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RESEARCH ARTICLE

TRANSFERABILITY OF AN APPROACH TO CALIBRATE BACKGROUND AIR POLLUTION CONCENTRATIONS

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ABSTRACT

The aim of this research paper is to investigate the transferability of an approach to calibrate background air pollution concentrations for improving the accuracy of air pollution modelling results. Using the central area of the City of Nottingham in the UK as a case study, an air pollution model in ADMS-Roads was created for investigating the applicability of this approach to a study area different from the one that was used in the initial development of this approach. The iterative application of this approach to the input background concentrations effectively reduced the error between the annual mean, and the hourly, calculated and monitored air pollution concentrations. This confirmed the transferability of this approach to the Nottingham City Centre study area. A mathematical algorithm was developed, and implemented by computer programming, to improve further the effectiveness of this approach. The application of this algorithm to the calibrated background concentrations reduced further the error between the hourly calculated and monitored air pollution concentrations.

INTRODUCTION

Ambient air quality in a geographic area is usually evaluated by modelling the air quality in that area. When air pollution levels exceed national standards, air pollution modelling is used to evaluate the effectiveness of the proposed air quality action plans. Also, it can be used to evaluate the national plans such as local transport plans (NCC and NCC, 2006). Accurate annual mean and hourly air quality predictions are required for the comparison with the air quality objectives, which are usually in the form of annual mean and hourly air pollution concentrations (AEA, 2010). Recent air pollution dispersion modelling research validates air quality predictions be determining the error between calculated and monitored air pollution concentrations. However, the potential sources of this error has not been investigated in this recent research (Cai and Xie, 2010, Ginnebaugh *et al*., 2010, Jain and Khare, 2010, Majumdar *et al*., 2009, Parra *et al*., 2010). Nottingham City Council calibrated the results of its air pollution dispersion model using an adjustment factor (PCS, 2008). The factor was the average ratio of monitored to calculated annual mean concentrations at three monitoring sites. The multiplication of the model results by this factor improved the annual mean results, but the hourly calculated results were not improved.

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Another approach used the hourly predictions of ADMS-Urban and the hourly observations for the first half of 1993 to derive a multiplicative adjustment factor (Namdeo *et al*., 2002). The output results for the second half of 1993 were multiplied by the factor, and were compared to the corresponding observations. Although the long-term results were improved over the second half of 1993, this approach did not show how much improvement was achieved on the short-term level. Moreover, Cambridge Environmental Research Consultants (CERC), the developers of ADMS software, has advised that the multiplication of the model results by such an adjustment factor should be avoided (CERC, 2009). Instead, CERC has recommended the adjustment of the model set-up, such as input data and modelling options, until the calculated results agree with the monitored concentrations.

Nottingham City Council used the approach developed by DEFRA (2009) to verify the annual mean NO_2 results of ADMS-Urban (PCS, 2010). If NO_2 results of the model do not fit the monitored concentrations, the approach states that NO_X (not NO_2) concentrations should be verified and adjusted. Using the LAQM Tools – NO_X to NO_2 spreadsheet, the adjusted results of NO_X and background NO_2 concentrations are used to derive the adjusted calculated total annual mean NO_2 concentrations (DEFRA, 2010). The calculated annual mean NO_2 concentrations, adjusted using this approach, did not fit the monitored annual mean NO_2 concentrations. In addition, this approach only adjusts the calculated annual

mean concentrations, and is not suitable for the adjustment of hourly concentrations (CERC, 2009). Li *et al*. (2010) applied a genetic algorithm to calibrate the emission rate inputs to an air pollution model. The application of this approach resulted in a non-significant reduction in the error between short-term calculated and monitored PM_{10} concentrations. The calculated results of the model, using the calibrated emission rates, were not validated against monitored concentrations, independent of the calibration process. The runtime of the genetic algorithm extended to several weeks on a single PC. This runtime, plus the model runtime which may extend to several days (Barrett and Britter, 2008, Barrett and Britter, 2009), constitutes a very expensive computing time. Zahran (2013) introduced a mathematical approach for adjusting the air pollution model set-up by the calibration of input background concentrations. For the broad variety of air pollution dispersion models, background concentrations are some of the most important input data (Venegas and Mazzeo, 2006). They account for uncertainties in the number and definition of input air pollution sources to the model. A 3D visualisation approach was used for the visualisation of the model output data in a 3D digital city model (Zahran *et al*., 2012, Zahran *et al*., 2010). The calibration of background concentrations improved significantly the accuracy of the annual mean and hourly model results. In addition, the application of this approach reduced significantly the computing time. This research paper investigates the transferability of this approach to a study area different from the one that was used in the initial development of this approach.

MATERIALS AND METHODS

As a study area, Nottingham City Centre Air Quality Management Area (AQMA) was used to set-up an air pollution model in ADMS-Roads software version 2.3 for investigating the transferability of the calibration approach. ADMS-Roads software was developed by CERC (CERC, 2006). City Centre AQMA is an urban study area in the city of Nottingham, as shown in Fig. 1, with NO_2 levels exceeding the permissible levels (PCS, 2001). NO_2 was selected as the modelled air pollutant. 2006 was selected as the modelling year of the air pollution model due to data availability for this year. The significant industrial air pollution sources relevant to the City Centre AQMA were identified and their emission rates were obtained from Nottingham City Council, which also provided the traffic flow and speed data of the road network in the study area. Since the road network was very dense, a GIS-based approach was used to automating the collection of geospatial road network input data to the air pollution model (Zahran *et al*., 2011). The Nottingham Watnall Weather Station (MO, 2010) provided the 2006 hourly sequential meteorological data which included surface temperature, wind speed at 10-metre height above the ground surface, wind direction, precipitation, cloud cover and degree of humidity.

The 2006 annual mean and hourly monitored NO_X, NO_2 and O_3 concentrations by the Automatic Urban and Rural Network (AURN) and Carter Gate continuous monitoring stations, located in the City Centre AQMA as shown in Fig. 1, were provided by Nottingham City Council. The 2003 DMRB traffic emission factors (DMRB, 2007), built-in in ADMS-Roads, were used to derive the traffic emission rates from the traffic flow and speed data. The Chemical Reaction Scheme (CRS) was used to model the atmospheric conversion of NO_X to NO_2 due to a number of chemical reactions with background O_3 (CERC, 2006). Modelling these atmospheric reactions was necessary to get accurate NO_2 results, so NO_X and O_3 were modelled in addition to NO_2. However, using this chemical scheme requires inputs for NO_2, NO_X and O_3 background concentrations. Therefore, Nottingham City Council provided the 2006 hourly sequential NO_2, NO_X and O_3 concentrations monitored by the Rochester air quality monitoring station. This is a rural monitoring station remote from the City Centre AQMA and far from urban air pollution, and hence it was advisable to use its monitoring data as the input background concentrations to the air pollution model to avoid double counting (CERC, 2009).

Calibration and validation of the background concentrations

Two output receptors were defined in the air pollution model at the geographical location of the AURN and Carter Gate monitoring stations. With reference to Run 1 in Table 1, the calculated 2006 annual mean NO_X and NO_2 concentrations underestimated the monitored ones by 45.4% and 26% respectively at the AURN monitoring station. The calculated 2006 annual mean of O_3 concentrations overestimated the monitored one by 17.6% at the AURN monitoring station. In addition, the calculated 2006 annual mean NO_X and NO_2 concentrations underestimated the monitored ones by 31.1% and 23% respectively at the Carter Gate monitoring station. This indicated the need for the calibration of the rural background concentrations.

RESULTS AND DISCUSSION

The calibration process started with the macro-calibration of NO_X, NO_2 and O_3 background concentrations, as explained by Zahran (2013). Since O_3 concentrations were not monitored by the Carter Gate monitoring station, the AURN-monitored NO_X, NO_2 and O_3 concentrations were used for the calibration of the background concentrations. The Carter Gate-monitored NO_X and NO_2 concentrations were kept independent of the calibration process for the validation of calculated concentrations at the Carter Gate output receptor. The 2006 annual mean NO_2, NO_X and O_3 concentrations calculated using the uncalibrated rural background concentrations were substituted, along with the 2006 annual means of the AURN-monitored NO_2, NO_X and O_3 concentrations, into Equations 8, 9 and 10 in Zahran (2013) to evaluate the macro-calibration adjustment values for the rural background concentrations. Using the macro-calibrated background concentrations greatly improved the macro-validation results of the air pollution model at both the AURN and Carter Gate monitoring stations, as indicated by the results of run 2 in Table 1.

The uncalibrated rural background concentrations were used for running the air pollution model in order to output the 2006 hourly calculated NO_2 concentrations at the AURN and Carter Gate monitoring stations. This was for the micro-validation of the model before any calibration as shown in Fig. 2 and Fig. 3. Then for the micro-validation after the macro-calibration, the model was run with the macro-calibrated background concentrations to output the 2006 hourly calculated NO_2 concentrations at the AURN and Carter Gate monitoring stations. Fig. 4 and Fig. 5 illustrate the micro-validation results of running the model after the macro-calibration of rural

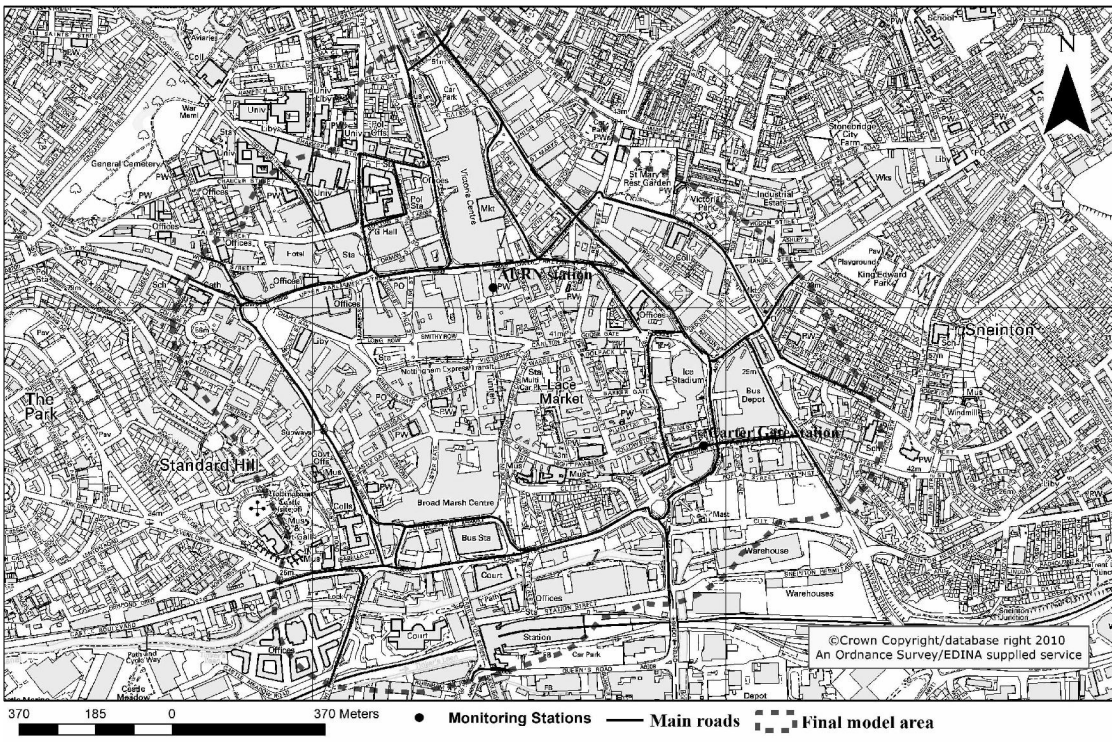

Figure 1. Central Nottingham Air Pollution Model Application Area

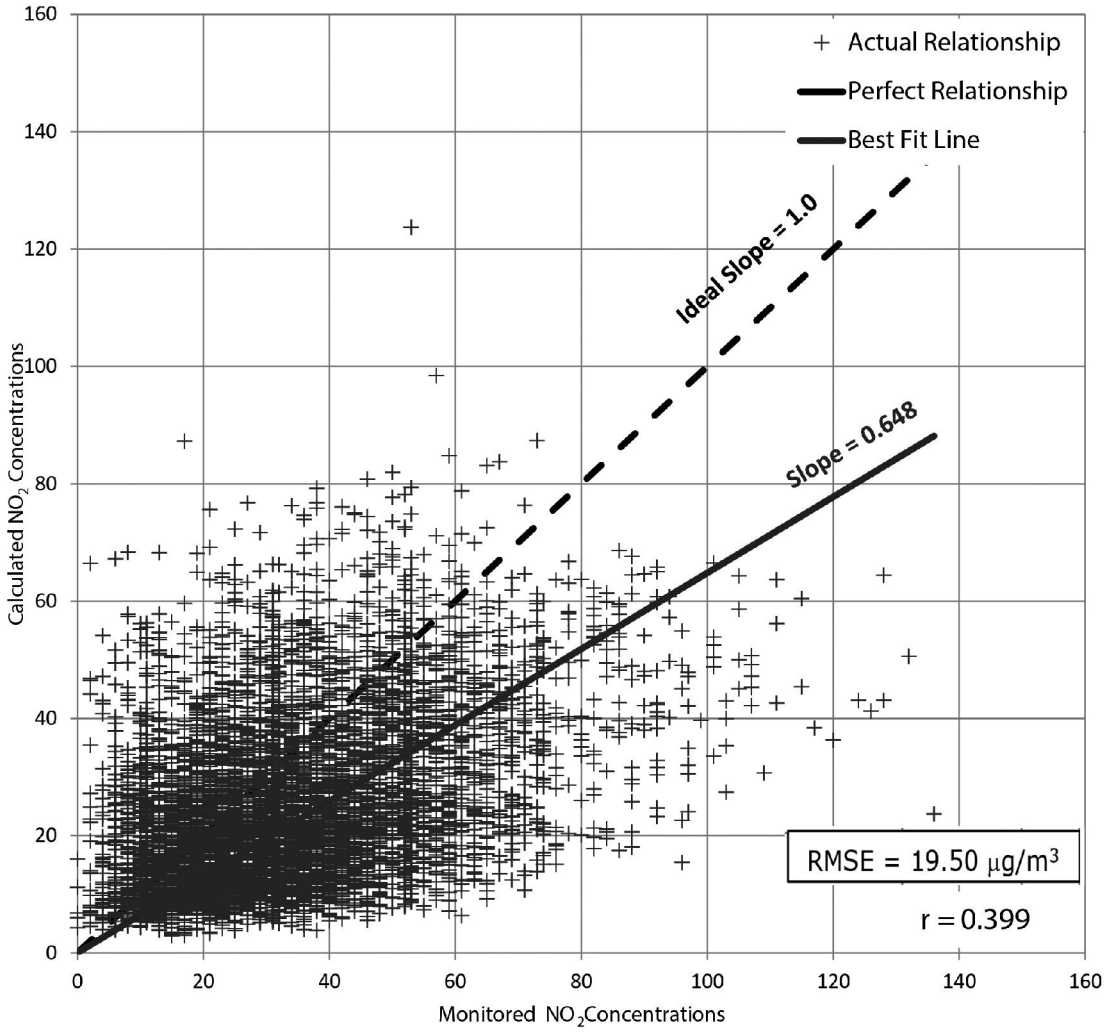

Figure 2. Scatter Diagram of Hourly NO_2 Concentrations at the AURN Station before Calibration

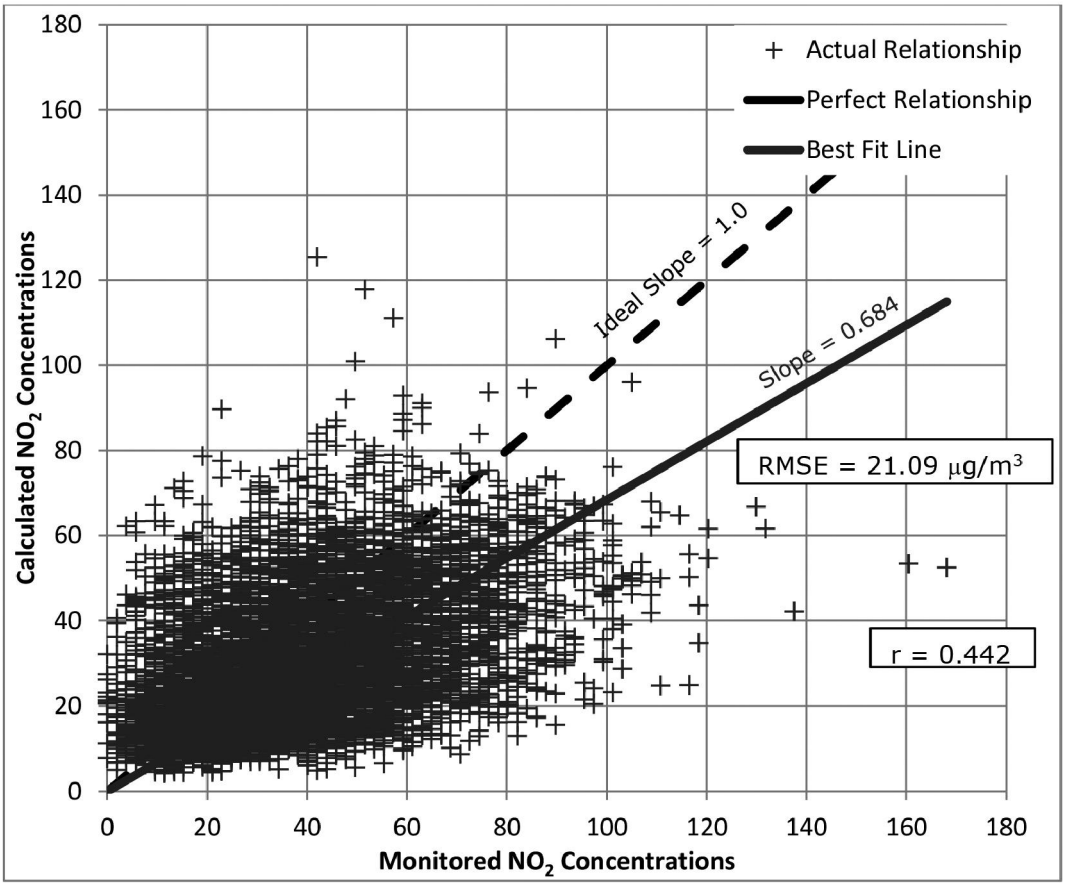

Figure 3. Scatter Diagram of Hourly NO_2 Concentrations at the Carter Gate Station before Calibration

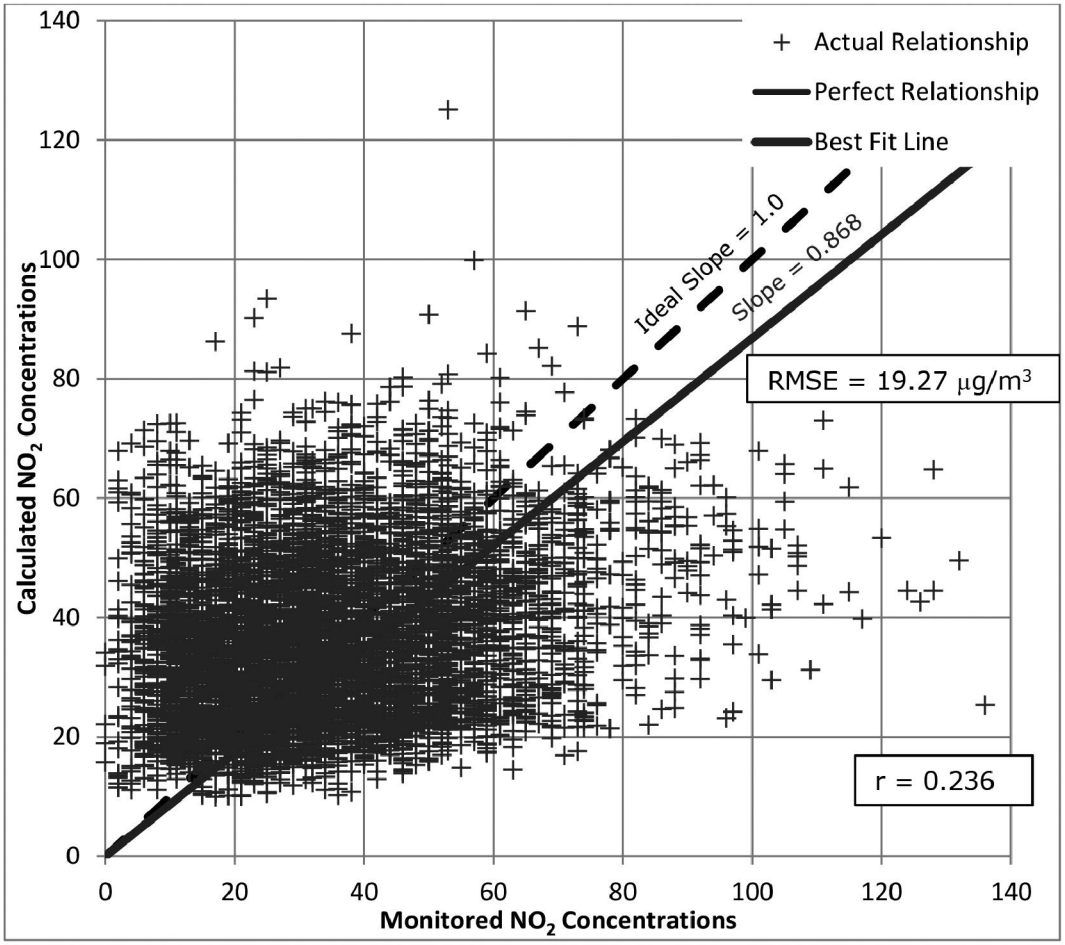

Figure 4. Scatter Diagram of Hourly NO_2 Concentrations at the AURN Station after Macro-calibration

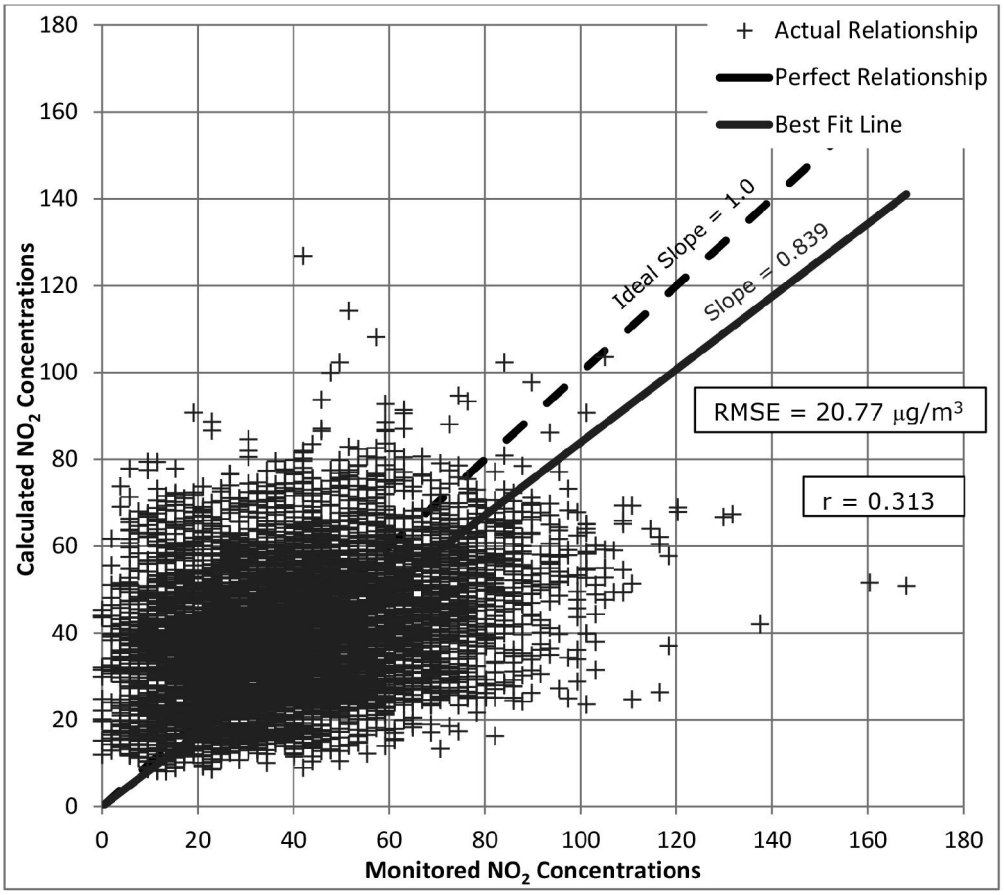

Figure 5. Scatter Diagram of Hourly NO_2 Concentrations at the Carter Gate Station after Macro-calibration

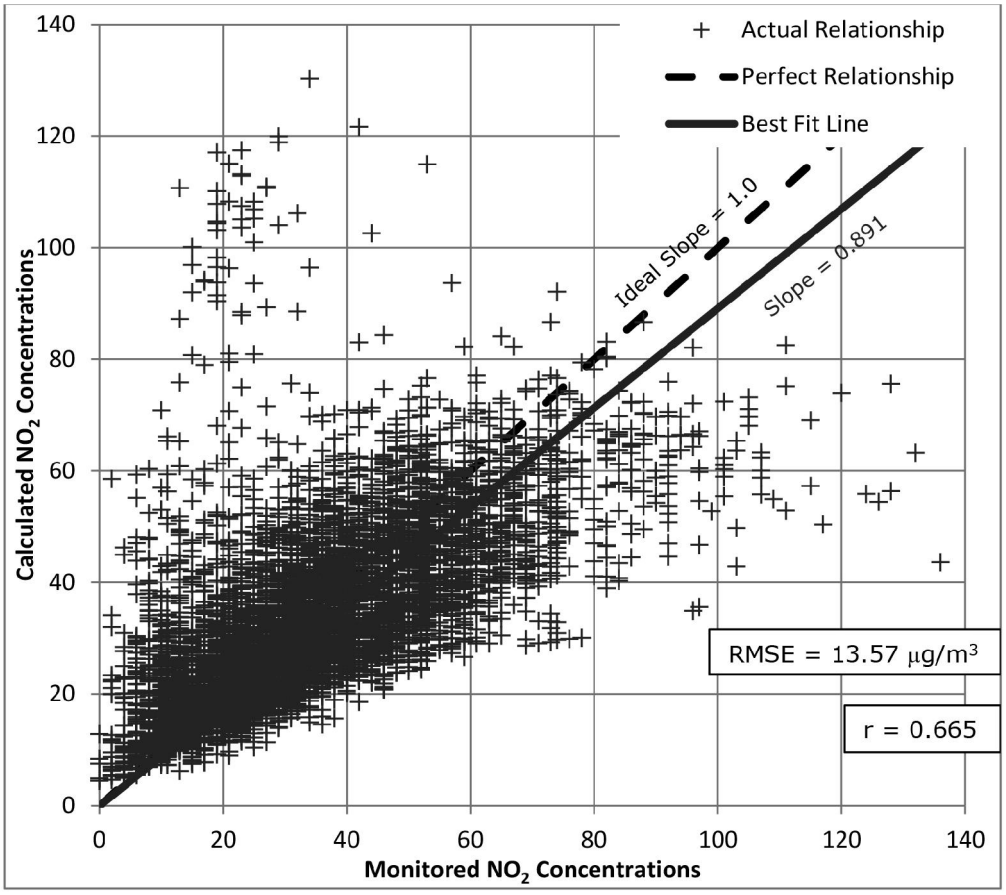

Figure 6. Scatter Diagram of Hourly NO_2 Concentrations at the AURN Station after the Micro-calibration based on Run 2

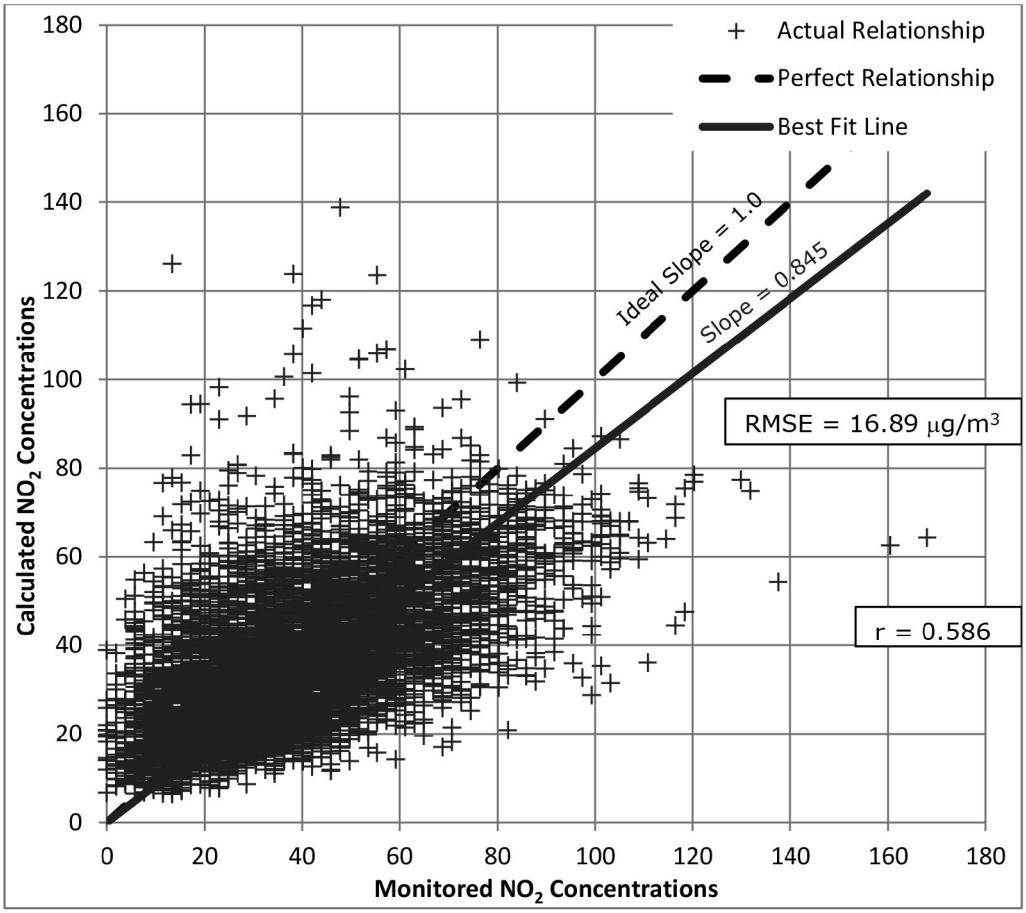

Figure 7. Scatter Diagram of Hourly NO_2 Concentrations at the Carter Gate Station after the Micro-calibration based on Run 2

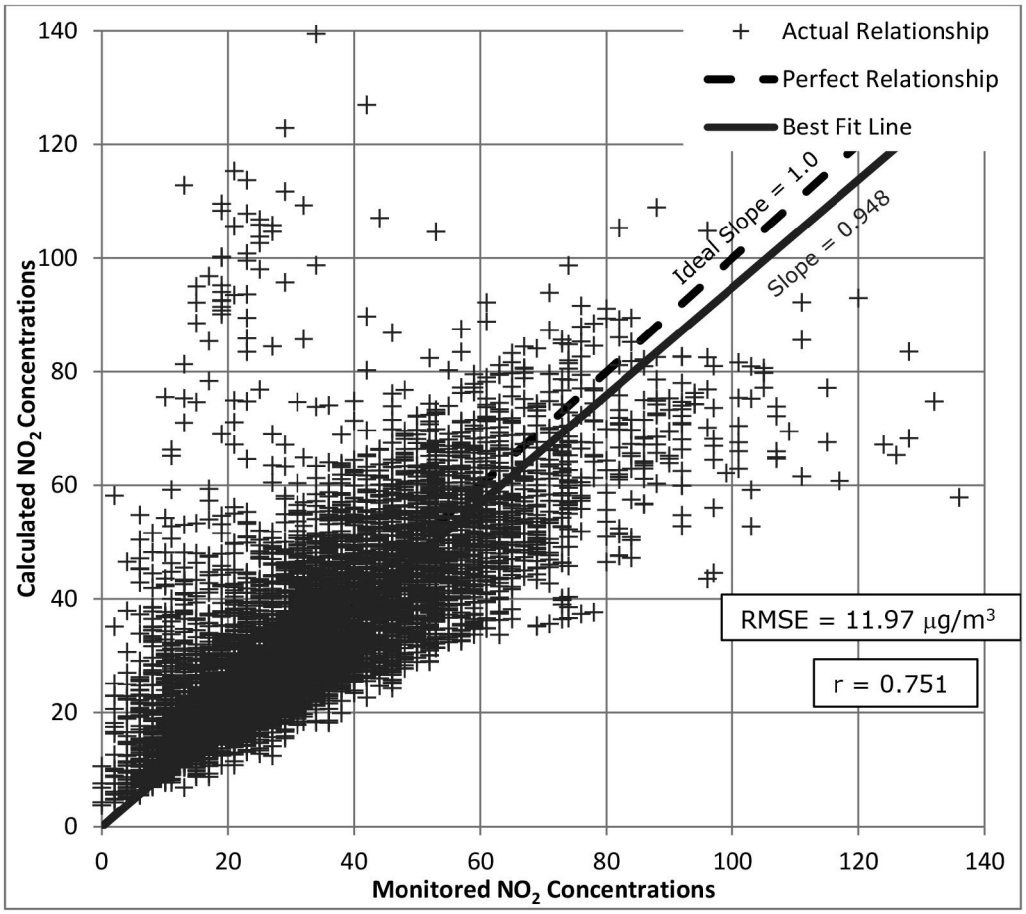

Figure 8. Scatter Diagram of Hourly NO_2 Concentrations at the AURN Station after the Micro-calibration based on Run 9

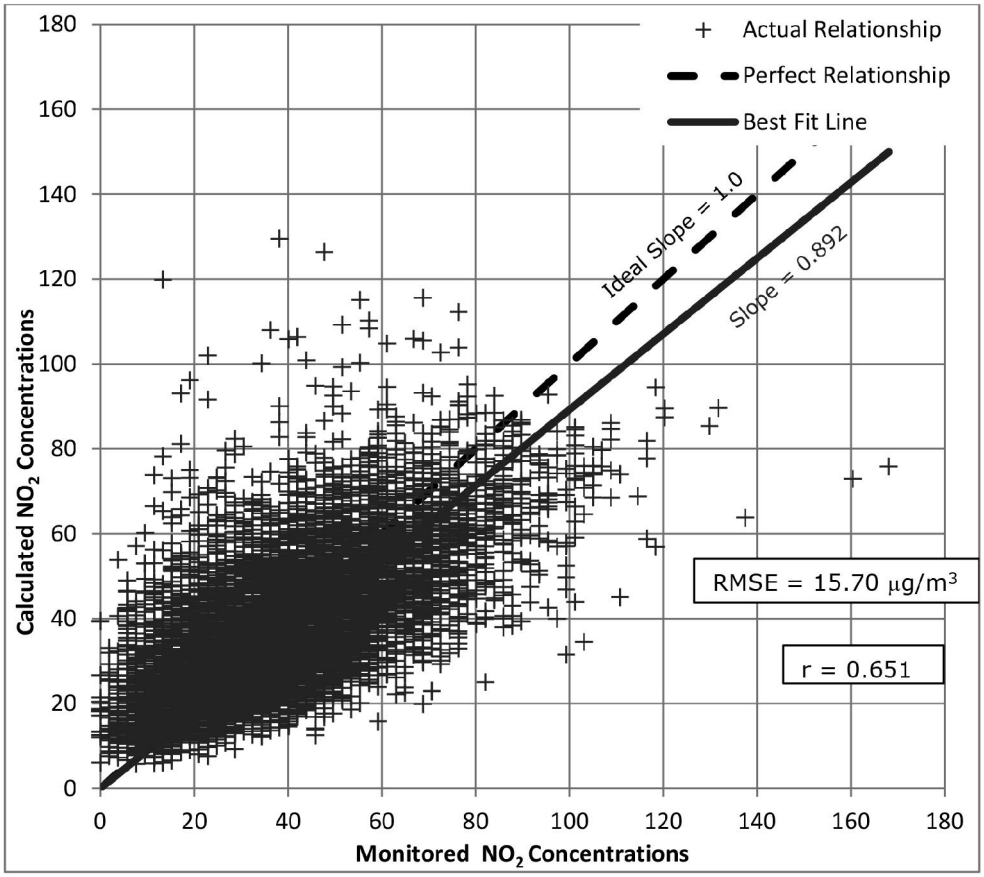

Figure 9. Scatter Diagram of Hourly NO_2 Concentrations at the Carter Gate Station after the Micro-calibration based on Run 9

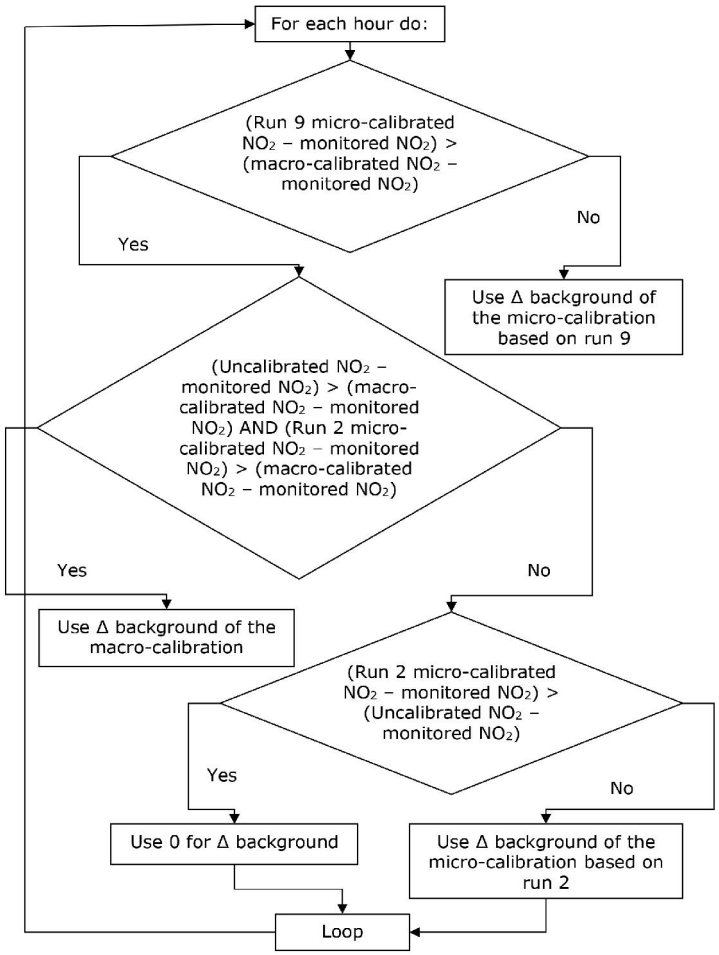

Figure 10. Adjustment Flowchart of Micro-Calibrated Background Concentrations based on Run 9

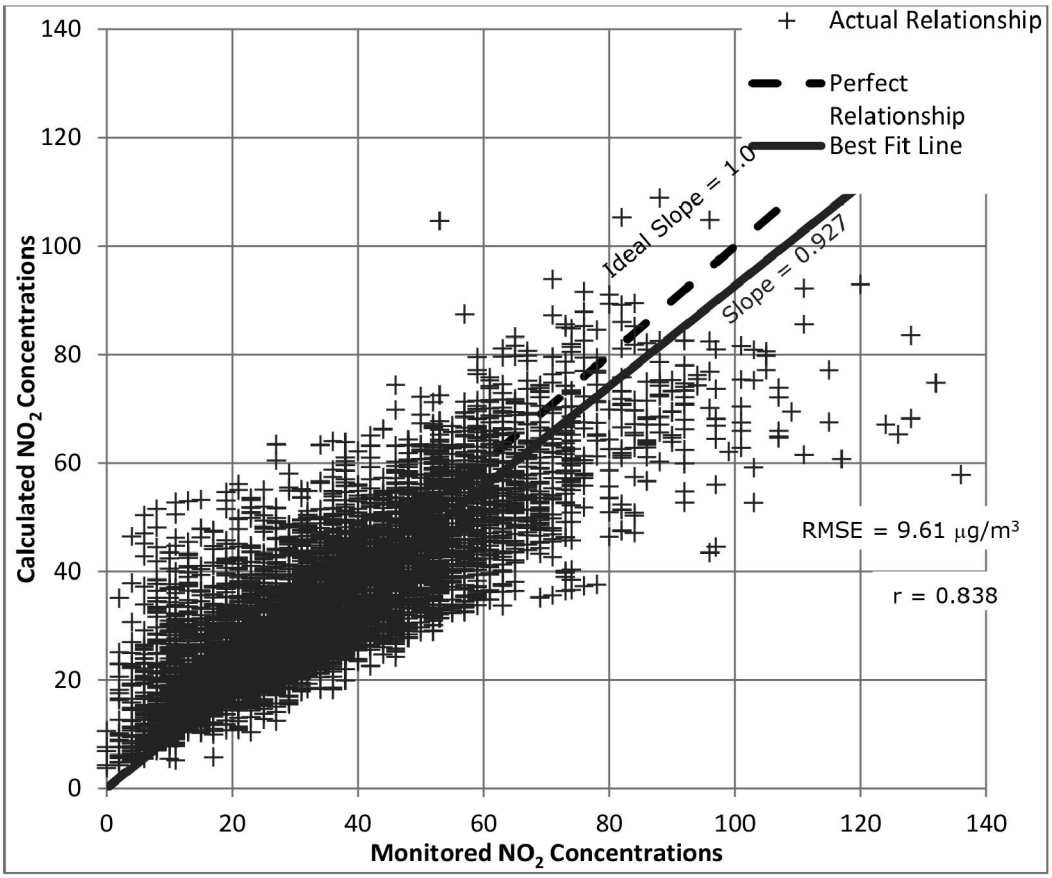

Figure 11. Scatter Diagram of Hourly NO_2 Concentrations at the AURN Station after the Micro-calibration based on Run 9 Adjusted

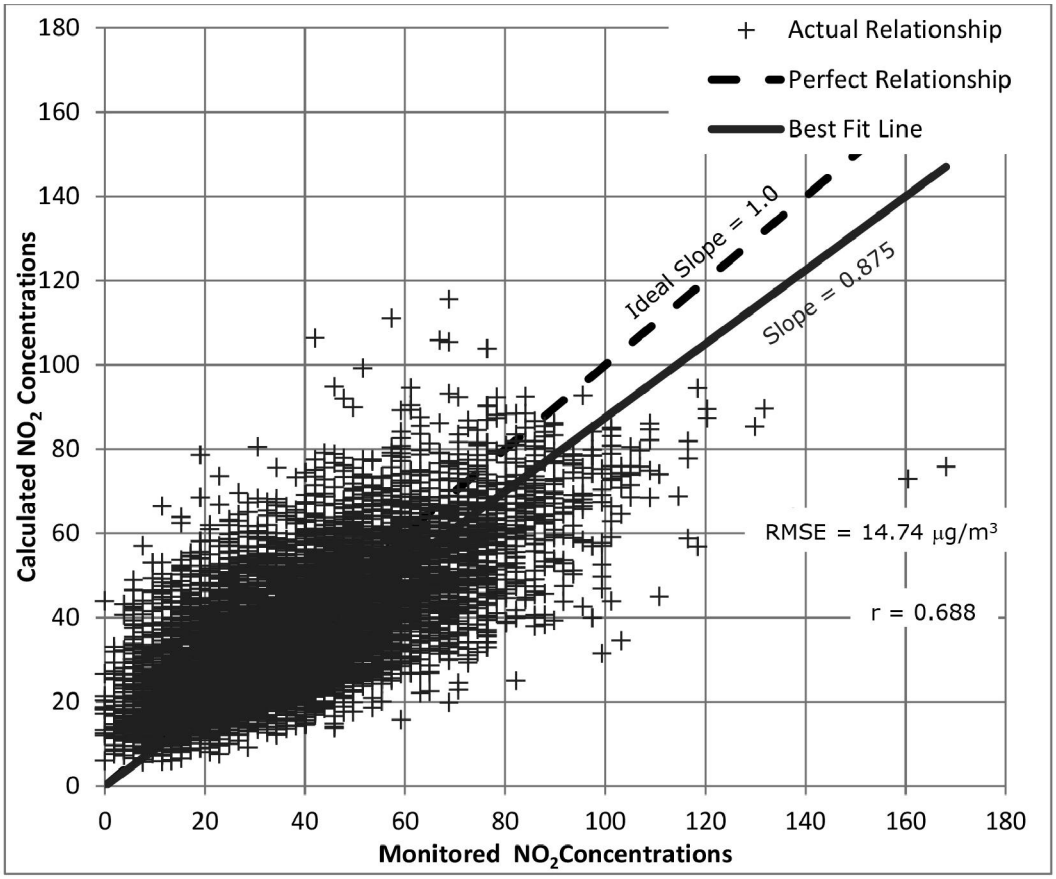

Figure 12. Scatter Diagram of Hourly NO_2 Concentrations at the Carter Gate Station after the Micro-calibration based on Run 9 Adjusted

Table 1. Macro-calibration Results of the City Centre Air Pollution Model

RUN 1	Background	Δ background	Calculated Concentrations at AURN	Δ Calculated	Target concentrations at AURN	Calculated Concentrations at Carter Gate	Target concentrations at Carter Gate
NO_2	0	0	24.86	0	33.6	30.34	39.4
NO_x	0	0	34.16	0	62.56	59.16	85.9
O_3	0	0	44.84	0	38.54		
RUN 2	**Background**	**Δ background**	**Calculated Concentrations at AURN**	**Δ Calculated**	**Target concentrations at AURN**	**Calculated Concentrations at Carter Gate**	**Target concentrations at Carter Gate**
NO_2	+1.406	+1.406	35.38	+10.517	33.6	39.20	39.4
NO_x	+28.41	+28.41	62.57	+28.407	62.56	87.57	85.9
O_3	-2.571	-2.571	32.85	-11.982	38.54		
RUN 8	**Background**	**Δ background**	**Calculated Concentrations at AURN**	**Δ Calculated**	**Target concentrations at AURN**	**Calculated Concentrations at Carter Gate**	**Target concentrations at Carter Gate**
NO_2	+3.406	+2.000	36.76	+11.898	33.6	40.75	39.4
NO_x	+28.41	0	62.57	+28.407	62.56	87.57	85.9
O_3	-1.571	+1.000	34.54	-10.299	38.54		
RUN 9	**Background**	**Δ background**	**Calculated Concentrations at AURN**	**Δ Calculated**	**Target concentrations at AURN**	**Calculated Concentrations at Carter Gate**	**Target concentrations at Carter Gate**
NO_2	+3.406	0	37.23	+12.371	33.6	41.31	39.4
NO_x	+28.41	0	62.57	+28.407	62.56	87.57	85.9
O_3	-0.500	+1.071	36.01	-8.823	38.54		

Table 2. Micro-calibration Development Stages of the City Centre Air Pollution Model

case description	Receptor name	annual mean NO_x		annual mean NO_2		annual mean O_3		uncalibrated RMSE	macro-calibrated RMSE	micro-calibrated RMSE
		calculated	monitored	calculated	monitored	calculated	monitored			
based on run	AURN	62.81	62.56	32.79	33.60	36.47	38.54	19.50	19.27	13.57
2	Carter Gate	87.73	85.90	36.87	39.40	34.83	–	21.09	20.77	16.89
based on run	AURN	62.59	62.56	33.66	33.60	37.37	38.54	19.50	19.27	12.16
8	Carter Gate	87.54	85.90	37.80	39.40	–	–	21.09	20.77	15.82
based on run	AURN	62.61	62.56	34.13	33.60	38.18	38.54	19.50	19.27	11.97
9	Carter Gate	87.55	85.90	38.29	39.40	36.44	–	21.09	20.77	15.70
Based on run	AURN	61.84	62.56	33.27	33.60	38.18	38.54	19.50	19.27	9.61
9 adjusted	Carter Gate	86.82	85.90	37.60	39.40	36.28	–	21.09	20.77	14.74

background concentrations. The macro-calibration of the background concentrations slightly improved the micro-validation results at the AURN monitoring station, as implied by the comparison between the values of the Root Mean Square Error (RMSE) in Fig. 2 and Fig 4. In addition, the comparison between the values of RMSE in Fig. 3 and Fig. 5 confirmed this slight improvement in the micro-validation results of the model at the independent receptor point of the calibration process, the Carter Gate monitoring station. This indicated the need for the application of the micro-calibration strategy in order to improve effectively the micro-validation results of the air pollution model. The 2006 hourly sequential rural background concentrations, monitored concentrations and the calculated concentrations at the AURN monitoring station before any calibration were used along with the macro-calibration results, corresponding to run 2 in Table 1, for the application of Equations (12), (14) and (15) given in Zahran (2013). These equations were applied to generate the micro-calibrated 2006 hourly sequential NO_2, NO_X and O_3 background concentrations. Running the air pollution model with these background concentrations significantly improved the micro-validation results at both the AURN and Carter Gate monitoring stations as shown in Fig. 6 and Fig. 7. The air pollution model (based on run 2) with these micro-calibrated background concentrations underestimated both the annual means of monitored NO_2 and O_3 concentrations at the AURN monitoring station as shown in Table 2. This underestimation tendency was confirmed by the underestimation of the annual mean of monitored NO_2 concentrations at the calibration-independent Carter Gate monitoring station. This indicated the need for the trial and error macro-calibration approach, explained in Zahran (2013), to undertake additional runs of ADMS-Roads, beyond run 2, as shown in Table 1. The purpose of these additional runs was to overestimate the annual mean NO_2 and O_3 concentrations after the macro-calibration, so that they would be well estimated after the micro-calibration based on these additional macro-calibration runs, at the AURN monitoring station. Running the model with micro-calibrated background concentrations based on the results of these additional macro-calibration runs improved the macro-validation of the model, as shown in Table 2. Moreover, the micro-calibration based on these additional macro-calibration runs improved further the micro-validation of the model results as shown in Fig. 8 and Fig. 9.

The micro-calibration development, from run 2 to run 9, increased the error between the calculated and monitored NO_2 concentrations at many hours, as implied by the comparison between the scatter in the overestimated points on the upper left side of Fig. 6 and Fig. 8. This increase in the error at many hours was also indicated by the comparison between the scatter in the overestimated points on the upper left side of Fig. 7 and Fig. 9. The potential reason for such unexpected behaviour of the micro-calibration process at these hours was explained, but not resolved, in Zahran (2013). In addition, the number of these hours from the air pollution model of Nottingham City Centre was higher than the number of these hours from the air pollution model of Zahran (2013).

Therefore, a mathematical algorithm was developed and implemented by VBA in MS Excel in order to mitigate this error as shown in Fig. 10. The adjustment of micro-calibrated background concentrations based on run 9, according to the implementation of this mathematical algorithm, mitigated the above-mentioned error and improved further the micro-validation results of the City Centre air pollution model as shown in Fig. 11 and Fig. 12.

Conclusions

The macro-calibration of background concentrations strategy, introduced in Zahran (2013), reduced effectively the error between the calculated and monitored annual means of NO_X, NO_2, and O_3 concentrations at the Nottingham City Centre study area, shown in Fig. 1. The iterative application of the micro-calibration equations, initially developed by Zahran (2013), reduced effectively the error between the calculated and monitored annual means of NO_X, NO_2, and O_3 concentrations, and also the error between the hourly calculated and monitored NO_2 concentrations. This indicated the transferability of the calibration of background concentrations approach, developed by Zahran (2013), to a study area different from the area that was used for the initial development of this approach. Despite of being a dense road network, the hourly and monthly traffic profiles of the road network in Nottingham City Centre were not included in the air pollution model due to the lack of detailed traffic data. Further research is recommended to investigate the impact of including the monthly and hourly traffic profiles on the micro-validation of an air pollution model that has a large number of road sources. This is to correlate between the number of road sources with traffic profiles in the air pollution model and the possible reduction in the RMSE between the hourly calculated and monitored NO_2 concentrations. The mathematical algorithm, implemented by VBA in MS Excel as shown in Figure 10, was helpful to eliminate the increase in the error between the calculated and monitored NO_2 concentrations at some hours after the micro-calibration at these hours. The application of this mathematical algorithm after the final iteration of the micro-calibration improved further the micro-validation of the air pollution model.

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