A STATIONARY 3D LAGRANGIAN STOCHASTIC NUMERICAL MODEL FOR CONCENTRATION FLUCTUATIONS

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SUMMARY

- LAGRANGIAN MICROMIXING MODELS
- THE MICROMIXING MODEL LAGFLUM
- THE MUST WIND TUNNEL TEST
- CONCLUSIONS

LAGRANGIAN MICROMIXING MODELS

- Concentration fluctuations (Reynolds' decomposition):

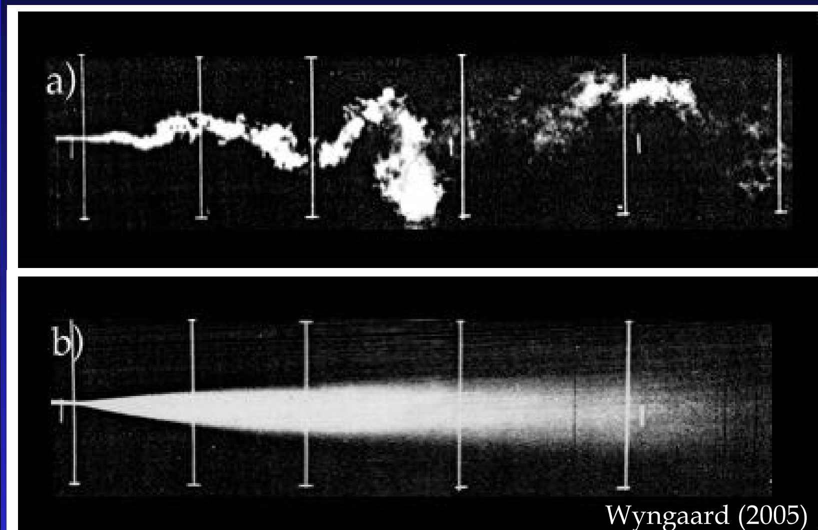
$$C = \overline{C} + C' \quad \text{E.1}$$

- Fields of interest of concentration fluctuations:
  - ✓Microscale dispersion ($t<T_L$)
  - ✓Reactive pollutants
  - ✓Strong non linear relationship between concentration and impact (accidents, odours)

- State of the art about Lagrangian micromixing models:
  - ✓1D dispersion: Sawford 2004 (grid turbulence), Sawford 2006 (reactants), Luhar-Sawford 2005 (CBL), Cassiani et al. 2005c (canopy)
  - ✓2D dispersion: Cassiani et al. 2005a (NBL), Cassiani et al. 2005b (CBL), Dixon-Tomlin 2007 (NBL and canopy), Cassiani et al. 2007a and Cassiani et al. 2007b (canopy), Amicarelli et al. (2007) (NBL)

LAGRANGIAN MICROMIXING MODELS

FIELDS OF INTEREST



Wyngaard (2005)

instantaneous vs mean plume


www.med.usf.edu/~npoor/3

microscale (reactive) dispersion


Chiverton (2008)

accidents


Messaggio (2007)

odours

LAGRANGIAN MICROMIXING MODELS

CONCENTRATION FLUCTUATIONS OF NON CONSERVATIVE PARTICLES

- Balance equation for the instantaneous concentration (C):

$$\frac{\partial C}{\partial t}+u_i\frac{\partial C}{\partial x_i}=D_M\frac{\partial^2 C}{\partial x_i^2}-rCC_B \qquad \text{E.2}$$

- Balance equation for the mean concentration $(\overline{C})$:

$$\frac{\partial \overline{C}}{\partial t}+\overline{u_i}\frac{\partial \overline{C}}{\partial x_i}+\frac{\partial \overline{u_i'C'}}{\partial x_i}=D_M\frac{\partial^2 \overline{C}}{\partial x_i^2}-r\left(\overline{C}\,\overline{C_B}+\overline{C'C_B'}\right) \qquad \text{E.3}$$

- Balance equation for the concentration variance (σ_C^2):

$$\frac{\partial \sigma_C^2}{\partial t}+\overline{u_i}\frac{\partial \sigma_C^2}{\partial x_i}+\frac{\partial \overline{u_i'(C')^2}}{\partial x_i}=-2\overline{u_i'C'}\frac{\partial \overline{C}}{\partial x_i}-2D_M\overline{\left(\frac{\partial C'}{\partial x_i}\right)^2}+D_M\frac{\partial^2 \sigma_C^2}{\partial x_i^2}+2\overline{C'T'} \qquad \text{E.4}$$

$$(\varepsilon_C<0)$$

dissipation of the concentration variance

THE MICROMIXING MODEL LAGFLUM

PHASES OF SIMULATION

1) MACROMIXING
Thomson 1987

- Conservative polluted particles released from the source (passive pollutants)
- Computation of the mean concentration, the conditional mean and the mixing time scale

2) MICROMIXING
Thomson 1987 + IECM (Pope 1998, Sawford 2004)

- Non conservative particles (polluted or clean) released all over the domain (or from the plume contour)
- Computation of the concentration fluctuations

THE MICROMIXING MODEL LAGFLUM
MACROMIXING OF CONSERVATIVE PARTICLES

- Balance equation for the mean concentration (passive):

$$D_M \frac{\partial^2 \overline{C}}{\partial x_i^2} \to 0, \quad \mathrm{Re} \to \infty \quad \Rightarrow \quad \frac{\partial \overline{C}}{\partial t} + \overline{u_i}\frac{\partial \overline{C}}{\partial x_i} + \frac{\partial \overline{u_i' C'}}{\partial x_i} = \overline{\frac{dC}{dt}} = 0 \qquad \text{E.5}$$

- Conservative particles satisfy the balance equation for $\langle \overline{C} \rangle$:

$$\frac{dC}{dt} = 0 \quad \Rightarrow \quad \overline{\frac{dC}{dt}} = 0 \qquad \text{E.6}$$

- Molecular diffusion (micromixing) doesn't alter the mean, the conditional mean $\langle C | \underline{U} \rangle$ and the pollutant flux in turbulent flows (Pope 1998)

THE MICROMIXING MODEL LAGFLUM

MACROMIXING SCHEME (THOMSON 1987)

- Thomson 1987 stationary well- mixed solution for independent gaussian eulerian velocity pdfs (C_0: Kolmogorov constant):

$$\underline{X}(t+dt)=\underline{X}(t,\underline{x})+\underline{U}(t)dt,\quad \underline{X}(t=0)=\underline{X}_0 \qquad \text{E.7}$$

$$U_i(t+dt)=\overline{u_i}(t+dt)+U_i^{'}(t)+dU_i^{'}(t) \qquad \text{E.8}$$

$$dU'=\left[-\frac{U'}{T_{Lx}}+\frac{1}{2}\frac{\partial\sigma_u^2}{\partial x}+\frac{U'}{2\sigma_u^2}\left(U'\frac{\partial\sigma_u^2}{\partial x}+V'\frac{\partial\sigma_u^2}{\partial y}+W'\frac{\partial\sigma_u^2}{\partial z}\right)\right]dt+\sqrt{C_0\varepsilon}d\xi_u \qquad \text{E.9}$$

$$dV'=\left[-\frac{V'}{T_{Ly}}+\frac{1}{2}\frac{\partial\sigma_v^2}{\partial y}+\frac{V'}{2\sigma_v^2}\left(U'\frac{\partial\sigma_v^2}{\partial x}+V'\frac{\partial\sigma_v^2}{\partial y}+W'\frac{\partial\sigma_v^2}{\partial z}\right)\right]dt+\sqrt{C_0\varepsilon}d\xi_v \qquad \text{E.10}$$

$$dW'=\left[-\frac{W'}{T_{Lz}}+\frac{1}{2}\frac{\partial\sigma_w^2}{\partial z}+\frac{W'}{2\sigma_w^2}\left(U'\frac{\partial\sigma_w^2}{\partial x}+V'\frac{\partial\sigma_w^2}{\partial y}+W'\frac{\partial\sigma_w^2}{\partial z}\right)\right]dt+\sqrt{C_0\varepsilon}d\xi_w \qquad \text{E.11}$$

THE MICROMIXING MODEL LAGFLUM

IECM MICROMIXING SCHEME

- IECM micromixing scheme (Pope 1998, Sawford 2004) for passive pollutants (molecular diffusion process):

$$\frac{dC}{dt} = -\frac{C - \langle C|\underline{U}\rangle}{t_m} \qquad \text{E.12}$$

- Mixing time (t_m):
  - ✓Source dimension (σ_0)
  - ✓Velocity of dissipation of turbulent kinetic energy (ε)
  - ✓Travel time (t)

$$t_m = 0.8\left(\frac{3}{2}\right)^{-\frac{1}{2}}\left[\left(\frac{3}{2}\right)^{\frac{1}{2}}\frac{\sigma_0^{\,2/3}}{\varepsilon^{1/3}} + \sqrt{2T_L t}\right] \qquad \text{E.13}$$

THE MICROMIXING MODEL LAGFLUM

IECM SCHEME WELL FOUNDED ON THE BALANCE EQUATION OF THE MEAN CONCENTRATION

- Balance equation for the mean concentrations:

$$\overline{\frac{dC}{dt}} = 0, \qquad \left\langle \frac{dC}{dt} \middle| \underline{U} \right\rangle = 0 \qquad \text{E.14}$$

- IECM micromixing scheme:

$$\frac{dC}{dt} = -\frac{C - \langle C|\underline{U}\rangle}{t_m} \qquad \text{E.15}$$

- IECM doesn't alter the mean concentration:

$$\overline{\frac{dC}{dt}} = -\frac{\overline{C - \langle C|\underline{U}\rangle}}{t_m} = -\frac{\overline{C} - \overline{C}}{t_m} = 0 \qquad \text{E.16}$$

- IECM doesn't alter the conditional mean concentration:

$$\langle \frac{dC}{dt} \Big| \underline{U}\rangle = \langle \left(-\frac{C - \langle C|\underline{U}\rangle}{t_m} \right) \Big| \underline{U}\rangle = -\frac{\langle C|\underline{U}\rangle - \langle C|\underline{U}\rangle}{t_m} = 0 \qquad \text{E.17}$$

THE MICROMIXING MODEL LAGFLUM

IECM SCHEME WELL FOUNDED ON THE BALANCE EQUATION OF THE CONCENTRATION VARIANCE

- Dissipation of the concentration variance:

$$\varepsilon_C = -2D_M \overline{\left(\frac{\partial C'}{\partial x_i}\right)^2} = 2\overline{C'\frac{dC}{dt}} \qquad \text{E.18}$$

- IECM micromixing scheme (Pope 1998, Sawford 2004):

$$\frac{dC}{dt} = -\frac{C - \langle C|\underline{U}\rangle}{t_m} \qquad \text{E.19}$$

- IECM satisfyes the balance equation of $\langle\sigma_C^2\rangle$ because t_m (mixing time) approximately respects:

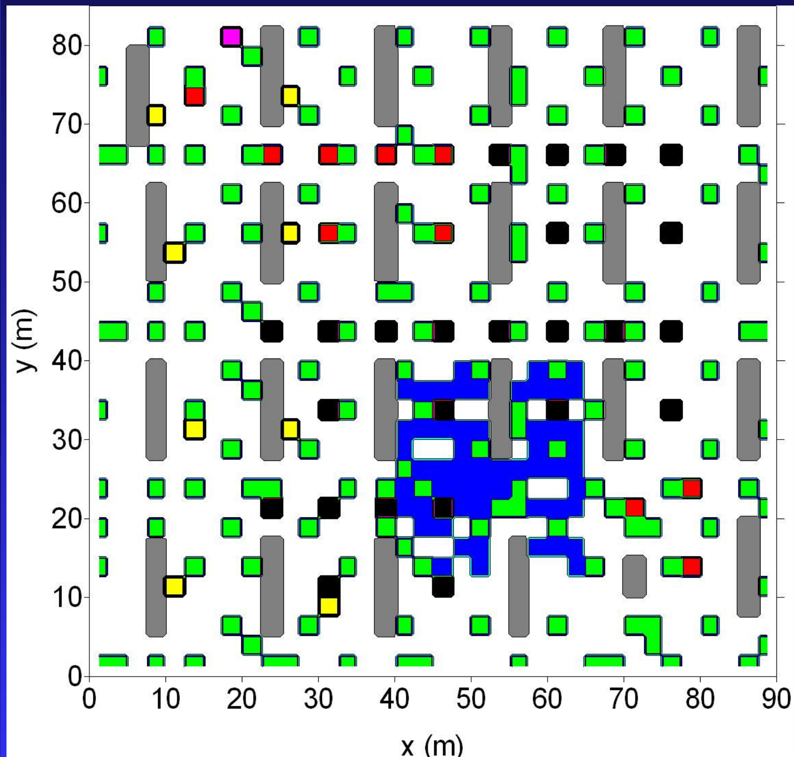
$$\varepsilon_C = -2\overline{C'\left(\frac{C - \langle C|\underline{U}\rangle}{t_m}\right)} \;\Rightarrow\; t_m = -\frac{2}{\varepsilon_C}\left[\sigma_C^2 - \overline{\left(C'\langle C|\underline{U}\rangle\right)}\right] \qquad \text{E.20}$$

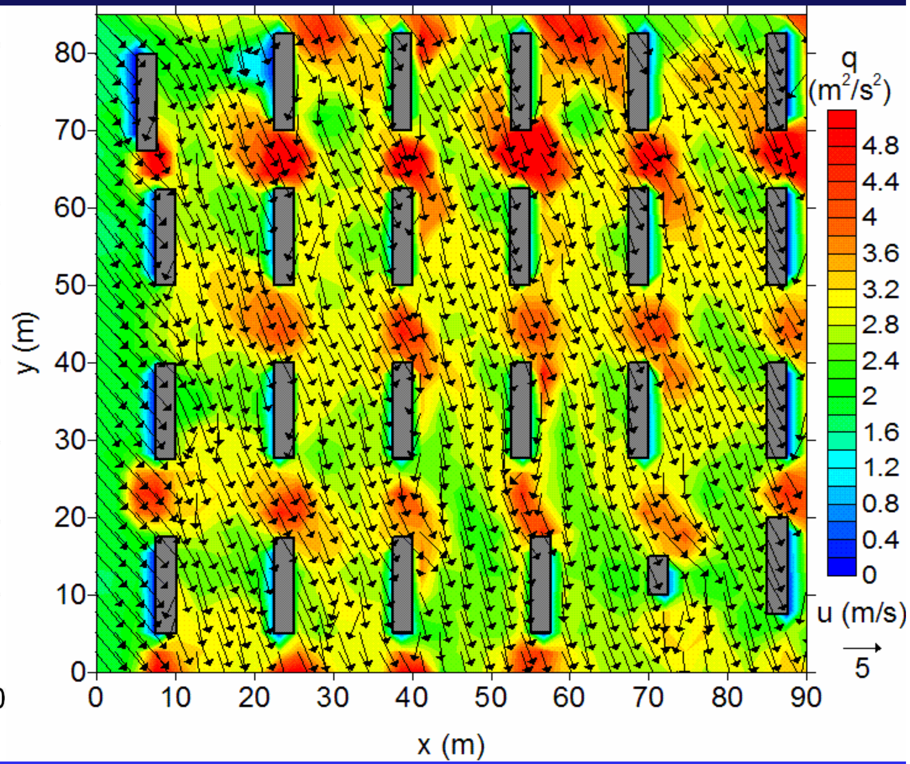
THE MUST WIND TUNNEL TEST
THE EXPERIMENTS

MUST WIND TUNNEL
Bezpalcova (2007),
Leitl et al. (2007)

MUST
(Mock Urban Setting Test)
Yee-Biltoft (2004)

THE MUST WIND TUNNEL TEST
METEOROLOGICAL DATA PROCESSING





Numerical domain, meteorological monitoring points and pollutant source

Elaborated horizontal mean wind and turbulent kinetic energy (z=H/2)

THE MUST WIND TUNNEL TEST
DATA PROCESSING AND CONFIGURATION

- Numerical domain: dx=dy=2.5m, dz=0.5m
- Buildings geometry: 12.5*2.5*2.5m^3
- 3D interpolation for the horizontal means and variances of veocity
- SNBL for horizontal mean velocity (z<1m), z_0=0.0165m
- Continuity equation for the vertical mean velocity
- (1D+2D) interpolation for the vertical variance of velocity
- (Simplified balance equation of turbulent kinetic energy + k-ε closure) for ε (Beljaars et al. 1987, Kitada 1987, Detering and Etling 1985):

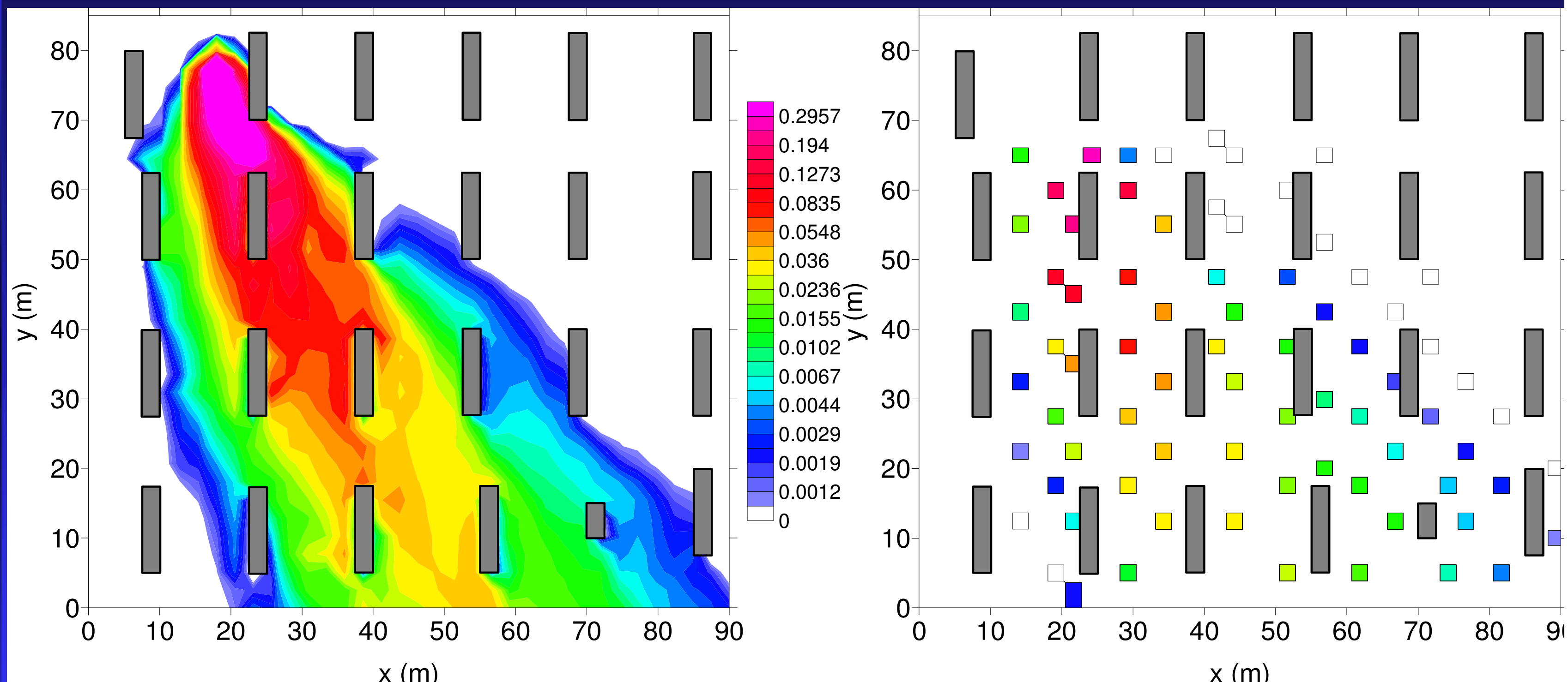
$$\varepsilon = 0.3q\sqrt{\left(\frac{\partial \overline{u}_i}{\partial x_j}\right)^2} \quad \text{E.21}$$

- Number of particles released: 20’000’000 (each phase)
- Kolmogorov constant (C_0)=3
- Scale concentration: (Q/H^2U_{ref})

THE MUST WIND TUNNEL TEST

RESULTS

MEAN CONCENTRATION (z=H/2)



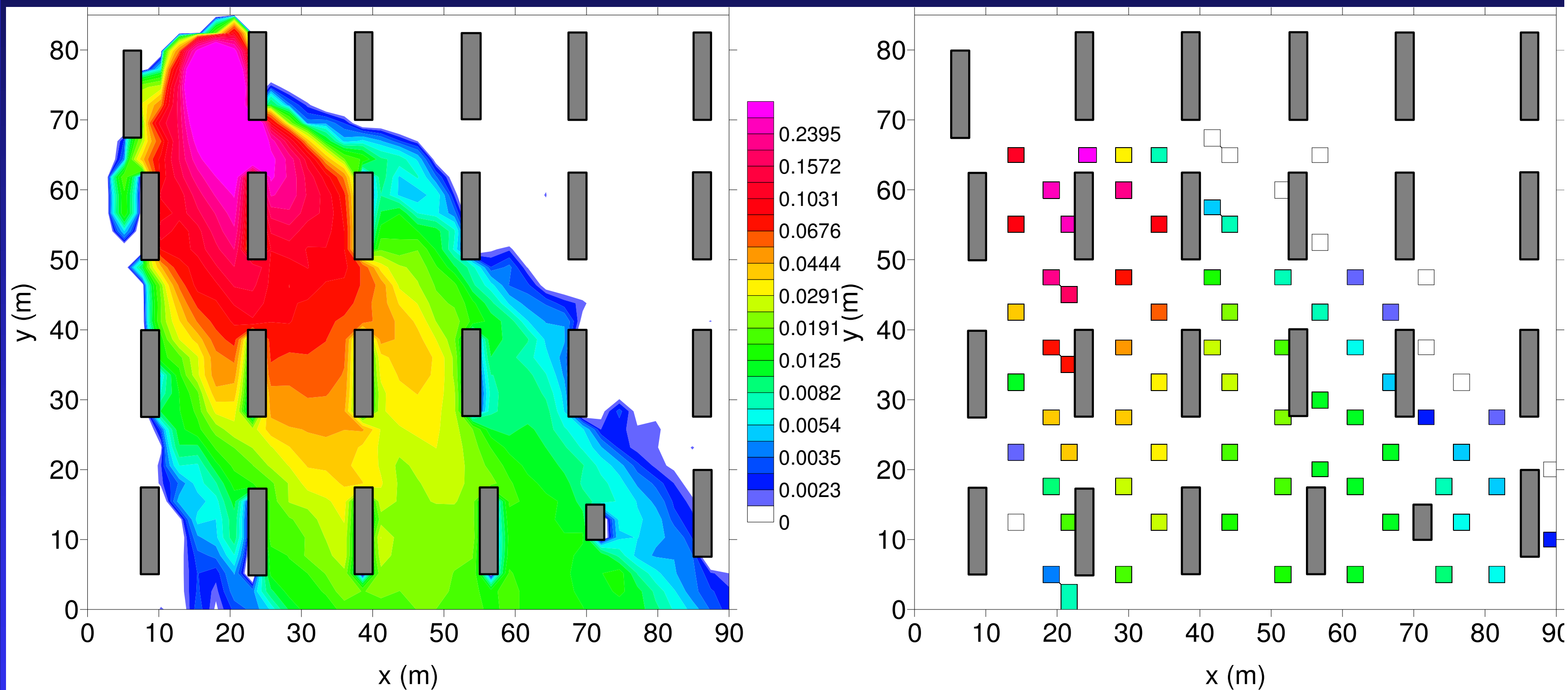
SIMULATED MEASURED

- Channelling effects
- Good agreement

THE MUST WIND TUNNEL TEST

RESULTS

STANDARD DEVIATION OF CONCENTRATION (z=H/2)



SIMULATED MEASURED

- Spread of maxima zone
- Channelling effects
- Intensity of fluctuations
- Good agreement

CONCLUSIONS

- The stationary 3D Lagrangian micromixing model LAGFLUM (LAGrangian FLUctuation Model) has been developed coupling Thomson 1987 macromixing scheme with the IECM micromixing scheme (Pope 1998, Sawford 2004)
- The model has been tested on the MUST wind tunnel experiment (Bezpalcova 2007, Leitl et al. 2007)
- The preliminary results of the concentration mean and variance are in good agreement with the measured values
- Possibility to interface LAGFLUM with k-ε (or similar) meteorological models
- Fields of applications: microscale dispersion, accidents, odours
- Developments: other pdfs for eulerian velocities, non stationary regimes, reactive pollutants

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