MODELLING THE DISPERSION OF NANOPARTICLES IN STREET CANYONS

PRASHANT KUMAR* & ALAN ROBINS

UNIVERSITY OF SURREY

HARMO 13: PARIS, FRANCE 1–4 JUNE 2010

OUTLINE

- BACKGROUND

- MEASUREMENTS
  - Application of a DMS500 for street canyon measurements

- MODELLING
  - Effect of wind speed and direction on the various size ranges of nanoparticles in street canyons (i.e. testing of inverse wind speed law; cut–off wind speed)?
  - Role of particle dynamics in street scale modelling
  - Formulation of a simple dispersion model (a modified Box model)
  - Comparison of measured and modelled concentrations of nanoparticles using OSPM, CFD (Fluent) and the modified Box model
  - Uncertainties in modelling due to particle number emission factors

- SUMMARY AND CONCLUSIONS

- ACKNOWLEDGEMENTS

BACKGROUND

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

- 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

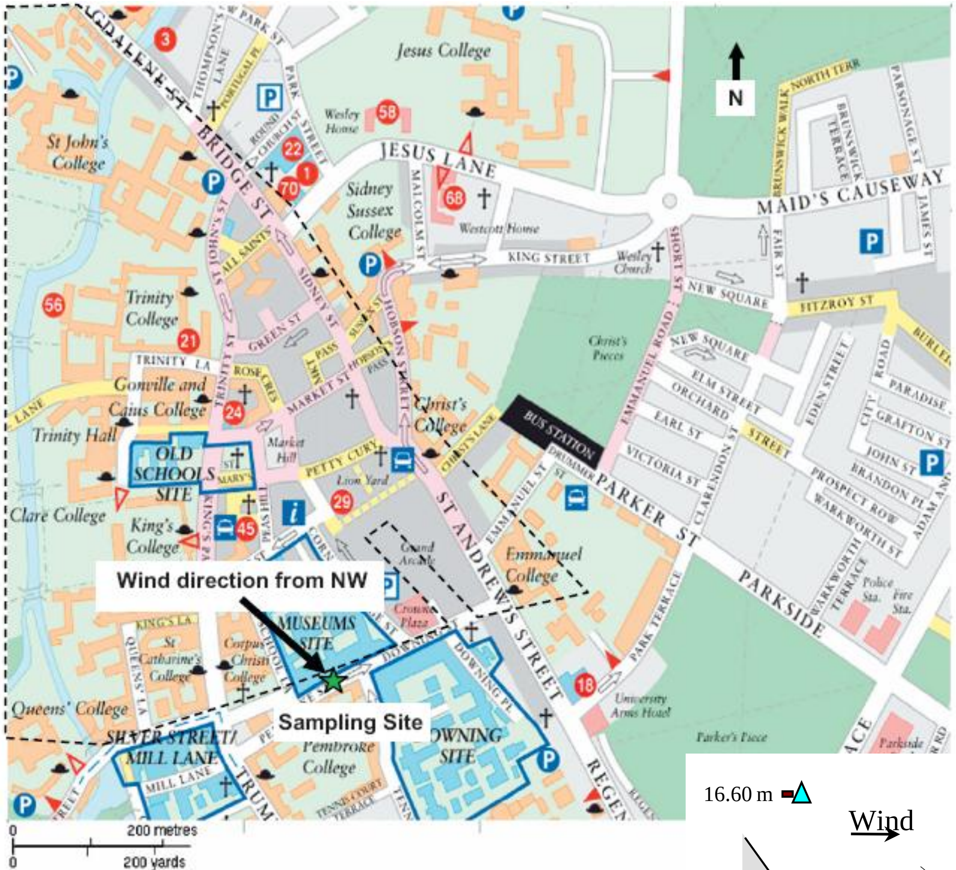
- Current regulations address atmospheric particulate matter as PM_{10}, $PM_{2.5}$ mass concentration; not particle number concentration (PNC)

- Recent inclusion of in vehicle emission standards Euro–5 and Euro–6 on a *particle number* basis – ambient air quality standards for nanoparticles also likely

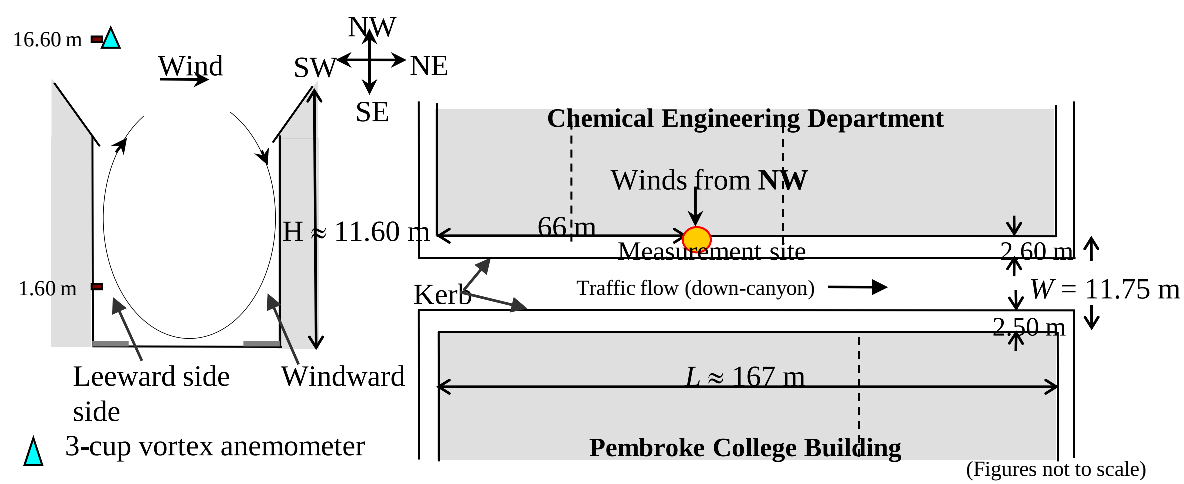
- Progress hampered by
  - lack of standard instruments for measurements,
  - limited understanding of nanoparticles dispersion, and
  - scientifically validated modelling tools

- **Measurement Campaigns:**
  - Street canyon (Pembroke Street, Cambridge)
- **Instrument:** Differential Mobility Spectrometer (DMS500)
  - Response: 10 Hz, real time continuous
  - 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 Instruments)

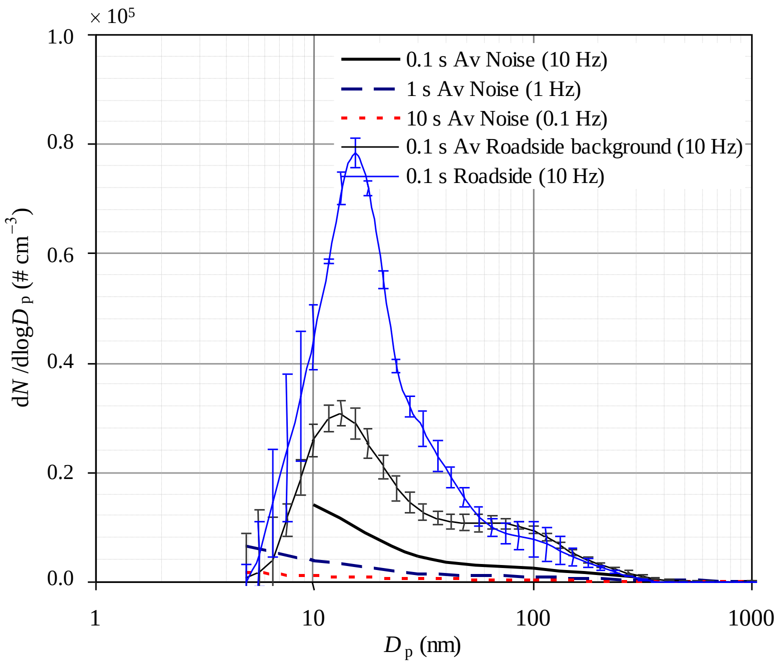
SAMPLING SITE



Site: Pembroke Street, Cambridge, UK



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



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

- 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–d, 2009a-c):
  - measured PNDs well above instrument's noise level
  - reduced size of data files to manageable proportions

EFFECT OF WIND DIRECTIONS & SPEED ON $N_{10\text{-}30}$ and $N_{30\text{-}300}$

- Measurements taken for 17 days continuously; sampling rate 1 Hz
- Range considered: $N_{10\text{-}30}$ (nucleation) and $N_{30\text{-}300}$ (accumulation)
- Measurements at 1.6 m with intention that effect of TPT's can be observed
- Objective was to test inverse-wind speed law on $N_{10\text{-}30}$ and $N_{30\text{-}300}$; ***important information for nanoparticle dispersion models***
- $U_{r,crit}$ is critical cut-off wind speed which divides zone of traffic-dependent and wind-dependent concentrations
  - $U_{r,crit}$ is generally considered as ≈ 1.2 m s^{-1} for gaseous pollutants (DePaul and Sheih, 1986).
  - What about $U_{r,crit}$ for $N_{10\text{-}30}$, $N_{30\text{-}300}$ and overall $N_{10\text{-}300}$ during various wind directions and speed?

- Two limiting cases for PNCs dilution $N_{i\text{-}j} = aT^m U_r^{-n} + C_{b,i\text{-}j}$
  - Traffic dependent PNCs case (during smaller U_r; $n=0$ & $m=1$)
  - Wind dependent PNCs case (during larger U_r; $n=1$ & $m=1$)

- **A model with two distinct regimes**, reflecting the role of both ***TPT*** and ***WPT***, was proposed and applied to the measured data:

$$\frac{N_{i-j}}{T^m} = \left(\frac{N_{i-j}}{T^m}\right)_{crit}$$

For $U_r \ll U_{r,crit}$ ($n = 0$; $m = 1$)

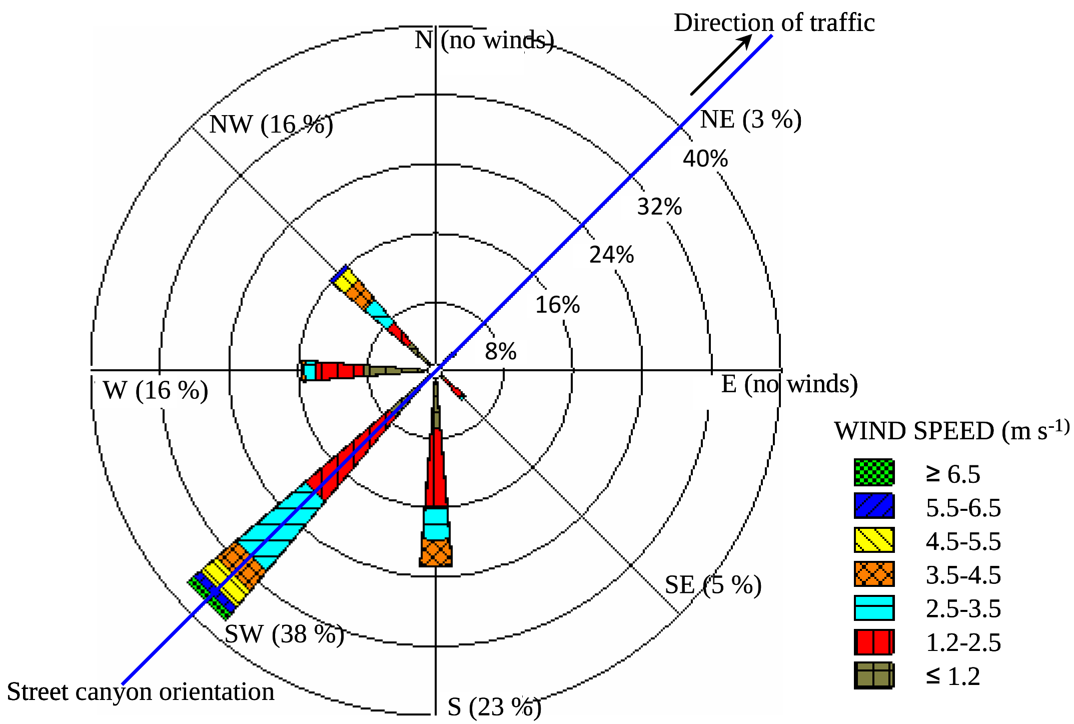
Traffic dependent regime: Normalised PNCs are independent of U_r up to $U_{r,crit}$

$$\frac{N_{i-j}}{T^m} = \left(\frac{N_{i-j}}{T^m}\right)_{crit} U_{r,crit} U_r^{-n}$$

For $U_r \gg U_{r,crit}$ ($n = 1$; $m = 1$)

U_r dependent regime: Norm PNCs are inversely dependent of U_r after $U_{r,crit}$

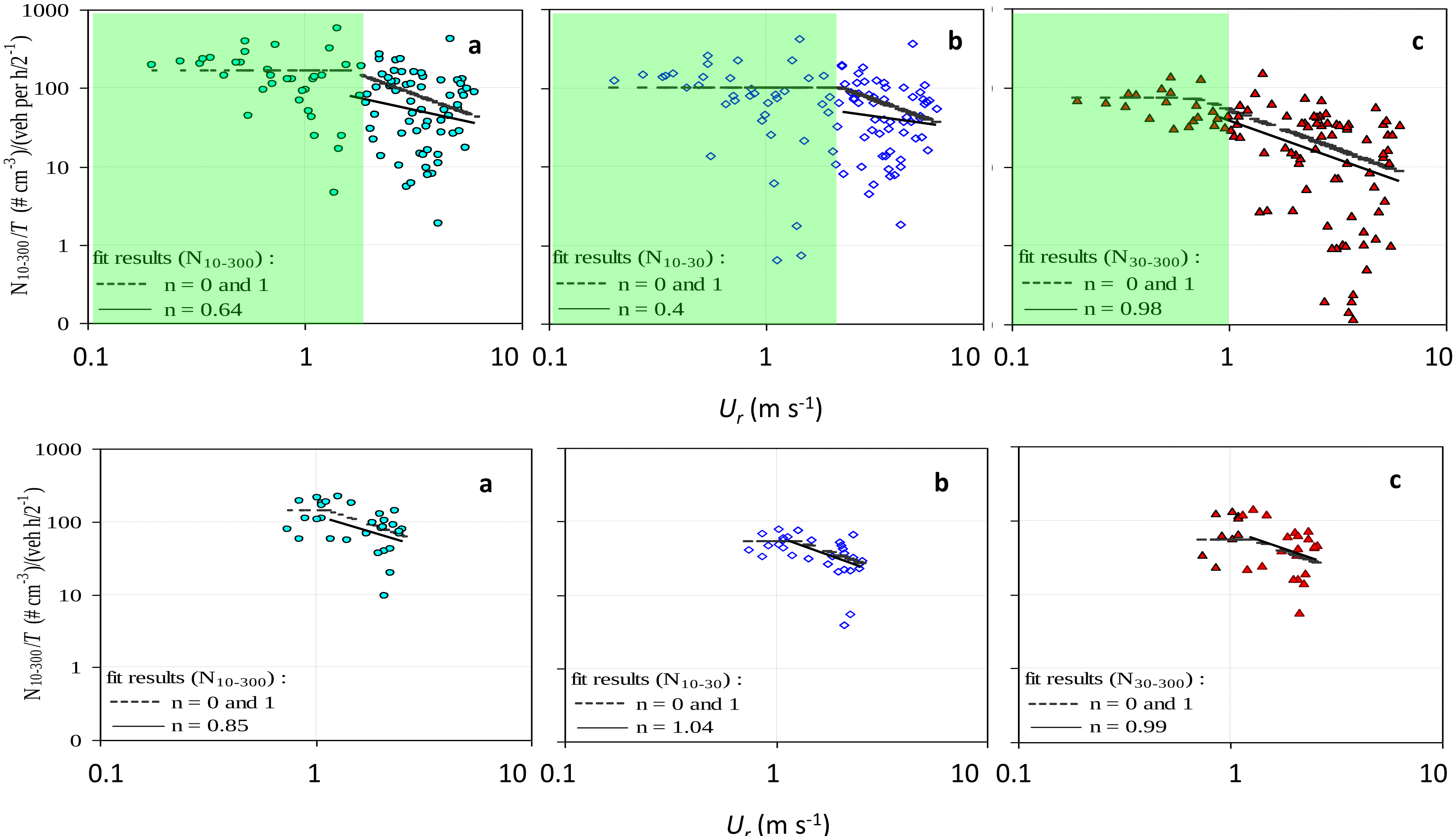
- Wind directions during the measurements were:
  - Cross Canyon (NW and SE)
  - Along canyon (SW and NE)
  - Period covered smaller and larger U_r's



EFECT OF WIND DIRECTIONS & SPEED ON N_{10-30} and N_{30-300}

NW

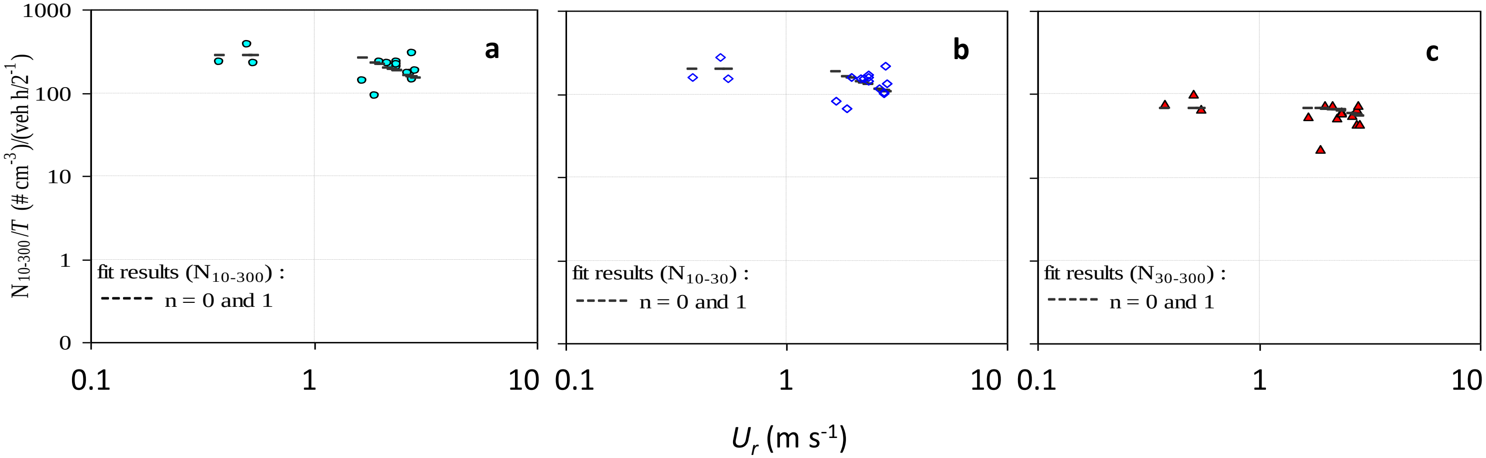
SE



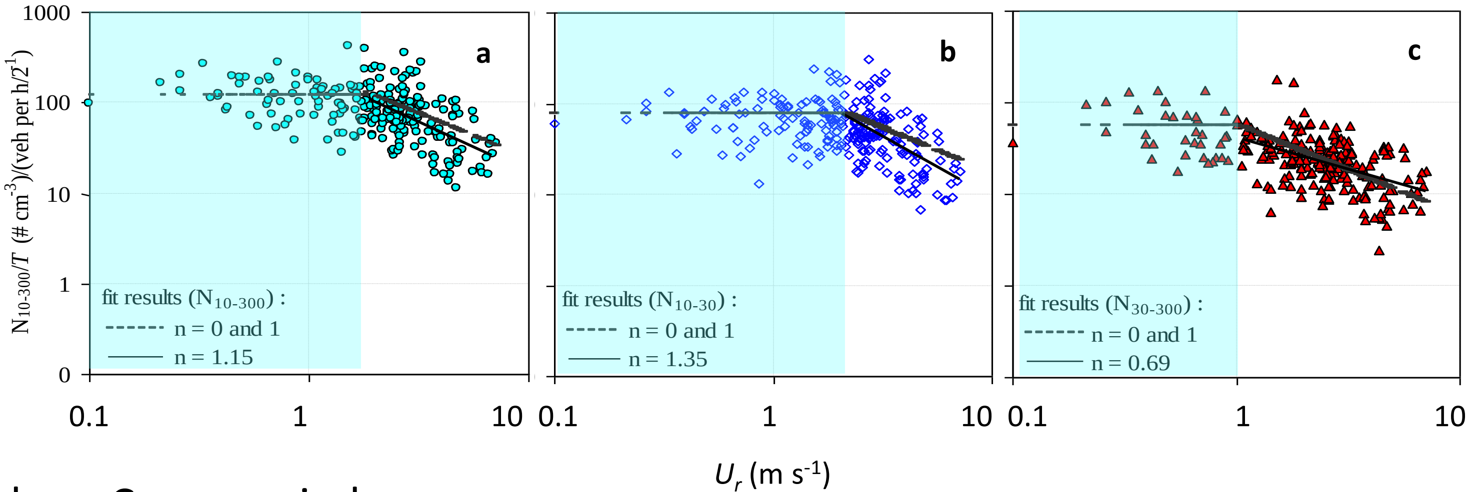
- Norm PNCs against U_r (logarithmic plots) for **cross-canyon wind direction**
  - Different best-fit model tried; proposed model fitted data best which split data into wind-independent (n=0) and wind-dependent (n=1) regions.
  - Minimising the diff. between model and experimental results yielded $U_{r,crit}$

EFECT OF WIND DIRECTIONS & SPEED ON $N_{10\text{-}30}$ and $N_{30\text{-}300}$

NE

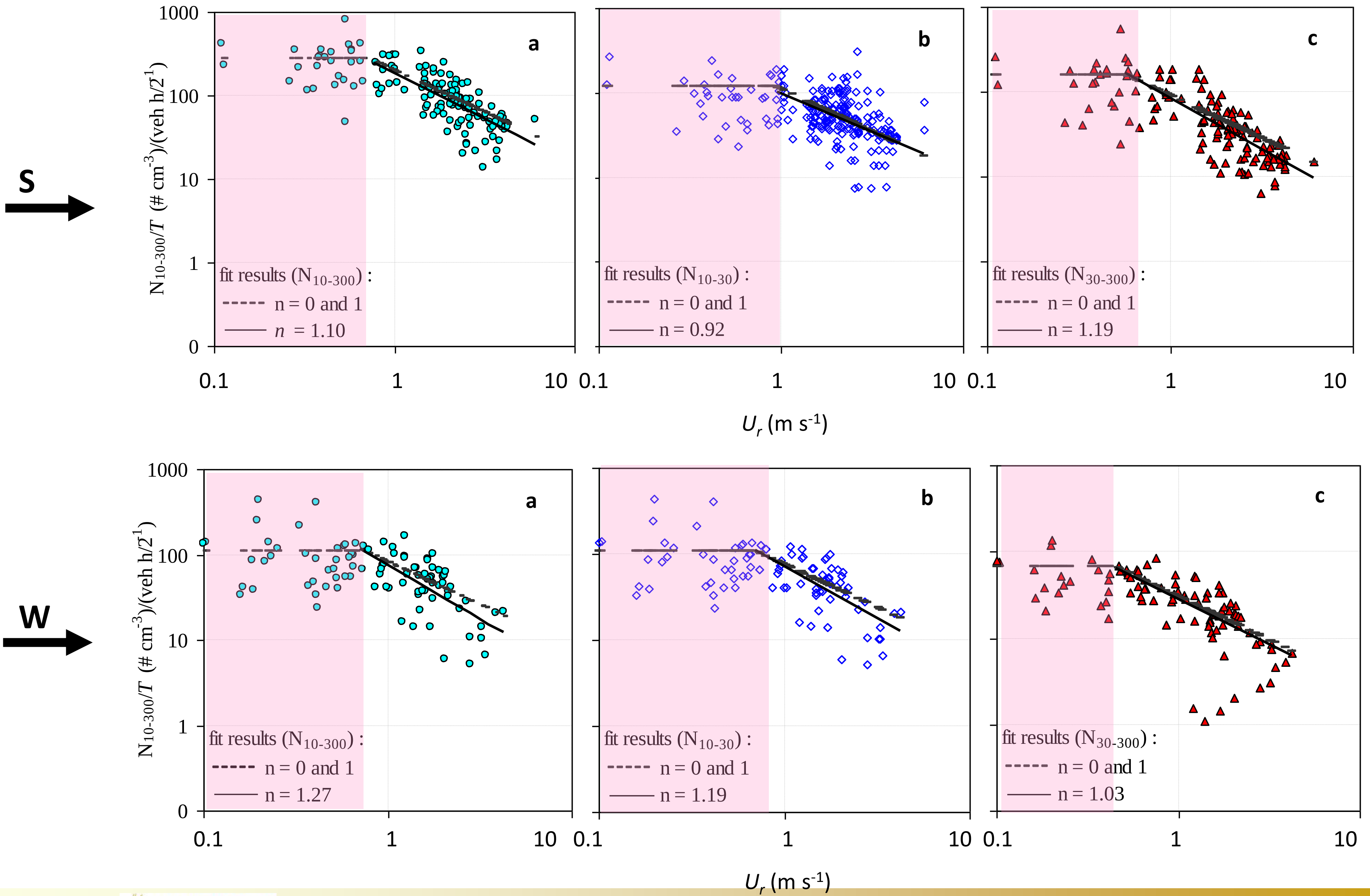


SE



- Along-Canyon winds
  - Till $U_{r,crit}$- dilution independent of U_r; here TPT governs dilution
  - After $U_{r,crit}$ - dilution independent of T; here WPT governs dilution

EFECT OF WIND DIRECTIONS & SPEED ON N_{10-30} and N_{30-300}



- **The values of *n* for:**

  $N_{10-300} = 1.00 \pm 0.25$
  $N_{10-30} = 0.98 \pm 0.36$
  $N_{30-300} = 0.94 \pm 0.14$

Irrespective of wind directions, results are consistent with unity exponent (i.e. follow Inverse wind speed law) in wind-dependent PNC regions

- **The $U_{r,crit}$ for:**

  $N_{10-300} = 1.23 \pm 0.55\ \text{ms}^{-1}$
  $N_{10-30} = 1.47 \pm 0.72\ \text{ms}^{-1}$
  $N_{30-300} = 0.78 \pm 0.29\ \text{ms}^{-1}$

- Spanned often quoted 1.2 ms^{-1} for gaseous pollutants.

THE MODIFIED BOX MODEL

Constant for exchange velocity ≈ 1% of U_r

$$C = \left[\frac{4\sigma_0\sqrt{\pi}}{U_r{}^n W} \sum_{x=1}^{n} E_{x,i-j} T_x + C_b \right] \exp\left(-k_1 z\right)$$

Vertical Concentration profile

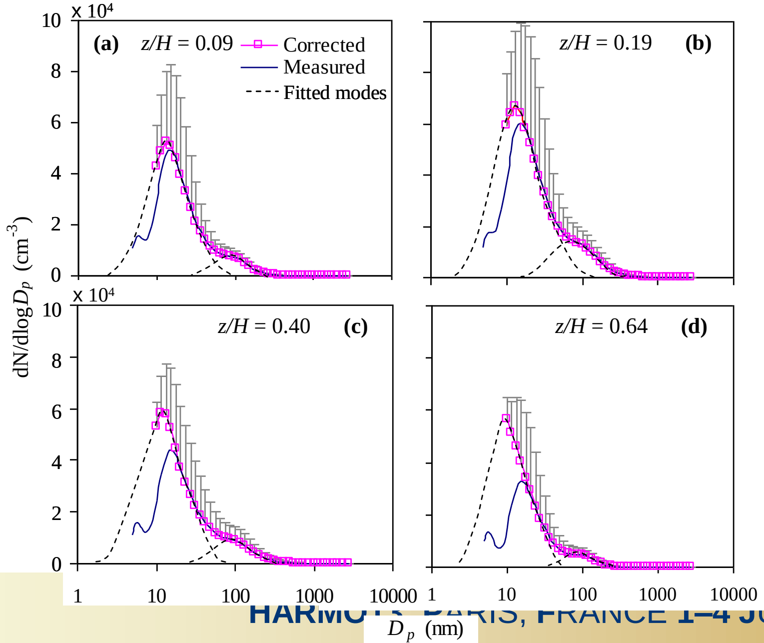
when z = max (z , h_0), U_r = max (U_r, $U_{r,crit}$) and $k_1 = 0.11\ m^{-1}$

For $U_r \ll U_{r,crit}$: $n = 0$ & $Ur \gg Ur,crit$: $n = 1$
$k_1 = 0$ when $z \leq 2$ m & For & $k_1 = 0.11\ m^{-1}$ when $z > 2$ m)

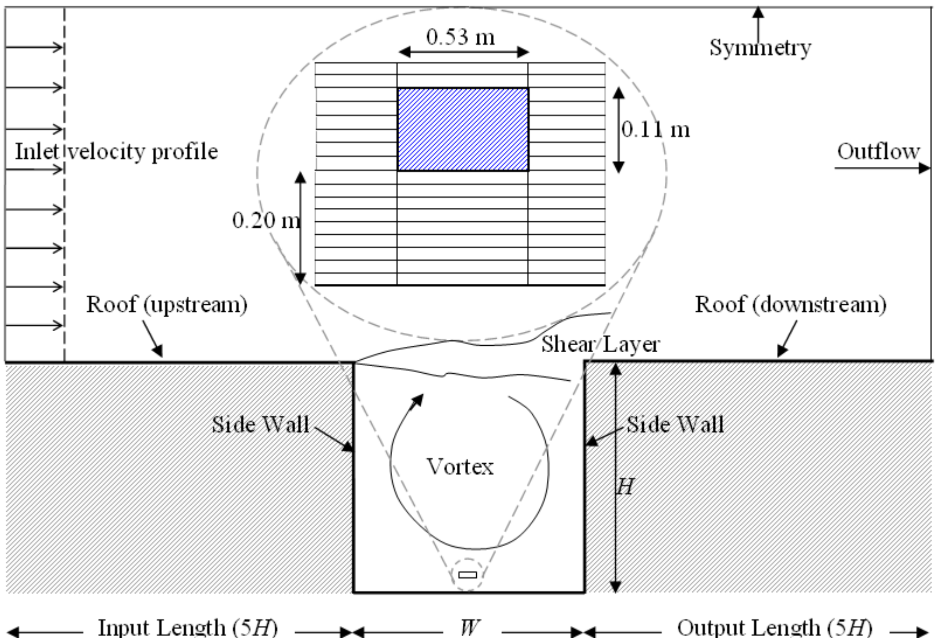
- C and C_b are the predicted and background PNCs (# cm^{-3})
- U_r and $U_{r,crit}$ are in cm s^{-1}, k_1 is exponential decay coefficient in cm^{-1}
- σ_0 = 11 dimensionless parameter (Rajaratnam, 1976)
- $E_{x,i\text{-}j}$ (PNEF # $veh^{-1}cm^{-1}$ in any particle size range of any vehicle class x)
- T_x = veh s^{-1} of a certain class
- h_0 (= 2 m) is assumed initial dispersion height close to road level
- W (width in cm); z (vertical height in cm above road level)

Ignored for street scale modelling because:

- Time scale analysis showed dilution was very quick (dilution ~40s; dry deposition on road surface (30–130 s) and street walls (600–2600 s); coagulation ~10^5 s and condensation ~10^4–10^5 s.
- Vehicle wake study (Kumar et al., 2009c) indicated that the competing influences of transformation processes was nearly over by the time particles reach from the tailpipe to the road side.
- Pseudo-simultaneous measurements at different heights found similarity in shape and the negligible shift in peak and geometric mean diameters of PNDs in both modes at each height, as shown below.



CFD SIMULATIONS

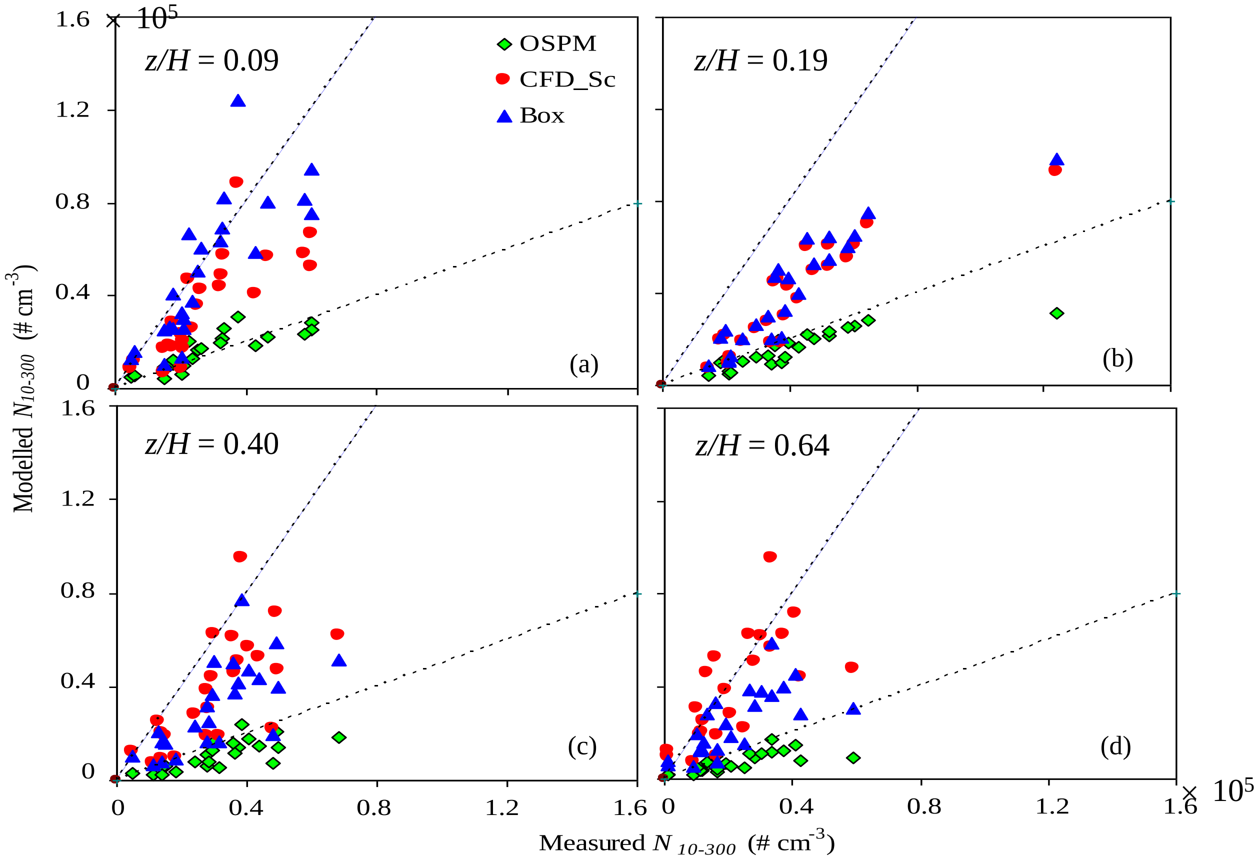


- CFD code: FLUENT
- Standard k-ε model
- 2D domain; Ht. = 6*H*
- Inlet U_r profile: constant
- 53824 grid cells, expansion factor 1.10 near walls
- TKE profile $k = IU_{in}^2$ ($I = 0.1$)
- Turbulent dissipation profile

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

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
- ρ and T_a changed every hour



- 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. (2009b) for details*

Summary & Conclusions

- An advanced particle spectrometer was successfully applied to measure PNDs and PNCs in street canyons and was found to be useful for fast response measurements.

- Nanoparticle number concentrations in each size range during all wind directions were better described a proposed two regime model (wind- and traffic-dependent mixing), rather than by simply assuming that the PNCs are inversely proportion to the wind speed.

  - In the traffic–dependent PNC region ($U_r << U_{r,crit}$), concentrations in each size range were approximately constant and independent of wind speed and direction.

  - In wind-dependent PNC region ($U_r >> U_{r,crit}$), concentrations were inversely proportional to wind speed, irrespective of any particle size range and wind direction – following a best-fit power law (or inverse wind speed law).

  - It is important to use the critical-cut off wind speed concept for nanoparticle dispersion models to avoid over-prediction of concentrations.

SUMMARY & CONCLUSIONS

- Particle dynamics at street-scale modelling can be neglected as competing influences of transformation processes seems to be over by the time particles are measured at road side.
  - However, it is important to consider it at above-rooftop and city scale modelling; not discussed here but details cane be seen in Kumar et al. (2009a).

- 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.
  - The particle number emission factor is one of the most important model input parameter which is not abundantly available for routine application.
  - This can result in large uncertainties (i.e. up to an order of magnitude), meaning that modelled results are likely to be affected by the similar degree irrespective of the accuracy of a model (not discussed here – see conference paper for details).

RELATED ARTICLES FOR DETIALED INFORMATION

- **Kumar, P.,** Robins, A., Vardoulakis, S., Britter, R., 2010. **A review of the characterstics of nanoparticles in the urban atmosphere and the prospects for developing regulatoy control.** *Atmospheric Environment (revised manuscript under review).*
- **Kumar, P.,** Fennell, P., Robins, A., 2010. **Comparsion of the behaviour of manufactured and other airborne nanoparticles and the consequences for prioritising research and regulation activities.** *Journal of Nanoparticle Research* 12, 1523-1530.
- **Kumar, P.,** Robins, A., Britter, R., 2009c. **Fast response measurements of the dispersion of nanoparticles in a vehicle wake and a street canyon.** *Atmospheric Environment* 43, 6110-6118.
- **Kumar, P.,** Garmory, A., Ketzel, M., Berkowicz, R., 2009b. **Comparative study of measured and modelled number concentration of nanoparticles in an urban street canyon.** *Atmospheric Environment* 43, 949-958.
- **Kumar, P.,** Fennell, P., Hayhurst, A., Britter, R., 2009a. **Street versus rooftop level concentrations of fine particles in a Cambridge Street Canyon.** *Boundary–Layer Meteorology* 131, 3-18.
- **Kumar, P.,** Fennell, P., Symonds, J., Britter, R., 2008d. **Treatment for the losses of ultrafine aerosol particles in long sampling tubes during ambient measurements.** *Atmospheric Environment* 42, 8831-8838.
- **Kumar, P.,** Fennell, P., Britter, R., 2008c. **Effect of wind direction and speed of the dispersion of nucleation and accumulation mode particles in an urban street canyon.** *Science of the Total Environment* 402, 82-94.
- **Kumar, P.,** Fennell, P., Britter, R., 2008b**. Pseudo-simultaneous measurements for the vertical variation of coarse, fine and ultrafine particles in an urban street canyon**. *Atmospheric Environment* 42, 4304-4319.
- **Kumar, P.,** Fennell, P., Britter, R., 2008a. **Measurements of the Particles in the 5-1000 nm range close to the road level in an urban street canyon.** *Science of the Total Environment* 390, 437-447.

- The Royal Society –travel grant

- Department of Civil, Chemical and Environmental Engineering, University of Surrey, UK –travel grant

- Prof. Rex Britter (*MIT, USA*), Dr. Paul Fennell (*Imperial College, London*), Dr. Matthias Ketzel (*NERI, Denmark*) and Dr. John Dennis (*Cambridge University, UK*) –helping in experiments, data analysis, discussions and publishing, and lending of the DMS500

THANK YOU

CONTACT

DR. PRASHANT KUMAR

Email: p.kumar@surrey.ac.uk

Webpage: http://www2.surrey.ac.uk/cce/people/prashant_kumar/

- **Why was $U_{r,crit}$ not same for N_{10-30} and N_{30-300}?**
  - Always smaller for N_{30-300} than for N_{10-30}.
  - N_{10-30} are relatively more affected by TPT than N_{30-300} for same level of TPT as these are formed in turbulent wake of a vehicle and TPT may play a much greater role in their measured number than does the wind.

- **Why was $U_{r,crit}$ in each size range different for various wind directions?**
  - Defined as the intersection of traffic-related and wind-related correlations.
  - First of these assumed to be independent of wind speed and direction.
  - Second varies the turbulence generating capacity of the mean wind in a particular geometry. Thus if second changes, then $U_{r,crit}$ must also be.

See Kumar et al. (2008c) for details

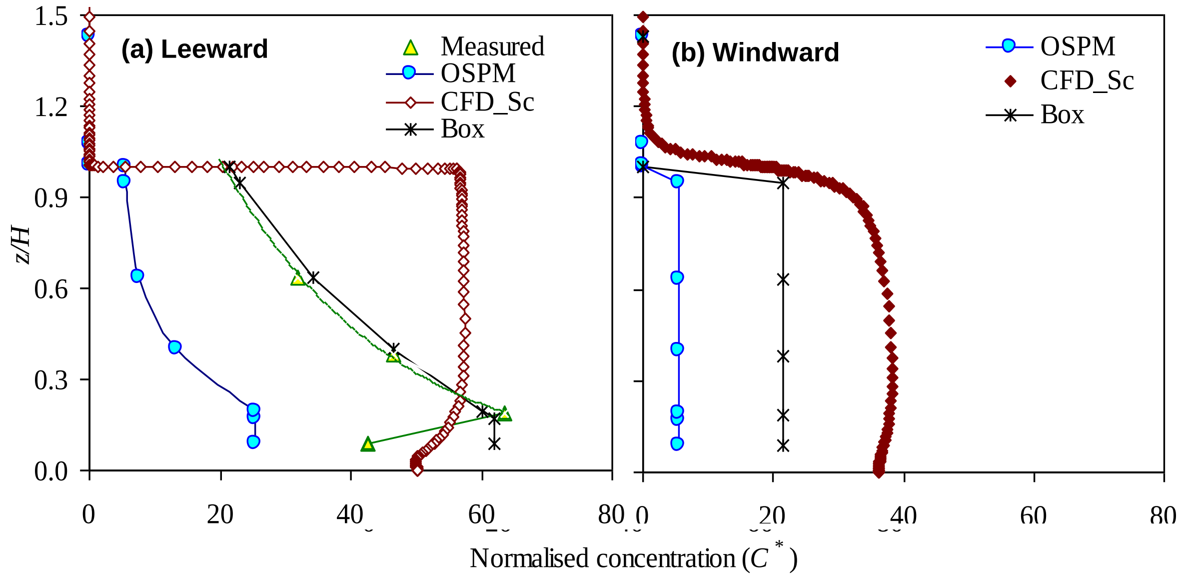
EFECT OF WIND DIRECTIONS & SPEED ON $N_{10\text{-}30}$ and $N_{30\text{-}300}$

Overall performance of proposed model (Eqs. 2 and 3) fitted on entire PNC data, and the best fit single power law fitted on entire PNC data. R is the regression coefficient, FAC2 is the fraction of predictions within a factor of 2 and FB is the fractional bias.

Wind directions		Proposed model (Eqs. 2 and 3) fitted on entire PND data			Other model (best fit single power law) fitted on entire PNC data		
		$N_{10\text{-}300}$	$N_{10\text{-}30}$	$N_{30\text{-}300}$	$N_{10\text{-}300}$	$N_{10\text{-}30}$	$N_{30\text{-}300}$
NW	**R**	0.35	0.31	0.54	0.41	0.23	0.51
	FAC2	53%	61%	52%	48%	48%	40%
	FB	-0.02	-0.01	-0.04	-0.36	-0.46	-0.21
SE	**R**	0.48	0.52	0.42	0.44	0.49	0.38
	FAC2	77%	90%	70%	80%	87%	57%
	FB	0.01	0.01	0.01	-0.15	-0.11	-0.21
NE*	**R***	0.42*	0.40*	0.42*	0.34*	0.31*	0.32*
	FAC2*	93%*	81%*	94%*	93%*	81%*	93%*
	FB*	-0.03*	-0.03*	-0.03*	-0.04*	-0.05*	-0.04*
SW	**R**	0.56	0.55	0.58	0.49	0.41	0.54
	FAC2	76%	74%	75%	75%	74%	75%
	FB	0.01	0.01	-0.05	-0.15	-0.18	-0.15
S	**R**	0.79	0.68	0.79	0.59	0.50	0.61
	FAC2	84%	80%	79%	77%	79%	67%
	FB	0.03	0.00	0.04	0.11	0.01	0.37
W	**R**	0.64	0.64	0.79	0.53	0.54	0.68
	FAC2	72%	73%	80%	66%	66%	78%
	FB	0.03	-0.01	-0.01	-0.19	-0.16	-0.27

*Based on very little available data, therefore these are not considered or estimated for analysis.

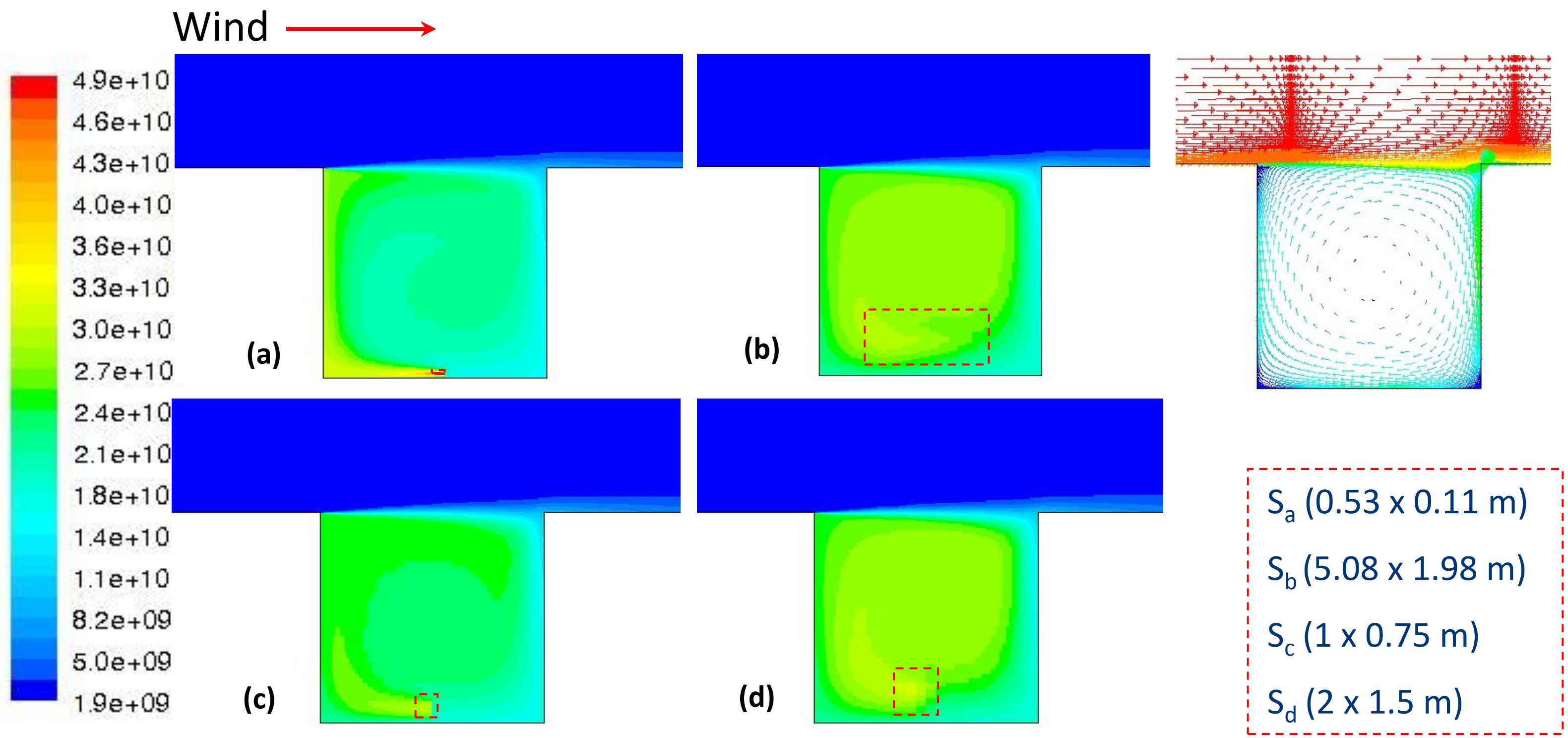
COMPARISON OF VERTICAL PNC PROFILES



- 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. (2009b) for details

CFD SIMULATIONS



- 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 ≈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.