Prepared for NZ Transport Agency Waka Kotahi

MODEL VERIFICATION GUIDANCE

FOR DETAILED ASSESSMENT OF AIR QUALITY IMPACTS FROM ROAD TRANSPORT PROJECTS

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Prepared for NZ Transport Agency Waka Kotahi

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1 INTRODUCTION

Where road traffic emissions factors are estimated, and dispersion models used to simulate the dispersion of those emissions to air, it is important that errors and uncertainty are minimised as much as possible; model verification is a process by which this can be achieved.

Model verification comprises a comparison of model predictions to measured pollutant concentrations at a set of monitoring locations. This enables an assessment of model performance. It also determines whether adjustment factors should be applied to model results at selected sensitive receptor locations, to bring the model in line with observations.

This guidance provides an in-depth methodology to undertake model verification for detailed dispersion modelling of road traffic emissions. It aims to compliment NZ Transport Agency Waka Kotahi's Air Quality guidance document[1] on the assessment of road traffic impacts on air quality in relation to State Highway schemes. NZ Transport Agency Waka Kotahi's guidance states that the purpose of comprehensive technical assessment *'is to comprehensively evaluate the air quality impacts (and opportunities) arising from the project*". Model verification is a key process to ensure that potential impacts are comprehensively assessed, and appropriate mitigation recommendations made.

The methodology presented here follows the principles of the United Kingdom's (UK) Local Air Quality Management Technical Guidance document (TG22)[2], adapted to make it more applicable to road projects in New Zealand.

The guidance focusses on the completion of model verification of predicted annual-mean nitrogen dioxide (NO_2) concentrations, to align with the annual monitoring data available or anticipated to be available from NZ Transport Agency Waka Kotahi's NO_2 diffusion tube monitoring network and project-specific monitoring.

The principles of the methodology presented within this document can also be applied for the verification of modelled annual mean particulate matter predictions (PM_{10} and $PM_{2.5}$), where sufficient monitoring data exists. In the absence of sufficient monitoring data, the adjustment factor for modelled road NO_x can be applied to modelled road contributions of particulate matter.

This guidance is accompanied by the following tools, which have been developed on behalf of NZ Transport Agency Waka Kotahi to assist users of this guidance with applying the methodologies detailed.

- A **NO_x to NO_2 Tool** – for conversion between modelled and monitored road NO_x and NO_2.
- A **Verification Template** – for use when completing model verification and calculating model adjustment factors.
- An **Adjustment Template** – used to adjust modelled predictions.

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1 NZ Transport Agency Waka Kotahi (2019) Guide to assessing air quality impacts from state highway projects v2.3, October 2019.

2 Department for Environment Food & Rural Affairs (2022) Local Air Quality Management Technical Guidance (TG22).

2 PURPOSE OF MODEL VERIFICATION

Model verification is undertaken to validate dispersion modelling results (modelled concentrations) against monitored concentrations. Undertaking model verification will give credibility to predicted model concentrations by checking, adjusting where necessary, and confirming that model performance is acceptable across the study area. Model verification is an important step to ensure that exceedances of guideline values are not predicted where they do not exist, or conversely that exceedances of guideline values are captured where they do – for example, in locations where local dispersion effects (such as multiple street canyons) or features impacting real-world emissions (e.g., very steep gradients or congestion) are not accurately accounted for in the model.

Model uncertainty can be investigated and reduced by undertaking dispersion model verification with the modelled base year traffic scenario and ambient monitoring site data (if available). This is supported by international guidance from Department for Environment Food & Rural Affairs (Defra) in the UK, (TG22[2]) which outlines that "*to ensure a robust Detailed Assessment for road traffic sources, it is recommended that model verification is carried out*".

The verification process considers model performance through the comparison of predicted against total monitored concentrations, and the application of statistical analysis to guide this comparison. The process of model verification determines whether model adjustment factors, based on the relationship between modelled and monitored values, should be applied to model results to improve overall model performance.

The model is being used to predict road traffic contributions, which are added to background values to provide predicted total concentrations. Model adjustment factors are based on, and applied to, only the modelled road-traffic contributions and not the background concentrations.

Adjustment factors can be calculated and applied for the entire study area, or for specific model zones where there are known local effects. This process is described in more detail in Section 6 of this technical guidance.

3 MONITORING SITE SELECTION

As verification involves the direct comparison between modelled and measured pollutant concentrations at monitoring locations to confirm model performance and provide adjustment factors if needed, appropriate monitoring site selection is one of the most important steps.

It is recommended that as many monitoring sites as possible across the study area are used for model verification, with a minimum of 6 sites being included, and more for larger study areas.

Early engagement of a suitably experience air quality professional to review available monitoring data is important to identify if there is a requirement for project specific monitoring to be completed.

This could include a combination of both continuous and passive monitoring. It is recommended that where diffusion tubes are co-located with continuous monitors, data from the continuous monitor is used to develop a local bias adjustment factor for application to the diffusion tube results. Where there is no local co-location to provide a project specific bias adjustment factor, a national bias factor may be available from NZ Transport Agency Waka Kotahi's Annual monitoring report, and the use of this should be discussed with their air quality specialist at NZTA.

3.1 SITE TYPE

To decide on which monitoring sites are to be included in the model verification, the site type firstly needs to be understood and defined. It is unlikely that all available monitoring data will be classified consistently by site type. It is therefore recommended that the descriptors in Figure 3-1 and Figure 3-2 of this technical guidance are used to broadly classify monitoring sites as either 'roadside', or 'background' – these are the sites most important to be defined for road traffic dispersion model verification and adjustment. Further details for each are provided below.

3.2 ROADSIDE SITES

Figure 3-1 of this technical guidance presents an extract from the Ministry for the Environment (MfE) '*Good Practice Guide (GPG) for Air Quality Monitoring and Data Management 2009*'[3] with New Zealand specific monitoring site classifications, site type classifications from Defra's TG22[2] are shown in Figure 3-2 of this technical guidance.

In the context of this guidance, and for the purposes of dispersion model verification of road traffic predictions, 'roadside' sites are monitoring locations typically between 1 m and 15 m from the kerb, which are therefore suitable for use in the model verification process for road traffic emissions (it is noted that in some instances it may be appropriate to use sites located further

[3] Ministry for the Environment (2009) Good Practice Guide for Air Quality Monitoring and Data Management 2009. Wellington: Ministry for the Environment.

than 15 m from the kerb if there are no other significant sources of pollution nearby and monitoring sites are limited).

It is important not to over or under-adjust at traffic/roadside sites, as they are of most interest in road modelling projects, being the most likely locations at which modelling predicts exceedances of the air quality guidelines. Dispersion models struggle to predict concentrations within the first metre of a roadside accurately. As outlined in Defra's technical guidance (TG22) the inclusion of kerbside sites as part of the model verification calculations could lead to an "*over-adjustment of modelling at roadside sites*". As such 'kerbside' sites, which are defined in the context of this guidance as locations within one metre of the kerb of a busy road, **should not** be used for model verification and adjustment of predictions in locations which are further than 1 m from the kerb, and only considered for use if there is exposure within a kerbside location.

Whilst it is considered unlikely, if there is representative exposure at kerbside sites within the study area (e.g. there are sensitive receptors located less than a metre from the kerbside) a zonal approach to verification and adjustment may be necessary to allow for model adjustment of kerbside locations in isolation from those in traffic/roadside locations.

Unless there are sensitive receptors located at the kerbside in the study area, the model verification calculations will likely be based only on traffic/roadside monitoring locations.

Background sites:

The site type classifications from TG22 (Figure 3-2 of this technical guidance) should be applied to define 'urban background', 'suburban' or 'rural' sites. These sites will be used as a check on the background concentration added to the modelled road traffic contribution when calculating total predicted pollutant concentrations.

Recommended site category	Site scale equivalent	Typical area
Traffic	Peak (metres to 10s of metres)	Typically very close to high-traffic-use roads and intersections. Site should be between 2 to 5 m from the roadside.
Industrial	Peak (metres to 10s of metres) or Neighbourhood (10s of metres to 0.5 km)	Peak – close to one large point source or fugitive emissions. Typically used for compliance monitoring. Neighbourhood – with large and varied point source industry emissions and high population density. Such areas may contain heavy commercial and processing industries.
Residential	Peak (metres to 10s of metres) or Neighbourhood (0.5 to 10s of kilometres)	Peak – a monitoring site located somewhere not truly representative (so it is not neighbourhood scale) but does not exactly fit the 'traffic' or 'industrial' peak site descriptions. Neighbourhood – suburban areas in larger cities with a relatively high population density, but not in the immediate vicinity of congested roads or industry. This category also includes residential areas in smaller towns in rural areas.
Special (site description)	Regional (10s to 100s of kilometres)	Airsheds that are distinct in their geographical, meteorological and emissions characteristics. Included are the effects of any point sources or urban plumes on the regional air quality. Could include places where natural emissions are significant (eg, Rotorua), in which case the category would be *Special (Geothermal)*.
	National	National background sites that contribute to the global network; eg, *Special (National)*.

Figure 3-1: New Zealand-specific monitoring site type classifications, as presented in Section 6 of MfE's GPG[3].

Site Type	Description
Urban centre	An urban location representative of typical population exposure in towns or city centres, for example, pedestrian precincts and shopping areas
Urban background	An urban location distanced from sources and therefore broadly representative of city-wide background conditions, e.g. urban residential areas
Suburban	A location type situated in a residential area on the outskirts of a town or city
Roadside	A site sampling typically within one to five metres of the kerb of a busy road (although distance can be up to 15 m from the kerb in some cases)
Kerbside	A site sampling within one metre of the kerb of a busy road
Industrial	An area where industrial sources make an important contribution to the total pollution burden
Rural	An open countryside location, in an area of low population density distanced as far as possible from roads, populated and industrial areas
Other	Any special source-orientated or location category covering monitoring undertaken in relation to specific emission sources such as power stations, car-parks, airports or tunnels

Figure 3-2: Monitoring site type classifications, as presented in Section 7 of TG22[2].

3.3 OTHER CONSIDERATIONS

In addition to being too close to the modelled road source (kerbside sites or locations on traffic islands) there may be other reasons why monitoring sites should not be included in the model verification calculations. This may be due to local characteristics which are influencing the dispersion of pollutants that could skew the results of that monitoring site. It is important to include in the reporting a detailed reasoning for the inclusion or exclusion of monitoring sites in model verification calculations. Examples of some reasons to exclude monitoring sites include the following:

- Low data capture for the ‘base’ year.
- Other nearby emissions sources directly influencing the concentrations at the monitoring location that are not explicitly included in the dispersion model or accounted for within the background concentrations used (e.g. ventilation shafts/heater flues/generators on building sites nearby/car parks/bus stops).
- The road link next to a monitoring site not being modelled due to lack of traffic data, therefore that monitoring location not being defined as ‘roadside’ for modelling purposes.
- Location (e.g. height or distance from kerb) unable to be confirmed and suspected to be not accurate.
- Local pollutant dispersion disrupted at monitoring site (e.g. obscured by vegetation, buildings, or traffic signs).

The aim is to use monitoring sites that are representative of the environment at the receptors being modelled. Some of the reasons for exclusion outlined above can be eliminated through completing a site visit to confirm the existing environment and ensuring any factors that may be influencing the air quality at a specific monitoring location are being accounted for in the dispersion model.

3.4 DISPERSION MODEL EXTENT

If insufficient road traffic data is available to include all main and arterial roads within 200 m of a monitoring site (as a minimum), that site should be excluded from the verification as the modelled road traffic impacts are likely to be underestimated. It is anticipated that the study area will include those roads within the traffic model for the project.

3.5 MONITORING DATA PERIODS

Ideally each monitoring site should have twelve months of data for the chosen 'base' year to capture representative conditions from across the year. All monitoring sites with data capture less than 75 %, or less than a full year, should be annualised. This will allow practitioners to account for seasonal variation. Where possible, if scheme specific monitoring is co-located with a reference monitor, a local bias adjustment factor should be applied.

Whilst not ideal, a minimum of three months of monitoring data could be used to provide annual mean equivalent concentrations for use in model verification and adjustment, through annualisation of monitoring results being completed following guidance within Box 7.9 of Defra's LAQM guidance[2]. This is expected to provide more confidence in modelled predictions than if model verification/and adjustment was not completed, but it is important to acknowledge that the short period monitoring would increase uncertainty in the results, particularly where predicted concentrations are near to the air quality objectives or guidelines being considered.

3.6 MONITORING DATA CHECKS

Checks should be undertaken on all monitoring data before it is used in model verification calculations.

Initial checks of location, distance to kerb and a general understanding of any features that could affect local dispersion around the monitoring sites can be obtained from open-source data as previously mentioned.

If there is a more complex environment around the monitoring location (e.g. features noticed on aerial mapping such as congestion that is not described within the traffic data), a site visit may be necessary to confirm the monitoring environment.

Whilst only the 'base' year monitoring concentrations are used in model verification calculations, it is recommended that where possible five years of data for each site are reviewed to ensure that the 'base' year concentration is part of the trend at that monitoring site and not an anomaly. If the data from one site has an unusually high or low value in a year, that is not consistent with the rest of the dataset, the reasoning should be obtained from the territorial local authority (TLA) that undertook the monitoring and, in some cases, if there is no reason the data may need to be excluded from the monitoring verification calculations to avoid skewing both the verification and resulting adjustment factors.

It is expected that monitoring data obtained from the TLA will not need to be updated, but there could be cases where data has been incorrectly recorded in monitoring reports (e.g. 2.3 $\mu g/m^3$ rather than 23 $\mu g/m^3$, or changes to locations and heights following site visit checks). Any changes made to the monitoring data should be recorded in the modelling report.

Any data used from the NZTA national survey is expected to have had a national bias adjustment factor already applied and not require additional bias adjustment prior to use. For scheme specific or TLA data, the use of a local or NZTA national bias adjustment factor may be appropriate, and this should be discussed and confirmed with the NZTA air quality specialist.

3.7 PROJECT-SPECIFIC ROADSIDE MONITORING

If detailed dispersion modelling is to be undertaken and there are limited suitable representative monitoring locations in the study area with concentrations for the 'base' year, project-specific monitoring should be undertaken.

Monitoring should ideally be undertaken for 12 months to account for seasonal variability, however where the timeline is constrained a minimum of three months of monitoring data can be used to provide annual mean equivalent concentrations, as outlined earlier within Section 3.4 of this technical guidance.

4 BACKGROUND CONCENTRATION DATA SELECTION AND CONSIDERATIONS

For detailed dispersion modelling of road sources, the contribution from the road source is calculated by the model, and an appropriate background concentration is added to the road contribution to derive a total predicted concentration at the modelled location, prior to comparison with the relevant air quality guidelines.

The NZ Transport Agency Waka Kotahi mapped background concentrations[4] can be used in the model verification calculations. Where this data is used it should be compared against background monitoring sites which are representative of the study area, such as ‘urban background’, ‘suburban’ or ‘rural’ locations (see site type definitions in Section 3 of this technical guidance). The sites used for comparison should be appropriately distanced from road emission sources in the region (greater than 200 m) such that they broadly represent the background environmental conditions of that area, without the influence of road traffic. It may be appropriate to vary the background values used within an assessment to represent the urban and rural regions of an overall study area.

There should be a good correlation between the mapped and monitored background concentrations (mapped within 10-15% of monitored). If not, further investigation into the mapped concentrations may be needed and consideration given to whether the use of local background monitoring concentrations in preference to, or to adjust, the NZ Transport Agency Waka Kotahi mapped background values. This is particularly important where there are significant non-road sources within a study area (e.g. airports, seaports, railyards, industrial areas).

4.1 PROJECT-SPECIFIC BACKGROUND MONITORING

Following the methodology presented in Section 3.7 of this technical guidance, if “*there are no suitable representative monitoring locations in the study area with concentrations for the ‘base’ year, project-specific background monitoring should be undertaken*”. This is especially important in more complex environments with additional sources of NOx, where the NZ Transport Agency Waka Kotahi background maps may not accurately represent all non-road sources.

[4] NZ Transport Agency Waka Kotahi, Background air quality. Available from: Background air quality | NZ Transport Agency Waka Kotahi (nzta.govt.nz).

5 DISPERSION MODEL SET-UP CONSIDERATIONS

Prior to completing model verification and any adjustment of modelled results, the dispersion model set-up and inputs should first be reviewed in-depth, and any uncertainties minimised where possible.

When setting up the detailed dispersion model in preparation for completing model verification, consideration should be given to the following aspects:

- A 'base' year has been defined and there is suitable traffic data and local air quality monitoring data for that year.
- Monitoring data is appropriate for the 'base' year, taking into consideration trends in concentrations from previous years.
- The spatial extent of the dispersion model is appropriate to include the monitoring locations and receptor locations. Ideally, road coverage should extend 500 m in all directions around the monitoring and receptor locations for major roads and arterial routes, and 200 m as a minimum for all other roads (Figure 5-1 of this technical guidance).
- All monitoring locations used are included in the dispersion model at the correct location including their relative distance to the kerb and height above ground as stated in the reporting by local authorities or administrative bodies. Where the distance and height are presented in annual monitoring reports, check that this is consistent with the model set-up. Where they are not presented, aim to determine the distance from the kerb and height through a site visit or online mapping.
- Road widths included in the model are correct and any variation along a road link is accounted for, especially in the vicinity of monitoring locations to be used in the model verification or sensitive receptor locations included in the model (Figure 5-2 of this technical guidance).
- Features that will influence local dispersion characteristics have been included and accounted for in the model where possible (for instance, street canyons, road gradients, flyovers, or elevated or depressed sections of road).
- Traffic data including fleet mix, volumes and speeds are appropriate for the locations modelled (Figure 5-3 of this technical guidance). Attention should be paid to congestion and flows around junctions and intersections, where traffic models may have more uncertainty and modelling the emissions from queuing traffic may be necessary.
- Model input parameters are suitable for the study area (in terms of terrain, land use and meteorological data).
- Appropriate estimates of background concentrations have been used.

It is recommended that for spatial checks the data is imported into a Geographic Information System (GIS) such as ArcMap or QGIS. Figure 5-1 to Figure 5-3 of this technical guidance present examples of some of the above model set-up spatial checks when using GIS.

In particularly complex environments, iterations of modelling and model refinements may need to be undertaken to improve model performance. A general understanding of any features that could affect dispersion can be obtained from open-source data such as 'Google Streetview' or 'Google Earth', however it may be necessary to conduct a site visit to confirm the existing environment and any factors that may be influencing the air quality at that location. It may also be necessary to complete location specific monitoring in these complex environments to allow a zonal approach to model verification and adjustment to be completed (i.e. split into multiple separate areas of similar model performance), as discussed further in Section 6 of this technical guidance.

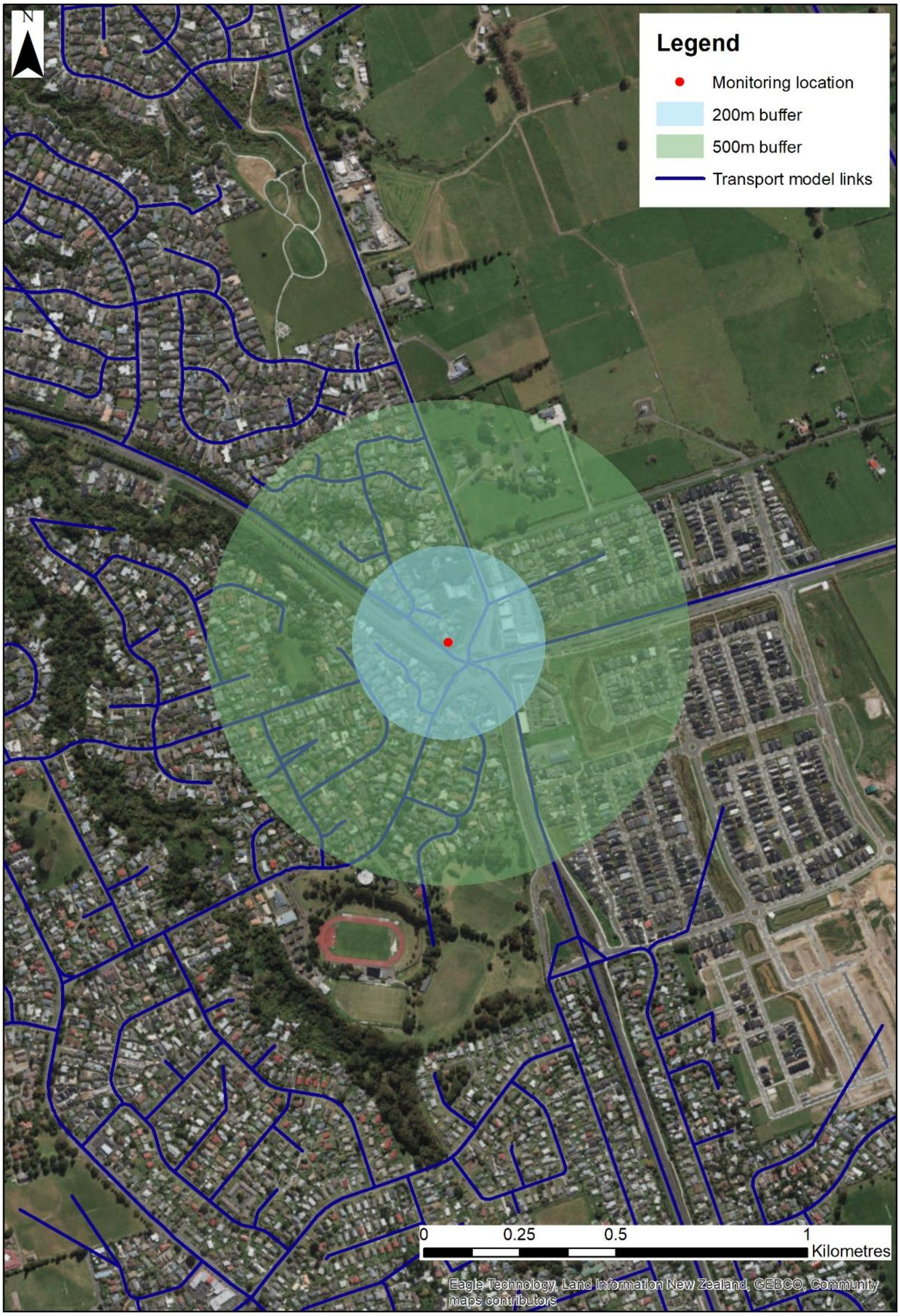

Figure 5-1: Example of the use of buffers to ensure 500m extent around a monitoring location.

Figure 5-2: Example of modelled road network refinements around a junction to better represent the widths and alignments of the road network.

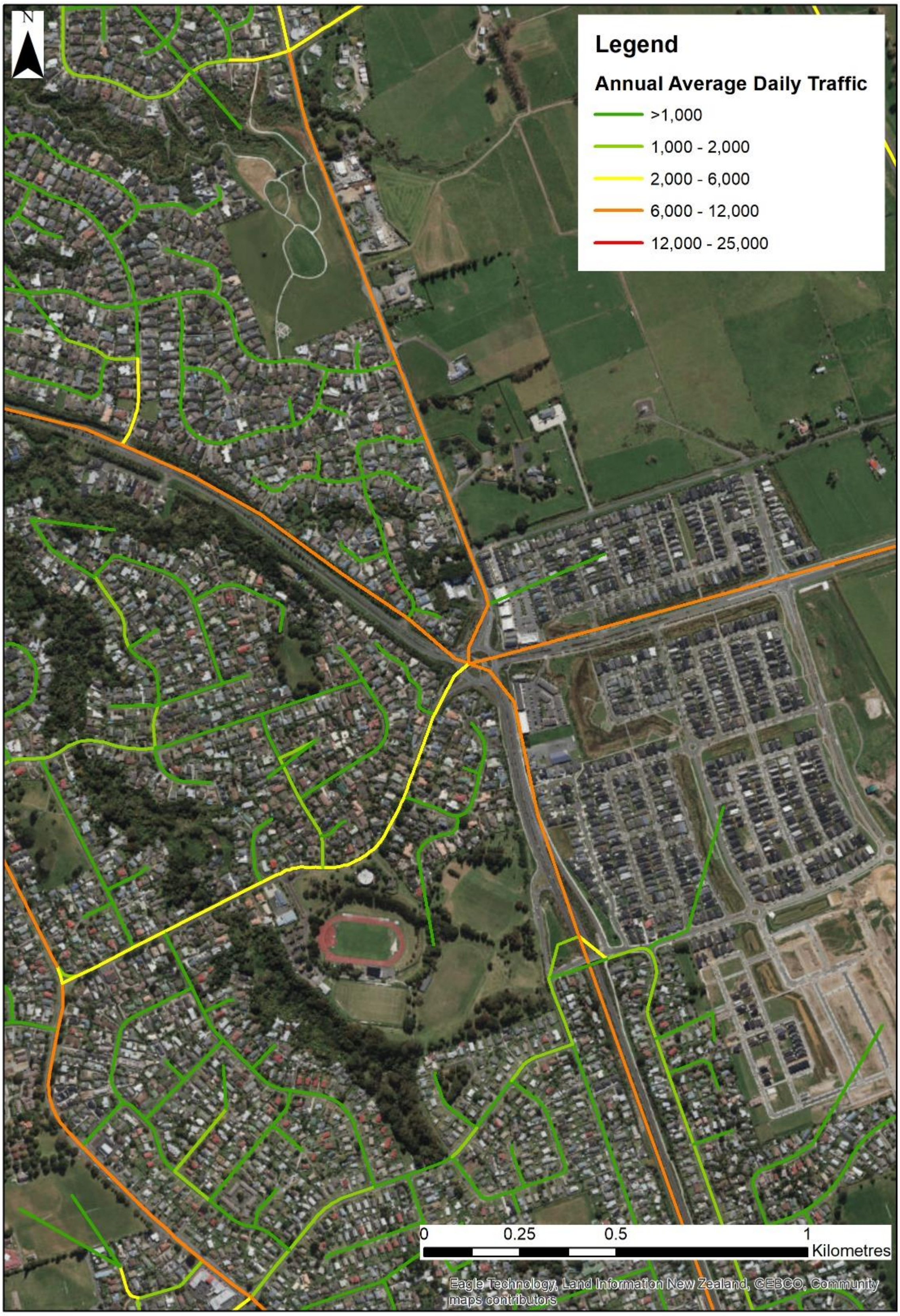

Figure 5-3: Example of the use of colour banding symbology to investigate traffic flow volumes.

6 DETAILED VERIFICATION METHODOLOGY

The model verification method comprises the steps shown in Table 6-1.

Table 6-1: Step-by-step detailed verification methodology.

Step	Details	Tools used
1	Predict total concentrations of NO_2 at selected monitoring locations. The total is calculated from the modelled NO_x due to traffic emissions (termed 'Road NO_x'), and background NO_2. Verification determines if the modelled Road NO_X component has been modelled within an acceptable range of uncertainty.	Verification Template , NO_X to NO_2
2	Compare the total predicted NO_2 concentrations with the total monitored NO_2 concentrations at each roadside/traffic monitoring location. Evaluate the model performance using the following statistical parameters: Root Mean Square Error (RMSE), Fractional Bias, and Correlation Coefficient. Also check to see if the majority of sites have modelled concentrations within 25% (and ideally 10%) of the monitored concentration. This step will confirm if the model performs without further work, or alternatively if it requires steps 3 and 4 to be carried out.	Verification Template , NO_X to NO_2
3	If required, consider whether model set-up refinements could be made to improve model performance and update the modelling if necessary.	Modelling software, GIS
4	If following Step 3 the model still does not perform adequately, calculate and apply a 'Road NO_x' adjustment factor, then re-calculate the same statistics using the adjusted total NO_2 predictions to further evaluate model performance.	Verification Template , NO_X to NO_2
5	Apply adjustment factors from verification to model predictions at sensitive receptors	Verification Template, NO_X to NO_2, Adjustment Template.

The following subsections provide further information on each of the assessment steps, for which the relevant tools developed to accompany this guidance (outlined in Table 6-1) should be used.

Step 1: Predict total concentrations of NO_2 at selected monitoring locations.

Set up a model with receptors for each of the roadside monitoring sites within the project study area. The model is used to predict the contribution of NO_x from the road traffic at each monitoring site. This 'Road NO_x contribution is then input alongside the background NO_2 to the NO_x to NO_2

Tool, which converts the Road NO_x component to NO_2 and provides predicted total NO_2 concentrations at the monitoring site.

Step 2: Compare the predicted total NO_2 against monitored NO_2 concentrations using statistical analysis and graphs.

Compare all predicted total NO_2 concentrations at the selected roadside monitoring locations against the monitored total NO_2 concentrations from those monitoring sites, for the whole model study area.

This can be done using some simple statistical analysis alongside creating a graph with trendlines as a visual aid to the comparison.

The statistical measures that are used to assess model performance include the following:

- Root Mean Square Error: the average error/uncertainty of the model.
- Fractional Bias: to identify any systematic under- or over-prediction of the model.
- Correlation Coefficient: evaluates the linearity in the relationship between predicted and observed data.

The RMSE is calculated in the same units as the criteria to which it is applied. NZ Transport Agency Waka Kotahi currently considers 40 $\mu g/m^3$ as the annual mean NO_2 criteria. An acceptable RMSE is considered to be less than 25% of the criterion (i.e. 10 $\mu g/m^3$) and an ideal RMSE less than 10% (4 $\mu g/m^3$) when modelled concentrations are compared to monitored concentrations.

For the fractional bias, the ideal value is zero. Below zero is a systematic overprediction, and above zero is systematic underprediction.

For the correlation coefficient, the ideal value is 1. However, it should be noted this statistic should not be relied on for small datasets as the outliers could influence the overall result unduly.

Further details on the interpretation of these statistical parameters and the formulas used to calculate them are presented in Section 7 of this technical guidance.

Table 6-2 presents an example comparison using statistical analysis for consideration of model performance. As outlined above, the comparison of total concentrations can also use a graphical approach to help with interpreting the data, an example based on the values in Table 6-2 is shown in Figure 6-1 of this technical guidance.

Table 6-2: Example comparison between non-adjusted total monitored and total modelled NO_2 concentrations.

Site ID	Monitored total NO_2 concentration (µg/m³)	Non-adjusted total modelled NO_2 concentration (µg/m³)	Percentage difference before adjustment ([modelled – monitored] / monitored)	Root mean square error (RMSE)	Fractional Bias	Correlation Coefficient
1	18.8	9.9	-47.3%	6.78	0.42	0.74
2	19.3	13.0	-33.6%			
3	19.6	11.4	-41.8%			
4	16.0	12.3	-23.1%			
5	23.1	12.4	-46.3%			
6	10.7	9.3	-13.1%			
7	11.3	9.0	-20.4%			
Taken directly from monitoring data.	*Taken directly from monitoring data.*	*Derived from the input of Road increment NO_x alongside background NO_2 concentrations in the NO_x to NO_2 Tool.*	*Calculated from ([modelled – monitored] / monitored) *100. The majority of modelled concentrations should be within 25%, and ideally within 10% of the monitored values.*	*Average error or uncertainty of the model calculated as per equation stated in Section 7.2 of this technical guidance. Ideal value is less than 4.*	*Used to identify any systematic under- or over-prediction of the model. Calculated as per equation stated in Section 7.3 of this technical guidance. Ideal value is zero, below zero is systematic overprediction, above zero is systematic underprediction.*	*Used to compare the linear relationship between predicted and observed data. Calculated as per equation stated in Section 7.4 of this technical guidance. The ideal value is 1. Note: this statistic should not be used for small datasets as the outliers could influence the overall result.*

Figure 6-1 provides the graphical comparison between modelled and monitored concentrations, based on the data in Table 6-2. Plotting the monitored values against the model predictions is useful for an initial review of model performance, allowing easy identification of whether the model is performing within 10 % or 25 % at each site modelled. Ideal after the verification process is complete, most sites will come within 25 %, as well as the RMSE being below 10 % of the annual NO_2 criterion. Negative percentage would show that the model is underestimating and positive, overestimating.

This approach is particularly useful for large datasets allowing easy identification of systematic under- or over-prediction of the model, single site outliers, or where there are groups of monitoring sites performing similarly.

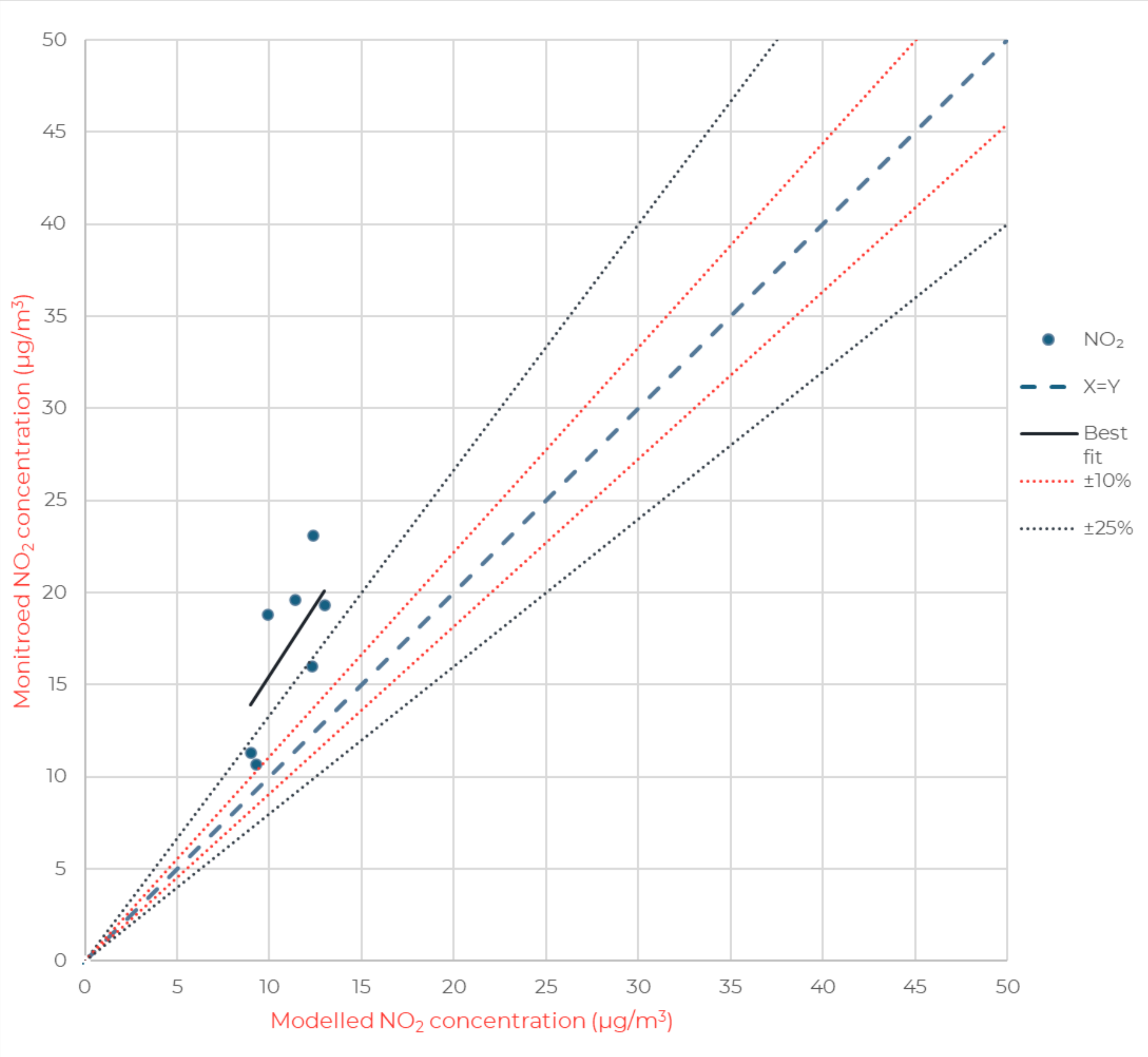

Figure 6-1: Example of graphical comparison between non-adjusted total monitored and total modelled NO_2 concentrations.

Figure 6-1 shows clearly that for all sites considered, the model is underpredicting compared to the monitoring.

Step 3: Consider whether model refinements could improve model performance

If, after the initial 'whole model' verification calculations have been completed, the model is found to not perform well enough, it should be investigated and model refinements as outlined in Section 5 of this technical guidance undertaken to see if any of those refinements improve model performance.

In particular, the aim should be for the model to show good performance where the predicted concentrations are close to or above the air quality guideline values, where the risk of human health impacts is therefore highest.

If model refinements do not improve the comparison of modelled to monitored results sufficiently, adjustment of results using a verification factor can be undertaken. This is not considered an unusual requirement for road traffic modelling, where there are numerous uncertainties within the calculation of emission rates and modelling that can cause under- or over-estimates.

Step 4: Calculate and apply Road NO_x adjustment factor, then re-compare the modelled and monitored values using statistical parameters.

Table 6-3 shows an example of the data needed to compare and adjust the Road NO_x contribution.

Table 6-3: Example of data needed to undertake verification calculations for Road NO_x adjustment.

Site ID	Background NO_2 concentration (μg/m³)	Non-adjusted modelled road NO_x concentration (μg/m³)	Non-adjusted monitored road NO_x concentration (μg/m³)	Ratio of monitored road NO_x to modelled road NO_x	Adjustment Factor
1	5.7	10.7	38.9	3.6	2.4245
2	5.7	19.6	41.0	2.1	
3	5.7	14.8	42.3	2.9	
4	5.7	17.3	28.9	1.7	
5	5.7	17.8	56.9	3.2	
6	5.7	8.9	12.7	1.4	
7	5.7	8.3	14.6	1.8	
	Taken directly from background maps used in modelling as per Section 4.	*Taken directly from the modelled road output results.*	*Derived from the input of monitored NO_2 and background NO_2 concentrations in the NO_x to NO_2 Tool.*	*Calculated from (monitored road contribution/modelled road contribution).*	*Calculated through 'least squares' regression analysis of modelled to monitored Road NO_x, or by applying a trend line to the plotted results.*

The regression analysis can be completed using the "least squares" method in a spreadsheet. The adjustment factor is the resulting slope of the regression line of monitored Road NO_x on modelled Road NO_x, plotted through the data (and imposing a zero intercept). The regression line through the data is included in Figure 6-2 of this technical guidance.

With Monitored Road NO_x plotted on the vertical axis and Modelled Road NO_x on the horizontal axis, the gradient of the trendline is the adjustment factor to apply to the modelled road NO_x contribution.

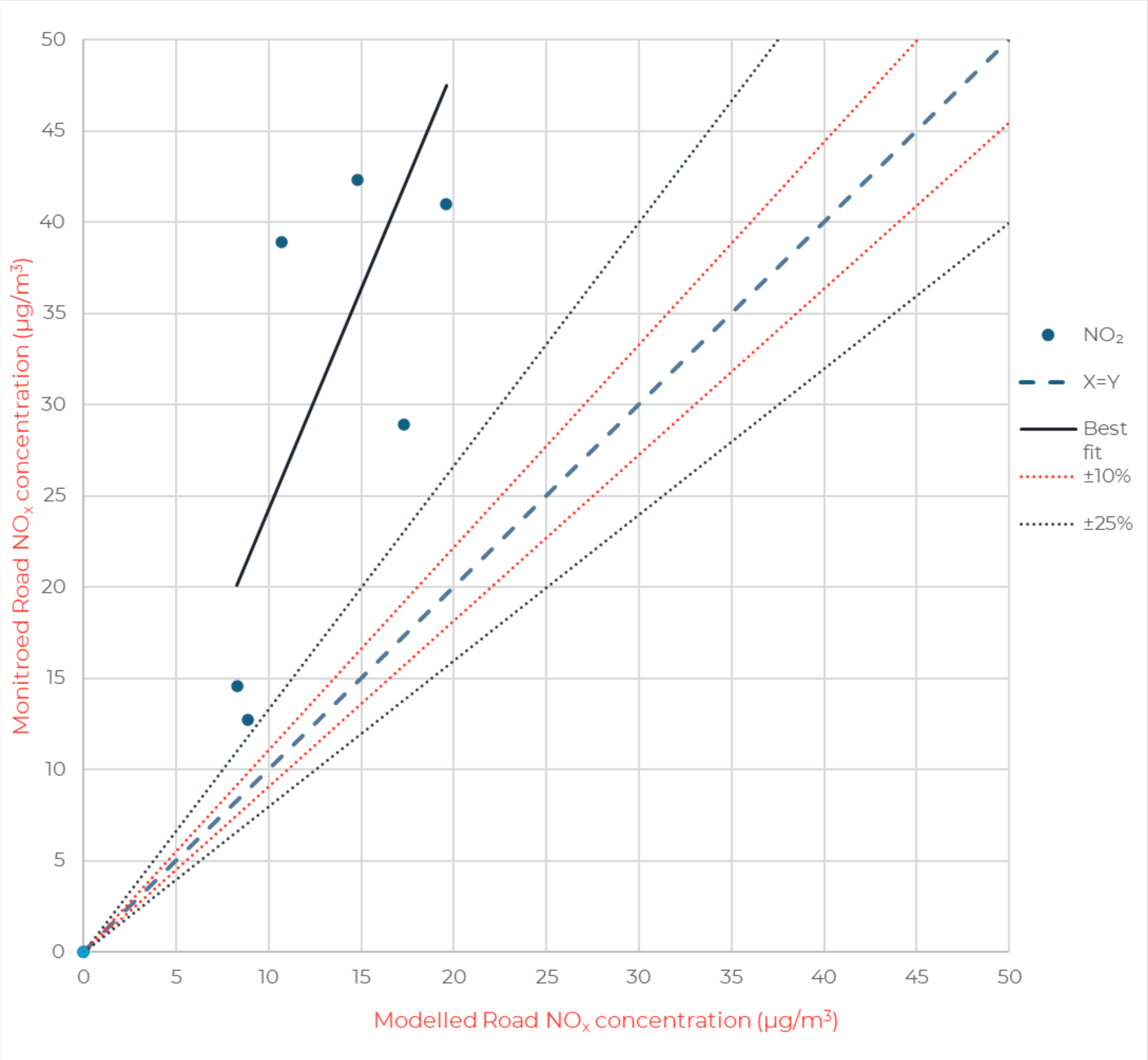

Figure 6-2: Example of graphical comparison between monitored Road NO_x and modelled Road NO_x pre-adjustment.

Once the adjustment factor has been applied to the modelled road NO_x contribution, recalculate the values and statistical parameters presented in Table 6-2 and Figure 6-1 of this technical guidance. The recalculated values, as shown in Table 6-2 and Figure 6-3 of this technical guidance, should be considered again to determine whether further model adjustments or verification calculations need to be undertaken.

If, following this initial model verification and adjustment the following have been confirmed, then the model verification and adjustment process can be considered complete:

- Modelled concentrations predicted at the majority of monitoring sites are within 25% (and ideally within 10 %) of the monitored concentrations,
- The model predictions and monitored concentrations are showing acceptable correlation,
- There is no systematic under- or over-prediction.

For the worked example, as shown in Table 6-4 and Figure 6-3 of this technical guidance, the adjusted results look appropriate. The RMSE is less than 4 µg/m^3 and all data points are within 10 % with no systematic under-/over prediction. Therefore, no further model adjustments or verification calculations are needed. The adjustment factor derived (2.4232 for this example) would then be applied to all modelled NO_x concentrations before using the NO_x to NO_2 Tool to predict total NO_2 concentrations for modelled receptor locations.

Table 6-4: Example of comparison between total monitored and adjusted total modelled NO_2 concentrations.

Site ID	Monitored total NO_2 concentration (µg/m^3)	Non-adjusted modelled road NO_x concentration (µg/m^3)	Adjusted modelled road NO_x concentration (µg/m^3)	Adjusted total modelled NO_2 concentration (µg/m^3)	Percentage difference after adjustment ([modelled – monitored] / monitored)	Root mean square error (RMSE)	Fractional Bias	Correlation Coefficient
1	18.8	10.7	25.9	15.1	-19.7%			
2	19.3	19.6	47.5	20.9	8.3%			
3	19.6	14.8	35.8	17.9	-8.7%			
4	16.0	17.3	42.0	19.6	22.5%	2.82	-0.01	0.75
5	23.1	17.8	43.1	19.8	-14.3%			
6	10.7	8.9	21.6	13.7	28.0%			
7	11.3	8.3	20.1	13.2	16.8%			
Taken directly from monitoring data.	*Taken directly from monitoring data.*	*Taken directly from the modelled road output results.*	*Calculated from non-adjusted values multiples by the gradient value of the trend line (2.4232).*	*Derived from the input of adjusted Road increment NO_x alongside background NO_2 or NO_x concentrations in the NO_x to NO_2 Tool.*	Calculated from adjusted ([modelled – monitored] / monitored) *100. *The majority of modelled concentrations should be within 25%, and ideally within 10% of the monitored values.*	*Average error or uncertainty of the model calculated as per equation stated in Section 7.2 of this a technical guidance. Ideal value is less than 4.*	*Used to identify any systematic under- or over-prediction of the model. Calculated as per equation stated in Section 7.3 of this technical guidance.*	*Used to compare the linear relationship between predicted and observed data. Calculated as per equation stated in Section 7.4 of this technical guidance. The ideal value is 1. Note: this statistic should not be used for small datasets as the outliers could influence the overall result.*

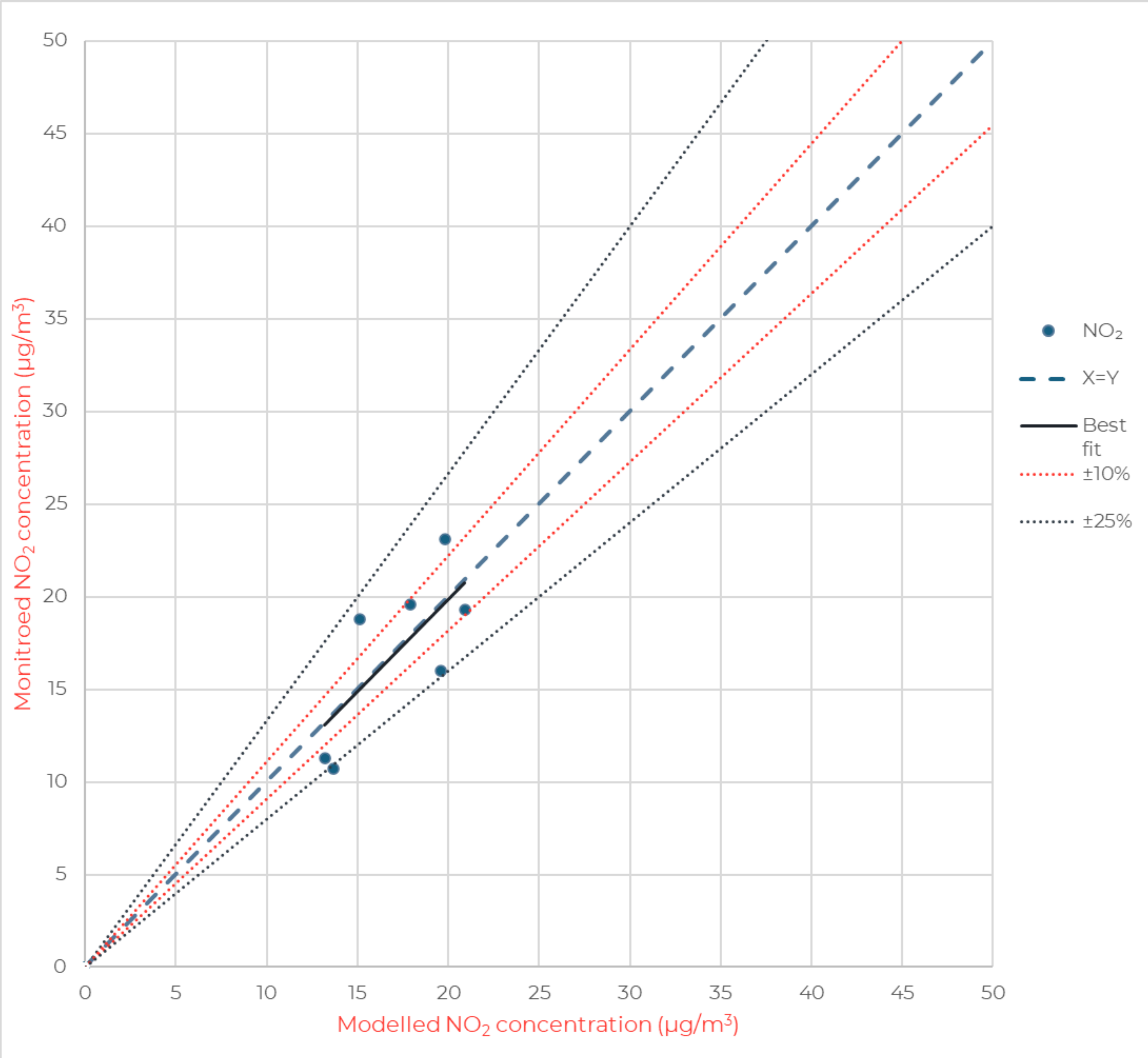

Figure 6-3: Example of graphical comparison between total monitored and adjusted total modelled NO_2 concentrations.

6.1 ZONAL VERIFICATION FACTORS

Following 'whole model' verification calculations, the comparison between modelled and monitored concentrations may show some clear outliers within the data, with subsets of monitoring sites performing similarly, but not within the range of uncertainty required overall.

This can be indicative of a zonal approach to verification being necessary. A zonal approach to verification is one where the verification and adjustment process is completed for monitoring sites and model predictions within zones of the study area.

The verification and adjustment zones defined will be individual to every project and dispersion model, and can be based on a variety of aspects such as:

- Road type (e.g. motorways).

- Spatial extent (e.g. urban centre).
- Traffic composition (e.g. bus lanes).
- Physical features (e.g. road gradients, areas with monitoring and receptors within street canyons).

Zonal verification factors will help to minimise the model under- or over-predicting concentrations at certain locations across a study area. Each zone will have its own verification calculations and adjustment factor to apply to the road contribution of the modelled NO_x concentrations, and the spatial extent of the zone will need to be defined to ensure the correct receptor locations are having the appropriate zonal adjustment factor applied to them.

The ratio of monitored road contribution to modelled road contribution (last column in Table 6-3 of this technical guidance) can be used to help define these zonal areas where ratios are similar but should not be relied on in isolation when defining zones. There should be common physical features or dispersion characteristics identified within a zone that results in similar model performance in that area.

7 STATISTICAL ASSESSMENT OF MODEL PERFORMANCE

7.1 USE OF STATISTICAL PARAMETERS

There are a variety of statistical methods that can be used to assess model performance, and to determine whether adjustment of modelling results is required. As outlined within Section 6 of this technical guidance, the recommended methods for assessing road traffic dispersion model uncertainties are root mean square error (RMSE), fractional bias and correlation coefficient. The calculation of these statistics is outlined within the following sections. The definitions that apply to the equations presented are:

- 'N' is the total number of data points, summed over index 'i'.
- 'Obs' is the observed concentration; 'Avg.Obs' is the average of all observed concentrations.
- 'Pred' is the predicted concentration; 'Avg.Pred' is the average of all predicted concentrations.
- 'Stdev.Obs' is the standard deviation of the observed concentrations with 'Stdev.Pred' being the standard deviation of the predicted concentrations.

Care should be taken when applying statistical parameters to small datasets. For example, fractional bias is recommended for larger not smaller datasets and therefore should not be relied upon individually for model verification with a smaller number of data points.

The statistical parameters outlined within the following sections are all calculated automatically within the accompanying Verification Template.

7.2 ROOT MEAN SQUARE ERROR (RMSE)

The formula for the RMSE is :

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(Obs_i - Pred_i)^2}$$

This method is used to quantify the average difference (error/uncertainty) between the precited and actual data, in this case modelled to observed pollutant concentrations. The ideal value for RMSE is 0 but as the units are the same at the data inputted it also depends on the standard that the data is being assessed against. As with the other verification calculations if the RMSE value is greater than +/- 25% of the guideline value it is being assessed against then the model should be re-evaluated, and refinements made to produce a 'better' model performance.

The aim would be to get within 10 %. Therefore, as stated in Step 4 of the detailed methodology in Section 6 of this technical guidance, with the data being assessed against 40 μg/m^3 (annual mean NO_2 concentration) then model adjustment would be advised if an RMSE greater than 10 μg/m^3 was calculated. The ideal RMSE for this example would be results within 10 % of 40 μg/m^3 (less than 4 μg/m^3).

7.3 FRACTIONAL BIAS

The formula for the fractional bias (FB) is: $FB = \frac{(Avg.Obs - Avg.Pred)}{0.5\ (Avg.Obs + Avg.Pred)}$

This method is used to determine whether a model has a systematic tendency to deviate from the actual results and under- or over-predict. The ideal value for fractional bias is 0 where there is no systematic under- or over-prediction (negative values imply the model is over predicting and positive, underpredicting). This statistic evaluates the whole model and therefore if should be used alongside the detailed comparison of performance at each site considered, especially where predictions are close to or above the air quality guideline.

7.4 CORRELATION COEFFICIENT

The formula for the correlation coefficient (r) is: $r = \left[\frac{\sum_{i=1}^{N}(Obs_i - Avg.Obs)(Pred_i - Avg.Pred)}{Stdev.Obs \times Stdev.Pred}\right]$

This method is used to compare the linear relationship between predicted and observed data. The ideal value for correlation coefficient is 1 which indicates a perfect linear relationship between predicted and observed data, a value of 0 mean there is no relationship. This statistical parameter can be useful for comparison if the model has many data points. This statistic is most useful with a large amount of data and is not recommended for smaller datasets as the outliers could sway the overall result.

8 CONSIDERATIONS FOR IMPROVING MODEL PERFORMANCE

If the model performance is still not acceptable following the model refinement process outlined in Section 5 of this technical guidance and the model zoning approach (where appropriate) in Section 6 of this technical guidance, then it may be necessary to complete a more detailed review of input data such as traffic, meteorological, emissions calculations and monitoring data. This might involve detailed discussions of traffic data with transport engineers, or those carrying out the monitoring across the study area.

9 REPORTING

Where detailed dispersion modelling is undertaken, it is recommended that the model verification is completed and documented in the project air quality assessment report. This reporting should include, but not necessarily be limited to:

- Full details of monitoring sites used (including aspects such as XY co-ordinates, site ID, site type, distance to kerb, height, whether it is in a polluted airshed).
- A map of the monitoring locations considered with respect to the detailed modelling area extent.
- Detailed reasoning for inclusion or exclusion of monitoring sites in the model verification process.
- Graphs and tables summarising the verification process, such as the examples presented in Section 6 of this technical guidance, as produced by the accompanying Verification and Adjustment Template tools.