Street Scale Modelling of Nanoparticles Using a Simplified Approach and An Operational Model

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7th Int. Conf. on Air Quality – Science & Application, Istanbul, 24-27 March 09
POINTS FOR DISCUSSION

☐ BACKGROUND

☐ MEASUREMENTS
  ▪ Application of a DMS500 for street canyon measurements

☐ MODELLING
  ▪ Formulation of a simple dispersion model (a modified Box model)
  ▪ CFD (FLUENT) simulations, and OSPM
  ▪ Comparison of measurements with CFD, OSPM and Box models

☐ SUMMARY AND CONCLUSIONS

☐ ACKNOWLEDGEMENTS
BACKGROUND

- Stringent emissions: particle mass emissions (↓), number (↑)

- Current regulations address atmospheric particulate matter as PM$_{10}$, PM$_{2.5}$ mass concentration; not particle number concentration (PNC)

- Ultrafine particles (< 100 nm); main component of ambient particles by number, produced mainly by vehicles, contribute most to PNC but little to PMC; these are more toxic than coarse particles per unit mass (Brugge et al., 2007)

- Progress hampered by lack of proven methods and instrumentation to measure PNCs

- **This work addresses:**
  - Application of a fast response DMS500, its suitability and best operating conditions for the measurements of PNDs in street canyons
  - To apply an operational (OSPM), a CFD (using FLUENT) and the modified Box model to one of our previously studied street canyon and to compare the model predictions with measured PNCs
  - To investigate the effect of different sizes of emission sources on the distribution of the mean PNCs in CFD simulations
  - To compare measured and modelled vertical PNC profiles
MEASUREMENTS

- **Measurements:**
  - Street canyon (Pembroke Street, Cambridge)

- **Instrument:** Differential Mobility Spectrometer (DMS500)
  - Response: 10 Hz, real time continuous (used 0.5 Hz)
  - Sampling flow rate: 8.0 lpm at 250 mb for 5-1000 nm
    - 2.5 lpm at 160 mb for 5-2738 nm

- **Movie:** [Diesel drive by](#) (Courtesy: Cambustion Ltd.)
Check the sensitivity level of the instrument

Identify the suitable operating conditions (mainly sampling frequency) of the instrument which maximised its utility

Smaller (1 Hz or lower) rather than maximal (10 Hz) sampling frequencies found appropriate, unless experiments relied critically upon fast response data

Suggested sampling frequencies used in later experiments (Kumar et al., 2008a-c, 2009a-c):

- measured PNDs well above instrument’s noise level
- reduced size of data files to manageable proportions

Sensitivity of the DMS500. Both typical roadside and background PNDs were measured at the fastest (10 Hz) sampling frequency.

See Kumar et al. (2009d) for details
**MEASUREMENTS**

**STREET CANYON**

- **Pseudo-simultaneous measurements**
  - Measurements at four heights \( z/H = 0.09, 0.19, 0.4 \) and 0.64
  - Lengths of sampling tubes: 5.17, 5.55, 8.9 and 13.4 m
  - Switching time: 60 s; Sampling frequency: 0.5 Hz
  - Size range: 5–2738 nm (range considered here 10-300 nm)
  - Sampling tunes i.d.: 7.85 mm
  - Cross-canyon winds (NW)

**Pembroke Street, Cambridge**

See Kumar et al. (2008b) for details
THE MODIFIED BOX MODEL

\[ C = \sum_{x=1}^{n} \frac{E_{x,i-j}T_x}{b_1 U_r W} \exp(-k_1 z) + C_b \]

when \( z = \max(z, h_0) \), \( U_r = \max(U_r, U_{r,crit}) \) and \( k_1 = 0.11 \text{ m}^{-1} \)

- \( C \) and \( C_b \) are the predicted and background PNCs (# cm\(^{-3}\))
- \( U_r \) and \( U_{r,crit} \) are in cm s\(^{-1}\), \( k_1 \) is exponential decay coefficient in cm\(^{-1}\)
- \( b_1 = 1/4 \sigma_0 \sqrt{\pi} \) \( \sigma_0 = 11 \) dimensionless parameter (Rajaratnam, 1976)
- \( E_{x,i-j} \) (PNEF # veh\(^{-1}\)cm\(^{-1}\) in any particle size range of any vehicle class \( x \))
- \( T_x = \text{veh s}^{-1} \) of a certain class
- \( h_0 (= 2 \text{ m}) \) is assumed initial dispersion height close to road level
- \( W \) (width in cm); \( z \) (vertical height in cm above road level)

Empirical constant for exchange velocity = 1% of \( U_r \)
(Bentham and Britter, 2005)
**MODELLING**

**CFD SIMULATIONS – COMPUTATIONAL DOMAIN**

- **CFD code**: FLUENT
- **Standard k-ε model**
- **2D domain; Ht. = 6H**
- **Inlet $U_r$ profile**: constant
- **53824 grid cells, expansion factor 1.10 near walls**
- **TKE profile $k = lU_{in}^2$ ($l = 0.1$)**
- **Turbulent dissipation profile**

\[
\varepsilon(z) = C_\mu^{0.75} k^{1.5} \kappa^{-1} z^{-1}
\]

with $C_\mu = 0.09$ and $\kappa = 0.40$

- **Constant discharge emission sources of 4 various sizes used**
- **24 set of simulations were made for 24 h selected data**
- **$\rho$ and $T_a$ changed every hour**
Shows the advection of PNCs from the sources to the leeward side of the canyon; selection of the source size is critical to determine PNC distributions.

In case of smallest source $S_a$, largest concentrations in the bottom corner of the canyon and the region near to the street wall up to $\approx 0.50$ m in the leeward side.

In other cases with larger source area, particles first accumulate on the leeward side corner of the source, where concentrations are largest, and then advected upwards in the leeward side by the canyon vortex.
Important aspects *shape* and *magnitude*; General trend – conc. (↓) with (↑) height

Box and OSPM assume constant PNCs up to ≈ 2 m and then follows general trend, but CFD profiles does not show this decrease, suggesting that it does not predict enough mixing in region of leeward wall

Measurements showed positive concentration gradient; reasons identified were: dry deposition, recirculating vortex, trailing vortices (Kumar et al., 2008b)

This gradient was not shown by Box and OSPM, but reproduced by CFD suggesting that *size of source which is closest to vehicle dimensions* may be a better representation for setting up a source in CFD simulations

See Kumar et al. (2009c) for details.
The measured PNCs at different heights compared well within a factor of 2-3 to those modelled using OSPM, Box model and CFD simulations, suggesting that if model inputs are given carefully, even the simplified approach can predict the concentrations as well as more complex models.

See Kumar et al. (2009c) for details
SUMMARY AND CONCLUSIONS

- An advanced particle spectrometer was successfully applied to measure PNDs and PNCs in street canyons and was found to be quite useful when fast response nature of an instrument is essential.

- Model comparison suggested that if model inputs are given carefully, a simplified approach can predict the PNCs to accuracy comparable with that obtained using more complex models.

- Study for the selection of the source size in CFD simulations showed that a source size scaling the vehicle dimension, not the size of the exhaust pipe, better represented the measured PNC profiles.

- The PNC differences were largest between idealised (CFD and Box) and operational (OSPM) models at upper sampling heights; these were attributed to weaker exchange of clean air between street and roof-above in the upper part of canyon in case of idealised models.
RELATED ARTICLES FOR DETIALED INFORMATION

**JOURNAL**


**CONFERENCE**

- **Kumar, P.,** Fennell, P., Britter, R., 2007c. The measurement of fine particles for the study of their dispersion and of street-scale air quality. *UK Atmospheric Aerosol Network (UKAAN) Workshop, University of Reading, Berkshire (UK)*, 6-7 June 2007.
ACKNOWLEDGEMENTS

- World Meteorological Organisation – bursary award

- Cambridge Nehru Scholarship and ORS Award – PhD funding

- Dr. Paul Fennell (Imperial College, London) – helping in experiments
THANK YOU

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Considerably larger PNC variations in leeward side, but modest on windward side (≈ 0.50 m), while changing size of the source.

PNCs increases from road level to a certain height; the height at which this maximum occurs could be related to the height of various sources used.

The largest sources shows similar profile suggesting that effect of source size is minimal after a certain cross-sectional area.

Unlike leeward side, concentration profiles in windward side shows similar trend with consistent increase in concentrations with increasing distance from windward wall.

See Kumar et al. (2009c) for details.