

## Calibration of Background Concentrations versus the Use of Grid Sources in Air Pollution Dispersion Modelling

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### ABSTRACT

*The aim of this research paper is the comparison of an approach to calibrate background air pollution concentrations to the use of grid air pollution sources for improving the performance of air pollution models. Using the Dunkirk area of the City of Nottingham in the UK as a case study, an air pollution model in ADMS-Urban was created for this comparison. First, air pollution dispersion in the study area was modelled using grid sources and rural background concentrations. Then, it was modelled using calibrated background concentrations. For the two model set-ups, the air pollution model was validated by comparing both the hourly and annual means, of monitored and calculated concentrations by the model. The output hourly and annual mean results of the air pollution model with calibrated background concentrations were more accurate than those of the air pollution model with grid sources and rural background concentrations. The runtime of the air pollution model with calibrated background concentrations was much less than that of the air pollution model with grid sources and rural background concentrations.*

**Keywords:** Calibration, Background concentrations, Modelling, Air pollution

### 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 proposed air quality action plans. Also, it can be used to evaluate 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 by determining the error between calculated and monitored air pollution concentrations. However, the potential sources of this error has not been investigated by 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.

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<sub>2</sub> results of ADMS-Urban (PCS, 2010). If NO<sub>2</sub> results of the model do not fit the monitored concentrations, the approach states that NO<sub>x</sub> (not NO<sub>2</sub>) concentrations should be verified and adjusted. Using the Local Air Quality Management (LAQM) Tools – NO<sub>x</sub> to NO<sub>2</sub> spread sheet, adjusted results of NO<sub>x</sub> and background NO<sub>2</sub> concentrations are used to derive adjusted calculated total annual mean NO<sub>2</sub> concentrations (DEFRA, 2010). The calculated annual mean NO<sub>2</sub> concentrations, adjusted using this approach, did not fit the monitored annual mean NO<sub>2</sub> 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<sub>10</sub> 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 personal computer. 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.

A grid air pollution source in ADMS-Urban model consists of a matrix of identically sized cells, where each can have a different emission rate (CERC, 2006). Concentrations calculated using a grid source is modelled as if each cell in the grid source was modelled as an individual volume source, which reduces significantly the model runtime. The trajectory model of the Chemical Reaction Scheme (CRS) is used along with a grid air pollution source in ADMS-Urban to adjust the background concentrations in the main model domain, the model application area, on the basis of the grid source emissions. This converts the rural background concentrations within the model application area to urban background concentrations, accounting for residual, poorly-defined or diffused emissions in urban areas, which cannot be entered explicitly into the air pollution model. This reduces effectively the error between monitored and calculated concentrations by the air pollution model.

Zahran (2013a) introduced a mathematical approach for adjusting the air pollution model set-up by the calibration of input background concentrations. This approach offered two options for the calibration of input background concentrations: macro-calibration and micro-calibration. Macro-calibration refers to the adjustment of rural background concentrations, so that the error between the annual means of calculated and monitored air pollution concentrations can be effectively reduced. Micro-calibration refers to the adjustment of rural background concentrations so that the error between not only the annual means of, but also the hourly, calculated and monitored air pollution concentrations can be effectively reduced. 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., 2010; Zahran et al., 2013). 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 runtime of the model. Also, this approach was found transferrable to study areas different from the one that was used in its initial development (Zahran, 2013b). This research paper compares the application of this mathematical approach to the use of grid sources in air pollution dispersion modelling in terms of the accuracy of output results and the model runtime.

## MATERIALS & METHODS

Dunkirk Air Quality Management Area (AQMA) was used as a study area to set-up two air pollution models in ADMS-Urban version 2.3, one with calibrated background concentrations and another with a grid air pollution source. ADMS-Urban was developed by CERC (CERC, 2006). As an urban study area in the city of Nottingham, Dunkirk AQMA has NO<sub>2</sub> levels exceeding the permissible levels (PCS, 2001). Therefore, the majority of the available air pollution monitoring data, required to calibrate the background concentrations and validate the air pollution models, was NO<sub>2</sub> data, and hence NO<sub>2</sub> was selected as the modelled air pollutant.

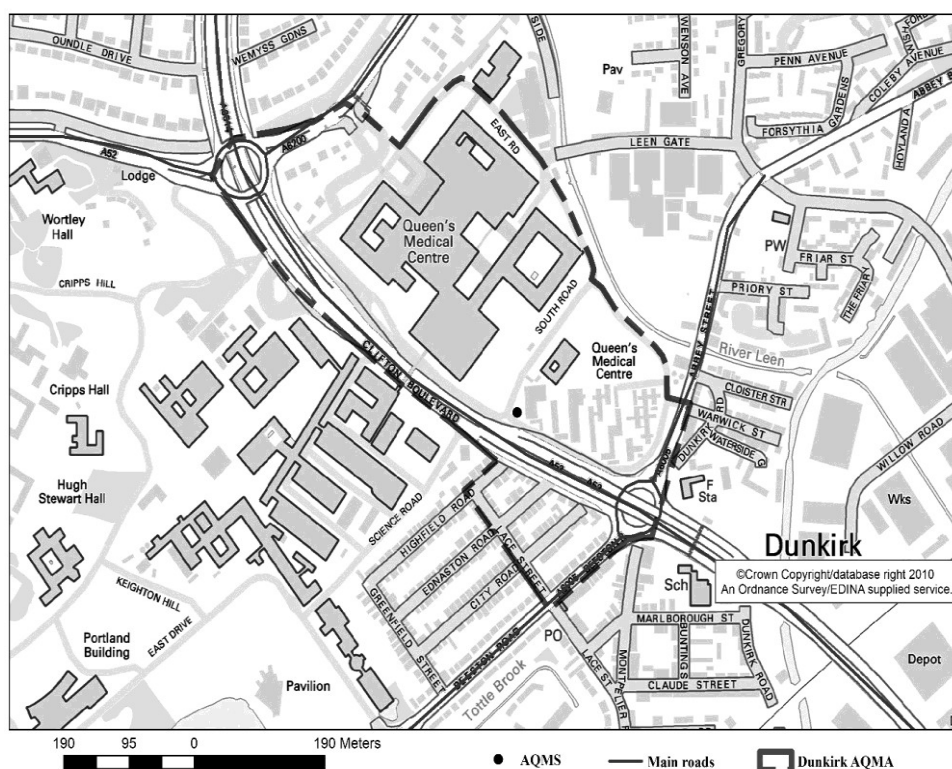


Figure 1. The Dunkirk AQMA

Due to data availability, 2006 was selected as the modelling year of the two air pollution models. Nottingham City Council provided the emission rates of significant industrial air pollution sources, and the traffic speed data of the main roads, relevant to the Dunkirk AQMA. The traffic on the main roads within, and close to, the Dunkirk AQMA, and the relevant significant industrial air pollution sources were the emission sources defined explicitly in the two air pollution models, as shown in Figure 1. The 2006 hourly sequential meteorological data was provided by The Nottingham Watnall Weather Station (MO, 2010). The meteorological data included surface temperature, wind speed at 10-metre height above the ground surface, wind direction, precipitation, cloud cover and degree of humidity. Nottingham City Council provided the 2006 annual mean and hourly monitored NO<sub>x</sub>, NO<sub>2</sub>

and O<sub>3</sub> concentrations by the Air Quality Monitoring Station (AQMS), located in the Dunkirk AQMA as shown in Figure 1.

Nottingham City Council provided the traffic flow data of the main roads in the Dunkirk AQMA. The provided data was the traffic count every five minutes collected automatically using detector loops embedded in the main roads. Using computer programming in MS Excel, a Visual Basic for Applications (VBA) computer program was written to calculate automatically the 2006 Annual Average Daily Traffic (AADT) flow and the 2006 hourly and monthly traffic flow profiles from the five-minute traffic counts, using the following mathematics:

For each day, the five-minute flow data was automatically aggregated to yield hourly flow data.

Let  $f_{ijk}$  = the total traffic flow in both directions in hour  $i$  of day  $j$  of month  $k$ , and let  $N_k$  = the number of days in month  $k$ , such that  $i = 0, \dots, 23$ ,  $j = 1, \dots, N_k$  (where  $N_k = 28, 29, 30$  or  $31$  as appropriate), and  $k = 1, \dots, 12$ .

Therefore

$$\text{AADT (vehicles/hour)} = \frac{\sum_{k=1}^{12} \sum_{j=1}^{N_k} \sum_{i=0}^{23} f_{ijk}}{[\sum_{k=1}^{12} N_k] \times 24} \quad (1)$$

$$\text{Monthly Average}_k(\text{vehicles/hour}) = \frac{\sum_{j=1}^{N_k} \sum_{i=0}^{23} f_{ijk}}{N_k \times 24} \quad \forall k, k = 1, \dots, 12 \quad (2)$$

$$\text{Monthly Factor}_k = \frac{\text{Monthly Average}_k}{\text{AADT}} \quad \forall k, k = 1, \dots, 12 \quad (3)$$

Let  $p_k$ ,  $q_k$  and  $r_k$  = the number of weekdays, Saturdays and Sundays, respectively, in month  $k$ , such that  $p_k + q_k + r_k = N_k \forall k, k = 1, \dots, 12$ . Therefore, the Hourly Average <sub>$i$</sub> (vehicles/hour):

$$\text{For weekdays (if } j \text{ denotes weekdays)} = \frac{\sum_{k=1}^{12} \sum_{j=1}^{p_k} f_{ijk}}{\sum_{k=1}^{12} p_k} \quad \forall i, i = 0, \dots, 23 \quad (4)$$

$$\text{For Saturdays (if } j \text{ denotes Saturdays)} = \frac{\sum_{k=1}^{12} \sum_{j=1}^{q_k} f_{ijk}}{\sum_{k=1}^{12} q_k} \quad \forall i, i = 0, \dots, 23 \quad (5)$$

$$\text{For Sundays (if } j \text{ denotes Sundays)} = \frac{\sum_{k=1}^{12} \sum_{j=1}^{r_k} f_{ijk}}{\sum_{k=1}^{12} r_k} \quad \forall i, i = 0, \dots, 23 \quad (6)$$

Hence there are  $3 \times 24 = 72$  different day-related hourly average traffic flows so, correspondingly, there are 72 hourly factors, such that:



$$\text{Hourly Factor}_i = \frac{\text{Hourly Average}_i}{\text{AADT}} \quad \forall i, i = 0, \dots, 23 \quad (7)$$

Therefore, the full traffic flow data processing output for each main road was:

- I. 24 hourly factors for weekdays, in order, from hour 0 to hour 23.
- II. 24 hourly factors for Saturdays, in order, from hour 0 to hour 23.
- III. 24 hourly factors for Sundays, in order, from hour 0 to hour 23.
- IV. 12 monthly factors for the 12 months, in order, from January to December.

Lack of data from some detectors for some time periods during the year 2006 had to be addressed. If the corresponding traffic data was available for another year, then that was used, factored using traffic data from the nearest detectors, for that other year and 2006. Steps were taken in the code to avoid zero division in factoring the traffic data of that other year. If the corresponding traffic data from another year was not available, then 2006 traffic data from the nearest available detectors were used. The traffic flow profiles were compiled to a special text file, a FAC file, which was used in ADMS-Urban to reflect the hourly and monthly variations in the AADT flow on traffic air pollution emissions. The traffic emission rates were derived from the traffic flow and speed data using the 2003 DMRB traffic emission factors (DMRB, 2007), built-in in ADMS-Urban.

The CRS with trajectory model was used to model the atmospheric conversion of  $\text{NO}_x$  to  $\text{NO}_2$  due to a number of chemical reactions with background  $\text{O}_3$  (CERC, 2006).  $\text{NO}_x$  and  $\text{O}_3$  were modelled in addition to  $\text{NO}_2$ , in order to model these chemical atmospheric reactions, and hence get accurate  $\text{NO}_2$  results. However, using the CRS with trajectory model requires inputs for  $\text{NO}_2$ ,  $\text{NO}_x$  and  $\text{O}_3$  background concentrations. Therefore, the 2006 hourly sequential  $\text{NO}_2$ ,  $\text{NO}_x$  and  $\text{O}_3$  concentrations, monitored by the Rochester air quality monitoring station, were provided by Nottingham City Council. This is a rural monitoring station remote from the Dunkirk AQMA and far from urban air pollution, and hence it was advisable to use its monitoring data as the input background concentrations to avoid double counting (CERC, 2009).

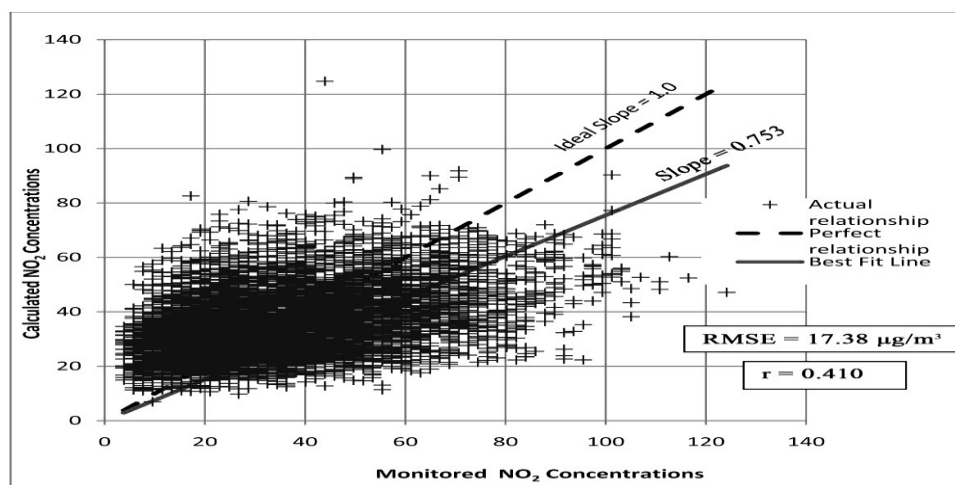
For the first air pollution model, the rural  $\text{NO}_2$ ,  $\text{NO}_x$  and  $\text{O}_3$  background concentrations were once macro-calibrated, and another time micro-calibrated, as explained by Zahran (2013a). For the second air pollution model, the rural background concentrations were used uncalibrated in addition to a grid air pollution source, defined using ADMS-Urban model interface. The air pollution emissions of the grid source were obtained from the UK National Atmospheric Emissions Inventory (NAEI). An output receptor was defined in the two air pollution models at the geographical location of the AQMS.

## RESULTS & DISCUSSION

The first air pollution model, with calibrated background concentrations, was run to output the 2006 annual mean concentrations of  $\text{NO}_2$ ,  $\text{NO}_x$  and  $\text{O}_3$  at the AQMS as shown in Table 1. The 2006 hourly  $\text{NO}_2$  concentrations calculated by the first air pollution model were compared to the 2006 hourly monitored  $\text{NO}_2$  concentrations at the AQMS as shown in Figure 2 and Figure 3. The second air pollution model, with a grid source and rural background concentrations, was run to output the 2006 annual mean concentrations of  $\text{NO}_2$ ,  $\text{NO}_x$  and  $\text{O}_3$  at the AQMS as shown in Table 1. The 2006 hourly  $\text{NO}_2$  concentrations calculated by the second air pollution model were compared to the 2006 hourly monitored  $\text{NO}_2$  concentrations at the AQMS as shown in Figure 4.

**Table 1. Monitored versus calculated annual mean concentrations at the AQMS**

Case Description	<i>NO<sub>2</sub> Annual Mean</i> $\mu\text{g}/\text{m}^3$		<i>NO<sub>x</sub> Annual Mean</i> $\mu\text{g}/\text{m}^3$		<i>O<sub>3</sub> Annual Mean</i> $\mu\text{g}/\text{m}^3$	
	<i>Calculated</i>	<i>Monitored</i>	<i>Calculated</i>	<i>Monitored</i>	<i>Calculated</i>	<i>Monitored</i>
ADMS-Urban + Macro-calibrated background concentrations	35.45	35.29	67.60	67.6	31.01	31
ADMS-Urban + Micro-calibrated background concentrations	35.19	35.29	67.47	67.6	30.96	31
ADMS-Urban + CRS with trajectory model + rural background concentrations + the grid source	37.77	35.29	69.31	67.6	35.07	31
ADMS-Urban + CRS + rural background concentrations + the grid source	37.65	35.29	69.31	67.6	35.18	31

Figure 2. Scatter diagram of hourly NO<sub>2</sub> concentrations at the AQMS after macro-calibration

With reference to Table 1, the calculated annual mean NO<sub>2</sub>, NO<sub>x</sub> and O<sub>3</sub> concentrations from the first air pollution model, with micro-calibrated background concentrations, were closer to the corresponding annual means of monitored concentrations than were the calculated annual means from the second air pollution model, with a grid source and rural background concentrations. This indicated that the first air pollution model, with micro-calibrated background concentrations, was more precise than the second air pollution model, with a grid source and rural background concentrations, on the annual mean level.

Comparing Figure 3 with Figure 4, the results of the second air pollution model, with a grid source and rural background concentrations, gave a much higher Root Mean Square Error (RMSE) than did the results of the first air pollution model, with micro-calibrated background concentrations. In addition, the results of the second air pollution model gave a much lower Pearson Correlation Coefficient (*r*), and a lower slope of the best-fit line through

the origin, than did the results of the first air pollution model. Therefore, the results of the first air pollution model, with micro-calibrated background concentrations, were much closer to the 2006 hourly NO<sub>2</sub> concentrations monitored by the AQMS than were the results of the second air pollution model, with a grid source and rural background concentrations.

With reference to Table 1, the calculated annual mean NO<sub>2</sub>, NO<sub>x</sub> and O<sub>3</sub> concentrations from the first air pollution model, with macro-calibrated background concentrations, were closer to the corresponding annual means of monitored concentrations than were the calculated annual means from the second air pollution model, with a grid source and rural background concentrations. In respect of the 2006 hourly NO<sub>2</sub> concentrations, comparing figure 2 with figure 4, the results of the second air pollution model, with a grid source and rural background concentrations, gave a slightly higher RMSE than did the results of the first air pollution model, with macro-calibrated background concentrations. Both the first and second air pollution models generally underestimated the 2006 hourly monitored NO<sub>2</sub> concentrations, which was indicated by the best-fit line through the origin having a slope of less than 1.0 in both figure 2 and figure 4. However, the slope of the best-fit line in the second air pollution model case (in Figure 4) was closer to 1.0 than was the slope of the best-fit line in the first air pollution model case (in Figure 2). Therefore, the tendency of the second air pollution model, with a grid source and rural background concentrations, to underestimate the hourly monitored NO<sub>2</sub> concentrations was less than that of the first air pollution model, with macro-calibrated background concentrations.

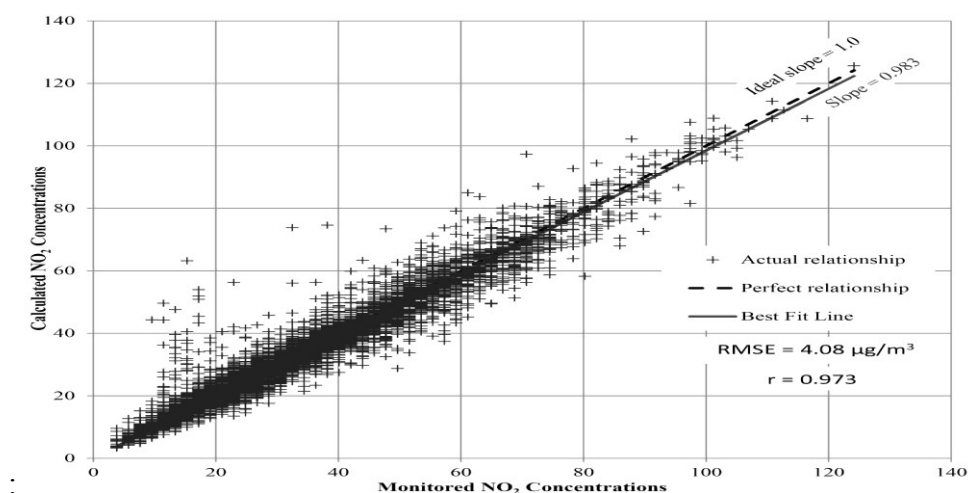


Figure 3. Scatter diagram of hourly NO<sub>2</sub> concentrations at the AQMS after micro-calibration

Continuing the comparison of figure 2 with figure 4, the results of the second air pollution model, with a grid source and rural background concentrations, gave a slightly higher  $r$  than did the results of the first air pollution model, with macro-calibrated background concentrations. This implied that the use of grid sources with rural background concentrations slightly increased the degree of linearity of the actual relationship between the calculated and monitored hourly NO<sub>2</sub> concentrations at the AQMS. Hence, the actual relationship between the calculated and monitored hourly NO<sub>2</sub> concentrations was slightly closer to the perfect straight-line relationship in the case of using a grid source with rural background concentrations than it was in the case of using macro-calibrated background concentrations.

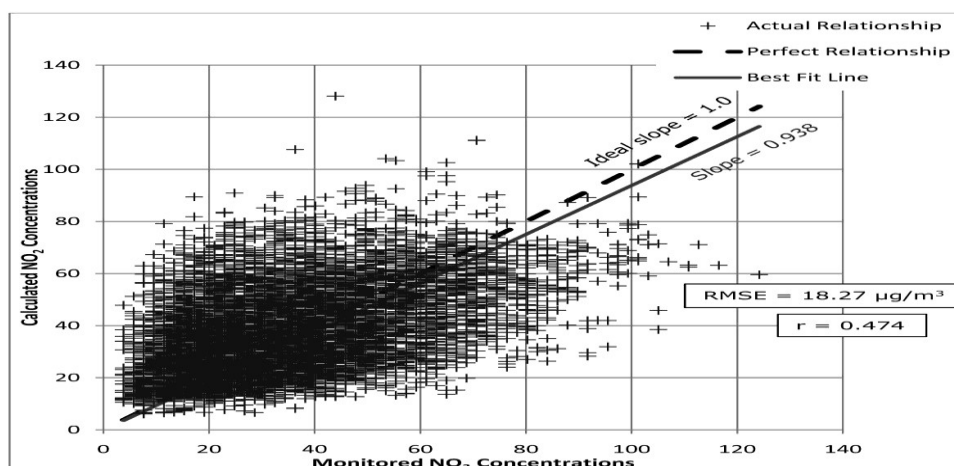


Figure 4. Scatter diagram of hourly NO<sub>2</sub> concentrations at the AQMS after using a grid source and rural background concentrations

The set-up of the second air pollution model, with a grid source and rural background concentrations, was adjusted to use the CRS, instead of the CRS with trajectory model, for modelling the atmospheric conversion of NO<sub>x</sub> to NO<sub>2</sub>. The adjusted air pollution model was run to output the 2006 annual mean concentrations of NO<sub>2</sub>, NO<sub>x</sub> and O<sub>3</sub> at the AQMS as shown in Table 1. The 2006 hourly NO<sub>2</sub> concentrations calculated by the adjusted air pollution model were compared to the 2006 hourly monitored NO<sub>2</sub> concentrations at the AQMS as shown in Fig. 5. The calculated annual mean NO<sub>2</sub>, NO<sub>x</sub> and O<sub>3</sub> concentrations at the AQMS by the adjusted air pollution model did not significantly change from the calculated annual means of these concentrations by the second air pollution model. Comparing Fig. 4 with Fig. 5, running the second air pollution model without the trajectory model of CRS did not significantly change the RMSE, *r* or the slope of the best-fit line through the origin of the actual relationship between the hourly calculated and monitored NO<sub>2</sub> concentrations at the AQMS.

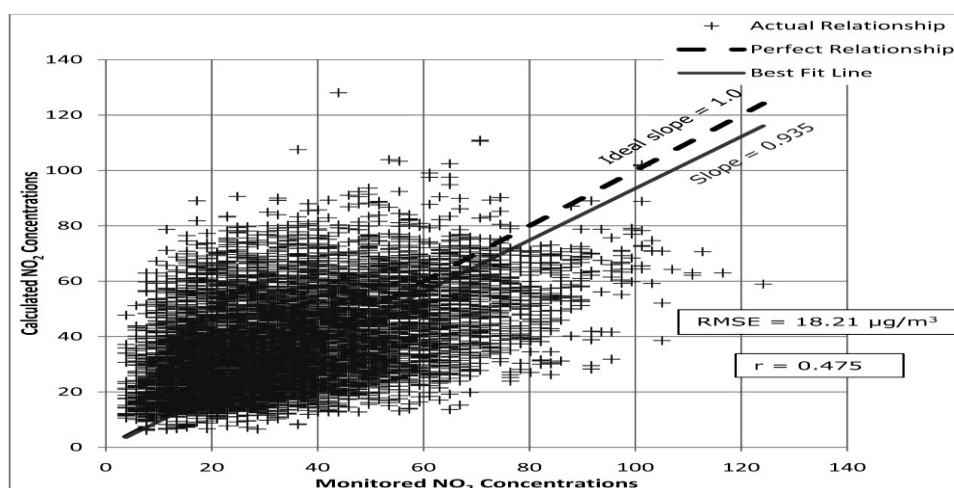


Figure 5. Scatter diagram of hourly NO<sub>2</sub> concentrations at the AQMS after using a grid source and rural background concentrations without the trajectory model of CRS

In terms of the model runtime, running the second air pollution model, with a grid source, rural background concentrations and either the CRS or the CRS with trajectory model,



required 44 minutes to calculate the annual mean and hourly concentrations of NO<sub>2</sub>, NO<sub>x</sub> and O<sub>3</sub> at a single output receptor point, the site of the AQMS. On the other hand, running the first air pollution model, with either the macro-calibrated or micro-calibrated background concentrations, required 9 minutes to calculate the annual mean and hourly concentrations of NO<sub>2</sub>, NO<sub>x</sub> and O<sub>3</sub> at the same output receptor point. To investigate the air pollution dispersion in an urban area such as the Dunkirk AQMA, an approximate number of 11610 output receptor points were defined in the air pollution model at and above the ground surface (Zahran et al., 2013). With simple mathematics, the total savings in the air pollution model runtime could be  $11610 \times (44 - 9) = 406350$  minutes  $\approx 9.4$  months.

## CONCLUSION

A comparison has been undertaken between the calibration of background concentrations approach, introduced by Zahran (2013a), and the use of grid sources in air pollution dispersion modelling, in terms of the accuracy of output results and the model runtime. In terms of the error between the annual means of calculated and monitored NO<sub>2</sub> concentrations, running the air pollution model with the macro or micro-calibrated background concentrations was more accurate than using a grid source and rural background concentrations. Moreover, in terms of the error between the hourly calculated and monitored NO<sub>2</sub> concentrations, running the air pollution model with the micro-calibrated background concentrations was much more accurate, although slightly less accurate with the macro-calibrated background concentrations. Using the trajectory model of CRS in ADMS-Urban did not significantly change the error between the monitored and calculated concentrations otherwise obtained, and so effectively did not change the comparative results between the calibration of background concentrations and the use of grid sources.

Replacing the grid source with either the macro or micro-calibrated background concentrations can save up to 9.4 months of the model runtime in order to investigate the air pollution dispersion, at and above the ground surface, in an urban area such as the Dunkirk AQMA. The micro-calibration mathematical approach did not require any input data to start the iterations, apart from the monitored air pollution concentrations. In comparison, the grid air pollution sources require precise input data for the air pollution emissions, which may impede their usage in air pollution modelling of areas without a precise emissions inventory.

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