density (kg m ⁻³)
ρ_s	stack gas density (kg m ⁻³)
σ	Stefan–Boltzmann constant (s ⁻¹ m ⁻² K ⁻⁴)
	absorption cross-section (cm ² molecule ⁻¹ or simply cm ²)
σ_n	standard deviation of perturbation function (m s ⁻¹)
σ_u	turbulent velocity in the x direction (m s ⁻¹)
σ_v	turbulent velocity in the y direction (m s ⁻¹)
σ_w	turbulent velocity in the z direction (m s ⁻¹)
σ_{w1}	turbulent velocity in the z direction of updraft (m s ⁻¹)
σ_{w2}	turbulent velocity in the z direction of downdraft (m s ⁻¹)
σ_x	dispersion parameter along the horizontal wind direction (m)
σ_y	dispersion parameter across the horizontal wind direction (m)
σ_z	dispersion parameter in the vertical direction (m)
τ	shear stress (Pa)
	time constant (s)
τ_0	shear stress at the surface (Pa)
τ_s	Taylor microscale (s)
φ	solar elevation (rad)
ϕ	latitude (rad)
	angle between plume path and the horizontal (rad)
	quantum yield (—)
ϕ_h	Monin–Obukhov similarity function for heat transfer (—)
ϕ_m	Monin–Obukhov similarity function for momentum transfer (—)
φ_y	dilution factor due to lateral dispersion (m ⁻¹)
φ_z	dilution factor due to vertical dispersion (m ⁻¹)
ω	angular frequency (rad s ⁻¹ or simply s ⁻¹)
Ω	angular velocity of Earth (s ⁻¹)

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