Modelling concentration variances in air quality models at mesoscale.

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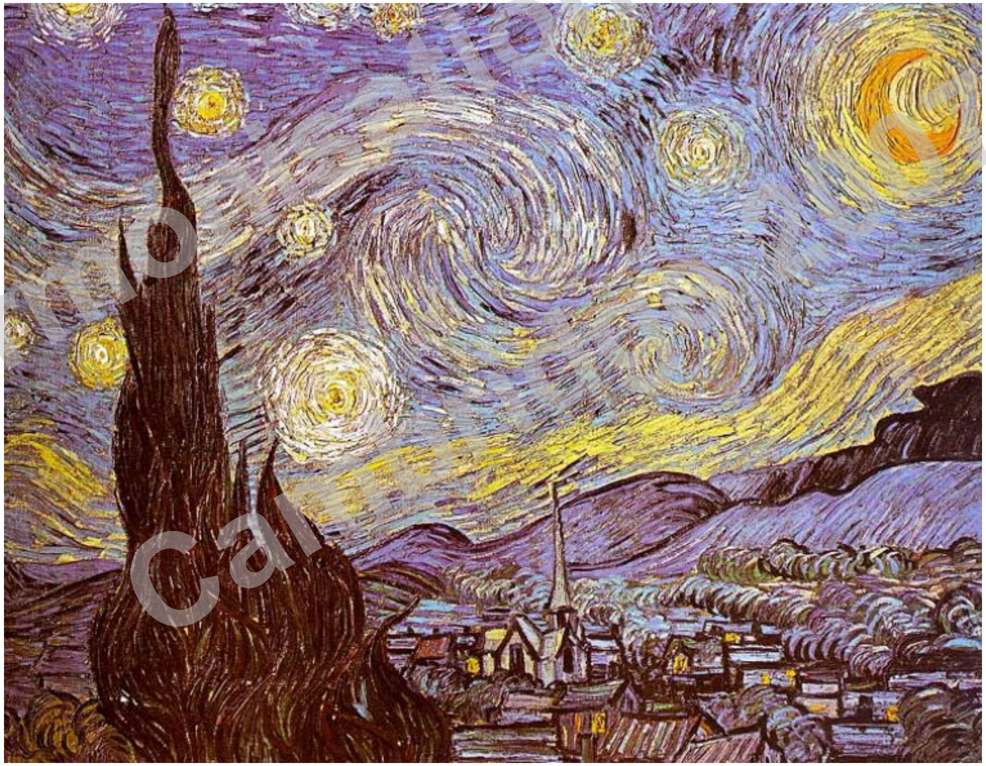

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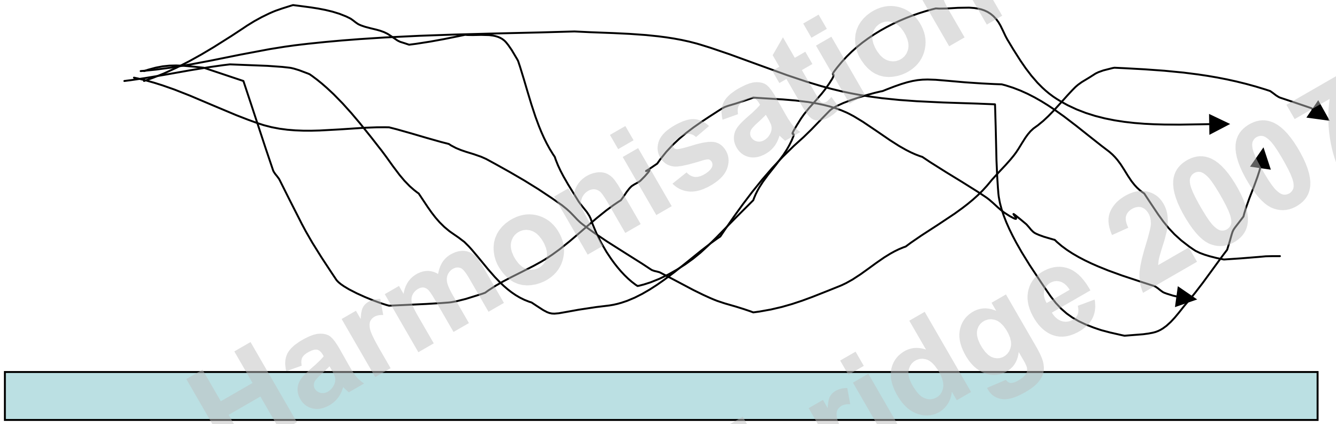
Most of the time atmosphere is turbulent. Turbulent motions are stochastic, which means that the next state of the atmosphere is partially but not fully determined by the previous state of the atmosphere.



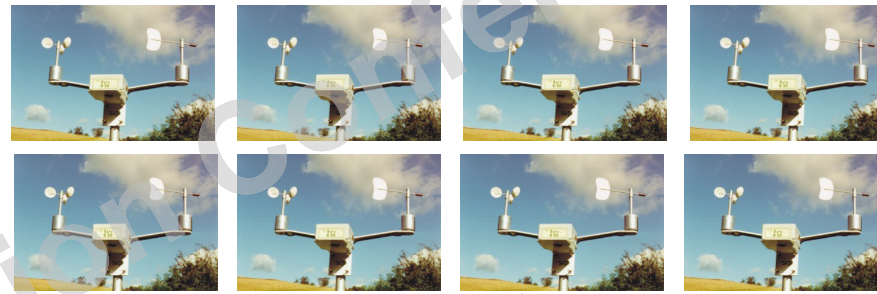
This limits the preditcability of air quality models. In fact they can only predict ‘mean’ values, not exact values.

Rigourously, mean values should be defined in a probabilistic way. For a variable ϕ, *we define* the probability to get the value η as $f(\eta)$ (probability density function). Then the mean is (Pope, 2000)

$$\overline{\phi} = \int_{-\infty}^{+\infty} \eta f(\eta) d\eta$$

The best way to 'measure' mean values is through an ensemble average (over many realizations)

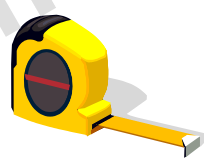
$$\overline{\phi}(x,t) \cong \frac{1}{N} \sum_{n=1,N} \phi_n(x,t)$$



If the flow is relatively homogenous in space and time, the mean can be considered similar to the space and time averages.

$$\overline{\phi}(x,t) \cong \frac{1}{T} \int_{t}^{t+T} \phi(x,t')dt'$$

$$\overline{\phi}(x,t) \cong \frac{1}{V} \int_{V} \phi(\vec{x}',t)d\vec{x}'$$



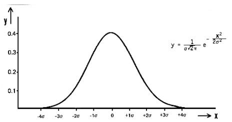
In the following we will consider this case.

However, the impact of air pollution on human health does not depend on the mean pollutant concentration, but on the actual concentration. It can be useful, then, *to estimate how much the actual concentration can differ from the mean value.*

This can be done by estimating the *variance* of the concentration. The *variance* is, by definition, the mean of the square of the departures from the mean. Or,

$$\overline{\phi'^2} = \overline{\left(\phi - \overline{\phi}\right)^2}$$

Morever, *if the distribution of the variable is normal*, there is a probability of about 68% to have values within the range:



$$\overline{\phi} - \sqrt{\overline{\phi'^2}} < \phi < \overline{\phi} + \sqrt{\overline{\phi'^2}}$$

It is possible to write a prognostic equation for the variance of pollutant concentration.

$$\frac{\partial \rho \overline{c'^2}}{\partial t} = -\frac{\partial \rho \bar{u}_i \overline{c'^2}}{\partial x_i} - \frac{\partial \rho \overline{u_i' c'^2}}{\partial x_i} - 2\rho \overline{c' u_i'} \frac{\partial \bar{c}}{\partial x_i} - 2\rho \varepsilon_c$$

tendency

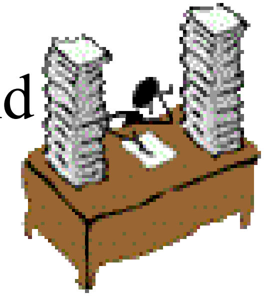
Mean transport

Turbulent transport

dissipation

Production term, (assuming downgradient turbulent transport). This is formally equivalent to the shear term in the TKE equation

How to parameterize turbulent transport, production term and dissipation?



Turbulent transport

Keeping only the vertical component

$$\overline{w'c'^2} = -K_h \frac{\partial \overline{c'^2}}{\partial z} \Rightarrow \frac{\partial \rho \overline{w'c'^2}}{\partial z} = -\frac{\partial}{\partial z}\left(\rho K_h \frac{\partial \overline{c'^2}}{\partial z} \right)$$

The turbulent coefficient K_h is estimated using the *K-l* closure of Belair et al. 1999. In this closure a prognostic equation for the turbulent kinetic energy *E* is solved, and dissipation and turbulent coefficients are derived using length scales as follows:

$$\varepsilon = c \frac{E^{3/2}}{l_\varepsilon}$$

$$K_h = a l_k E^{1/2}$$

where

$$\int_z^{z+l_{up}} \beta(\theta(z) - \theta(z'))dz' = E(z)$$

$$\int_{z-l_{down}}^{z} \beta(\theta(z') - \theta(z))dz' = E(z)$$

$$l_\varepsilon = (l_{up} l_{down})^{1/2}$$

$$l_k = l_\varepsilon \left(\frac{2B + S}{B + S} \right)$$

B, S are buoyancy and shear term, respectively, in the TKE equation

In analogy with what it is done for the TKE equation the other terms are paramterized as follow

Production term

$$-2\rho\overline{c'w'}\frac{\partial \bar{c}}{\partial z} = 2\rho K_h \left(\frac{\partial \bar{c}}{\partial z}\right)^2$$

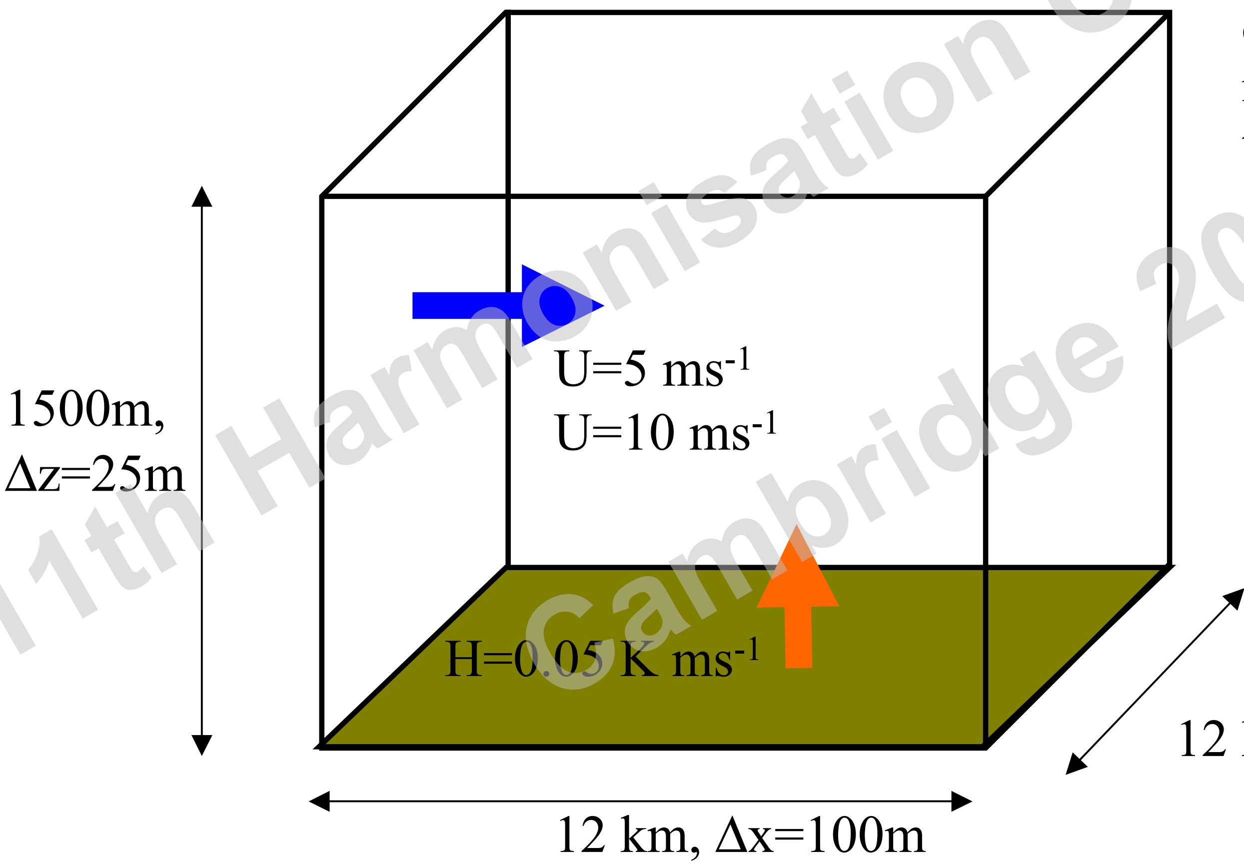
Dissipation

$$\varepsilon_c = c_\varepsilon \frac{\overline{c'^2} E^{1/2}}{l_\varepsilon}$$

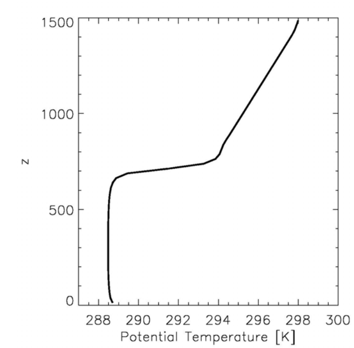
How to validate the parameterization?

Large Eddy Simulation *(The LES used here is the one developed by Cuypers and Duynkerke, 1993).*

Periodic lateral boundary conditions are assumed. The maximum time-step used in the calculations is 0.5 s



Potential temperature



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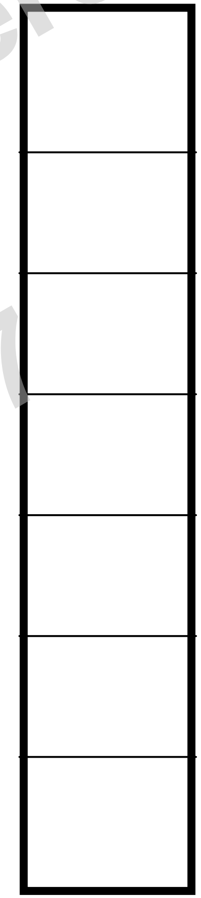
The new parameterization is run over a column in 1-D

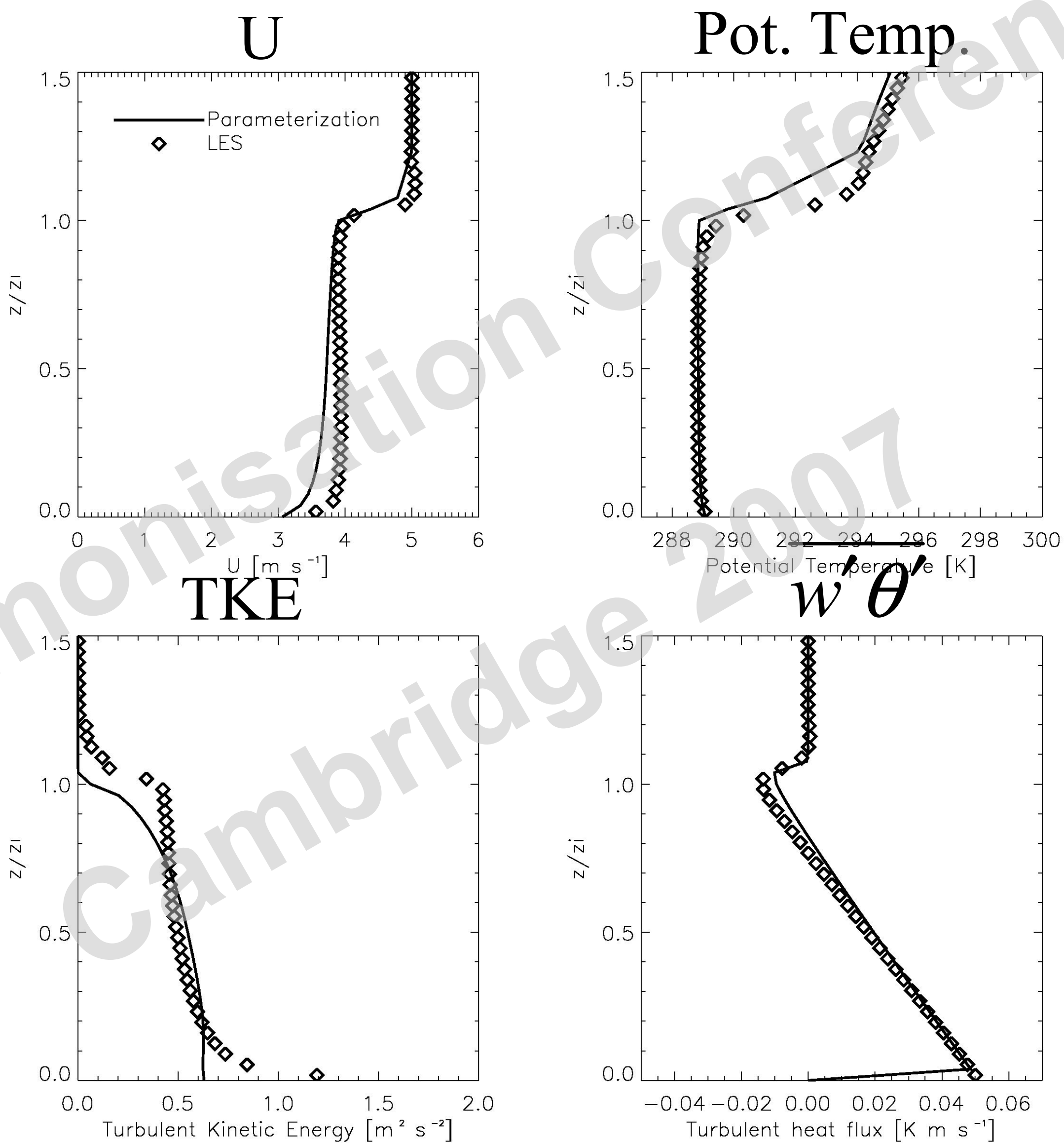
All the horizontal derivatives are neglected.

The vertical resolution is 25m, equal to the resolution of LES.

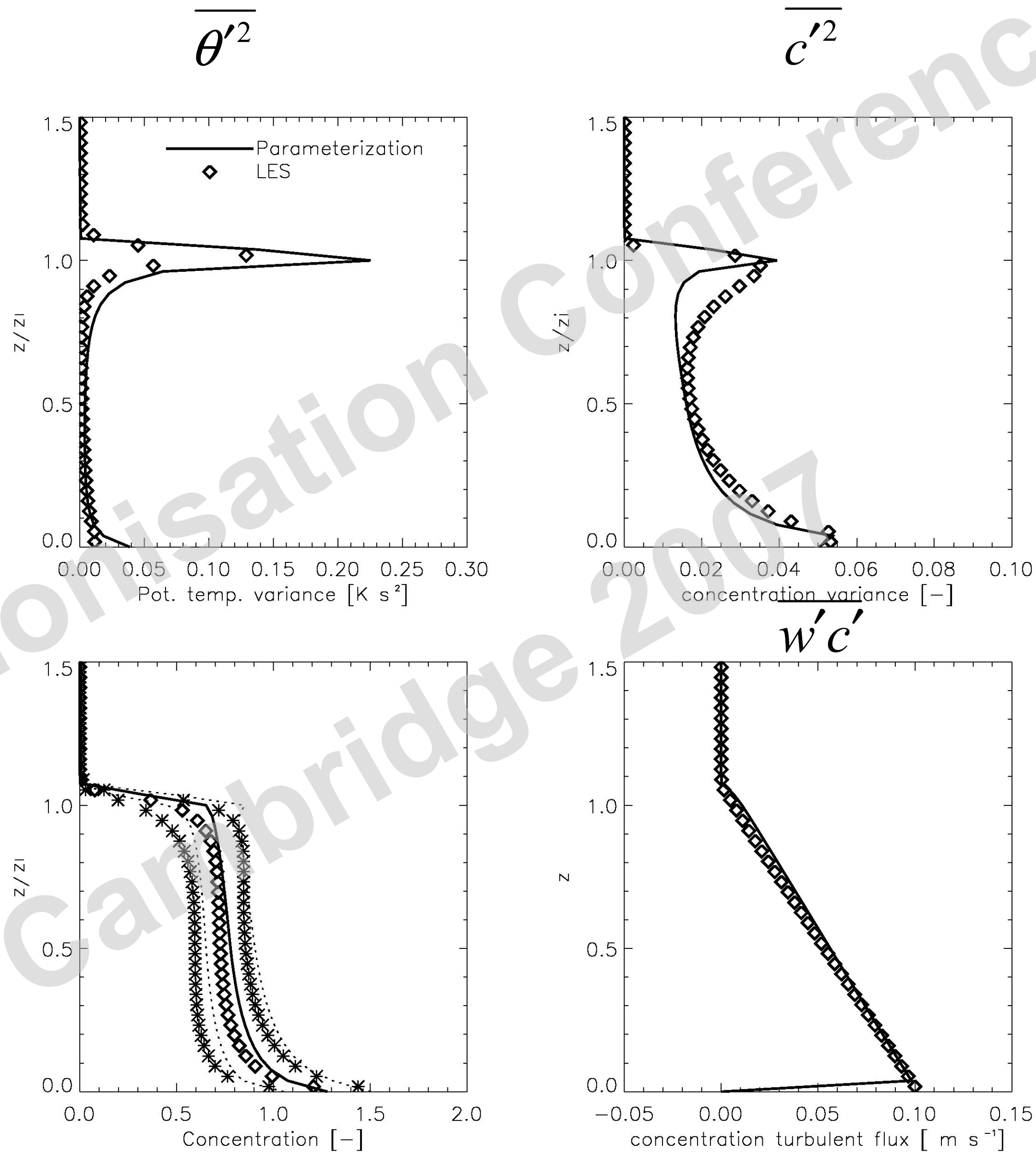
The initial conditions are equal to those used for the LES.



Results – comparison. 5m/s case



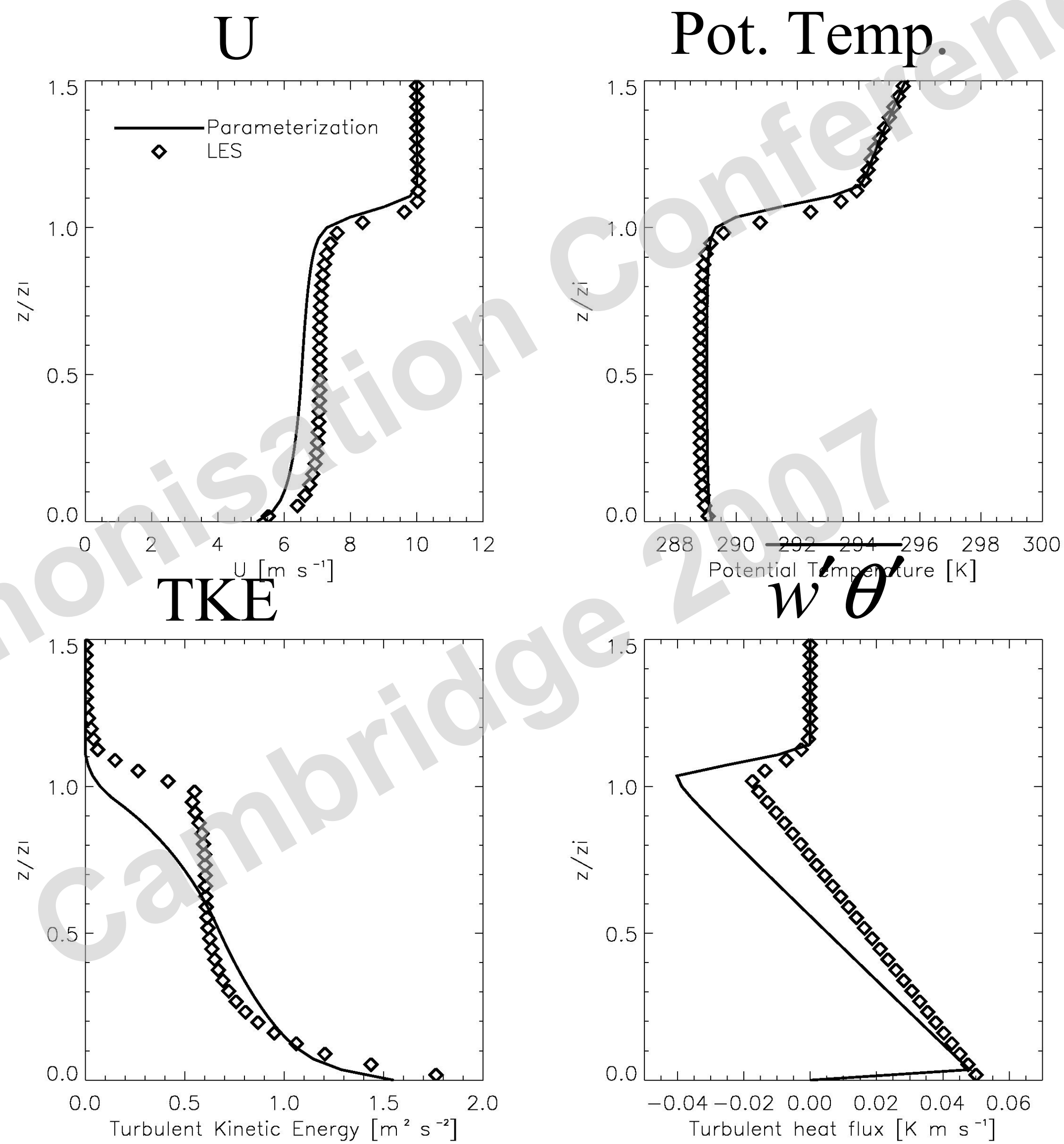
Results – comparison. 5m/s case



.... $\bar{c} \pm \sqrt{\overline{c'^2}}$ param

**** $\bar{c} \pm \sqrt{\overline{c'^2}}$ LES

Results – comparison. 10m/s case



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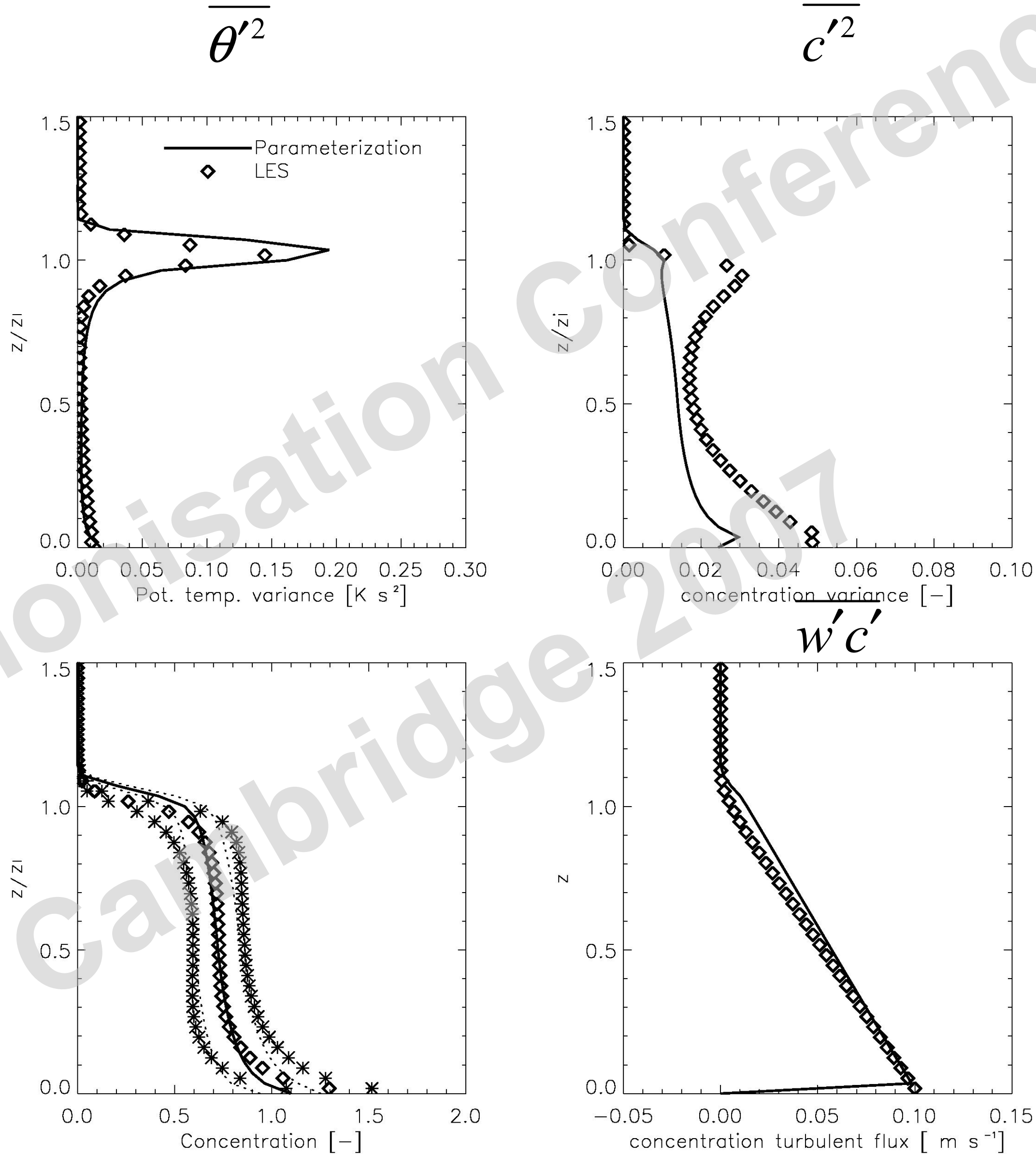
Results – comparison. 10m/s case



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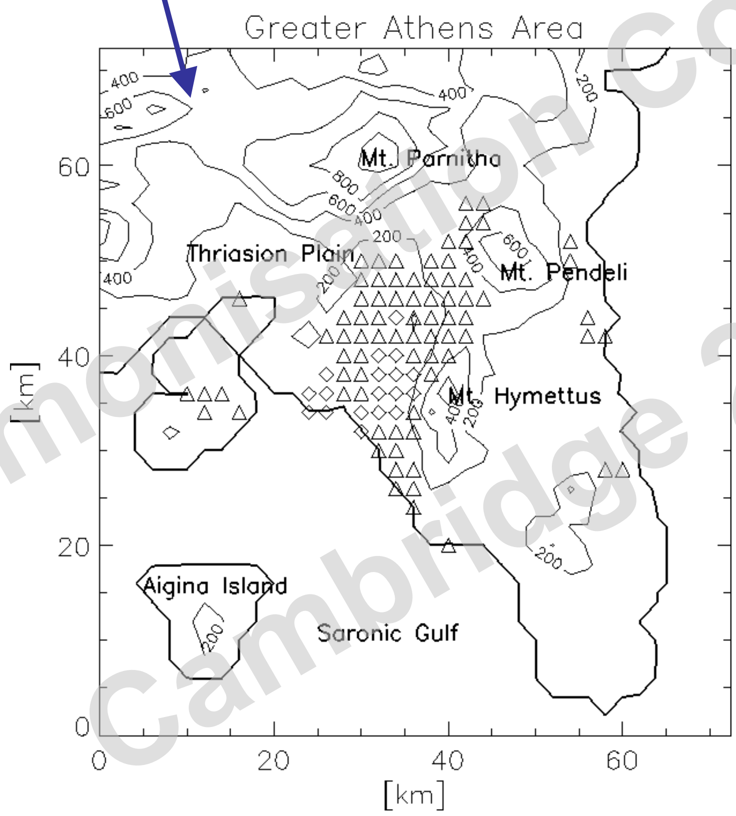
Test over a real case. Athens

Synoptic wind speed 340 deg., 1-2 m/s

14th September 1994
Medcaphot

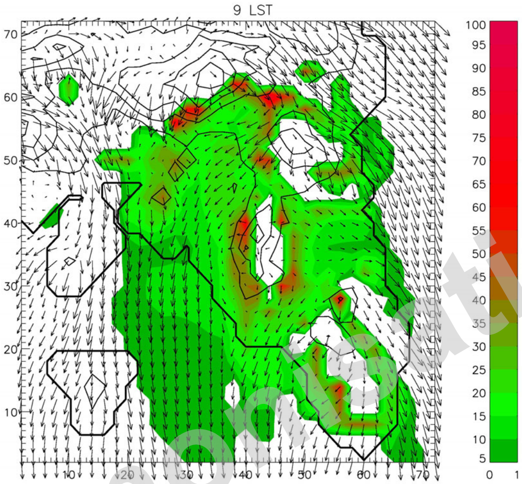


Dx=2km,Dz=10m near ground

CO emissions

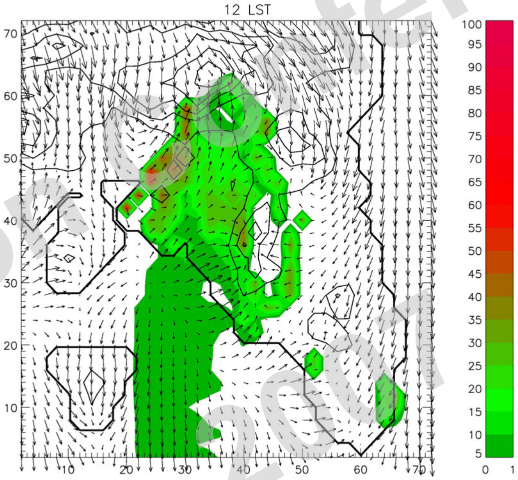
Maps of $$\frac{\sqrt{\overline{c'^2}}}{\overline{c}}\times 100$$

900 LST



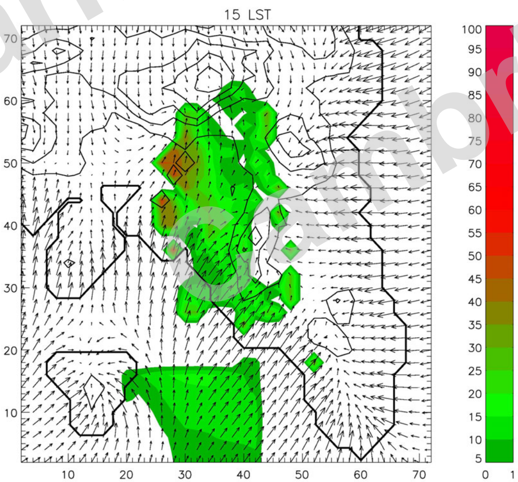
Max.=81%

1200 LST



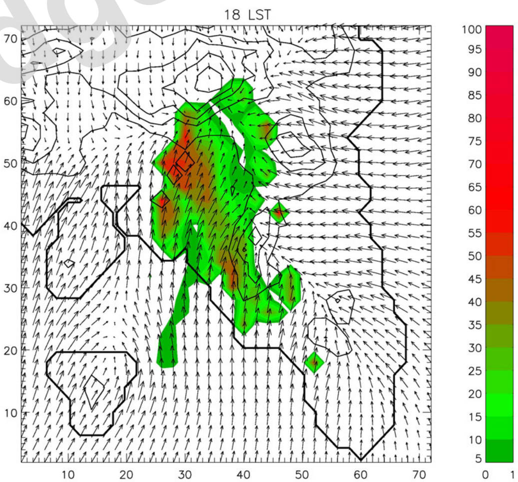
Max.=57%

1500 LST



Max.=51%

1800 LST



Max.=59%

Conclusions

A parameterization to model concentration variance of passive tracers in air quality models has been presented.

The parameterization has been tested against LES results for shear convective cases. Results are encouraging, but more investigation is needed.

The parameterization was implemented in a mesoscale model and tested over Athens. Results show that the variance can reach a significative percentage of the mean concentration, in particular during morning hours.

Future work

Improve the scheme for the cases analyzed, and test it for other atmospheric conditions (stable cases, free convection)

How to account for emissions variability ? Can we model in this way the subgrid variability of emissions?

If we introduce spatial hetereogenity in emissions, the space average is not equal anymore to the others averages. Is this a problem?

Thank you