

Recent developments inside a Lagrangian Particle Dispersion Model for the estimation of concentration peaks

Gianni Tinarelli and Roberto Sozzi

ARIANET Srl Milano



Structure of the presentation

- **1.** General description of the problem
- 2. Peak-to-mean formulations
 - a) Longitudinal
 - b) Variance-transport
- 3. Model implementations into the SPRAY LPDM
- 4. Results in controlled/real conditions and comparisons between different methods
- 5. Conclusions

1. General description of the problem



Some fundamental remarks

- Olfactory problems are perceived by an individual through a single respiratory act, lasting about 5 seconds
- it is the concentration averaged during this brief sampling period that does matter in principle, and not the relatively long-term average concentration (eg one hour)





⁸⁵Kr emitted in air(Lung e al. 2002)

It is therefore necessary to model the "instantaneout" values (or at least at a frequency of the order of 5 seconds) of the concentration

1. General description of the problem



Various way to compute the concentrations





The method consists in estimating the peak (short time/instantaneous) concentration values through the average values calculated by the model, using a multiplication factor (Peak-to-mean factor)

Some reference guidelines provides for the use of a **constant Peak-to-mean factor F** (independent from space, time, met)

For example: F=4 (Germany), F=2.3 (Italy)

2. Peak-to-mean formulations



a) Longitudinal Peak-to-mean Ratio



It is assumed that the p/m at the source position is a function of the atmospheric stability α , the typical average time t_m (3600 s) and to the average time t_p over a short period (e.g. 5 s)

2. Peak-to-mean formulations



b) Simplified Variance-Transport equation

Considering $C = \langle C \rangle + c'$ and starting from the general transport equation for c'^2

$$\frac{\partial \overline{c'^2}}{\partial t} + U_j \frac{\partial \overline{c'^2}}{\partial x_j} = -2\nu_c \left(\frac{\partial c'}{\partial x_j} \right)^2 - \frac{\partial}{\partial x_j} \left(\overline{u'_j c'^2} \right) - 2\overline{u'_j c'} \frac{\partial \langle c \rangle}{\partial x_j}$$

Following Oettl and Ferrero (2017): A simple model to assess odour hour for regulatory purposes, *Atmospheric Environment*, G155, **162-173**

- neglecting the transport terms
- neglecting the diffusion term
- comparing the rest to the lagrangian equations

the Variance-Transport equation Is reduced to:

$$\frac{\partial \overline{c'^2}}{\partial t} = -2\sigma_{ui}T_{Li}\left(\frac{\partial \langle C \rangle}{\partial x_j}\right)^2 - \frac{\overline{c'^2}}{2T_{Lw}} \quad \text{having the} \quad \overline{c'^2} = 2\sigma_{ui}T_{Li}(2T_{Lw})\left(\frac{\partial \langle C \rangle}{\partial x_j}\right)^2$$

the p/m is estimated from $\langle C \rangle$, $\overline{c'^2}$ computed at each point and a PDF of a given form



The SPRAY-3 Lagrangian Particle Dispersion Model is considered

Longitudinal P/M

- a value $\Psi(p)$ is associated to each computational particle
- the previous equation is applied in differential form, considering $\Delta x = U \Delta t$
- each particle contributes with its own $\Psi(p)$ inside a concentration cell to the computation of an averaged Peak-to-mean factor
- U and T_L are space/time dependent, computed on each particle position

Variance-transport P/M

- each 'sampling Δt ' a $\frac{\partial \langle C \rangle}{\partial x_j}$ field is computed on an Eulerian grid
- the simplified equation is applied to compute $\overline{c'^2}$
- using $\overline{c'^2}$ and $\langle C \rangle$, a p/m is computed using a Weibull PDF (other options are possible)
- the peak concentration values are estimated as the 98 percentile of the Weibull PDF with the given $\overline{c'}^2$ and $\langle C \rangle$



Setup of the numerical experiments in simple controlled conditions

Homogeneous and stationary conditions, 12 x 12 km² domain, flat terrain, 1 and 4 m/s wind, 2 different stability conditions, point source

| Point source characteristics | |
|------------------------------|---------------|
| Stack height | = 10 m |
| Diameter | = 0.5 m |
| Exit temperature | = environment |
| Emitting flow | = 70000 UO/s |



Unstable conditions, 1 m/s, concentrations

Average concentration <C>





Unstable conditions, 1 m/s, concentrations



3. Numerical experiments - results



Unstable conditions, 1 m/s, Peak-to-mean ratio





Unstable conditions, 4 m/s, concentrations





Unstable conditions, 4 m/s, concentrations



3. Numerical experiments - results



Unstable conditions, 4 m/s, Peak-to-mean ratio



Lateral behavior of the fluctuation intensity, $\sigma_c/<C>$, experimental data





From Lofstrom et al., 1994

A concentration fluctuation model for decision-makers based on joint tracer and lidar measurements from a non-buoyant elevated plume – Trans. Ecology and Environ., 3, 571-579

Lateral Peak to mean from the interpolated curve 400m from the source,



SPRAY 1 m/s unstable peak to mean



Lateral behavior of the fluctuation intensity, $\sigma_c/<C>$, experimental data







Stable conditions, 1 m/s, Peak-to-mean ratio



Stable conditions, 1 m/s, Peak-to-mean ratio

Realistic case over complex terrain

- 16 x 18 km² area
- Same emissions previously described
- 10 days during winter and 10 days during summer

98 percentile derived from hourly averaged concentrations

98 percentile <C>

98 percentile derived from hourly averaged concentrations

Peak-to-mean ratio of the 99.8 percentile

Some concluding remarks

- two P/M different approaches, having different spatial behaviours
- VART P/M seems to better follow some experimental evidences compared to the LONG approach, moving in a direction transverse to the plume
- stable cases: both approaches do not solve the problem of meandering to capture realistic peak values
- VART is oriented to a σ_c estimation, it has still some degrees of freedom moving to P/M (choice of the distribution and of the peak threshold)
- VART has the advantage to take into account multiple sources (it mainly depends on the concentration structure)

Thanks for your attention