

Urban emission inventory optimisation using sensor data, an urban air quality model and inversion techniques

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Abstract: An optimisation scheme has been developed that applies a Bayesian inversion technique to a high resolution (street-level) atmospheric dispersion model to modify pollution emission rates based on sensor data. The scheme minimises a cost function using a non-negative least squares solver. For the required covariance matrices, assumptions are made regarding the magnitude of the uncertainties in source emissions and measurements and the correlation in uncertainties between different source emissions and different measurement sites. The scheme has been tested in an initial case study in Cambridge using monitored data from four reference monitors and 20 AQMesh sensor pods for the period 30 June 2016 to 30 September 2016. Hourly NO_x concentrations from road sources modelled using ADMS-Urban and observed concentrations were processed using the optimisation scheme and the adjusted emissions were re-modelled. The optimisation scheme reduced average road emissions on average by 6.5% compared to the original estimates, changed the diurnal profile of emissions and improved model accuracy at four reference sites.

Keywords: inversion; optimisation; emissions; ADMS-Urban; sensors.

Reference to this paper should be made as follows: Carruthers, D., Stidworthy, A., Clarke, D., Dicks, J., Jones, R., Leslie, I., Popoola, O.A.M. and Seaton, M. (2019) 'Urban emission inventory optimisation using sensor data, an urban air quality model and inversion techniques', *Int. J. Environment and Pollution*, Vol. 66, No. 4, pp.252–266.

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This paper is a revised and expanded version of a paper entitled 'Urban emission inventory optimisation using sensor data, an urban air quality model and inversion techniques' presented at 18th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes. Bologna, Italy, October, 9–12 October 2017.

1 Introduction

Atmospheric emissions inventories are essential both to understand the absolute and relative contributions of the different source sectors of emissions and as input to chemical transport models and dispersion models. Traditionally emission inventories are compiled using either a bottom-up methodology where activity data for the different sources is used together with emission factors to calculate emissions for each source, or a top down methodology, where total emissions are estimated from 'global' data in a domain (e.g., total fuel use by road transport) and the emissions distributed according to proxy data (e.g., population density), and sometimes a combination of the two approaches (e.g.,

Tsagatakis et al., 2017). Either way the uncertainty of the compiled inventory is often large: for example the high uncertainty in published NO_x emission factors for light-duty diesel vehicles (Anenberg et al., 2017) or for PM from residential burning (Denier van der Gon et al., 2015).

In order to assess emission inventory uncertainty and to optimise emissions at the regional scale, measured concentrations of species in the atmosphere have been used with inversion techniques applied to both Eulerian and Lagrangian chemical transport models (Mulholland and Seinfeld, 1995; Polson et al., 2011; Rigby et al., 2011; Ganesan et al., 2014; Breon et al., 2015), however the application of such methodologies to source resolving emission inventories at the urban and local scale has been limited. An example at these scales involved the use of inverse methods to estimate emissions from a small number of sources using a rearranged version of the Gaussian plume model (Ropkins et al., 2009), however, more usually, dispersion models used in urban areas are first validated by comparing measured and modelled concentrations at well-established monitoring sites (Stocker et al., 2014); then at best, modellers manually refine inputs to the dispersion modelling to minimise error at these locations; at worst, modellers calculate ‘adjustment factors’ and apply these to modelled concentrations.

Meanwhile, the increasing availability of relatively low cost air pollution sensors that are easy to install and to maintain is allowing networks of such sensors to be installed across urban areas (Kumar et al., 2015; Reis et al., 2015). Although these sensors have reduced reliability and accuracy compared with traditional monitors, they allow much greater spatial coverage. This trend requires the dispersion modelling community to examine how data from these networks can be used most effectively to assess and improve dispersion models because the accepted model validation methods may not be appropriate. A systematic method that integrates data from these low cost sensors with models could deliver real benefits in terms of understanding and improving the quantification/verification of emissions of both air quality pollutants and greenhouse gases, and improving model calculations of concentrations of pollutants. It also offers the opportunity to examine important questions such as: what spatial separation or number of sensors is sufficient to optimise emissions through inverse modelling; and what is the relative effectiveness of a small number of reference monitors and a larger number of sensors.

This paper presents an inversion technique (e.g., Webster et al., 2016) implemented in the street scale resolution urban dispersion model ADMS-Urban (Owen et al., 2000; Hood et al., 2018). The methodology has been tested using data from four reference monitors and 20 AQMesh sensor pods.

2 Methodology

The inversion method (e.g., Webster et al., 2016) requires minimisation of the cost function $J(\mathbf{x})$ defined in equation (1); the equation parameters together with their dimensions are defined in Table 1.

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

In this equation the first term represents model error taking into account observation uncertainty and model uncertainty due to dispersion but not due to emissions; the second term represents emissions error taking into account emissions uncertainty. Given an initial set of emissions data, this cost function is minimised using a non-negative least squares solver to find revised emissions data which have the best fit to the measurements taking account of the estimated uncertainty in the measurements, model and first guess (a priori) emissions.

Table 1 Definition of cost function equation parameters. n is the number of sources and k the number of measurement sites

<i>Quantity</i>	<i>Definition</i>	<i>Dimensions</i>
x	Vector of emissions (result)	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 and model	k by k
e	Vector of first guess (a priori) emissions	n
B	Error covariance matrix for the first guess emissions	n by n

In order to implement the methodology, it is necessary to quantify the error covariance matrices R and B . In these matrices the diagonal values represent estimated variances σ^2 of observations and model error (R) at each monitoring site, and emissions error (B) for each source. The off-diagonal values are error covariances with the values representing the extent to which observation/model errors at different monitoring sites and emissions for different sources are correlated. For monitors we might expect that similar types of monitors may show some correlation, whilst model error is likely to be correlated for similar sites. In the case of emissions of road sources, one source of correlated error of source emissions is the error in the emissions factors (e.g., road traffic emissions factors where the same factors are used by all sources). Uncorrelated error might be, for example, an error in the traffic count on a particular road. For the Cambridge case study we make some pragmatic estimates of these error covariances as presented in Section 3.

2.1 ADMS-Urban

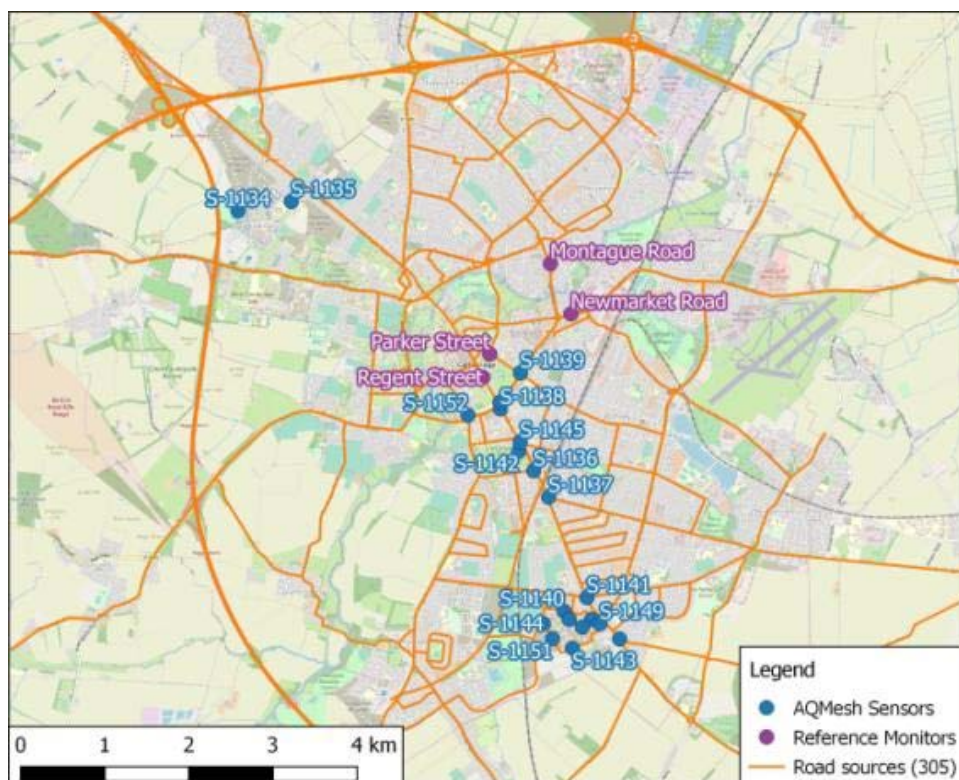
The model we use to generate the transport matrix is the quasi Gaussian plume dispersion model ADMS-Urban (Owen et al., 2000; Hood et al., 2018). In the model, emissions from all sources within the model domain are included, either explicitly with detailed time-varying profiles, for instance major road and industrial sources, or as grid-averaged emissions, representing diffuse sources such as those from heating and minor roads as a grid of regular volume sources, with simpler time variation. Allowance is made for the effect of buildings including street canyons on the flow and hence dispersion. The dispersion calculations are driven by hourly meteorological profiles of wind speed and direction, among other parameters, which are characterised using Monin-Obukhov length similarity; meteorological input data may be derived from measurements or output from a mesoscale model such as WRF. The ADMS-Urban model has been used to simulate air quality within cities worldwide; applications include testing of emission-reduction scenarios and forecasting (Stidworthy et al., 2017). The module has been validated

extensively by comparison with measurements from monitoring networks in Hong Kong and London (Hood et al., 2014; Stocker et al., 2014).

3 Case study

During 2016, 20 AQMesh sensor pods were deployed across Cambridge in addition to four reference monitors already in situ (see Figure 1). The sensors measure NO, NO₂, NO_x, O₃, CO, SO₂, PM₁, PM_{2.5}, PM₁₀ and total particle count (TPC) at intervals of 15 minutes. For the optimisation scheme case study, only hourly averaged NO_x concentrations were considered and it was assumed that local emissions were dominated by road traffic emissions; no other emission sources were considered. The initial (a priori) emission inventory thus comprised emissions from 305 road sources across Cambridge. These emissions were based on traffic flow data from the UK Department for Transport and from Cambridge County and City Councils. National traffic fleet composition data was supplemented with Cambridge-specific bus fleet data. Hourly time varying profiles are used separately for weekdays, Saturdays and Sundays. Standard emission factors for NO_x were adjusted for real driving emissions (Hood et al., 2018).

Figure 1 Map of Cambridge showing the locations of the AQMesh sensors, the reference monitors and the 305 road sources modelled (see online version for colours)



Background levels of NO_x were subtracted from the local monitored levels to remove any contribution from non-local sources; these “background” levels were taken from Defra AURN measurements, mainly from the station at Wicken Fen but from the station at St Osyth where Wicken Fen data were not available. The period analysed was 30 June 2016 to 30 September 2016. Wicken Fen is in a rural location approximately 15 km north east of Cambridge; St Osyth is in a rural location near the coast approximately 80 km south east of Cambridge.

The stages in the analysis were as follows: the dispersion of road emissions were modelled using ADMS-Urban for each hour of the three month period using meteorological data from the Andrewsfield weather station 40 km to the south-east of Cambridge and the road traffic emission inventory for Cambridge (a priori emissions inventory); the transport matrix, emissions vector and monitored data vectors were formed; the covariance matrices were constructed; the optimisation scheme was executed for each hour independently to determine the adjusted emissions for each hour; and finally the adjusted road emissions were re-modelled with ADMS-Urban keeping all other inputs unchanged. The optimisation was performed three times: firstly including both the reference monitor data and AQMesh sensor data in the optimisation scheme; secondly including only the AQMesh sensor data in the optimisation scheme; thirdly including only reference monitor in the optimisation scheme.

Table 2 Variance and co-variance uncertainty factors

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

The uncertainty and covariance factor values used to construct the covariance matrices are shown in Table 2. In this initial study these factors are taken to be constant across all sources, all reference monitors and all sensors and no account is taken of model error due to dispersion. It is assumed that the standard deviation σ represents the uncertainty in the emission or measurement and that this is proportional to the magnitude of the emission or measurement. The calculation of σ and the construction of the error covariance matrices \mathbf{B} and \mathbf{R} is described in equations (2) and (3) respectively.

$$i = [1, n]; j = [1, n]; \sigma_{B_i} = U_E |e_i|; B_{ij} = \begin{cases} \sigma_{B_i}^2 & i = j \\ U_{EF}^2 \sigma_{B_i} \sigma_{B_j} & i \neq j \end{cases} \quad (2)$$

$$\begin{aligned}
 i &= [1, k]; j = [1, k]; U_{O_i} = \begin{cases} U_{OR}, T_i = r \\ U_{OS}, T_i = s \end{cases}; \sigma_{R_i} = U_{O_i} |y_i|; \\
 U_{OF_{ij}} &= \begin{cases} U_{ORF} & T_i = T_j = r \\ U_{OSF} & T_i = T_j = s \\ 0 & T_i \neq T_j \end{cases}; \\
 R_{ij} &= \begin{cases} \sigma_{R_i}^2 & i = j \\ U_{OF_{ij}}^2 \sigma_{R_i} \sigma_{R_j} & i \neq j \end{cases}
 \end{aligned} \tag{3}$$

U_E is the fraction of the emission rate for each source that represents the uncertainty in the emissions; we have taken a value of 0.5 which is consistent with the uncertainty in reported NO_x emissions (e.g., Hood et al., 2018). It is assumed that a fraction U_{EF} of the error is systematic or correlated between two sources. For U_{EF} we take a plausible value of 0.4 which implies 40% of the error is correlated, for example error due to uncertainty associated with emissions factors which are used across all road sources to calculate emissions, whereas 60% is associated with road specific errors (e.g., traffic flow and speed).

U_{OR} and U_{OS} are fractions of the measured concentrations that represent the uncertainties in the observations at the reference monitors ($T = r$) and sensors ($T = s$) respectively. For the reference monitors we have assumed a value of 0.1 for the fractional uncertainty which is typical of quoted values (e.g., Pernigotti et al., 2013); for the sensors, collocation at the reference monitors suggested broadly comparable performance, however allowing for instrumental drift we have assumed a higher value of 0.3. We assume that there is zero error covariance between monitors of different types (e.g., between reference monitors and sensors) and we assume that a fraction U_{ORF} of reference monitor uncertainty U_{OR} is systematic and a fraction U_{OSF} of sensor uncertainty U_{OS} is systematic. It was assumed that the error covariance factors for both the sensors and reference instruments were small, which means that their influence on the calculations is very small.

Considering all the factors in Table 2 together we would expect that because $U_E \gg \gg U_{OR}$, the reference monitors may have a large influence on emissions which will extend beyond the immediate vicinity of the monitors because of the large value of U_{EF} . The influence of the sensors will be less because of the larger value of U_{OS} relative to U_E .

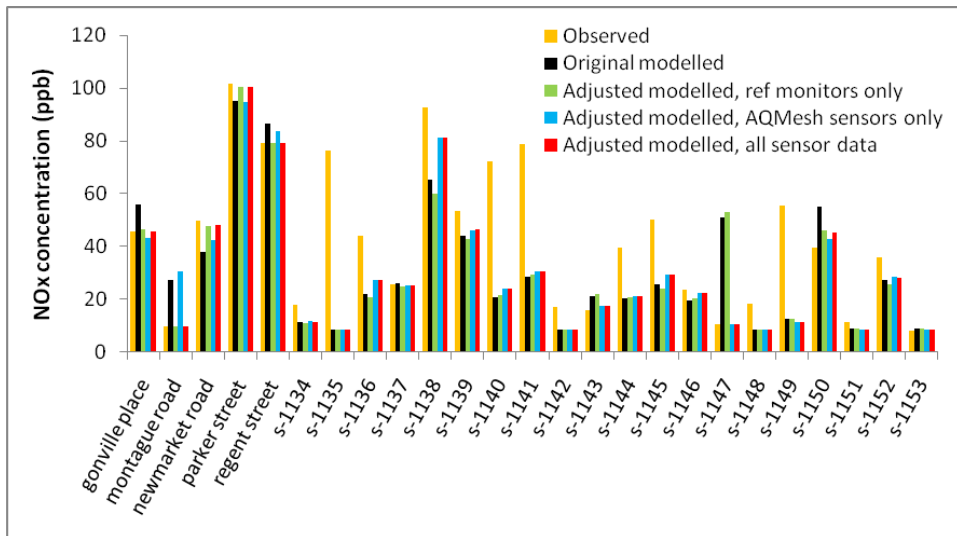
4 Results

The analysis of the case study results focuses on two aspects: firstly on how the modelled concentrations using adjusted emissions compare with observed concentrations and the original modelled values in the three cases; and secondly how the adjusted emissions compare with the original emissions.

4.1 Effect of the optimisation on modelled concentrations

Figure 2 shows an example for one hour only of modelled NO_x concentrations using adjusted emissions for each of the three cases compared with observed concentrations and the original modelled concentrations. At the reference monitors, when the reference monitors are included in the optimisation, the adjustment in emissions and hence concentrations are in all cases sufficient to ensure that the adjusted concentrations are in close agreement with observed concentrations; this is because the error in the observed concentrations at the reference monitors is assumed to be small (10%), both in absolute terms and relative to the assumed error of the emissions, so that they strongly constrain the emissions. However this is not always the case for sensor sites with sensors included in the optimisation (e.g., sites S1135, S1140 where there is little adjustment), or at the reference sites when only sensors are included in the optimisation (e.g., Montague Road); this is because the uncertainty of the sensors is assumed to be higher (30%). Note however that because of the assumed covariance between emissions from different roads that there is some adjustment in concentrations (sometimes small) at all sites.

Figure 2 Graph of NO_x concentration (ppb) for one hour of the simulation only (see online version for colours)

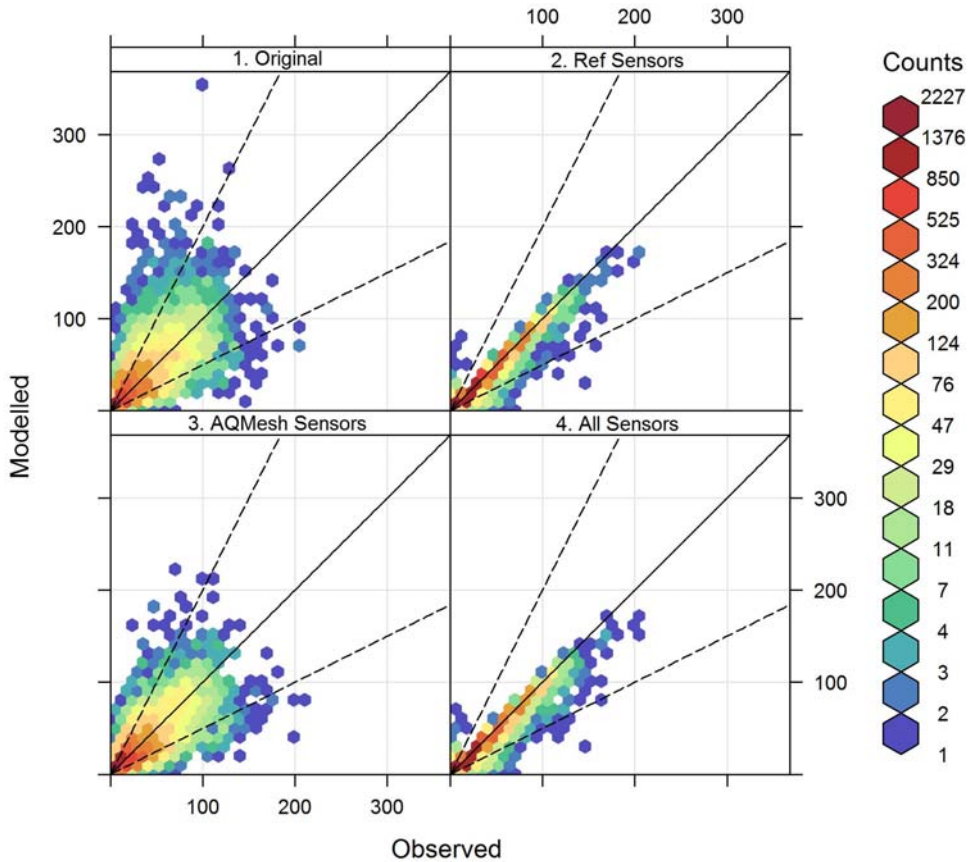


Note: Comparing observed levels with original modelled values and adjusted modelled values, where the adjustment either includes reference monitor data only, AQMesh data only or all sensor data.

To examine the effect of the optimisation on model performance, observed concentrations at the reference monitors were compared with modelled concentrations using: unadjusted emissions ('original'); emissions adjusted using reference monitor data ('adjusted, reference sensors'); emissions adjusted using sensor data only ('adjusted, AQMesh sensors') and emissions adjusted all sensors ('adjusted, all sensors'). Figure 3 shows scatter plots of the comparison; Table 3 shows model evaluation statistics for the same cases. Firstly the results show that, as expected, if the reference data are included in the optimisation then the model performance at the reference sites using the adjusted

emissions improves markedly. Of course, any monitor data being used for model validation should be excluded from the optimisation, but this result demonstrates that the scheme is behaving in the expected way. The few points above the $y = 2x$ line in this case represent data points that were omitted from the optimisation process because the monitored value was lower than the background concentration. The asymmetry in the scatter plots, where the reference monitors are used in the optimisation, is likely to be caused by the omissions of some sources other than road sources, the optimisation being unable to compensate for these omissions in some cases. The more important result is that if only the AQMesh sensor data are included in the optimisation the model performance at the reference sites improves noticeably, in particular the mean bias is reduced, is superior to that for the other two cases, and the correlation is increased.

Figure 3 Frequency scatter plots of modelled versus observed hourly NO_x concentrations (ppb) at the reference monitors for four emissions cases (see online version for colours)



Notes: Original emissions; adjusted emissions using reference monitor data only; adjusted emissions using AQMesh sensor data only; and adjusted emissions using all reference monitor and AQMesh sensor data. Results are shown for all hourly measurements over the study period. The solid black line represents $y = x$ and the dashed black lines represent $y = 0.5x$ and $y = 2x$.

Table 3 Model performance statistics at the reference sites for four emissions cases

Statistics		Original	Adjusted, reference monitors only	Adjusted, AQMesh sensors only	Adjusted, all sensors
Mean	Obs	31.2	31.2	31.2	31.2
	Mod	34.5	29.9	31.0	29.4
St. dev.	Obs	27.9	27.9	27.9	27.9
	Mod	31.0	26.6	27.0	26.1
MB (0)		3.30	-1.28	-0.23	-1.78
NMSE (0)		0.51	0.04	0.39	0.05
R (1)		0.70	0.98	0.75	0.97
Fac2 (1)		0.71	0.94	0.73	0.94

Notes: Original emissions; adjusted emissions using reference monitors only; adjusted emissions using AQMesh sensor data only; and adjusted emissions using all reference monitor and AQMesh sensor data. StDev is standard deviation, MB is mean bias, NMSE is normalised mean square error, R is correlation and Fac2 is the fraction of hourly model prediction points within a factor of 2 of observations. Numbers in brackets represent the perfect score for each statistic. Bold signifies the best statistic of the four cases.

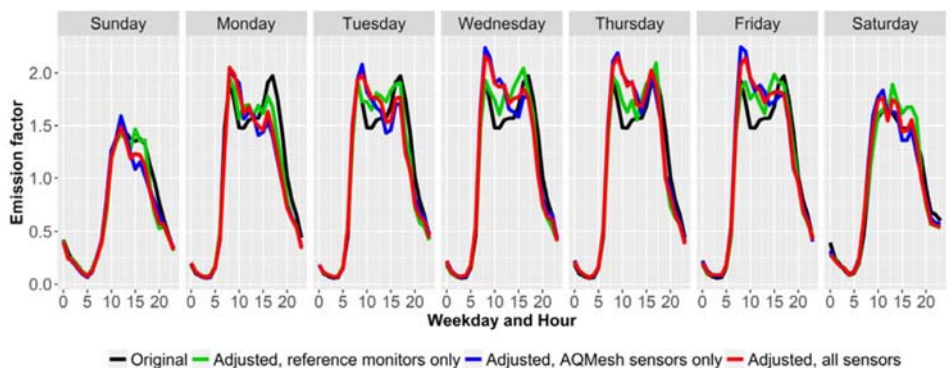
4.2 *Effect of the optimisation on emissions*

Whilst concentrations were recalculated from adjusted emissions for each source for each hour, in order to illustrate the broad effect of applying the optimisation scheme to the emissions, the average diurnal emission factors and average emission rates were calculated for the original emissions and for the three sets of adjusted emissions. Table 4 shows the emission rate average over all sources and over the measurement period. Figure 4a and Figure 4b compare the diurnal emission factors and Figure 5 shows a scatter plot of the change in the average emission rate for each road source for each of the cases. The table shows that the overall change in emissions is relatively modest, with the sensor-only case giving the largest change – a reduction for 90% of sources and an average change of -6.5%. This small change is perhaps to be expected since the emissions had already been adjusted to better reflect real world emissions. However Figure 4a shows that the changes in emissions for specific hours may be larger with the optimisation typically increasing the morning peak and reducing the evening peak in NO_x emissions. This effect is smaller when only the reference monitors are used in the optimisation, which may be connected to the fact that the reference monitors are located in the city centre whereas many of the sensors are on an arterial route with likely different diurnal cycles. Figure 4b also shows an example of the variability in calculated emissions as indicated by the standard deviation in the diurnal profile shown for each case for Mondays.

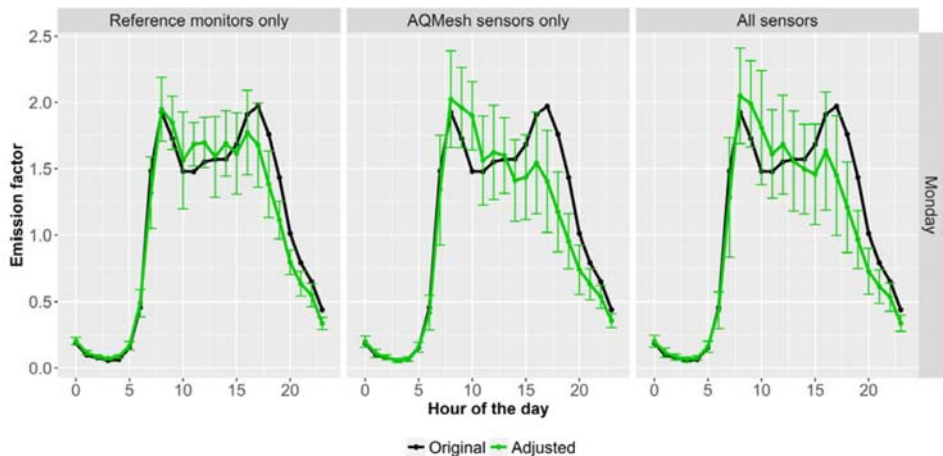
Table 4 Calculated mean emission rate of NO_x (g km⁻¹ s⁻¹) averaged over all sources for each case

	Mean	Change from original
Original	0.1552	
Reference monitors only	0.1551	-0.1%
AQMesh sensors only	0.1452	-6.5%
All sensors	0.1478	-4.8%

Figure 4 Comparison of mean diurnal emission factor profiles calculated from the original and adjusted emissions (see online version for colours)



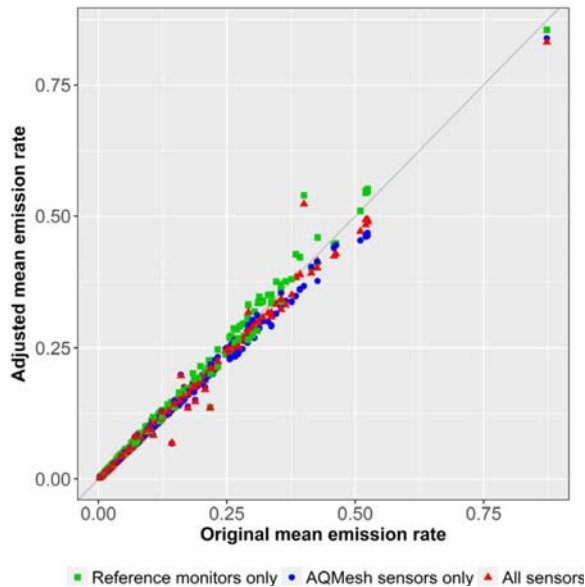
(a)



(b)

Notes: (a) The mean emission factors for each hour and each day are calculated over all road sources excluding those representing bus lanes. These are the emission factor profiles for British Summer Time (BST) expressed in UTC. (b) A comparison of mean diurnal emission factor profiles calculated from the original and adjusted emissions, in this case showing the results for an example weekday (Monday). The ‘Adjusted’ plots also show the standard deviation of the calculated mean. These are the emission factor profiles for British Summer Time (BST) expressed in UTC.

Figure 5 Scatter plot of adjusted versus original mean NO_x emission rates (g km⁻¹ s⁻¹) (see online version for colours)



Note: The $y = x$ line is shown in grey.

5 Conclusions

The optimisation scheme presented here, using inversion techniques to modify pollution emission rates based on sensor data, has been shown to predict changes to both the magnitude and diurnal patterns of emissions which in turn improves the accuracy of modelled concentrations despite a relatively simple representation of error covariance and sources other than roads being treated as ‘background’ in the case study presented. Indicators of emissions error covariance that were not yet accounted for include: distance between sources, differences in vehicle types between roads and meteorological factors such as temperature. Multiple pollutants and different source types also need to be accounted for; in the study presented here only road source emissions of NO_x have been considered, but a comprehensive ADMS-Urban modelling study of an urban area would also include pollutants such as PM₁₀ and PM_{2.5}, and point, line, area and volume sources in addition to road sources. Defining the error covariance between different pollutants and between difference source types presents a challenge, but the initial results presented here suggest that the approach presented could make use of large networks of low-cost sensors both to optimise/verify emissions inventories and to improve dispersion model results.

Acknowledgements

We are very pleased to acknowledge AQMesh who loaned the AQMesh sensor pods for this research at no cost.

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