Energy & Resources Research Institute (ERRI)

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EVALUATION OF A LAGRANGIAN MODEL FOR PREDICTING CONCENTRATION FLUCTUATIONS IN URBAN AREAS

Nick Dixon and Alison Tomlin

Motivation

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- Predicting pollution dispersion and exposure within urban areas requires representation of building structures which significantly affect air flows.
- 3-D effects such as vertical fluxes at intersections, corner vortices, flow convergence etc. all seen in field campaigns.
- Models used within air quality management context therefore need to represent such effects.
- Computational Fluid Dynamics (CFD) models are capable of representing the types of structures relevant to urban geometries.
- Non-steady models e.g. Large Eddy Simulations (LES) also capable of representing detailed structure of turbulent eddies at larger scales

  useful for predicting concentration fluctuations which affect exposure.
- LES computationally expensive → research rather than operational tool.
- Can steady Reynolds averaged models be used to model 3-D flow structures and concentration fluctuations adequately?

Concentration fluctuations

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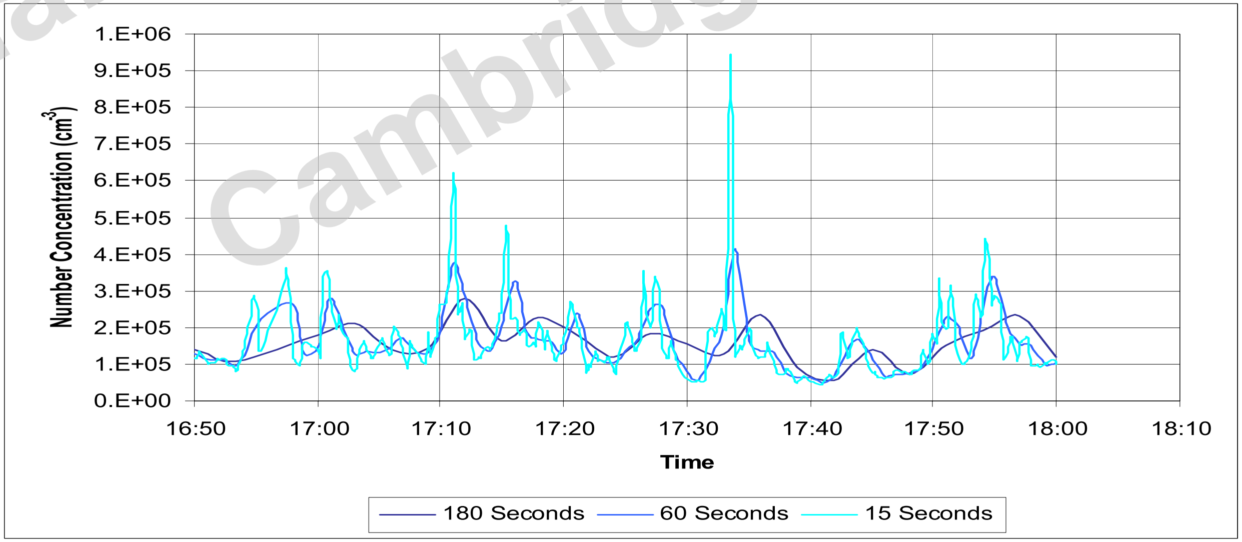
- Modelling concentration fluctuations important for several reasons:

    Exposure may be affected by short term peaks as well as longer term dosage.

    Fluctuations important for modelling interaction between turbulent mixing and chemical reactions e.g. prediction of secondary pollutants.



Model Choice

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- Motivation: to develop a practical model for predicting fluctuation intensities in urban areas that is far less computationally expensive than eddy-resolving models like LES.
- Requires an accurate description of the in-street flow as well as a dispersion model that can account for the widespread inhomogeneities.
- Here we use a microscale, *k*-ε CFD model to predict the flow between buildings and then model concentration fluctuations by combining a 1-particle Lagrangian Stochastic model with mixing using the interaction by exchange with mean (IEM) mechanism.
- Model tested against wind tunnel data:

  i) plume in open terrain i.e. a simple case without buildings;

  ii) concentration fluctuations from a line source in a street canyon.

Lagrangian Model

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- 1-particle model used to track fluid particles through the domain.
- Concentration probability density function evolves using a mixing model.
- Particles initially spread randomly throughout the domain with velocities randomly selected from Gaussian distribution about mean.
- Concentration assigned to those passing through source.
- Particle velocities and position evolve using Lagrangian Stochastic (LS) model of Thompson (1987) taking account of flow inhomogeneities.
- Concentration of particles evolves through the IEM mixing scheme:

$$\frac{dC_p}{dt} = -\frac{1}{t_m}(C_p - \langle C \rangle)$$

- C_p - concentration of particle, $\langle C \rangle$ - mean concentration, t_m - mixing timescale = $\alpha k/\varepsilon$, where α is a tuneable constant.
- Particles reflected off virtual reflection level z_{rfl} near solid boundaries with no loss of concentration or momentum.

i) Open Terrain

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- Comparison against wind tunnel study of dispersion from an elevated point source by Fackrell and Robins (1982).
- Flow fields in model derived from the mean flow and turbulent field profiles given in **FR**.
- Separate measurements of normal Reynolds stresses σ_u^2, σ_v^2 and σ_w^2 allowed inclusion of strong anisotropy of flow near the surface.
- Optimum model set-up found with Gaussian source distribution of σ_0 = 34mm (cf. experimental diameter of 8.5mm), c_0 = 5 and α = 0.75.
- Studies also carried out to test sensitivity to model parameters.
- 100,000 particle trajectories tracked for 100s using a timestep of 0.2s.
- Model grid used to segregate particles for mixing had gridspacing of 0.4m, 0.08m and 0.04m in the x, y and z directions respectively.

Normalised Mean Concentrations

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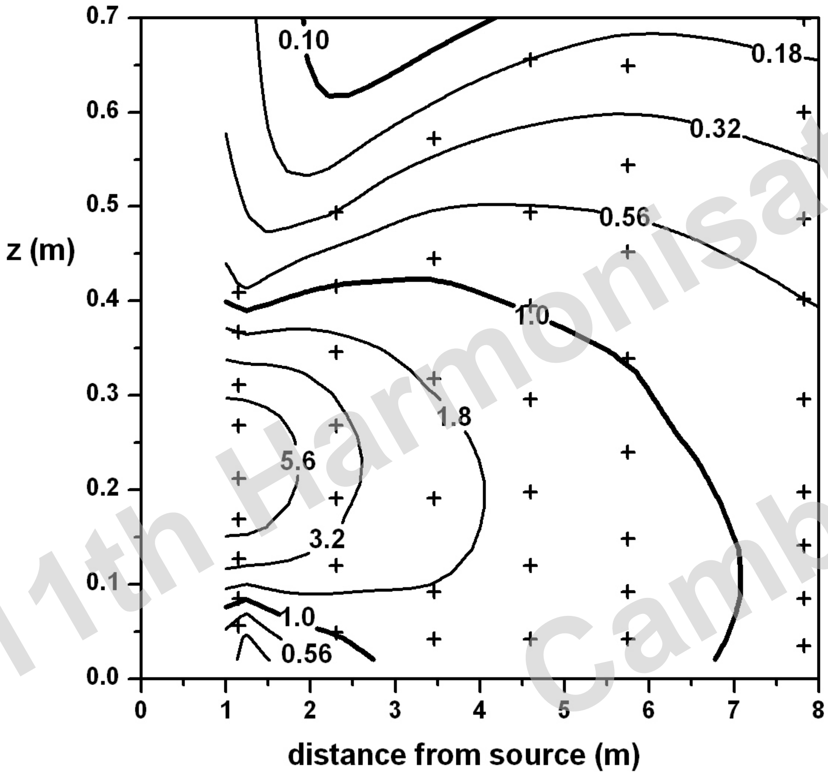
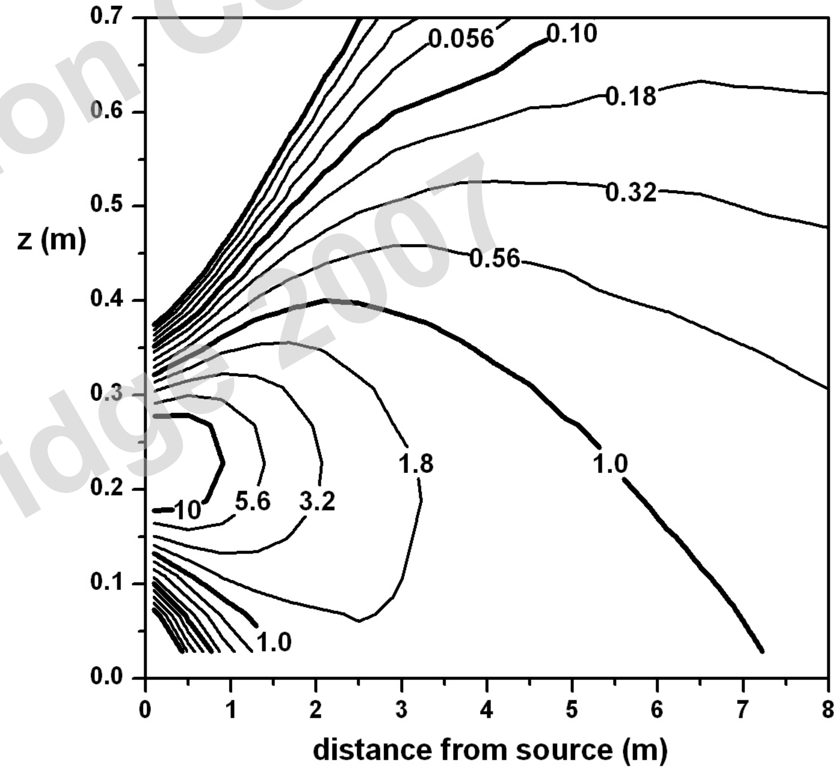


Wind tunnel experiment



Model simulation

Discussion

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- Model concentrations lower in top half of domain than measurements.
- Model plume reaches surface slightly nearer source than in experiment.
- Suggests that model underestimates vertical flux of tracer above the source level and overestimates the flux near the surface:

  model does not fully capture change in turbulence structure between the near surface region and at higher levels in the domain.
- Larger eddies at higher levels are transporting more tracer away vertically in experiment than model.
- Near surface, model is transporting too much tracer towards the surface and so possibly overestimating the size of eddies there.

Fluctuation Intensities $\sigma_c/\langle C\rangle$

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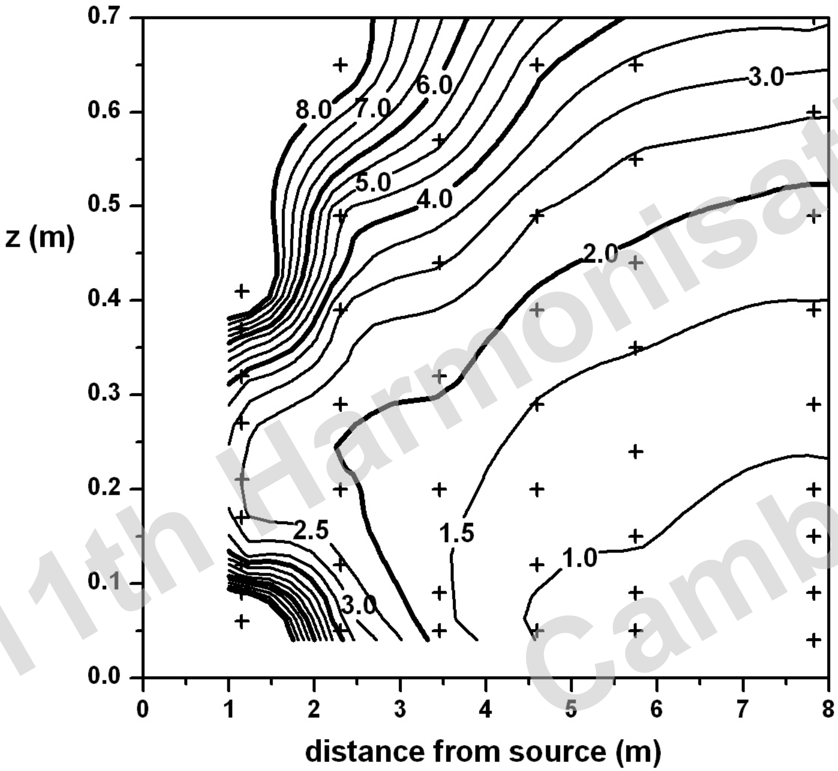
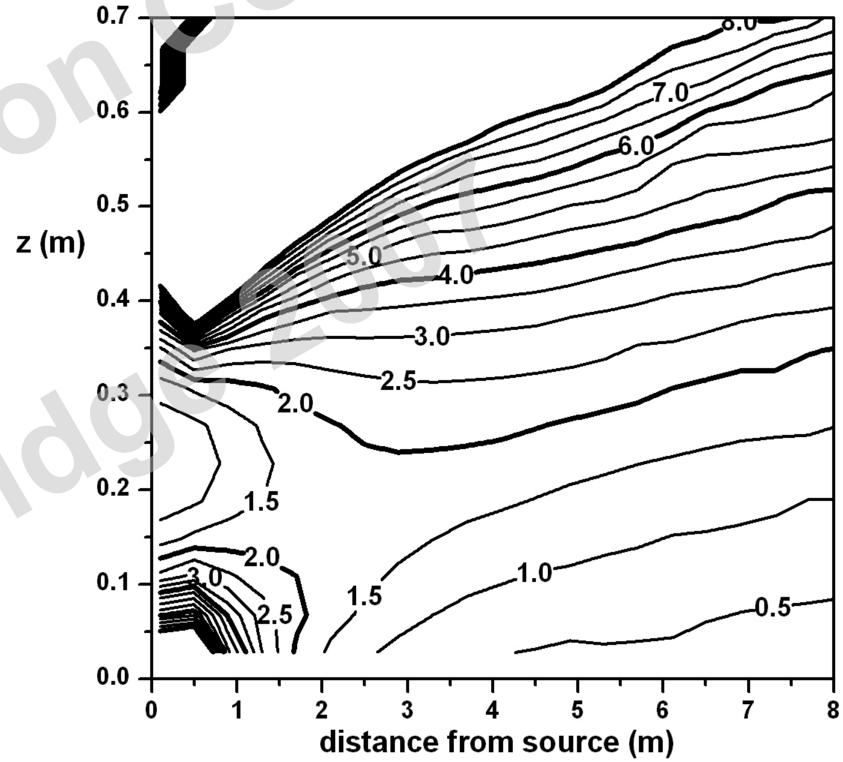


Wind tunnel experiment



Model simulation

Discussion

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- Model does reasonable job of predicting level of fluctuations.
- Model intensities higher than experimental ones in top of domain – partly due to lower mean concentration – partly due to lower mixing in model.
- Larger eddies at top of domain again appear to be important in wind tunnel.
- Model reproduces the low intensities at the surface well, although these low intensities are not penetrating quite as far into the flow as in the experiment.
- A basic mixing model with simple reflection can capture the development of the fluctuation intensities at the surface reasonably well.

Overall – Decision to use simple mixing model with general description of mixing time-scale has still allowed the main features to be captured.

Sensitivity Study

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- Crude sensitivity analysis performed to assess impact of changing input parameters.
- Geometric variance of outputs used as error measure.

Model run	α	σ_0 (mm)	C_0	Concentration error	Intensity error
Base	0.75	34	5	1.0950	1.3521
A1	0.25	34	5	1.0685	4.1839
A2	0.5	34	5	1.0785	1.6111
A3	1.0	34	5	1.1014	1.3751
B1	0.75	8.5	5	1.1092	6.0272
B2	0.75	17	5	1.0956	1.8522
B3	0.75	51	5	1.1192	1.7301
C1	0.75	34	3	1.1299	1.3440
C2	0.75	34	10	1.0761	1.3890
D1	No mixing	34	5	1.1197	3.6364

ii) Street Canyon Study

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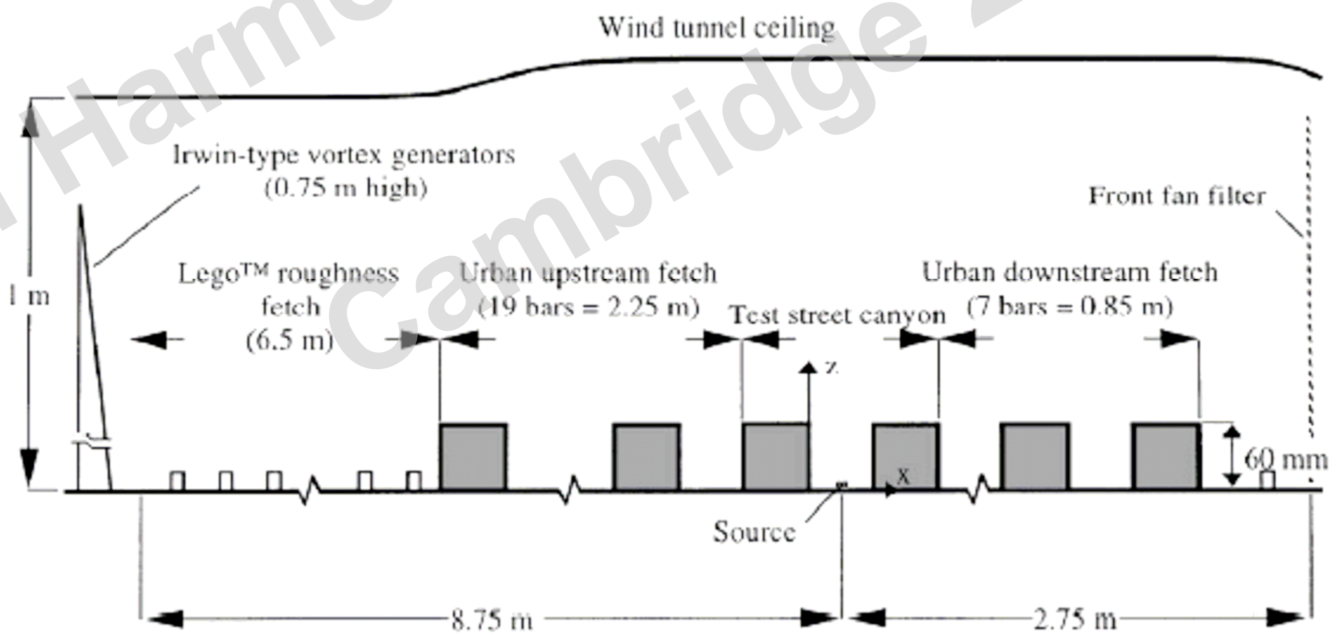
- Model now tested against wind tunnel data of Pavageau and Schatzmann (1999) - concentration fluctuations in an idealised street canyon.
- Continuous line source set up in 19th canyon downwind to simulate the pollution released from a steady stream of traffic.
- Measurements made at 70 points in and above test canyon using a high frequency, flame ionisation detector.



Model Setup

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- Flow field in wind tunnel experiment was modelled using the k-ε, CFD model MISKAM Version 4.21 (Eichhorn 1996).
- Since MISKAM designed for full-scale simulations, wind tunnel modelled at a scale one hundred times that in the real wind tunnel.
- Building height H = 6 m, inflow roughness = 17 cm, building and surface roughness = 5 cm.
- Inflow velocity profile logarithmic and $U_{ref} = 3\ ms^{-1}$ imposed at 3H.
- A top-hat distribution used for source and placed from the reflection level (z_{rfl} = 0.0333H) to a height of 0.0667H.
- Q = source strength.
- α = 0.75, as previously for consistency.
- 20,000 particles tracked through domain over 5,000 seconds with a timestep of 0.1 s.

Normalised Mean Concentrations

$\langle C \rangle U_{ref}HL/Q$

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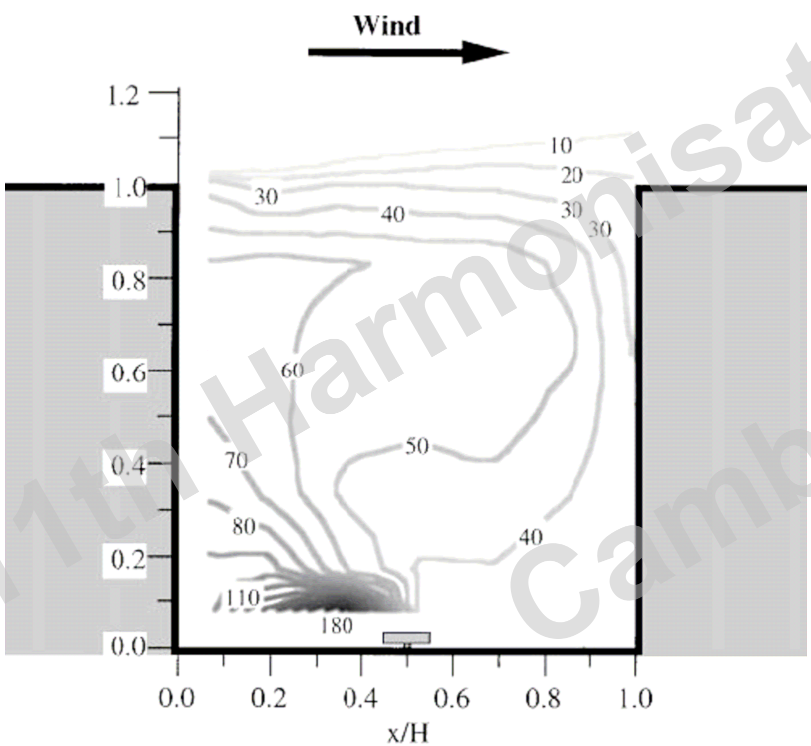
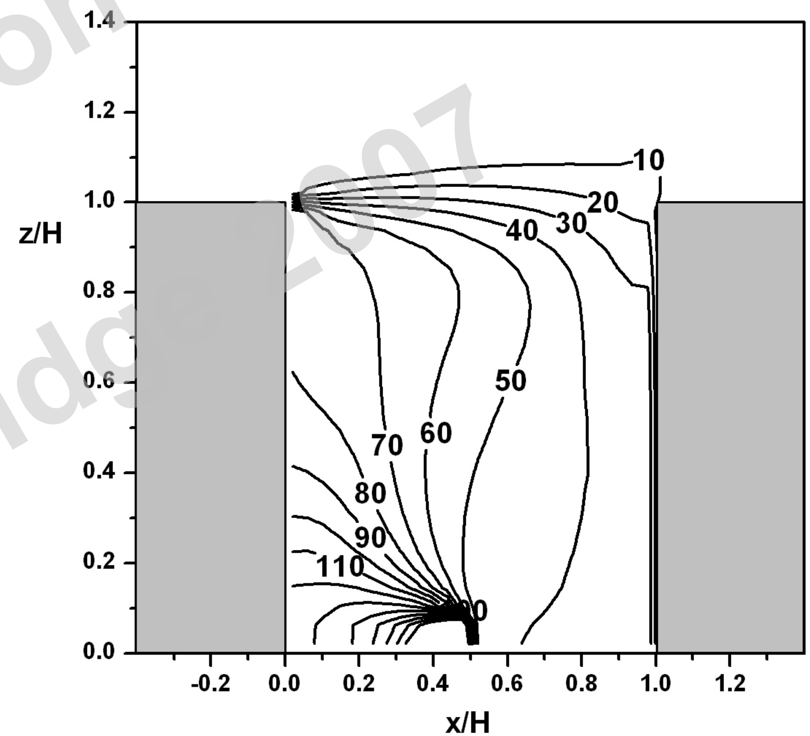


Wind tunnel experiment



Model simulation

Fluctuation Intensities $\sigma_c/\langle C\rangle$

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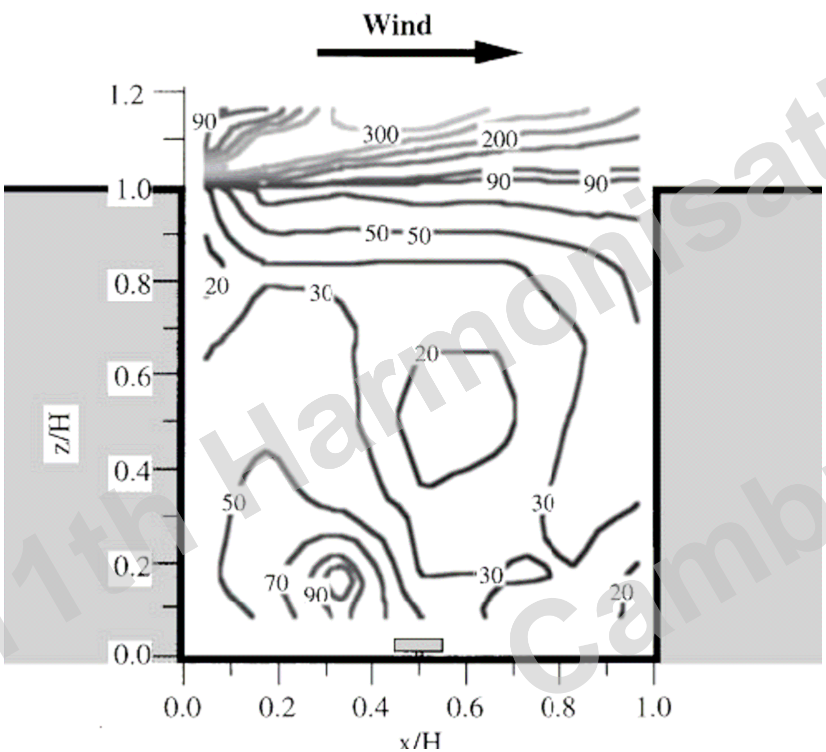
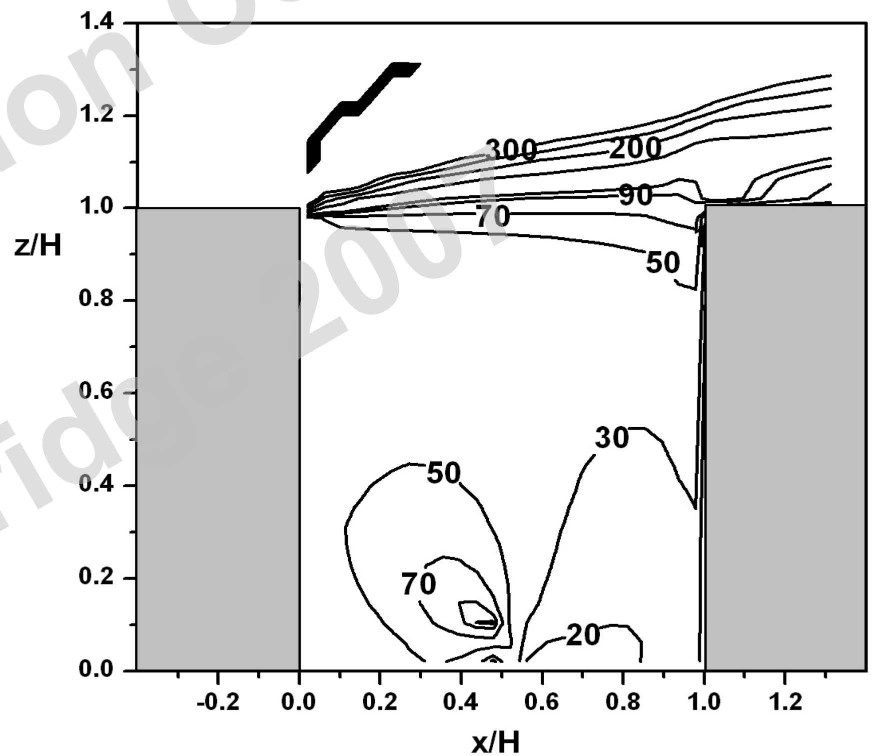


Wind tunnel experiment



Model simulation

Ratio of 99th Percentile values to <C>

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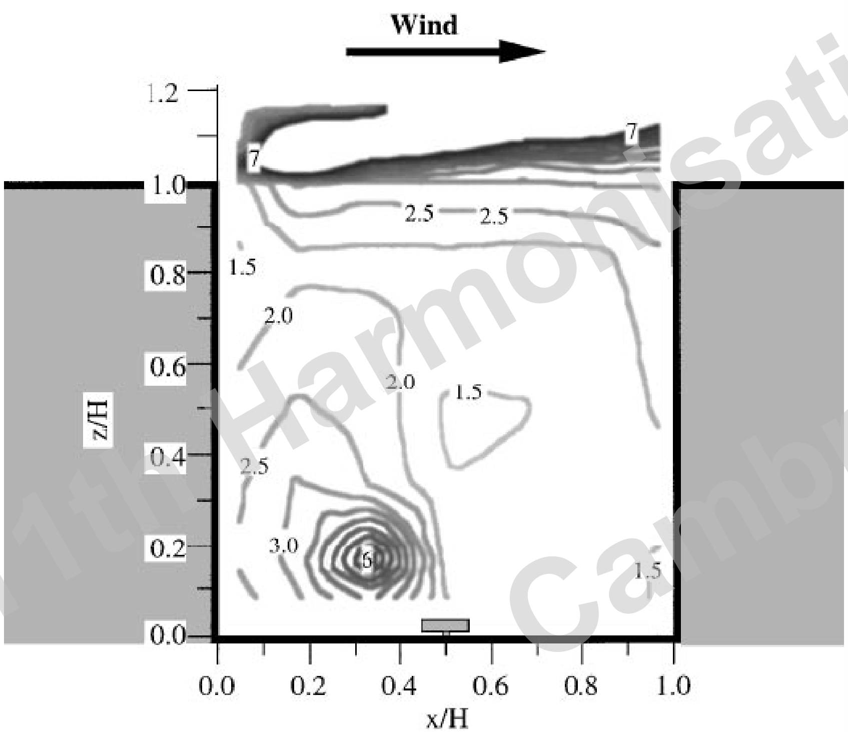
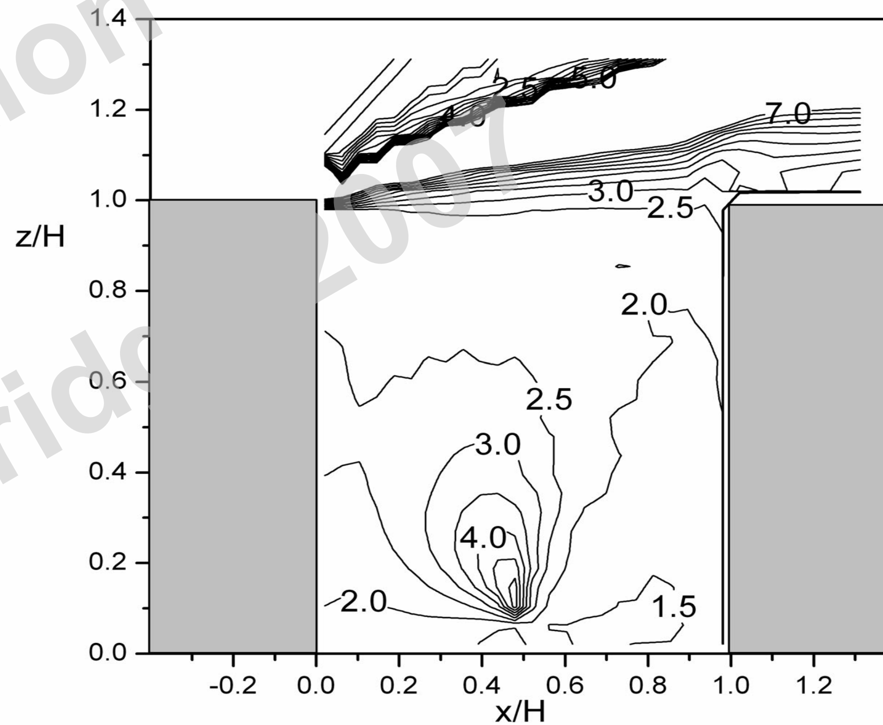
Indicates location of high peak values relative to mean



Wind tunnel experiment



Model simulation

Discussion

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- Model captures well regions of high mean concentration on the leeward canyon side i.e. downwind of source.
- Also captures regions of high fluctuation intensities on leeward canyon side and towards the top of canyon where air entrained from above within the sheer layer.
- Air entrainment extends slightly further down windward wall in experiment than in model leading to slightly lower fluctuation intensities there in the model compared to experiment.
- The modelled 99th percentile ratios agree well with experimental data:

  higher values on the leeward side of the canyon

  maximum of 5 at the bottom of canyon compared to 6 in the wind tunnel

  similar values for the minima of 1.5 in the bottom windward corner.
- Agreement for canyon better than for open terrain since confined canyon geometry reduces meandering. Simple description of mixing timescale therefore works well.

Conclusions

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- By choosing appropriate values for source size and mixing timescale coefficient, the practical LS model with simple IEM mixing scheme has reproduced the mean concentration and fluctuation intensity from the open terrain and the street canyon experiment reasonably well.
- The model inherits the limitations of its component parts:

  average representation of turbulence structures

  lack of ability to represent different eddy scales

  poor representation of very near field mixing
- These limitations are found to be less significant for the street canyon case due to the confined geometries.
- The ability of RANS/LS schemes to model fluctuations in real world scenarios has not been adequately tested. Requires further experimental data at wind tunnel and full scale.
- Simultaneous turbulence and concentration fluctuation measurements would help elucidate sources of discrepancy between model and experiment.
- Future work: evaluation of reactive flow model.