

# Observations on Air Quality Monitoring, Emissions Inventories and Source Apportionment Studies

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### **Content**

- SOURCE APPORTIONMENT
  - simple monitoring
  - receptor modelling
  - emission inventories and numerical models
  - conclusions for India



- SIMPLE MONITORING
  - triple site data
  - chemical mass closure
    - pragmatic mass closure model



### **Multi-Site Studies**

Simultaneous sampling ⇒

Roadside minus urban background = traffic increment

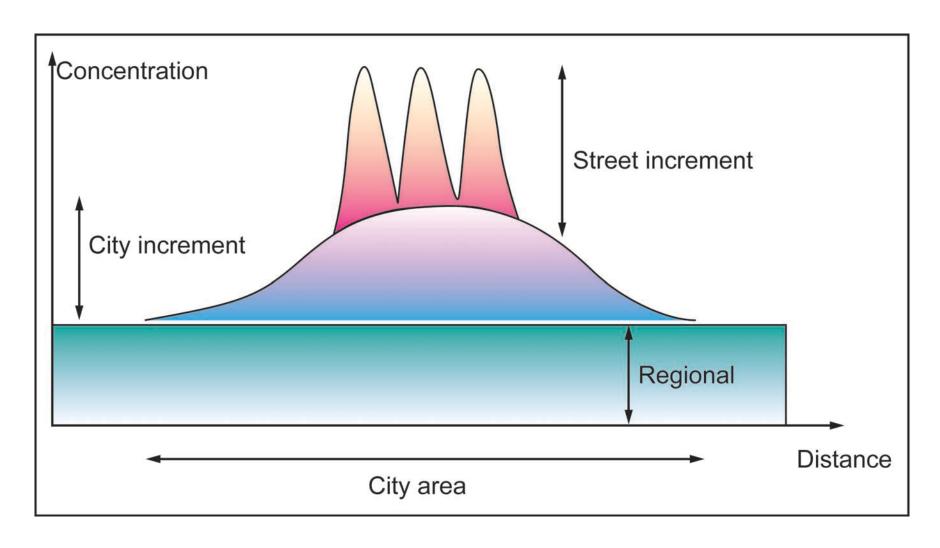
Urban background minus rural = urban increment

#### **Day of Week Studies**

Traffic volumes vary by day of week – may be used to infer traffic contribution

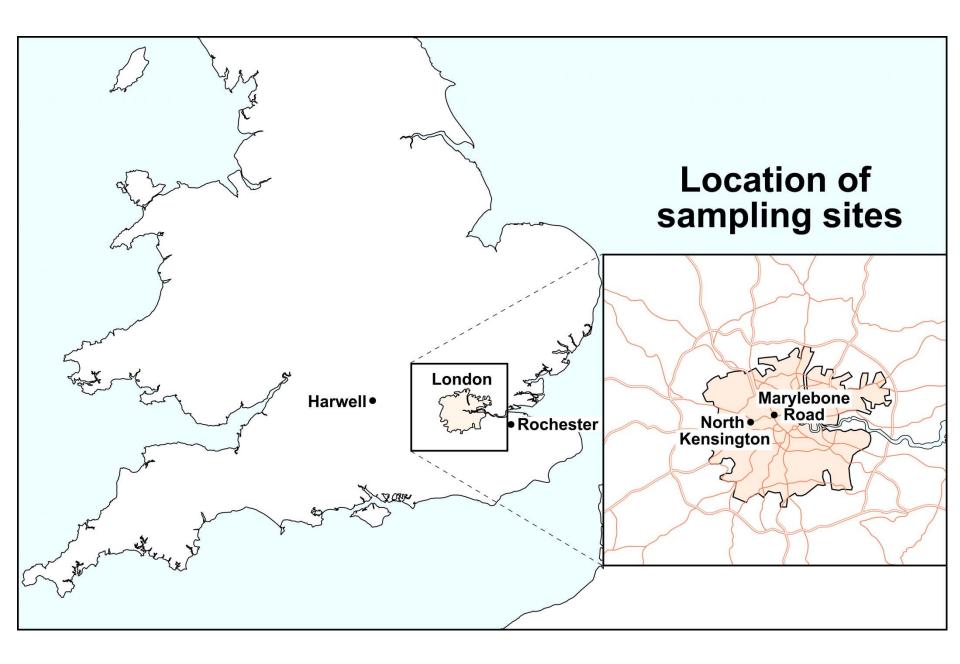




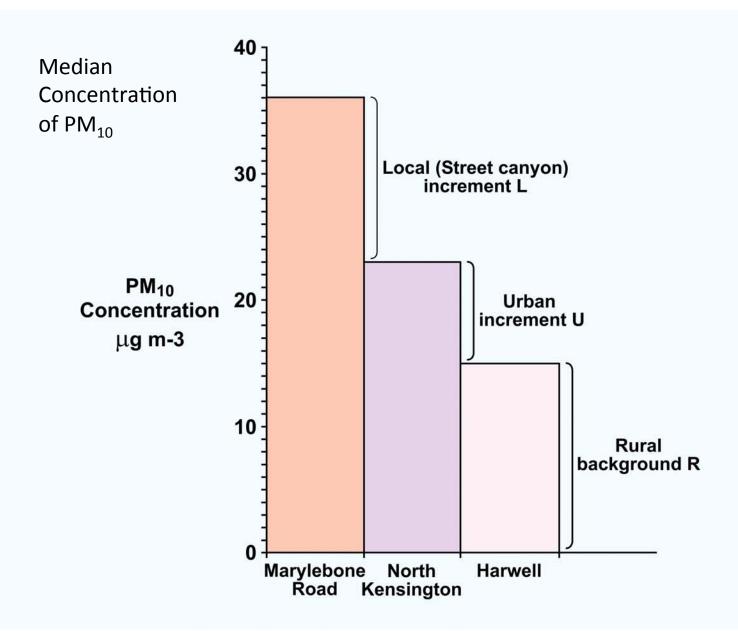


SCHEMATIC PROFILE OF POLLUTION ACROSS A CITY



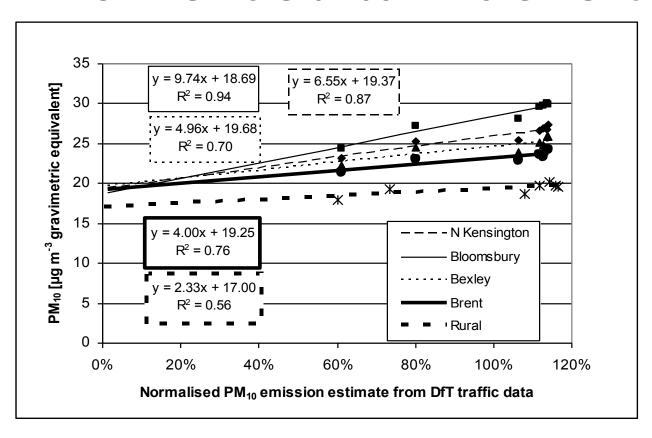








### Non-vehicle urban increment



PM<sub>10</sub> measured by TEOM v normalised daily emission calculated from DfT traffic data



# CHEMICAL COMPOSITION OF AIRBORNE PARTICLES

An essential indicator of the sources of airborne particles, and a determinant of toxicity

#### We can measure

- bulk chemical composition major components of an integrated sample of particles
- single particle composition



#### **URBAN AIR QUALITY: PARTICULATE MATTER**

Which sources are important?

<u>Source</u> <u>Chemical tracer (bulk samples)</u>

Local traffic exhaust elemental carbon and organic

compounds

Long range transport

- SO<sub>2</sub> oxidation sulphates

- NO<sub>x</sub> oxidation nitrates

- ammonia emissions ammonium

Soil and road dusts iron

Construction and demolition calcium

Sea salt sodium chloride



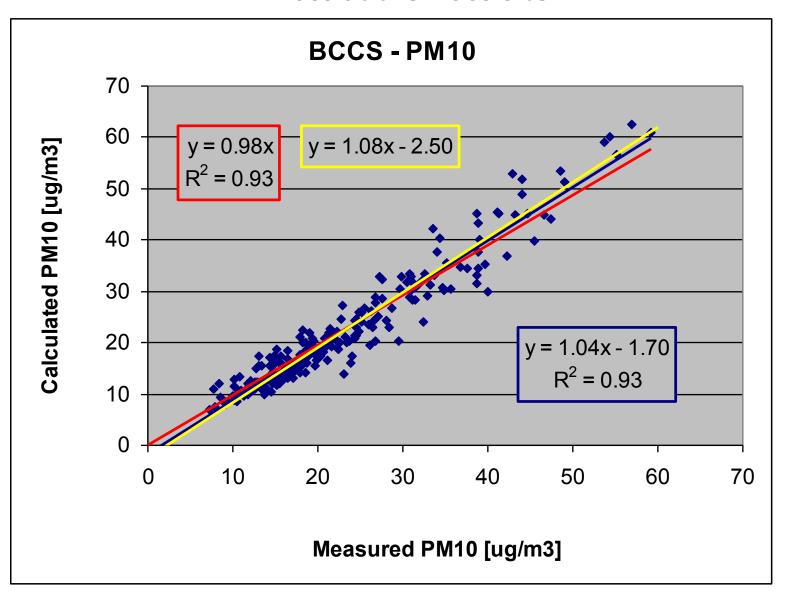
### AIRBORNE PARTICULATE MATTER: BULK CHEMICAL COMPOSITION

#### Mass closure is achieved in terms of the following components:

- Sulphate converted to ammonium sulphate mass
- Nitrate converted to ammonium nitrate (fine fraction) or sodium nitrate (coarse fraction) mass
- Chloride converted to sodium chloride mass
- Elemental carbon
- Organic carbon converted to organic matter mass
  - split into primary and secondary on the basis of OC/EC ratio
- Iron scaled to provide mass of traffic-related coarse dust
- Calcium converted to mass of gypsum, representing soil and construction/demolition dust
- Bound water estimated from sulphate and nitrate mass

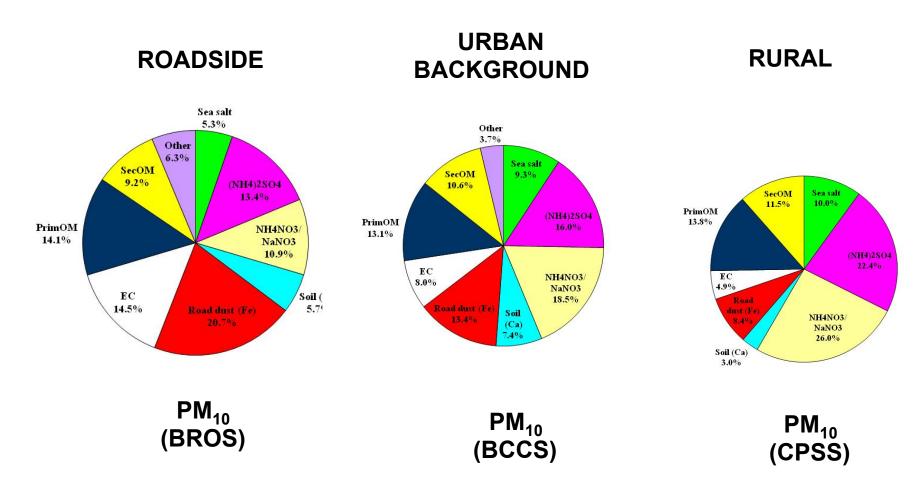


## Comparison between measured and calculated PM mass at the BCCS site





### **Major Component Composition of PM<sub>10</sub>**



From Pragmatic Mass Closure Model (Harrison et al., 2004)



### **Receptor Modelling Techniques**

#### These include:

- multicomponent analysis of many samples followed by factor analysis (usually PMF)
- Use of chemical tracers, including organic molecular markers and Chemical Mass Balance modelling
- Targeted studies
  - e.g. work on brake dust particles
- Aerosol mass spectrometry

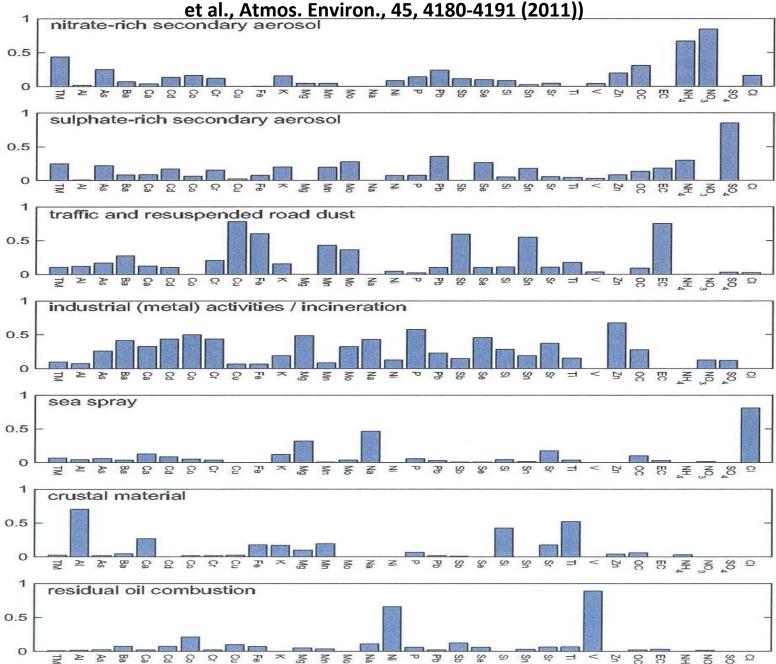


### **Use of PMF in Source Apportionment**

- Requires analysis of major and minor chemical components
- Technique is weighted according to the analytical uncertainties of specific components
- Key requirement is for number of samples to exceed number of analytical variables typically by a factor of > 3
- Has no *a priori* requirement for source composition profiles

Contribution F (in fractions)

Source Profiles of PM10 in the Netherlands (from D. Mooibrook





#### **Chemical Mass Balance Models**

- Consider atmospheric PM composition to be a linear sum of relevant source emission profiles
- Requires knowledge of the identity of all important sources and the chemical composition of emissions from each source
- Country-specific source composition data is not always available



# Chemical Mass Balance Study using Molecular Markers

- PM<sub>2.5</sub> samples were collected and analysed for
  - $\triangleright$  *n*-alkanes from  $C_{24} C_{36}$
  - 9 specific hopanes
  - > 13 PAH
  - > 14 carboxylic acids
  - levoglucosan
  - cholesterol
  - > inorganic marker elements (Si, Al)

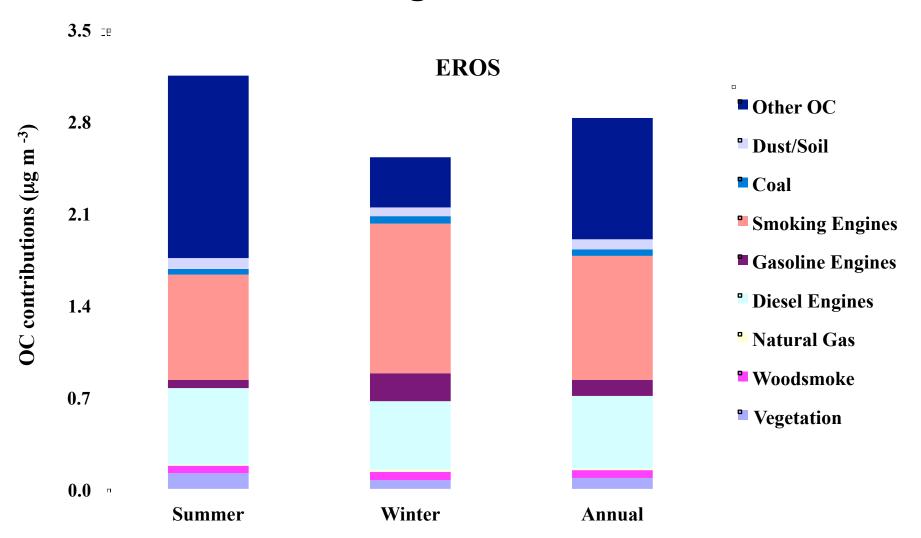


#### **CMB Model Results**

- Model used to apportion sources of organic carbon to:
  - diesel engine exhaust
  - gasoline engines
  - smoking gasoline engines
  - vegetative detritus
  - dust and soil
  - > wood smoke
  - coal combustion
  - > natural gas combustion

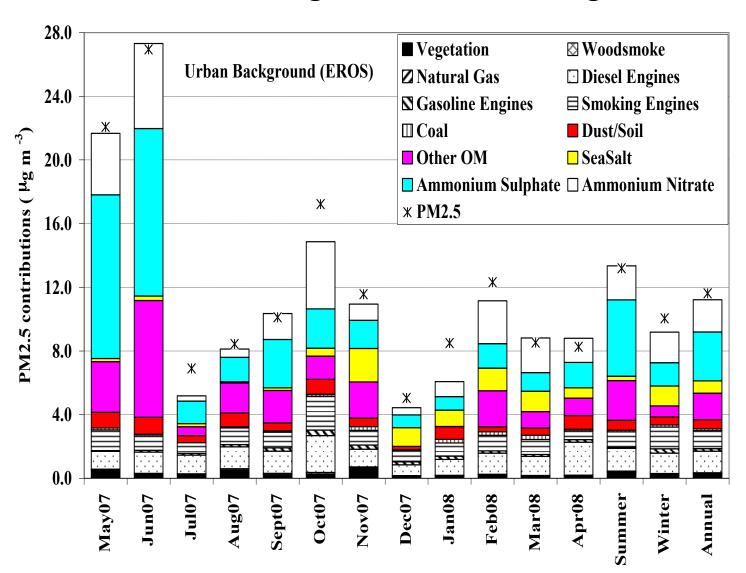


# Source Contributions to OC at Urban Background Site





# Results of Chemical Mass Balance/Pragmatic Mass Closure model for a background site in Birmingham





### **Emissions Inventories and Numerical Models**

Requires spatially disaggregated inventory of emissions

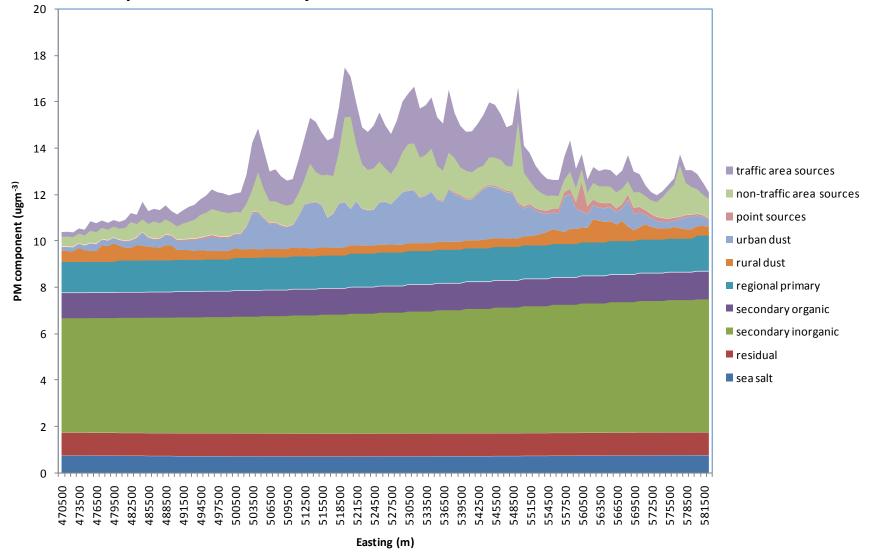
Application of dispersion model approach for primary particles

Application of chemistry-transport model for secondary particles

Specification of model boundary conditions is crucial



Transect through the PM<sub>2.5</sub> concentration distribution in London, showing a number of individual PM components from Henley-on-Thames in the west to Southend-on-Sea in the east



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# Estimates of PM<sub>2.5</sub> and PM<sub>10</sub> Emissions in Delhi, 2010

Source Category	PM <sub>2.5</sub> Emissions (Gg yr <sup>-1</sup> )	PM <sub>10</sub> Emissions (Gg yr <sup>-1</sup> )	
Power	2.87	11.02	
Vehicular (excl. road dust)	30.25	30.29	
Industrial	16.29	27.20	
Residential	18.65	36.07	
Road dust	18.35	131.27	

From: Sahu, S.K., Beig, G. and Parkki, Atmos. Environ., in press



### **Uncertainties in Dispersion Modelling**

- The results of dispersion model calculations are a linear function of source strength
- While it should be possible to estimate stack emissions from industry and exhaust emissions from traffic with reasonable confidence, other sources are far less certain
- Areas of particular uncertainty
  - non-exhaust emissions from road traffic
  - residential combustion
  - refuse burning
  - biomass burning
  - fugitive emissions from industry



# Example: Practical Application of Emission Inventory/ Dispersion Modelling

#### Prediction of Future Concentrations of Airborne Nanoparticles

Year	Population (x 10 <sup>6</sup> )	Vehicle Population (x 10 <sup>6</sup> )	Total Vehicle Kilometer Travelled (x 10 <sup>10</sup> )	Total Particle Number per annum (x 10 <sup>25</sup> )	Airborne Concentration (Background) (x 10 <sup>4</sup> )
2010	22.16	4.74	6.91	1.37	2.81
2030 (BAU)	30.87	25.6	38.56	5.77	10.44
2030 (BES)	30.87	9.26	20.41	0.078	0.17

P. Kumar, B.R. Gurjar, A.S. Nagpure and R.M. Harrison, Preliminary Estimates of Nanoparticle Number Emissions from Road Vehicles in Megacity Delhi and Associated Health Impacts, *Environ. Sci. & Technol.*, 45, 5514-5521 (2011).



#### CONCLUSIONS

- 1. Well designed monitoring strategies can provide vital insights into pollution sources.
- 2. Chemical composition provides complementary knowledge of major source types.
- 3. Receptor modelling methods have great potential and yield comprehensive information on major sources, but need great care in their implementation.
- 4. Emission inventories and dispersion modelling have the potential to explain ambient concentrations and source apportionment, but uncertainties in the inventories create large ranges in the results.

