

# Using sensor data and inversion techniques to systematically reduce dispersion model error

*D. J. Carruthers<sup>1</sup>, A. L. Stidworthy<sup>1</sup>, D. Clarke<sup>2</sup>, K.J. Dicks<sup>3</sup>,  
R. L. Jones<sup>4</sup>, I. Leslie<sup>5</sup>, O. A. M. Popoola<sup>4</sup>,  
A. Billingsley<sup>6</sup> and M. Seaton<sup>1</sup>*



<sup>1</sup>Cambridge Environmental Research Consultants

<sup>2</sup>Cambridgeshire County Council, Cambridge

<sup>3</sup>Cambridge City Council, Cambridge

<sup>4</sup>Department of Chemistry, University of Cambridge

<sup>5</sup>Computer Laboratory, University of Cambridge

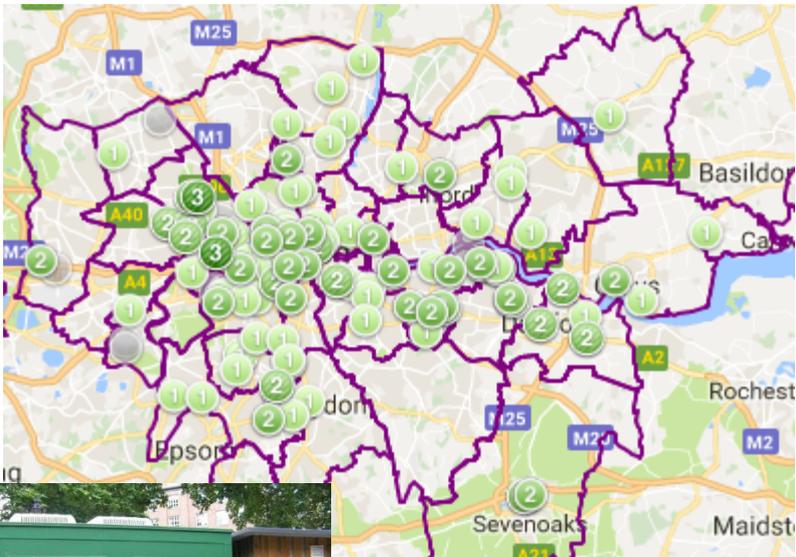
<sup>6</sup>AQMesh Environmental Instruments, Stratford-upon-Avon

Harmo18, Bologna, October 2017

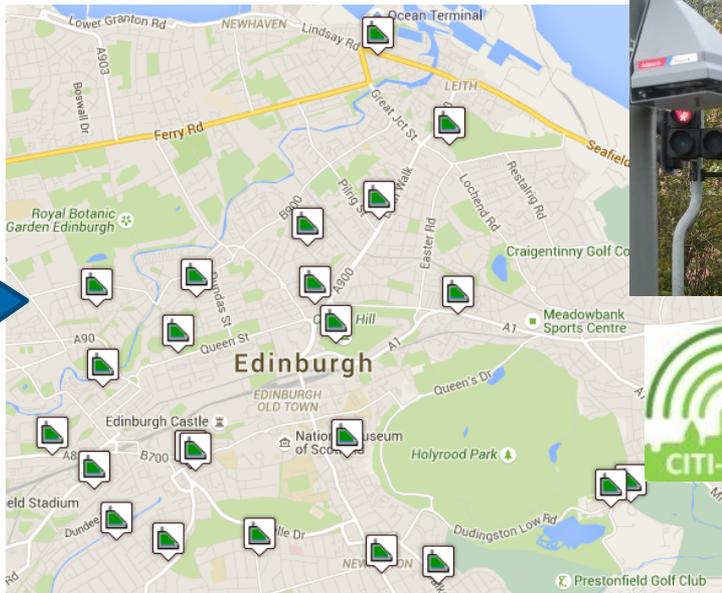
# Motivation



Traditional reference-standard air quality monitoring networks are high quality, but difficult to site and expensive to maintain, so the number of monitors is limited.



Could low-cost sensors, which are less accurate but easier to site and cheaper to buy and maintain, help to improve modelling?



# Motivation

- Emissions errors in urban areas account for a significant proportion of dispersion model error
- Traditionally, dispersion models such as CERC's ADMS-Urban model are validated against data from reference monitors:
  - Modellers either use the validation to improve model setup; or
  - Calculate and apply a model adjustment factor to model results
- New low cost air pollution sensors allow large networks of sensors to be installed across a city
- Accuracy and reliability is generally lower than reference monitors, but larger spatial coverage is possible
- How can we best use these sensor data in modelling?
- If the data are not accurate and reliable enough for model validation, maybe we can use the data in a different way...

Methodology

```
graph TD; A[Methodology] --> B[Case Study: Cambridge]; B --> C[Future development];
```

Case Study: Cambridge

Future development

# Methodology: Introduction

- The aim was to develop an inversion technique to use monitoring data from a network of sensors to automatically adjust emissions to improve model predictions
- Basic idea:
  - Run ADMS-Urban to obtain modelled concentrations at monitor locations in the normal way
  - Take these modelled concentrations and their associated emissions as a 'first guess', together with
    - a) monitored concentration data
    - b) information about the error in the monitored data and the proportion of that error that is systematic across all monitors
    - c) information about the error in the emissions data and the proportion of that error that is systematic across all sources
  - Use an inversion technique to calculate an adjusted set of emissions that reduces error in the modelled concentrations

# Methodology: Introduction

- There are some conditions that have to be satisfied for such a scheme to work:
  - a) The modelled concentration must be proportional to the emissions, which means that complex effects like chemistry have to be ignored
  - b) Each modelled source must contribute to the concentration at least one receptor (monitor)
  - c) Each receptor included must have non-zero modelled and monitored concentration
- The technique developed uses a Bayesian inversion approach following work by others, for example as used by the Met Office for estimating volcanic ash source parameters using satellite retrievals [Webster *et al*, 2016]

# Methodology: Cost function

We define a cost function  $J(\mathbf{x})$  with two terms: one that describes the error in the modelled concentration (left-hand term) and one that describes the error in the emissions (right-hand term):

$$J(\mathbf{x}) = (\mathbf{M}\mathbf{x} - \mathbf{y})^T \mathbf{R}^{-1} (\mathbf{M}\mathbf{x} - \mathbf{y}) + (\mathbf{x} - \mathbf{e})^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{e})$$

Quantity	Definition	Dimensions
$x$	<i>Vector of emissions (result)</i>	$n$
$M$	Transport matrix relating the source term to the observations	$n$ by $k$
$y$	Vector of observations	$k$
$R$	Error covariance matrix for the observations	$k$ by $k$
$e$	Vector of first guess emissions	$n$
$B$	Error covariance matrix for the first guess emissions	$n$ by $n$

The aim is to minimise  $J$  to obtain  $\mathbf{x}$ , a vector of adjusted emissions.

# Methodology: Cost function input

Quantity	Definition	Dimensions
$x$	<i>Vector of emissions (result)</i>	$n$
$M$	Transport matrix relating the source term to the observations	$n$ by $k$
$y$	Vector of observations	$k$
$R$	Error covariance matrix for the observations	$k$ by $k$
$e$	Vector of first guess emissions	$n$
$B$	Error covariance matrix for the first guess emissions	$n$ by $n$

- The  $y$  and  $e$  vectors are straightforward to form
- To find the transport matrix  $M$  we run ADMS-Urban with unit emission rates for all sources and obtain the concentration at the receptors due to each source; the concentration results give  $M$

# Methodology: Estimating error

## Estimating emissions error (B)

- For **emissions**, we need to estimate for each source (pair):
  - Emission error  
= Uncertainty Factor x Emission Rate
  - Co-varying emission error  
= Covariance Factor x Emission Error
- Example causes of co-varying error: common emissions factors, proximity of sources to each other
- Total Emission error includes both co-varying emission error and independent emission error

## Estimating sensor error (R)

- For **sensors**, we need to estimate:
  - Sensor error  
= Uncertainty Factor x Monitored Concentration
  - Co-varying sensor error  
= Covariance Factor x Sensor Error
- Example causes of co-varying error: same sensor type, ambient temperature, humidity
- Total Sensor error includes both co-varying sensor error and independent sensor error

# Methodology: Summary

Step 1: Run ADMS-Urban to obtain hourly modelled concentrations at monitoring site locations

Step 2: Form the transport matrix, error covariance matrices, emissions vector and monitored data vector for each hour

Step 3: Run the optimisation scheme independently for each hour

Step 4: Create an hourly factors (.hfc) file from the adjusted hourly emissions data

Step 5: Re-run ADMS-Urban using the adjusted emissions .hfc file

# Cambridge Case Study: Background

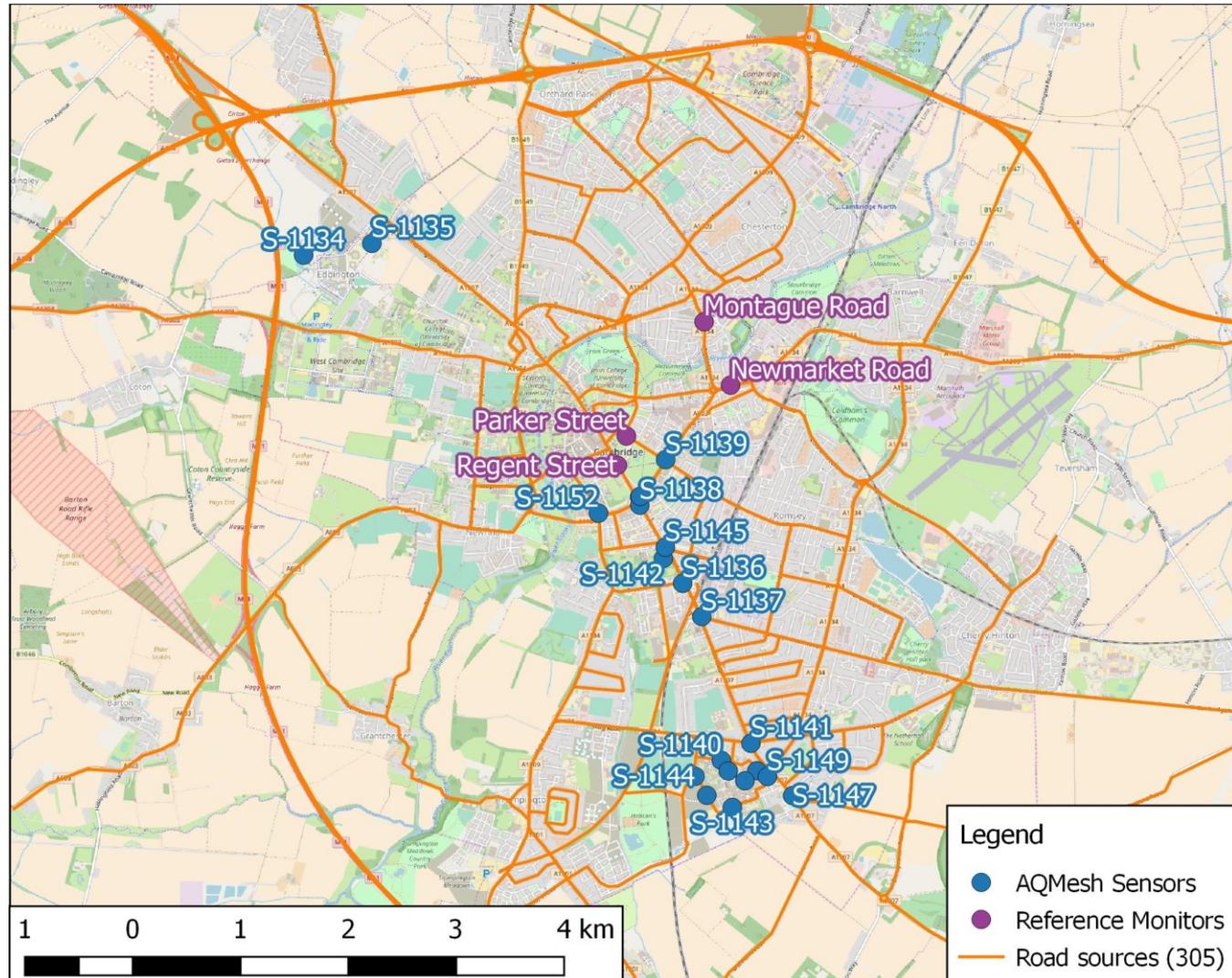


20 AQMesh sensor pods

4 Reference monitors

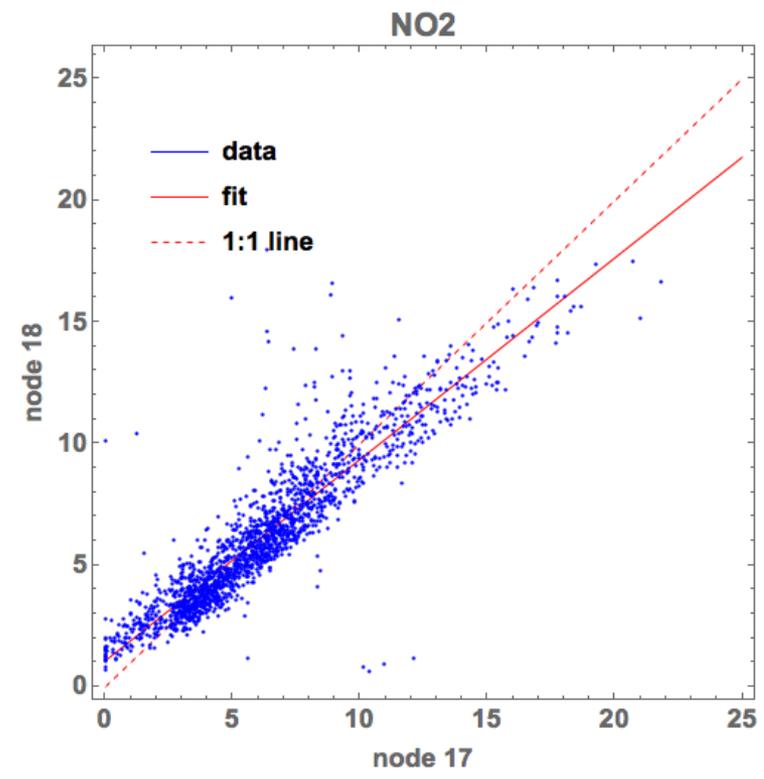
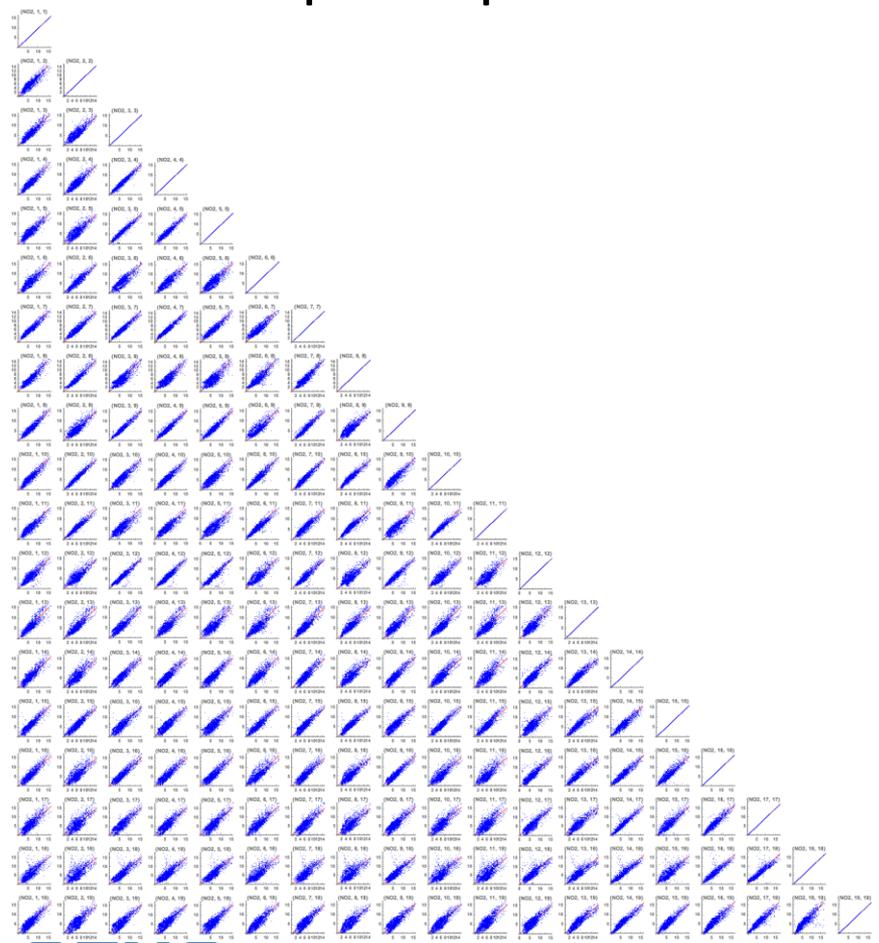
3-month analysis period, July-Sept 2016

305 road sources

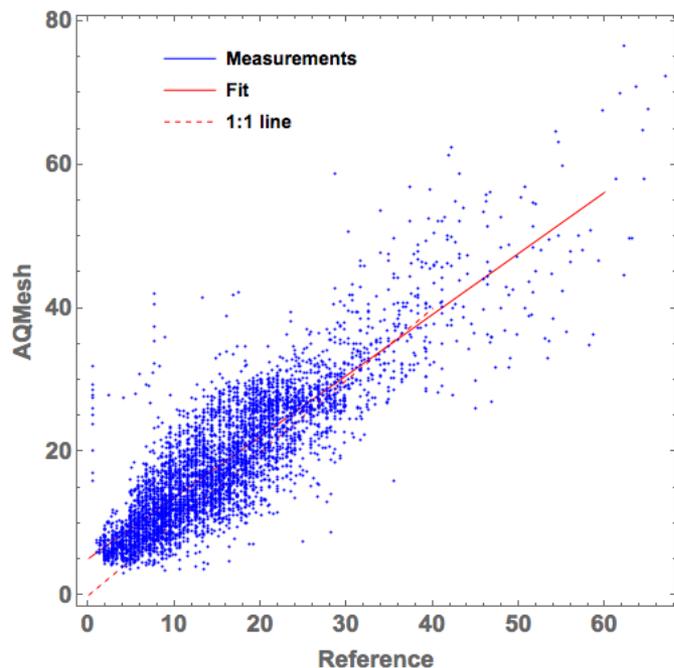
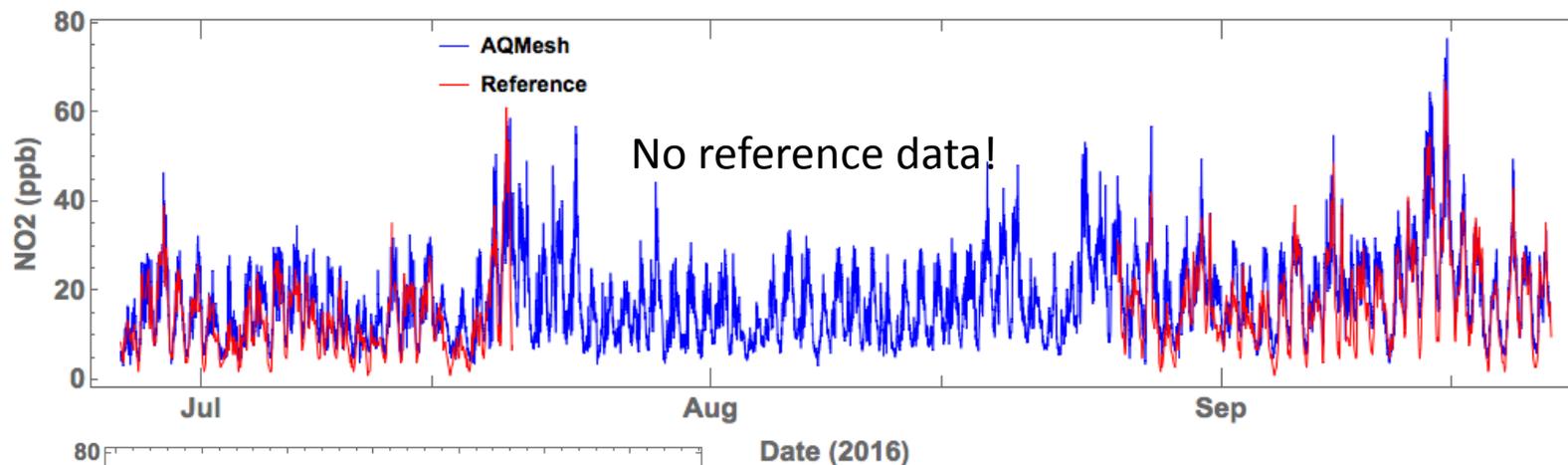


# AQMesh Sensors

- Used out of the box – no local calibration; pre-calibrated at AQMesh test facility
- Example of performance: NO<sub>2</sub> sensor-sensor comparison



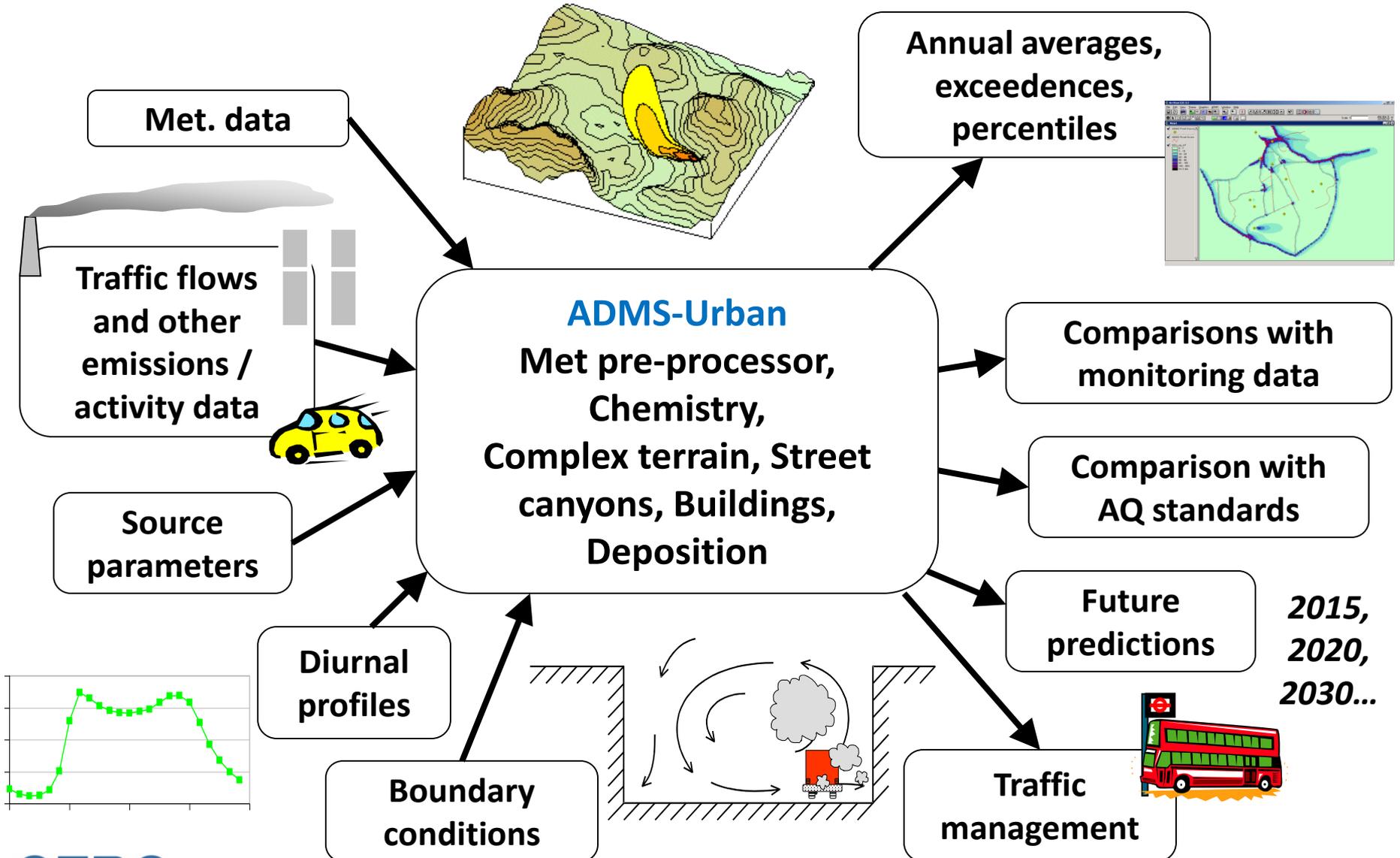
# NO<sub>2</sub> Gonville Place comparison



	Gradient	Intercept	R <sup>2</sup>
pre	1.07 (0.01)	10.0 (0.1)	0.50
post	0.82 (0.01)	5.1 (0.13)	0.74

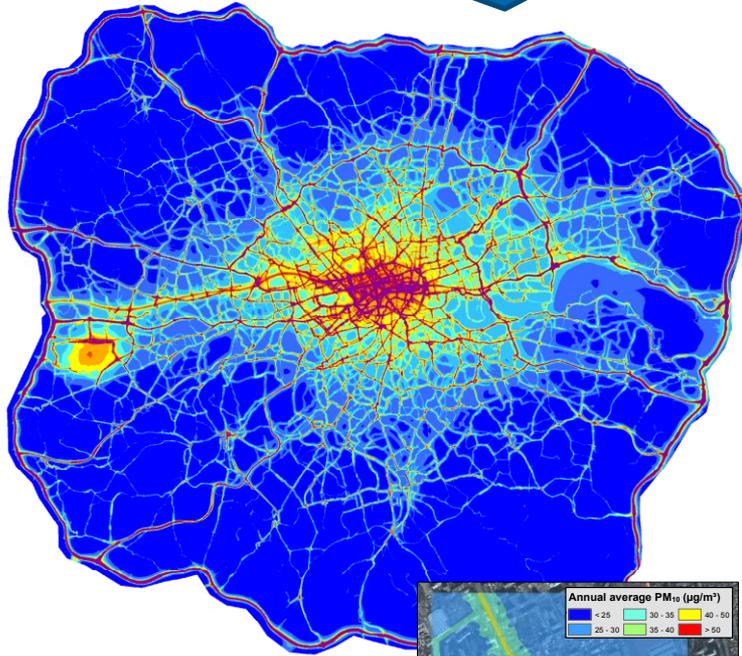
- Outliers removed (from reference)
- Significantly improved R<sup>2</sup>
- AQMesh ~ 0.82 of reference (unscaled)

# CERC's ADMS-Urban Model

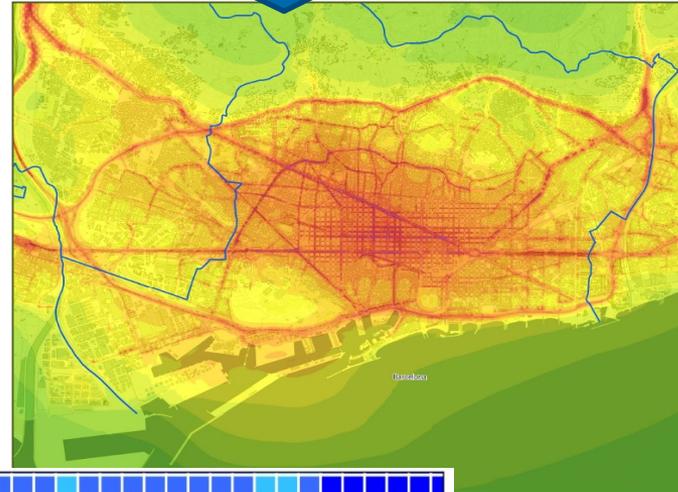


# CERC's ADMS-Urban Model

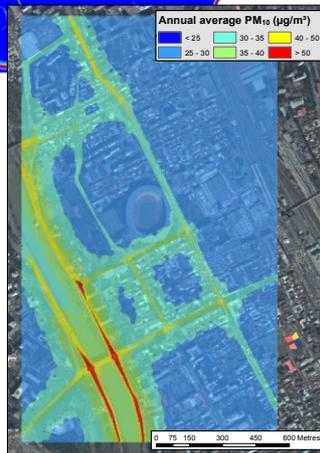
Annual average NO<sub>2</sub> concentrations in Greater London calculated using ADMS-Urban



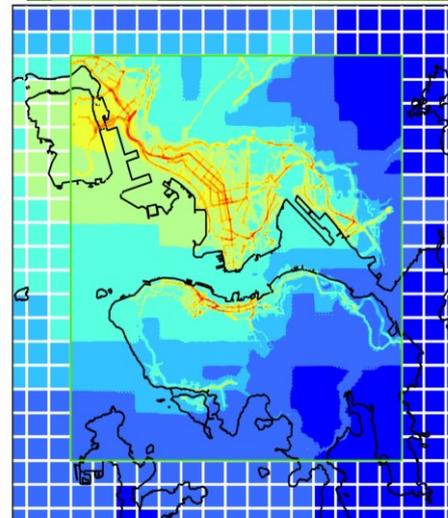
Annual average NO<sub>2</sub> concentration map of Barcelona calculated using ADMS-Urban. Modelling by Barcelona Regional.



Annual average PM<sub>10</sub> for Tblisi in Georgia calculated using ADMS-Urban



Annual average NO<sub>2</sub> over Hong Kong Island calculated using ADMS-Urban linked with CAMx regional model



# Cambridge Case Study: Aims

- Two aims:
  - Sense-check optimisation results, find and correct errors
  - Test this hypothesis: *Using inversion techniques, we can use sensor data to improve emissions and thereby improve model performance, judged at independent reference monitors.*
- Initial study -simple implementation
  - Only one source type: roads
  - Only one pollutant: NO<sub>x</sub>
  - Only 20 sensors – relatively small network
  - Simple representation of error covariance

# Methodology: Summary

**Step 1:** Run ADMS-Urban to obtain hourly modelled concentrations at monitoring site locations

**Step 2:** Form the transport matrix, error covariance matrices, emissions vector and monitored data vector for each hour

**Step 3:** Run the optimisation scheme independently for each hour

**Step 4:** Create an hourly factors (.hfc) file from the adjusted hourly emissions data

**Step 5:** Re-run ADMS-Urban using the adjusted emissions .hfc file

Steps 2 to 5 completed three times, for three different scenarios:

1. AQMesh sensor and reference monitors included in the optimisation.

- Including the reference monitors helps us to sense-check the results and identify any errors

2. Only reference monitors included in the optimisation

- This scenario is also included to sense-check results and identify errors

3. Only AQMesh sensors included in the optimisation.

- In this scenario, the reference monitor data is kept as an independent dataset for model validation.

# Cambridge Case Study: ADMS-Urban Setup

## Emissions

- Annual averages + diurnal profiles (weekdays, Saturdays, Sundays)
- Road traffic count data from UK Govt and County Council
- Guided bus flows
- Road traffic emission factors for 2016 from the UK National Atmospheric Emissions Inventory (NAEI), adjusted for real-world emissions

## Met data

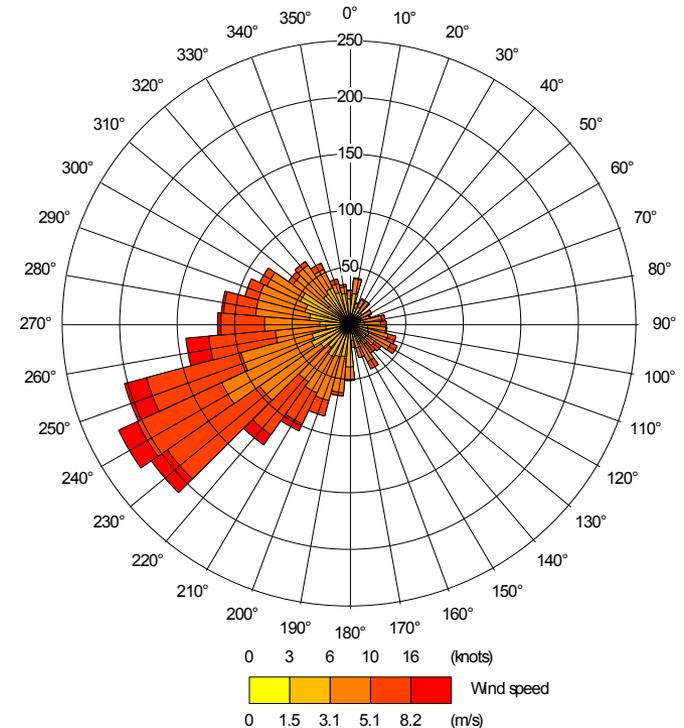
- Andrewsfield Met Office site, 21 June – 30 September

## Background data

- Background  $\text{NO}_x$  from Defra AURN measurements at rural sites

## Monitoring data used for validation

- All monitoring data are provisional apart from Gonville Place reference monitor; AQMesh data were obtained in real time.



Harmo18, Bologna, October 2017

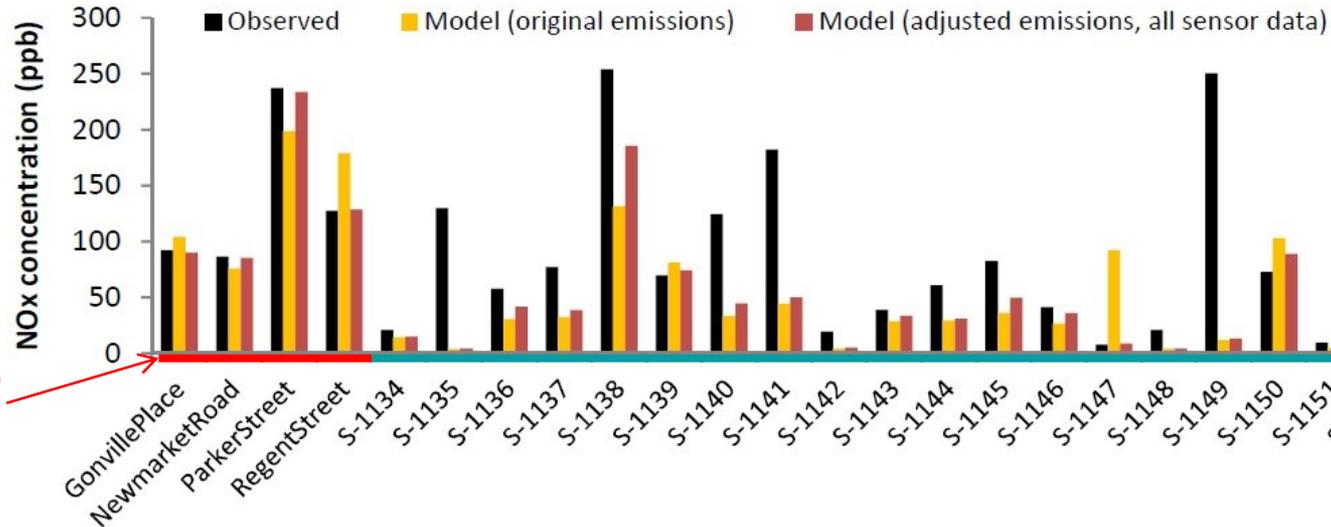
# Cambridge Case Study: Error Estimation

Parameter name	Description	Value
$U_{OR}$	Observation uncertainty factor (reference monitors)	0.1
$U_{OS}$	Observation uncertainty factor (AQmesh sensors)	0.3
$U_{ORF}$	Observation error covariance factor (reference monitors)	0.05
$U_{OSF}$	Observation error covariance factor (AQmesh sensors)	0.1
$U_E$	Emissions uncertainty factor	0.5
$U_{EF}$	Emissions error covariance factor	0.4

- Plausible estimates - would need refinement in any further study
- Assumed error covariance factors for both the sensors and reference instruments were small
- Assumed error covariance factors are more significant for emissions since depend on road traffic emission factors common to all sources

# Cambridge Case Study: Optimisation results

Example of observed, modelled and adjusted NO<sub>x</sub> concentration for one hour only

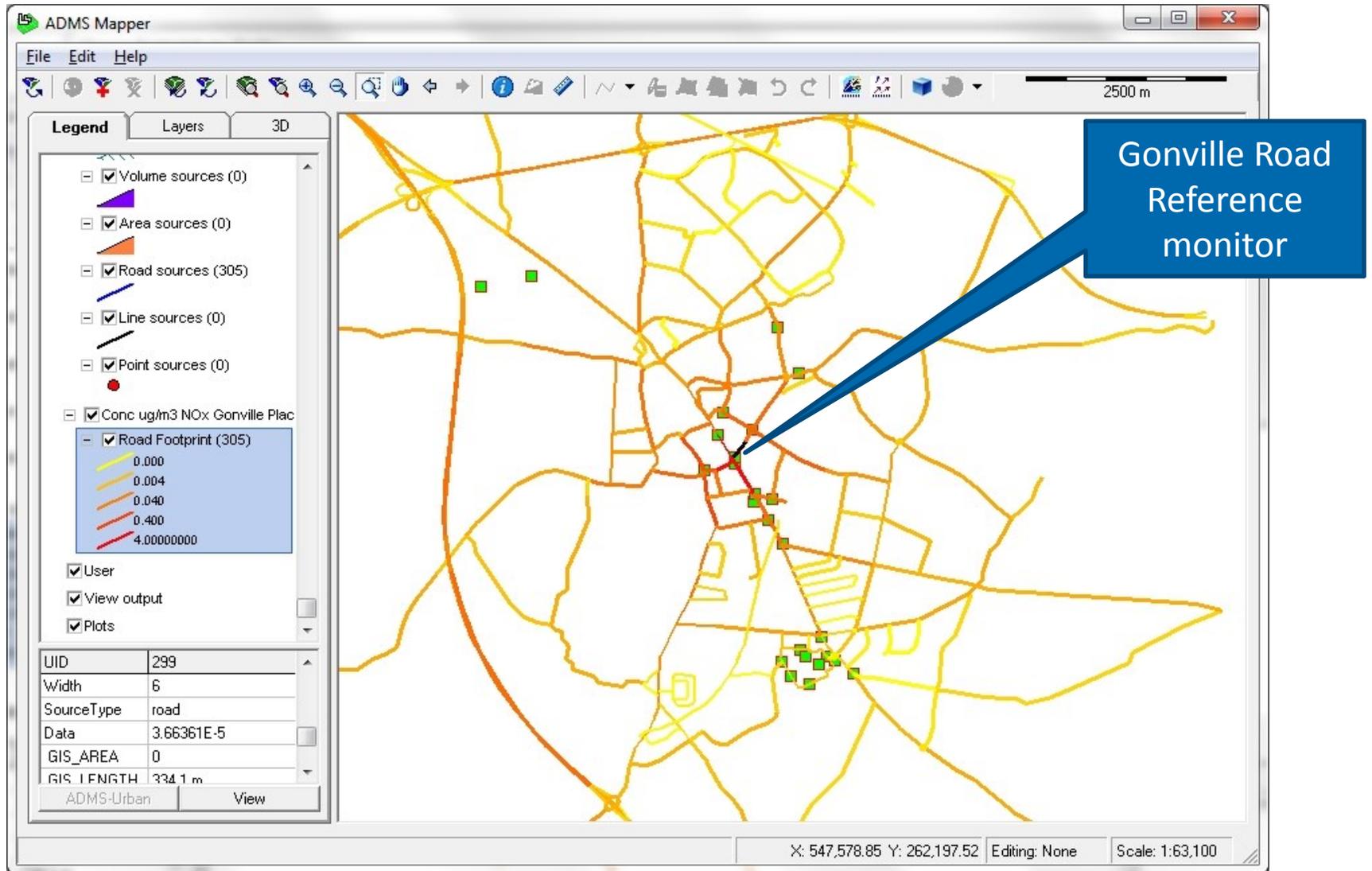


Reference monitors

AQMesh sensors

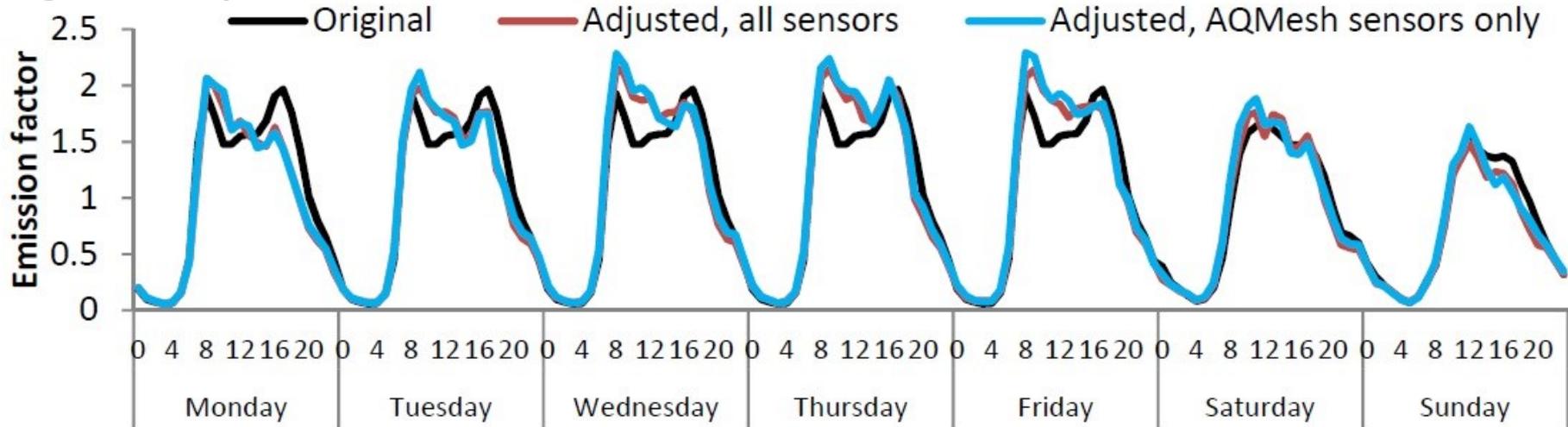
- The optimisation makes greater adjustment to the modelled concentration at the reference monitors than to the modelled concentration at the sensors - sensor uncertainty is higher than the reference monitor uncertainty
- The optimisation adjusts the modelled concentration at all sensors, not just at a selection of sensors - non-zero error covariance between sensors

# Footprint: Contribution of roads to receptor

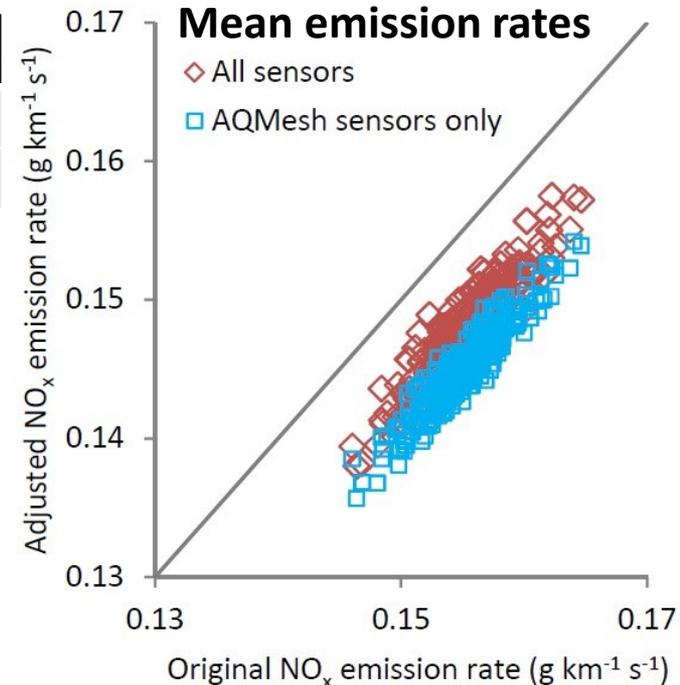


# Cambridge Case Study: Optimisation results

## Average diurnal profiles



Emission rate ( $\text{g km}^{-1} \text{s}^{-1}$ )	Original	Adjusted	Change
All sensors	0.1552	0.1478	-4.8%
AQMesh only		0.1452	-6.5%



Optimisation increases AM peak, decreases PM peak

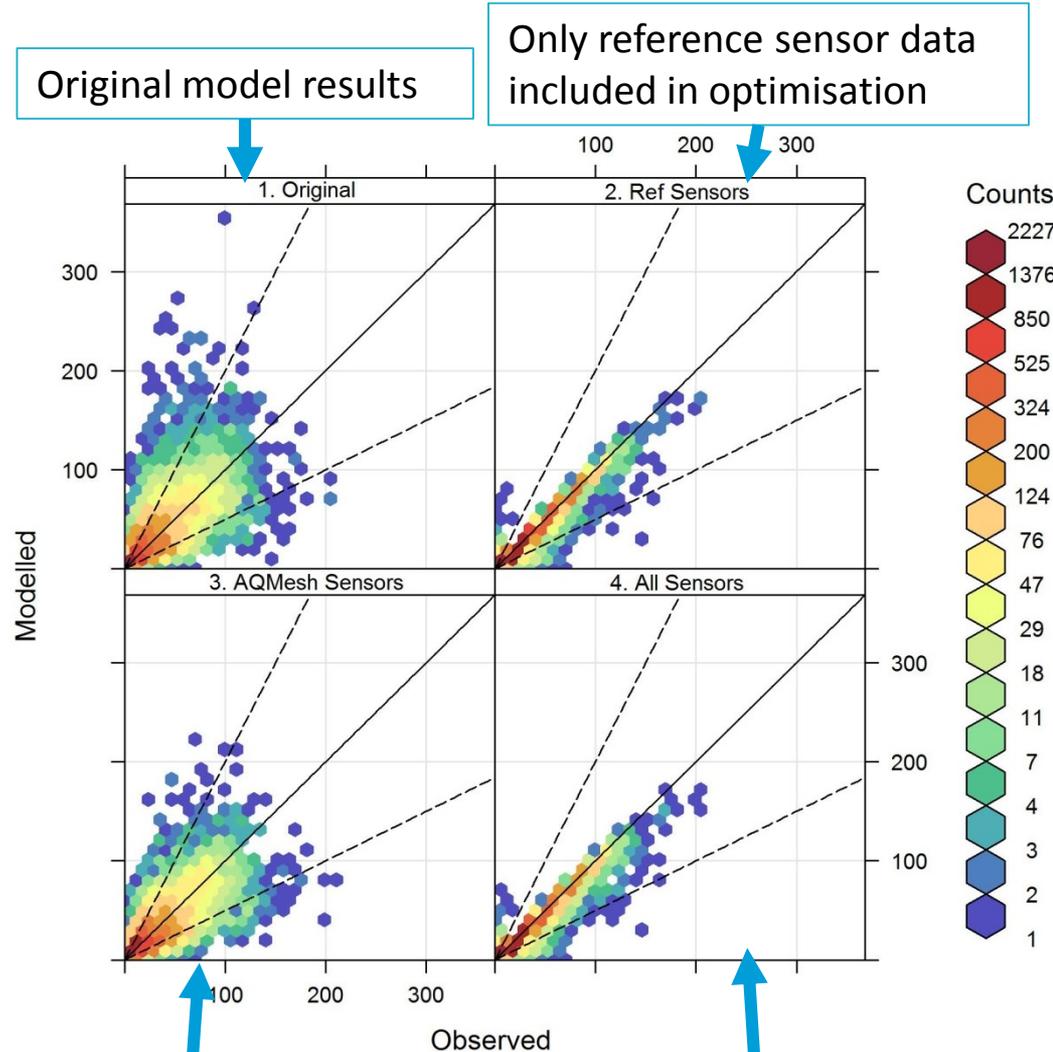
Optimisation reduces mean emission rate of all sources

Including reference monitors has only a small effect on overall emissions

# Cambridge Case Study: Model outcomes

Validation at Reference sites only

Statistics		1.	2.	3.	4.
Mean	Obs	31.2	31.2	31.2	31.2
	Mod	34.5	29.9	31.0	29.4
StDev	Obs	27.9	27.9	27.9	27.9
	Mod	31.0	26.6	27.0	26.1
	MB	3.30	-1.28	-0.23	-1.78
	NMSE	0.51	0.04	0.39	0.05
	R	0.70	0.98	0.75	0.97
	Fac2	0.71	0.94	0.73	0.94



Only AQMesh sensor data included in optimisation

All sensor data included in optimisation

# Conclusions

- The optimisation scheme presented here, using inversion techniques to modify pollution emission rates based on sensor data, has been shown to improve the accuracy of modelled concentrations.
- This study used a relatively simple representation of error covariance. Indicators of emissions error covariance that are not yet accounted for include:
  - Distance between sources
  - Meteorological factors such as temperature
  - Multiple pollutants (only NO<sub>x</sub> so far)
  - Different source types (only roads so far)
- Defining/refining the covariance in error between different pollutants and between different source types presents a challenge
- These initial results suggest that this approach could make practical use of large networks of low-cost sensors to improve dispersion model results and emission inventories.