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Hydrogen Pipeline

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Appendix 9G

Model inputs and Verification

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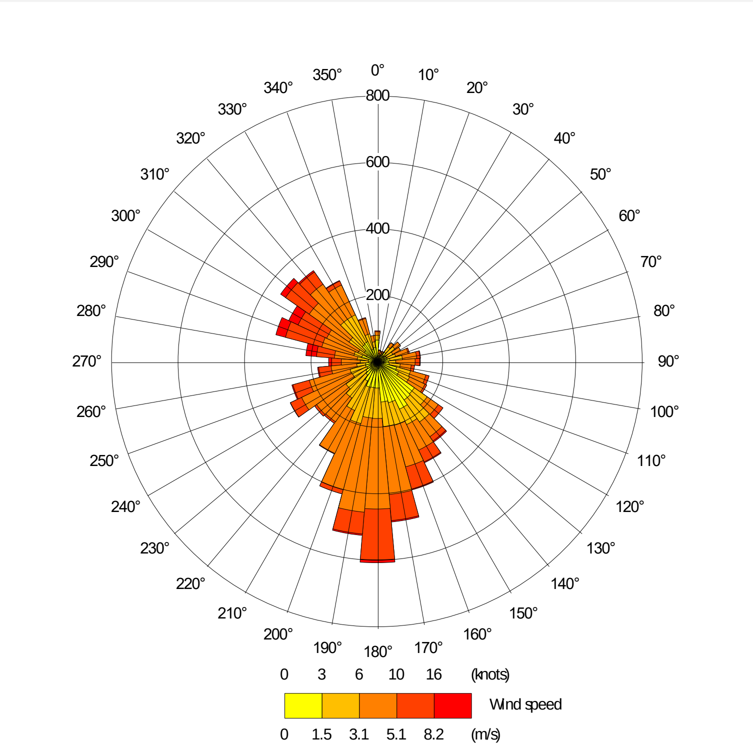
1. Model Inputs

1.1.1 **Table 9G 1.1** shows the model inputs used in the assessment presented in **Chapter 9: Air Quality**.

Table 9G 1.1 Model inputs

Input	Notes
Traffic data	The traffic data were provided by WSP Transport Consultants.
Vehicle Emissions Factors	NOx, PM_{10} and $PM_{2.5}$ emissions data for 2019 and 2028 were obtained from Defra's Emissions Factors Toolkit (EFT), version 12.0.1. For the predictions of future year emissions, the toolkit considers factors such as anticipated advances in vehicle technology and changes in vehicle fleet composition. Emissions data for 2022 (baseline) and 2028 (peak construction year) have been used with the following settings in EFT 12.0.1: • Area = England (not London). • Traffic format = Basic Split. • Road type = 'Motorway (not London)' for motorways and fast dual carriageways, 'Urban (not London)' for roads passing through urban areas and 'Rural (not London)' for roads outside urban areas. • Output = Air Quality Modelling (g/km/s) for NOx, PM_{10} and $PM_{2.5}$. NH_3 emissions data for 2022 and 2028 were obtained from Air Quality Consultants CREAMv1a tool which allows for the calculation of NH_3 emission factors arising from road traffic. Emissions data for 2022 (baseline) and 2028 (peak construction year) have been used with the following settings in CREAMV1A: • Area = England (not London). • Traffic format = Basic Split. • Road type = 'Motorway (not London)' for motorways and fast dual carriageways, 'Urban (not London)' for roads passing through urban areas and 'Rural (not London)' for roads outside urban areas. • Output = Air Quality Modelling (g/km/s) for NH_3.

Input	Notes
	‘NH_3GRASSLAND’ added to pollutant pallet with a deposition velocity of 0.02m/s, and ‘NH_3FOREST’ added to pollutant pallet with a deposition velocity of 0.03m/s (Note: deposition velocities taken from AQTAG06, GRASSLAND = short vegetation, FOREST = tall vegetation).
Road source geometry	All model links aligned to the carriageway centreline, set to true road width (kerb to kerb/edge of travelled lanes), road heights set to zero.
Meteorological data	Rostherne meteorological station 2022. Parameters include hourly sequential format: Julian date, hour, wind speed (m/s), wind direction (degrees from north), cloud cover (oktas), surface temperature (Celsius). • Meteorological site roughness length = 0.5m • Meteorological site minimum Monin-Obukhov length = 30m • Dispersion site latitude = 53.3˚ • Dispersion site roughness length = 0.5m • Dispersion site minimum Monin-Obukhov length = 30 
Background concentrations	From Defra 1 x 1km mapped datasets for 2022 and 2028.

Input	Notes
	(2018-based background maps for NOx, PM_{10} and $PM_{2.5}$). Background data for NH_3 and nitrogen deposition were taken from the Air Pollution Information System (APIS). Unlike the Defra background data, the data from APIS require manipulation to predict background concentrations in future years; this was done with reference to the Joint Nature Conservation Committee's Nitrogen Futures publication. For the assessment, the Nitrogen Futures 'business as usual' scenario was adopted whereby NH_3 background concentrations increase by approximately 0.08% year on year, and Nitrogen deposition (which depends on NOx and NH_3 levels) decreases by approximately -1.04% year on year.
Receptors	Specified points: • Discrete existing and future human receptors, see **Table 9E 1.1** (**Appendix 9E**). • Discrete ecological receptors, see **Table 9E.2.1** (**Appendix 9E**).
Model outputs	Annual mean (long-term) concentrations of NOx, PM_{10}, $PM_{2.5}$, 'NH_3grassland' and 'NH_3forest' (Note: grassland = short vegetation, forest = tall vegetation).
Post-processing	Verification (discussed below) to address systematic model error of road source contributions of annual mean NOx, PM_{10} and $PM_{2.5}$. NOx to NO2 conversion using Defra's calculator version 8.1. (NOx_to_NO_2_Calculator_v8.1). To indicate compliance with the 24-hour mean AQS for PM10 LAQM.TG(22) gives the following empirical equation that relates the annual mean concentration to the number of exceedances of the 50µg/m3 threshold, where up to 35 exceedances are allowed: • *Number of 24-hour mean exceedances of 50µg/m3 = -18.5 + 0.00145 × (annual mean)3 + (206 ÷ annual mean)* Note: where the annual mean PM_{10} concentration is less than 16.5µg/m3 then the number of exceedances of the 24-hour mean objective can be assumed to be zero (the relationship is invalid for annual mean concentrations less than 14.8µg/m3). To indicate compliance with the 1-hour mean NO2 standard, LAQM.TG(22) advises that compliance is likely if the annual mean concentration is less than 60µg/m3.

Input	Notes
	For NH_3, no adjustment was undertaken as there were no appropriate monitoring data to allow model verification for this pollutant. Nitrogen Deposition is calculated according to the following steps: • Step 1 – calculate dry deposition fluxes: ▸ Dry NO_2 deposition flux (µg/m2/s) = road source contributed NO_2 (µg/m3) * dry NO_2 deposition velocity for short vegetation (0.0015m/s) or tall vegetation (0.003m/s). ▸ Dry NH_3 deposition flux (µg/m2/s) = road source contributed NH3 (µg/m3) * dry NH_3 deposition velocity for short vegetation (0.02m/s) or tall vegetation (0.03m/s). • Step 2 – convert dry deposition fluxes to dry deposition rates: ▸ Dry nitrogen deposition due to NO2 (kg/ha/yr) = dry NO2 deposition flux (µg/m2/s) * 96. ▸ Dry nitrogen deposition due to NH3 (kg/ha/yr) = dry NH3 deposition flux (µg/m2/s) * 259.7. • Step 3 – calculate total dry deposition rate: ▸ Total dry nitrogen deposition (kg/ha/yr) = dry nitrogen deposition due to NO_2 (kg/ha/yr) + dry nitrogen deposition due to NH_3 (kg/ha/yr) + background nitrogen deposition for short or tall vegetation (kg/ha/yr).

2. Model Verification

2.1.1 The ADMS-Roads dispersion model has been widely validated for this type of assessment and is fit for purpose. The comparison of modelled concentrations with local monitored concentrations is a process termed ‘verification’. Model verification investigates the discrepancies between modelled and measured concentrations, which can arise due to the presence of inaccuracies and/or uncertainties in model input data, modelling and monitoring data assumptions.

2.1.2 This process of verification aims to minimise modelling uncertainty and systematic error by correcting modelled results by an adjustment or verification factor to gain greater confidence in the results. This was carried out following the methodology specified in the LAQM.TG(22).

2.1.3 The following are examples of potential causes of such discrepancy:

a) Estimates of background pollutant concentrations;

b) Meteorological data uncertainties;

c) Traffic data uncertainties;

d) Model input parameters, such as ‘roughness length’; and

e) Overall limitations of the dispersion model.

2.1.4 Monitoring results from National Highways National Air Quality Monitoring Network Annual 2022 Network Report, 2023 Air Quality Annual Status Report (ASR) for Warrington Borough Council, 2022 Air Quality ASR for Greater Manchester Combined Authority were analysed for the NO_2 monitoring around the study area.

2.1.5 The model was run for 2022 to predict the road source contribution to the annual mean NOx concentration at several diffusion tube sites. As the diffusion tube provides a measurement of NO_2 concentration only, it was necessary to derive an estimate of monitored road-NOx concentration using Defra’s NOx to NO_2 conversion calculator.

2.1.6 The data examined in the verification process are presented in **Table 9G 2.1.**

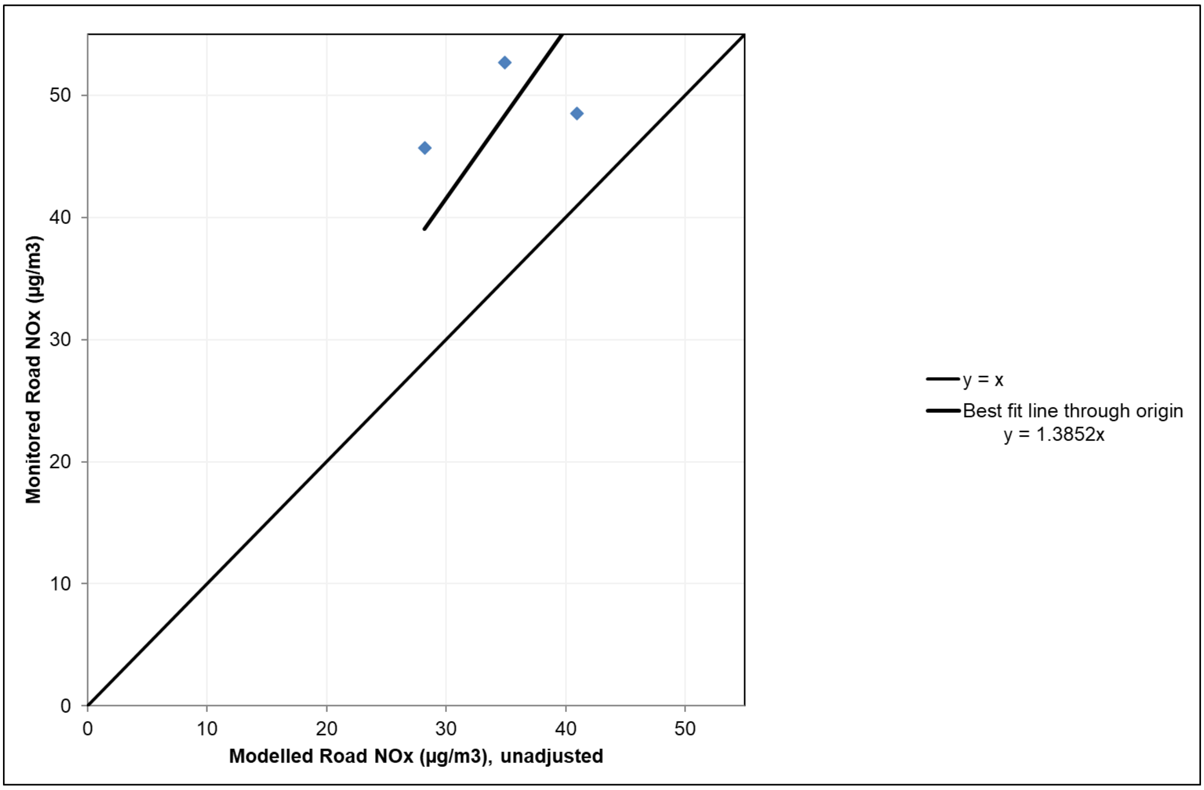
Table 9G 2.1Data used in model verification

Verification zone	Monitoring Site	Monitored Annual Mean NO_2 Concentration (µg/m^3)	Background NO_2 (µg/m^3)	Monitored Road-NOx (µg/m^3) (from NOx:NO_2 calculator)	Modelled Road-NOx (µg/m^3)	Ratio monitored / modelled road NOx
Motorway and fast dual carriageways	14	40.0	16.5	48.5	41.0	1.2
	15	41.8	16.5	52.7	34.9	1.5
	25	38.6	16.3	45.7	28.2	1.6
Urban environment	TR27NO	15.4	10.8	8.1	5.9	1.4
	TR29NO	17.6	12.8	9.0	4.9	1.8
Air quality management areas	CM3	24.0	12.8	21.3	21.4	1.0
	DT13	26.3	16.8	18.3	8.2	2.2
	DT14	23.6	12.8	20.5	10.1	2.0

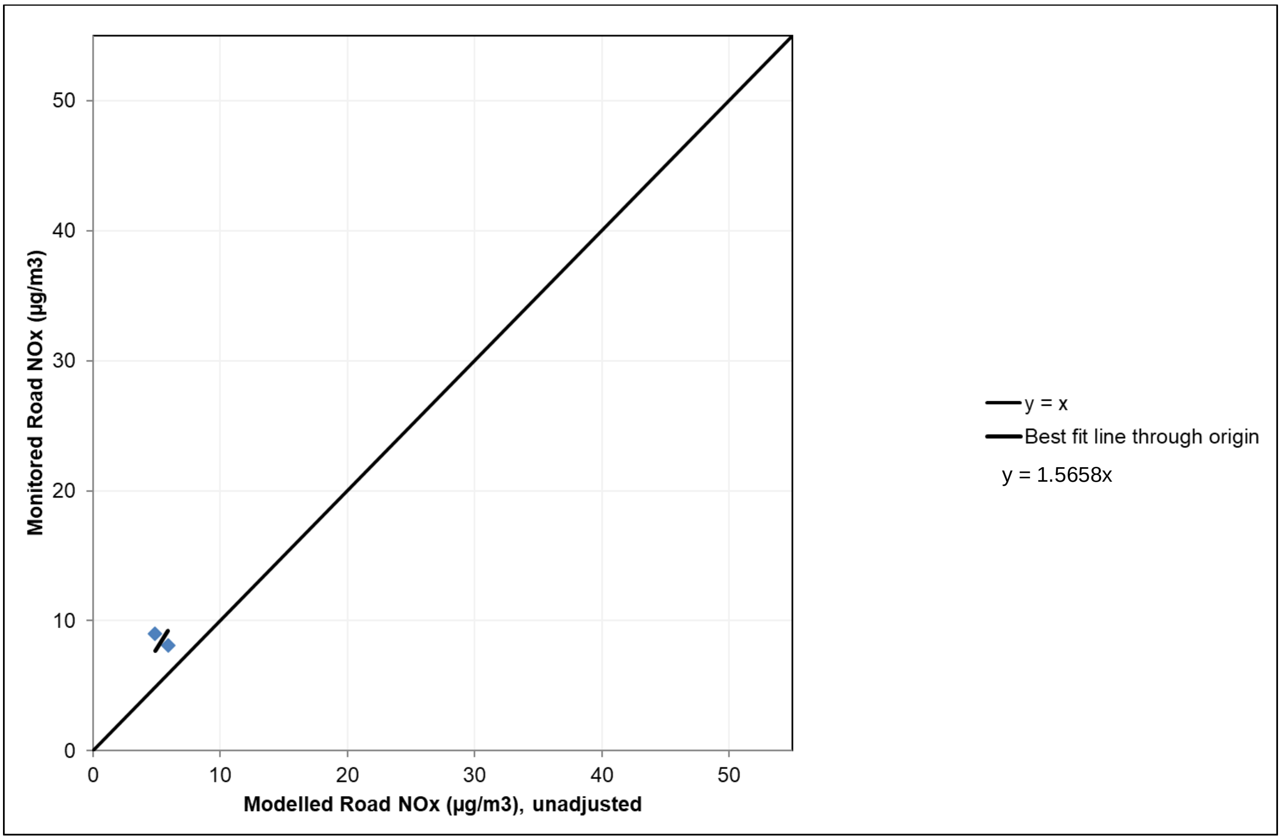
2.1.7 The road-NOx adjustment factor was determined as the slope of the best fit line between the ‘measured’ road contribution and the model derived road contribution, forced through zero (**Graphic 9G.1**). This factor was then applied to the modelled road-NOx concentration for each monitoring site to provide adjusted modelled road-NOx concentrations. The total nitrogen dioxide concentrations were then determined by inputting the adjusted modelled road-NOx concentrations and the background NO_2 concentration into the NOx to NO_2 calculator.

Graphic 9G.1 Comparison of Measured Road-NOx with Unadjusted Modelled Road-NOx

Motorway and fast dual carriageway



Urban environment



Air quality management area

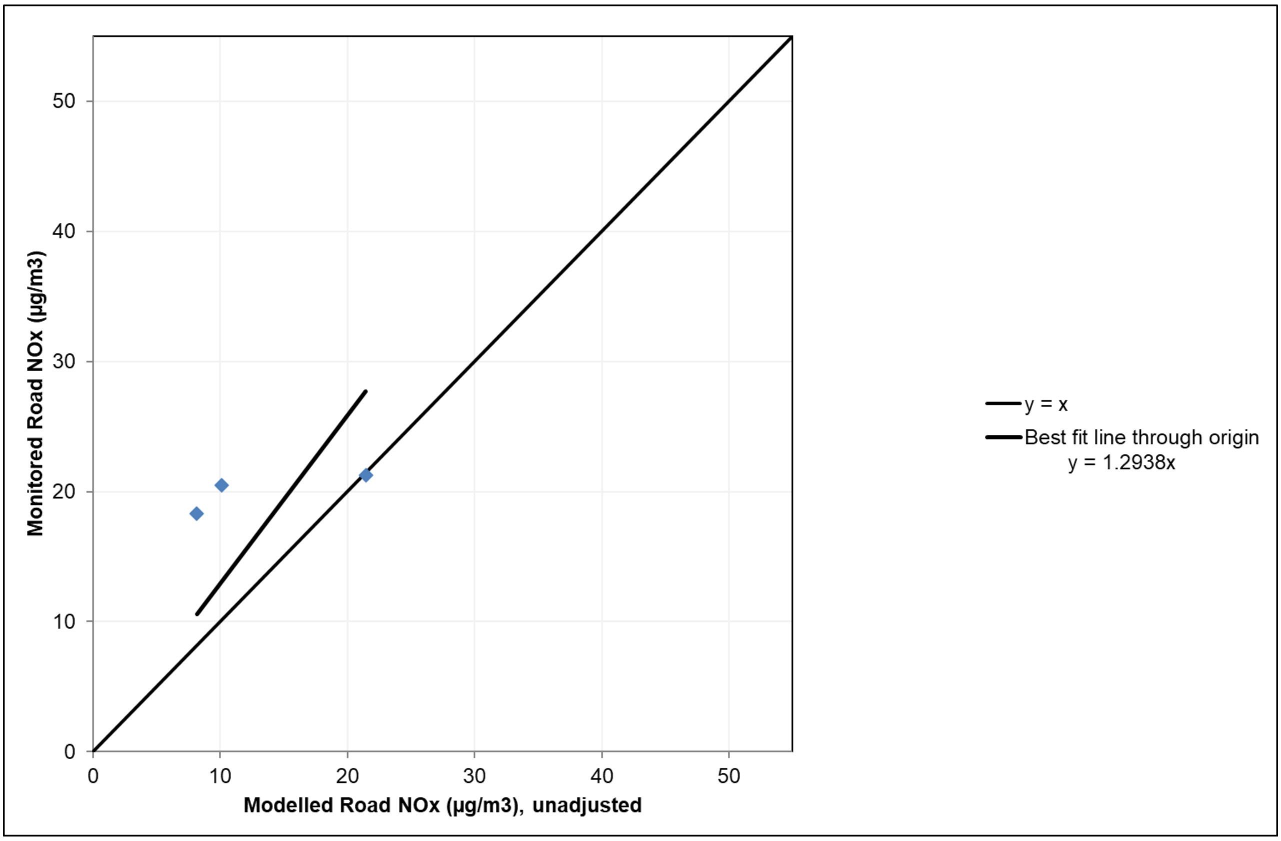


Table 9G 2.2 Data examined in model verification after adjustment

Verification zone	Monitoring Site	Monitored Annual Mean NO_2 Concentration (µg/m^3)	Background NO_2 (µg/m^3)	Adjusted modelled annual mean NO2 (µgm-3)	% (Modelled-Monitored)/Monitored
Motorway and fast dual carriageway	14	40	16.5	43.5	9%
	15	41.8	16.5	39.9	-4%
	25	38.6	16.3	35.6	-8%
Urban environment	TR27NO	15.4	10.8	15.8	2%
	TR29NO	17.6	12.8	16.9	-4%
Air quality management area	CM3	24.0	12.8	27.2	13%
	DT13	26.3	16.8	22.4	-15%
	DT14	23.6	12.8	19.8	-16%

PM_{10} and $PM_{2.5}$

2.1.8 There are no local PM_{10} or $PM_{2.5}$ monitoring data against which the model could be verified. Consequently, the verification factor determined above for adjusting the road-NO_x contribution has been applied to the predicted road-PM_{10} and road-$PM_{2.5}$ contributions, consistent with guidance set out in LAQM.TG(22).

Model Uncertainty

2.1.9 An evaluation of model performance has been undertaken to establish confidence in model results. LAQM.TG(22) identifies a number of statistical procedures that are appropriate to evaluate model performance and assess the uncertainty. These include:

a) Root mean square error (RMSE);

b) Fractional bias (FB); and

c) Correlation coefficient (CC).

2.1.10 These parameters estimate how the model results agree or diverge from the observations. These calculations can be carried out prior to, and after adjustment, or based on different options for adjustment, and can provide useful information on model improvement. A brief for explanation of each statistic is provided in **Table 9G 2.3**, and further **Table 9G 2.3** details can be found in Box 7.17 of LAQM.TG(22).

Table 9G 2.3 Methods for describing model uncertainty

Statistical Parameter	Comments	Ideal value
RMSE	RMSE is used to define the average error or uncertainty of the model. The units of RMSE are the same as the quantities compared. If the RMSE values are higher than 25% of the objective being assessed, it is recommended that the model inputs and verification should be revisited in order to make improvements. For example, if the model predictions are for the annual mean NO2 objective of 40µg/m3, if an RMSE of 10µg/m3 or above is determined for a model it is advised to revisit the model parameters and model verification. Ideally an RMSE within 10% of the air quality objective would be derived, which equates to 4µg/m3 for the annual mean NO2 objective.	0.01
Fractional Bias	It is used to identify if the model shows a systematic tendency to over or under predict. FB values vary between +2 and -2 and has an ideal value of zero. Negative values suggest a model over-prediction and positive values suggest a model under-prediction.	0.00
Correlation Coefficient	It is used to measure the linear relationship between predicted and observed data. A value of zero means no relationship and a value of 1 means absolute relationship. This statistic can be particularly useful when comparing a large number of model and observed data points.	1.00

2.1.11 To assess the uncertainty of a model, the RMSE is the simplest parameter to calculate providing an estimate of the average error of the model in the same units as the modelled predictions. It is also often easier to interpret the RMSE than the other statistical parameters and therefore it has been calculated in this assessment to understand the model uncertainty.

2.1.12 The RMSE value calculated after verification are summarised in **Table 9G 2.4**.

Table 9G 2.4 Root mean square values after verification

Verification zone	Root mean square value (µg/m3)
Motorway and fast dual carriageway	2.9
Urban environment	0.6
Air quality management areas	3.7

2.1.13 The derived verification factors used for each zone in the model are summarised in **Table 9G 2.5**.

Table 9G 2.5 Derived verification factors

Verification zone	Verification Factors
Motorway and fast dual carriageway	1.39
Urban environment	1.57
Air quality management areas	1.29

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