A LAGRANGIAN DISPERSION MODEL WITH A STOCHASTIC EQUATION FOR THE TEMPERATURE FLUCTUATIONS.

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18th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes 9-12 October 2017, Bologna, Italy

Talk outline

- Building Stochastic Differential Equations (SDEs) for plume rise: effect of temperature fluctuations on the spread of a buoyant plume.
- Parametrization of the SDEs coefficients.
- Variables initialisation.
- First implementation of the temperature SDE into an operating dispersion model: preliminary comparison of SPRAYWEB simulation with the convection tank experiment of Weil et al. (2002, *Boundary-Layer Meteorol.*)

Introduction

Plume rise

- Most of Lagrangian Stochastic Dispersion Models (LSDMs) for buoyant plume rise do not take into account the turbulence induced by the plume to the ambient, but only for the itself ambient turbulence.
- Webster and Thomson (2002, *Atmos. Environ.*) developed a hybrid approach in which:
    - The mean flow is calculated from a simple plume model.
    - The fluctuations are calculated from an LSDM.
- The turbulence generated by the plume is modelled by Webster and Thomson (2002, *Atmos. Environ.*) by an additional random increment to the position of a particle.
- Bisignano and Devenish (2015, *Boundary-Layer Meteorol.*) does not include this extra term, but they consider both fluctuations of the velocity and temperature to take into account the turbulence induced by the plume to the ambient.

Hybrids model for buoyant plume rise

$z(t+\Delta t) = z(t) + w(t)\Delta t +$ random displacement due to plume rise induced turbulence

$$\theta(t) = \overline{\theta}(t) + \theta'(t)$$

$w(t) = \overline{w}(t) + w'(t) +$ term of interaction between w' and θ'

Mean flow

Plume (mean particles) velocity $\overline{w}$

Plume (mean particles) temperature $\overline{\theta}$

Fluctuations

Velocity fluctuations w'

Temperature fluctuations θ'

Model for the mean flow

Standard plume equation (Briggs, 1984, *Atmospheric science and power production*; Weil, 1988, *Lectures on Air Pollution Modeling*)

Introduction of a second mass conservation equation

Model for the fluctuations

LSDM for w' (Thomson, 1987, *J. Fluid .Mech.*)

LSDM for w' and θ' (van Dop, 1992, *Atmos. Env.*; Das and Durbin, 2005, *Atmos. Env.*)

Legend: Webster and Thomson (2002, *Atmos. Environ.*), Bisignano and Devenish (2015, *Boundary-Layer Meteorol.*)

Building the stochastic differential equations: the plume equations

The equations governing the rise of a buoyant plume in a uniform crossflow U are given by (e.g. Briggs, 1984, *Atmospheric science and power production*; Weil, 1988, *Lectures on Air Pollution Modeling*)

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}s}(\pi v b^2) &= E \\ (1+k_v)\frac{\mathrm{d}}{\mathrm{d}s}(\pi v \overline{w} b^2) &= \pi b^2 \overline{g'} \\ \frac{\mathrm{d}}{\mathrm{d}s}(\pi v \overline{g'} b^2) &= -N^2 \pi b^2 \rho_p \overline{w} \end{aligned}$$

and respectively describe the evolution of the volume, momentum (per unit density) and buoyancy fluxes. It is possibile to re-express them in terms of w, b, θ and time t to get:

$$\begin{aligned} \frac{\mathrm{d}w}{\mathrm{d}t} &= \frac{g(\theta-\theta_a)}{\theta_0} - E\frac{w}{b^2} \\ \frac{\mathrm{d}b}{\mathrm{d}t} &= \frac{E}{2b} - \frac{bw}{2v^2}\frac{g(\theta-\theta_a)}{\theta_0} + E\frac{w^2}{2bv^2} \\ \frac{\mathrm{d}\theta}{\mathrm{d}t} &= -E\frac{(\theta-\theta_a)}{b^2} \end{aligned}$$

Reynolds decomposition

$w = \overline{w} + w'$ and $\theta = \overline{\theta} + \theta'$ (while $b' = \theta'_a = 0$). The overbar indicates a mean value. The prime indicates a fluctuating quantity. The Reynolds decomposition lead to:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\overline{w} + w') = \frac{1}{1+k_v} g \frac{\overline{\theta} - \theta_a}{\theta_0} + \frac{1}{1+k_v} g \frac{\theta'}{\theta_0} - E\frac{\overline{w}}{b^2} - E\frac{w'}{b^2}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(\overline{\theta} + \theta') = -E\frac{\overline{\theta} - \theta_a}{b^2} - E\frac{\theta'}{b^2}$$

Mean flow: differential equation

The averaged part of these equations provide the mean flow for the LSDM:

$$\mathrm{d}\overline{w} = \left(\frac{1}{1+k_v} \frac{g(\overline{\theta} - \theta_a)}{\theta_0} - E\frac{\overline{w}}{\pi b^2} \right) \mathrm{d}t$$

$$\mathrm{d}b = \left(\frac{E}{2\pi b} - \frac{1}{1+k_v} \frac{b\overline{w}}{2v^2} \frac{g(\overline{\theta} - \theta_a)}{\theta_0} + E\frac{\overline{w}^2}{2\pi b v^2} \right) \mathrm{d}t$$

$$\mathrm{d}\overline{\theta} = \left(-E\frac{\overline{\theta} - \theta_a}{\pi b^2} \right) \mathrm{d}t$$

Fluctuating part: Stochastic differential equation

The SDEs are constructed by analogy with the fluctuating part of previous equations and coupled with LSDMs for w' (Thomson, 1987, *J. Fluid .Mech.*) and θ' (van Dop, 1992, *Atmos. Env.*) to give:

$$
\begin{aligned}
dw' &= -E\frac{w'}{\pi b^2}\,dt + \frac{g\theta'}{(1+k_v)\theta_0}dt - \frac{w'}{T_L}dt + \frac{1}{2}\left[1+\left(\frac{w'}{\sigma_w}\right)^2\right]\frac{\partial\sigma_w^2}{\partial z}\,dt + \sqrt{C_0\varepsilon}\,dW \\
d\theta' &= \frac{w'}{w}d\overline{\theta} - E\frac{\theta'}{\pi b^2}\,dt - \frac{\theta'}{T_\theta}dt + \sqrt{C_\theta\varepsilon_\theta}\,dW_\theta
\end{aligned}
$$

- The terms involving E represent the effect on the turbulence of the entrainment whereas the terms like $\frac{X'}{T_X}$ the 'internal' turbulence of the plume.
- θ' contribute to the SDE for w' through the $w-\vartheta$ coupling term $\frac{g\theta'}{\theta_0}$ which therefore include the self-generated turbulence of the plume.
- the term $-\frac{w'}{w}d\overline{\theta}$ arises from $\frac{d\overline{\theta}}{dt}$ that implicitly contains fluctuations of velocity.
- We assumed that the turbulent temperature statistics are homogeneous.
- We neglect the covariance between velocity and temperature.

Entrainment rate assumptions

Additive entrainment assumption

$$E = 2\pi b \frac{|\overline{w}|}{v} \left[(\alpha |\overline{w}|)^m + (\beta U)^m \right]^{1/m}$$

- In a crosswind there are two entrainment additive mechanisms due to velocity differences normal and parallel to the plume axis and E is proportional to these differences
- The difference between the horizontal component of the plume velocity and U is small relative to U
- The effect of a crossflow can be characterised by $\tilde{U} = U/(F_0 N)^{1/4}$
  - In the weak-wind limit, $\tilde{U} \ll 1$, the first term on the right-hand side dominates.
  - In the bent-over limit, $\tilde{U} \gg 1$, the second term on the right-hand side dominates.
  - In both asymptotic limits E is independent of m.
- $m \geqslant 1$ is a tunable parameter, (Devenish et al., 2010, *Boundary-Layer Meteorol.*) found that $m = 3/2$ gave the best agreement with LES and field observations.

Parametrization of the plume turbulence variables: SDEs coefficients

The turbulence parameters σ_w, T_L, ε, σ_θ, ε_θ and T_θ have been choosen as function of z to be related to the approriate plume mean quantities. It is necessary to limit the turbulence parameters in order to avoid numerical overflow in the oscillating region.

- $\sigma_w = \alpha \max(|\overline{w}|, \overline{w}^*)$ where $\overline{w}^* = 2^{-5/8}\pi^{-1/4}\left(\frac{6\alpha}{5}\right)^{-1}\left(\frac{9\alpha}{10}\right)^{1/2} F_0^{1/4} N^{1/4}$
- $T_L = \dfrac{\min(b, b^*)}{\max(|\overline{w}|, \overline{w}^*)}$ where $b^* = \left(2^{3/4} - 2^{5/8}\right)\pi^{-1/4}\left(\frac{6\alpha}{5}\right)^{-1}\left(\frac{9\alpha}{10}\right)^{1/2} F_0^{1/4} N^{1/4}$
- $\varepsilon_w = 2\sigma_w^2/(C_0 T_L)$
- $\sigma_\theta = \gamma \max(|\overline{\theta} - \theta_a|, \overline{\theta}^*)$ where $\overline{\theta}^* = \left(\frac{\theta_0}{g}\right)\pi^{-1/4}\left(\frac{9}{10\alpha}\right)^{-1/2} F_0^{1/4} N^{-3/4}$
- $T_\theta = T_L$
- $\varepsilon_\theta = 2\sigma_\theta^2/(C_\theta T_\theta)$
- $C_0 = 6$ and $C_\theta = 1.6$ are the Kolmogorov and the Obukhov-Corrsin constants (Sreenivasan, 1996, *Phys. Fluids*; Das and Durbin, 2005, *Atmos. Env.*)
- γ is a tunable constant whose value is chosen to be 0.5. α is the same as in entrainment expression.
- $\overline{w}^* = \overline{w}(z_{eq})$, $\overline{\theta}^* = \overline{\theta}(z_{eq})$ and $b^* = b(z_{eq})$ where z_{eq} is the level of neutral buoyancy.

Initialisation of plume variables

The initialisation of $\overline{w}$, b and $\overline{g'}$ for a pure plume whose initial buoyancy flux is known is not straightforward.

- We estimate $b_0 = 2z$ so that $\overline{w}_0 = \sqrt{b_0 \overline{g'}_0}$.
- The initial buoyancy flux is known: $F_0 = \pi b_0^2 \overline{g'}_0 \overline{v}_0$
- We obtain a cubic polynomial for either $\overline{w}_0$ or $\overline{g'}_0$ for given b_0:

$$b_0 \overline{g'}_0^3 + U^2 \overline{g'}_0^2 - \frac{F_0^2}{\pi^2 b_0^4} = 0$$

- The nature of the roots of this equation can be inferred by analysing the discriminant:

$$\Delta = \frac{F_0^2}{\pi^2 b_0^4} \left(4U^6 - \frac{27 F_0^2}{\pi^2 b_0^2} \right).$$

- In the problem the values of F_0 and b_0 are such that Δ is always negative and so the roots consist of one real root and two complex roots (and can thus be discarded)

Introduction into a dispersion model

The above-described temperature SDE was implemented for the first time into an operating LSDM: SPRAYWEB (Tinarelli et al., 1994, *J. Appl. Meteor.*; Alessandrini et al., 2013, *Atmos. Environ.*; Bisignano et al., 2017, *IJEP*).

- It is designed to study the pollutants dispersion in complex terrain
- In the vertical direction the probability density function PDF is assumed to be non-Gaussian, so to deal with convective conditions

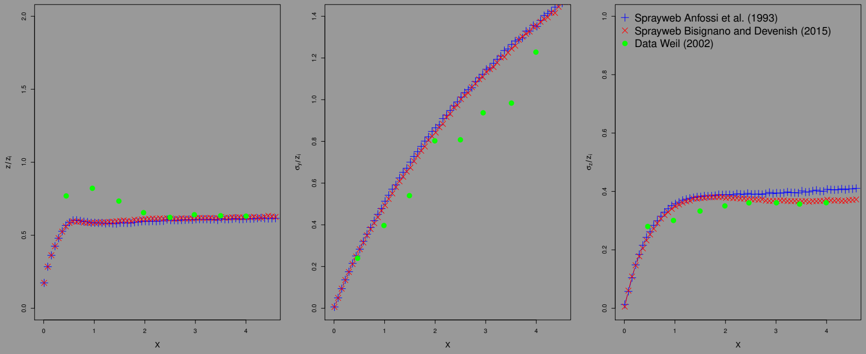
SPRAYWEB includes two methods for buoyant plume rise simulations.

- Anfossi et al. (1993, *Atmos. Environ.*): implemented into Lagrangian particle models by adding an additional velocity for taking into account buoyant rise. This extra-velocity is expressed as time differentation of empirical analitycal plume expression.
- Alessandrini et al. (2013, *Atmos. Environ.*): it makes use of two scalars transported by the particles (the temperature and vertical velocity difference between the plume and the environment). The entrainment derive from the plume-ambient interaction at the plume borders and each grid cell independently determines the rise increments of the particles.

The case study: Weil et al. (2002, *Boundary-Layer Meteorol.*) experiment

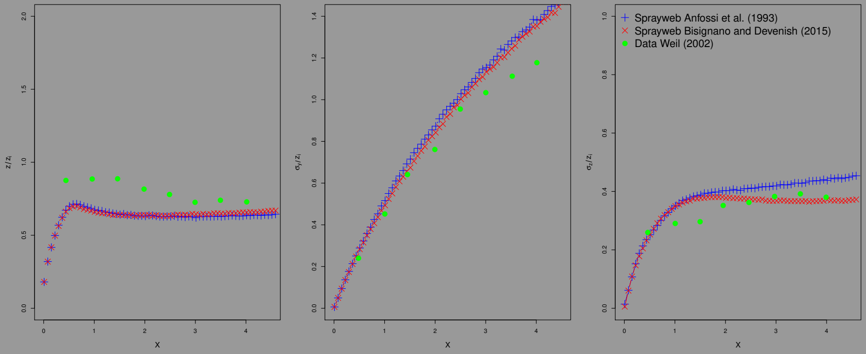
- Continuous buoyant releases in a convection tank.
- Plume dispersion in the convective boundary layer (CBL)
- Focus on highly-buoyant plumes trapped in the CBL capping inversion and resistant to downward mixing
- Dimensionless buoyancy flux $F^* = \dfrac{F}{U w_*^2 z_i} > 0.1$ (w_* is the convective velocity scale and z_i is the CBL depth).
- Different values of F^*: $F^* = 0$, $F^* = 0.1$, $F^* = 0.2$ and $F^* = 0.4$
- Results for lateral and vertical dispersion, mean and root-mean-square concentration fields as a function of F^*.

Comparison with Weil et al. (2002, Boundary-Layer Meteorol.) data. $F^* = 0.1$



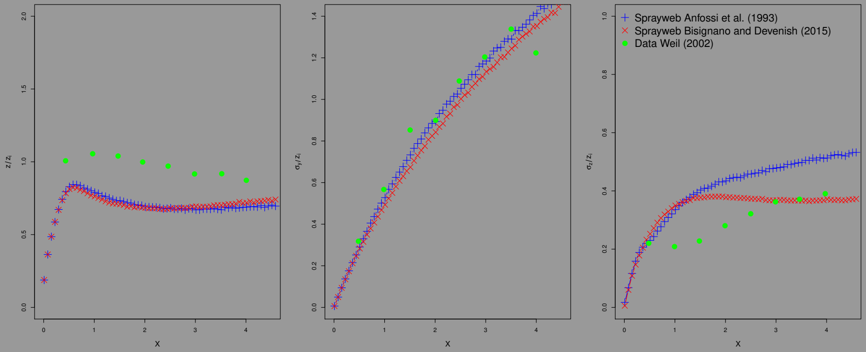
Comparison of the measured and the simulated mean height, horizontal and vertical standard deviations for $F^* = 0.1$, both with Anfossi et al. (1993, *Atmos. Environ.*) and Bisignano and Devenish (2015, *Boundary-Layer Meteorol.*) plume rise options.

Comparison with Weil et al. (2002, Boundary-Layer Meteorol.) data. $F^* = 0.2$



Comparison of the measured and the simulated mean height, horizontal and vertical standard deviations for $F^* = 0.2$, both with Anfossi et al. (1993, *Atmos. Environ.*) and Bisignano and Devenish (2015, *Boundary-Layer Meteorol.*) plume rise options.

Comparison with Weil et al. (2002, Boundary-Layer Meteorol.) data. $F^* = 0.4$



Comparison of the measured and the simulated mean height, horizontal and vertical standard deviations for $F^* = 0.4$, both with Anfossi et al. (1993, *Atmos. Environ.*) and Bisignano and Devenish (2015, *Boundary-Layer Meteorol.*) plume rise options.

Conclusion: plume rise model

- The hybrid model of buoyant plume rise combines coupled SDEs for vertical velocity and temperature with a classical plume model of buoyant rise in a crossflow.
- The novelty lies in the addition of the temperature SDE and of the consequent $w' - \theta'$ coupling term by means of which the model takes into account the turbulence generated by the plume itself.
- The model is able to reproduce the basic behaviour of the plume rise phenomenon in convective conditions and the numerical computation of the model compare well with Weil et al. (2002, *Boundary-Layer Meteorol.*) experiment data for dispersion parameters. In particular the model shows:
  - a little overestimation for the vertical standard deviation
  - a little underestimation in the mean height
- The agreement with the the vertical spread data is better than that evaluated with the Anfossi et al. (1993, *Atmos. Environ.*) plume rise characterised by the absence of temperature fluctuations.

Further development

- Better modelling of the inhomogeneity of the temperature fluctuations
- Evaluation of the effect of fluctuations on the mean flow.
- Modelling of the covariance between velocity and temperature
- Comparison of mean and root-mean-square concentration fields to Weil et al. (2002, *Boundary-Layer Meteorol.*) data.
- Comparison with Alessandrini et al. (2013, *Atmos. Environ.*) plume rise.

Acknowledgements

It is a pleasure to thank the Institute of Atmospheric Sciences and Climate (ISAC - CNR) and the Universitá del Piemonte Orientale, and expecially to Prof. Enrico Ferrero, Dr. Silvia Trini Castelli, Dr. Luca Mortarini and Dr. Domenico Anfossi.