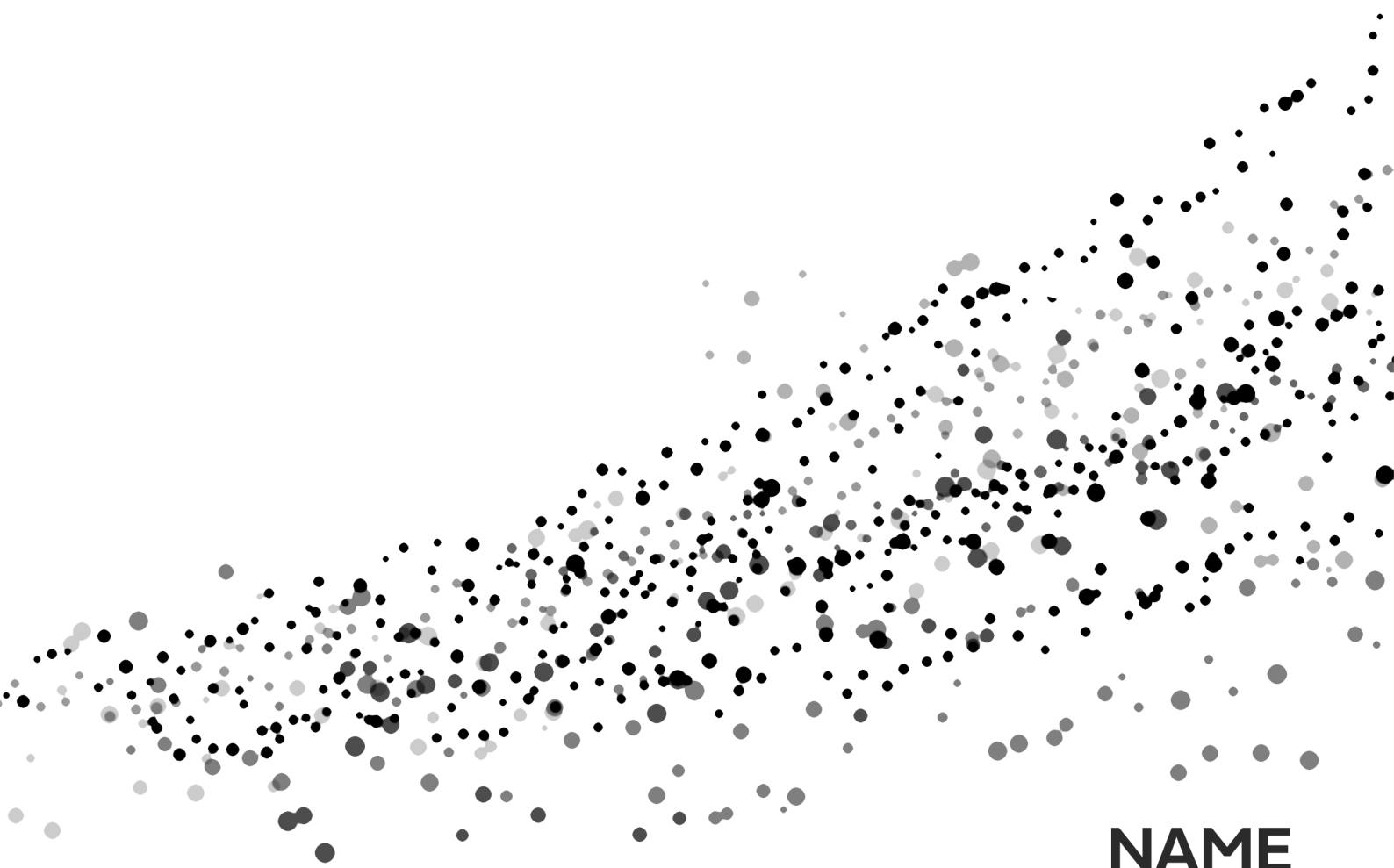

NAME Technical Specification Document C01

Physical and mathematical constants and functions

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NAME

Numerical Atmospheric-Dispersion Modelling Environment

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1 Introduction

This document summarises the values of various physical constants, mathematical constants and functions used.

2 Physical constants and functions

2.1 General physical constants

- Standard acceleration due to gravity $g = 9.806\,65\text{ m s}^{-2}$ (WMO 1988, appendix A; Abramowitz and Stegun 1965, table 2.4, page 8; Wilson 2000).
- Gas constant for dry air $R = 287.05\text{ J kg}^{-1}\text{ K}^{-1}$ (WMO 1988, appendix A; Wilson 2000).
- Specific heat of dry air at constant pressure $c_p = 1004.6\text{ J kg}^{-1}\text{ K}^{-1}$ (Gill 1982, page 43).
- Mean radius of the earth $R_E = 6,371,229.0\text{ m}$ (Meteorological Office 1991, page 99; Wilson 2000).
- von Karman's constant $k = 0.4$ (Pasquill and Smith 1983, page 42; Wilson 2000).
- Molecular mass of dry air $m_{air} = 28.966\text{ g/mole}$ (Gill 1982, page 597).
- Molecular mass of water $m_{water} = 18.016\text{ g/mole}$ (Gill 1982, page 597).
- Thermodynamic temperature at $0^\circ\text{C} = 273.15\text{ K}$ (WMO 1988, appendix A; Gill 1982, page 595; Wilson 2000).

2.2 Constants for the ICAO standard atmosphere

Taken from Meteorological Office 1991, page 153:

- Temperature at 0 km above mean sea level = 288.15 K.
- Temperature at 11 km above mean sea level = 216.65 K.
- Temperature at 20 km above mean sea level = 216.65 K.
- Lapse rate from 0 to 11 km above mean sea level = 0.0065 K m^{-1} .
- Lapse rate at more than 20 km above mean sea level = -0.001 K m^{-1} .
- Pressure at mean sea level = 101,325.0 Pa.

2.3 Reference pressure for potential temperature

- $p_{\theta ref} = 100,000.0\text{ Pa}$.

2.4 Non-SI units (in SI units)

- Feet to metres conversion factor: 1 foot = 0.3048 m (Abramowitz and Stegun 1965, table 2.5, page 8; Wilson 2000).

2.5 Humidity functions (Gill 1982)

- Specific humidity q and humidity mixing ratio r are related by $q = r/(1.0 + r)$ and $r = q/(1.0 - q)$.
- Relative humidity r_h (in percent) and humidity mixing ratio r are related by $r_h = 100.0 * r/r_w$ and $r = r_w * r_h/100.0$ where r_w is the saturated humidity mixing ratio.
- Saturation vapour pressure e_w is calculated from temperature using Wexler's (1976) formula.
- Humidity mixing ratio $r = \frac{m_{water}}{m_{air}} \frac{e}{p - e}$ where p is pressure and e is vapour pressure.
- Saturated humidity mixing ratio $r_w = \frac{m_{water}}{m_{air}} \frac{e_w}{p - e_w}$.



2.6 Gravitational settling of particulates

- Dynamic viscosity (μ) is calculated using

$$\mu = \begin{cases} (1.718 + 0.0049 T_c) \times 10^{-5}, & T_c \geq 0, \\ (1.718 + 0.0049 T_c - 1.2 \times 10^{-5} T_c^2) \times 10^{-5}, & T_c < 0, \end{cases}$$

where T_c is the temperature in degrees Celsius (Pruppacher and Klett 1997, page 417).

- The Reynolds number (Re) is given by

$$Re = \frac{\rho w_{sed} D}{\mu}, \quad (1)$$

where ρ is the density of the air, D is the particle diameter and w_{sed} is the sedimentation velocity (Maryon 1997).

- The drag coefficient (c_D) can be represented as a function of Re by the empirical equation

$$c_D = 0.25 + \frac{24}{Re} + \frac{6}{1 + \sqrt{Re}} \quad (2)$$

(Maryon 1997).

- The sedimentation velocity (w_{sed}) of a particle is given by

$$w_{sed} = \left(\frac{4}{3} \frac{D}{c_D} g \frac{\rho_p - \rho}{\rho} \right)^{1/2}, \quad (3)$$

where ρ_p is the density of the particle (Maryon 1997).

- For the Stokes' regime ($Re < 1$), $c_D = 24/Re$ and the sedimentation velocity is given by

$$w_{sed} = \frac{D^2 g (\rho_p - \rho)}{18\mu} \quad (4)$$

(Maryon 1997).

- Substituting for c_D and Re in Eq. (3) using Eqs. (1) and (2) yields an equation for w_{sed} which could be solved numerically. We choose, however, to adopt the following iterative procedure:

- Calculate the sedimentation value for the Stokes' regime using Eq. (4)
- Using this Stokes' regime sedimentation velocity as an initial value, iterate to obtain a revised sedimentation velocity:
 - * Substitute w_{sed} into Eq. (1) to obtain a revised Reynolds number.
 - * Substitute Re into Eq. (2) to obtain a revised drag coefficient.
 - * Substitute c_D into Eq. (3) to obtain a revised sedimentation velocity.
- The iteration procedure is iterated until the calculated sedimentation velocity converges to a fixed value.

- For small particles in the submicron range, the sedimentation velocity is modified by multiplying by the Cunningham slip-flow correction factor (CCF),

$$CCF = 1 + \alpha N_{Kn}$$

(Pruppacher and Klett 1997, page 450), where

$$\alpha = 1.257 + 0.4 \exp \left(- \frac{1.10}{N_{Kn}} \right),$$

N_{Kn} is the Knudsen number, $N_{Kn} = 2\lambda_a/D$ (Pruppacher and Klett 1997, page 448) and λ_a is the mean free path of air molecules

$$\lambda_a = \lambda_{a,0} \left(\frac{P_0}{P} \right) \left(\frac{T}{T_0} \right), \quad (5)$$

(Pruppacher and Klett 1997, page 417) where $\lambda_{a,0} = 6.6 \times 10^{-8}$ m, $P_0 = 1013.25$ mb, $T_0 = 293.15$ K, P is the pressure and T is the temperature.



3 Mathematical constants and functions

- $\pi = 3.141\ 592\ 653\ 589\ 793\ 238\ 462\ 643$ (Abramowitz and Stegun 1965, table 1.1, page 3)
- $\text{erf}(x)$ is calculated using the approximation given by Abramowitz and Stegun (1965, §7.1.26, page 299)
- NAME has an internal random number generator based on L'Ecuyer and Andres (1997). All requests for random values are implemented through calls to routines in the Maths module: `mathsRandomUniform()` for uniformly distributed random variables; and the pair of routines, `mathsRandomGaussian1()` or `mathsRandomGaussian2()`, for Gaussian distributed variables (which return 1 or 2 variates, as required). Gaussian variates are constructed from uniform random variables using the Box-Mueller method.

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