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Defra 2021 Air Quality Model Inter-Comparison Exercise

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21st International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes

27-30 September 2022,

Aveiro, Portugal

Cambridge Environmental Research Consultants
Environmental Software and Services

Project motivation & context

- **Policy makers** need to have confidence in the air quality (AQ) models used on their behalf for a range of applications
- **Model inter-comparison exercises** (MIE) quantify model performance, providing evidence that ensures selected **models are fit for purpose**
- UK takes a combined measurement and modelling approach to reporting associated with the **Air Quality Standards Regulations (AQSR, previously the EU Air Quality Directive)** pollutant metrics
- **Defra 2021 AQ MIE** focuses on the **suitability of models for AQSR reporting** by comparing the results from the model currently used for this purpose to three other models that have UK national AQ modelling capabilities
- Model performance and results have been explained using information on **models' formulations**, **configurations** and **inputs**

Project Tasks

Task	Brief description
0	Comparison of model formulation
1	Comparison of modelled compliance metrics
2	Comparison of modelled concentrations at measurement sites
3	Comparison of urban concentrations and compliance

- Focus of this presentation: Task 2 – comparison of modelled and measured data

Models & identifiers

Group	Modelling system	Identifiers	
Environmental Research Group, Imperial College London	CMAQ-Urban	ERG-ICL	CMAQ-Urban
Met Office	Air Quality Unified Model (AQUM)	MO	AQUM-SPPO
Ricardo*	Pollution Climate Mapping (PCM)	Ricardo	PCM
UK Centre for Ecology & Hydrology	EMEP	UKCEH	EMEP

Environmental Research Group
Imperial College London

Met Office

RICARDO

UK Centre for Ecology & Hydrology

*Ricardo currently perform AQ compliance modelling for Defra using PCM

Overview of model formulation

Modelling group	ERG-ICL	MO	Ricardo	UKCEH
Dispersion model	CMAQ-Urban	AQUM-SPPO	PCM	EMEP
Meteorological model	WRF		WRF (or measurements)	WRF
Temporal resolution	Hourly	Hourly	**Annual**	Hourly
Calibration	✗	✓	✓	✗
Explicit modelling of road sources	✓ (ADMS Kernel)	No, but calibration approach extended to roadside concentrations	✓ (ADMS Kernel)	✗
Street canyon modelling	✓	✗	✗	n/a
Scale	Multi-scale model, **high** (**20 m**) final grid resolution	**Low** resolution regular grid (~**12 km**)	**Mixed**: fine regular grid (**1 km**) plus urban roadsides	Fine regular grid (**1 km**)
Emissions	**Bottom-up road transport emissions**, differing from NAEI emissions / NAEI, EMEP in other sectors	NAEI, EMEP	NAEI, EMEP **(projected from 2017 to 2018)**	NAEI, EMEP, **MapEIRE** Integrated biogenic emissions; European biogenic vegetation emission factors
Computational expense	High	Medium	Low	High for meteorological modelling, lower for concentration modelling

Measurements – NO_X, NO_2, PM_{10}, $PM_{2.5}$, O_3

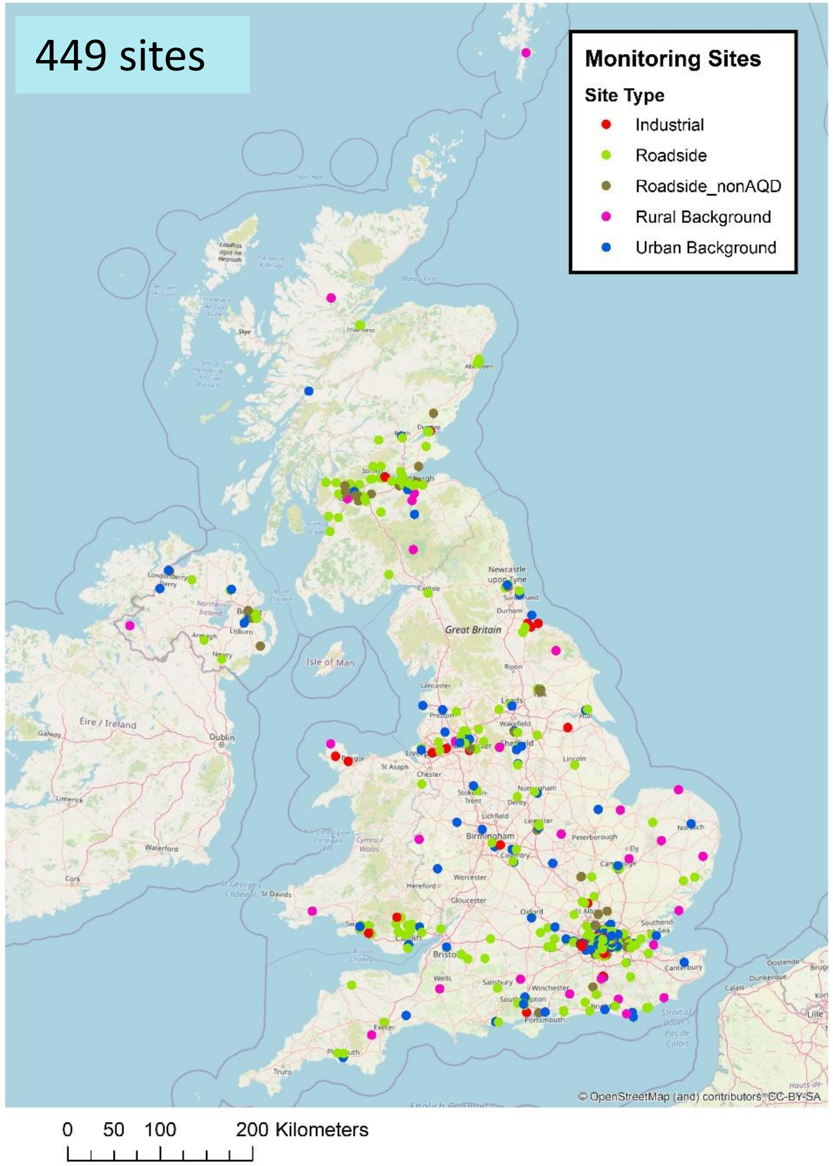
Hourly measurements from six automatic networks:

AURN	AQE	SAQN	WAQN	NIAQN	ICL (formerly KCL)
152	100	63	24	13	97

Analysed results for 5 pollutants for 5 site types:

Type	NO_X	NO_2	PM_{10}	$PM_{2.5}$	O_3
Rural Background	19	19	9	7	28
Urban Background	103	103	61	48	54
Roadside	223	224	154	66	15
Industrial	21	21	26	14	7
Roadside_nonAQD*	45	45	34	16	1

- All stations have at least 75% data capture in 2018 for the relevant pollutant
- Analysis includes sites used for calibration (PCM, AQUM-SPPO)



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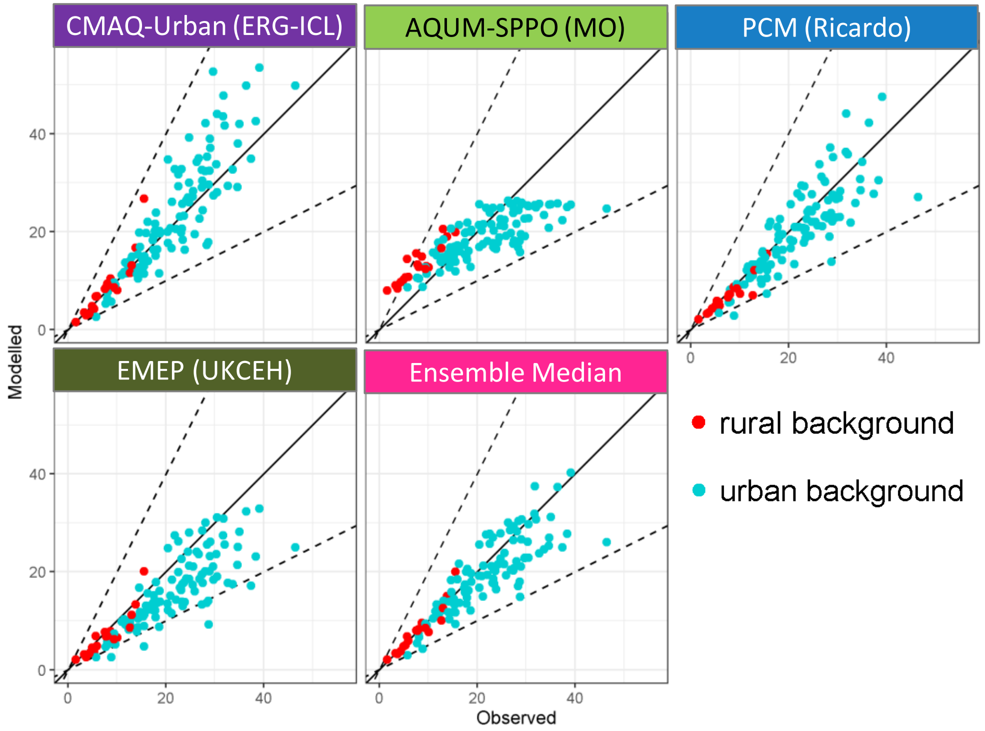
**Roadside sites that don't meet the AQD/AQSR siting criteria (Ricardo)*

Summary of model evaluation results for NO_2

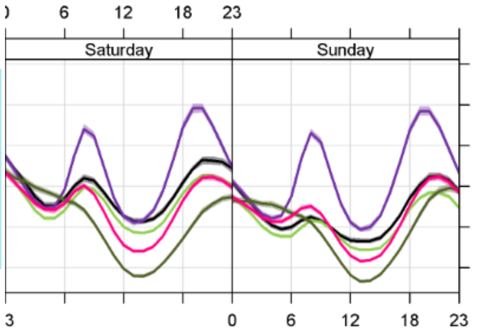
Concentrations in μg/m³

- Good overall agreement for **CMAQ-Urban** and **PCM**
- **EMEP** slightly underestimates at background sites and underestimates at roadside sites (no roadside model or increment)
- **AQUM-SPPO** overestimates at rural sites
- **AQUM-SPPO** and **EMEP** underestimate variability
- **CMAQ-Urban** overestimates variability; diurnal variation at weekends not well represented

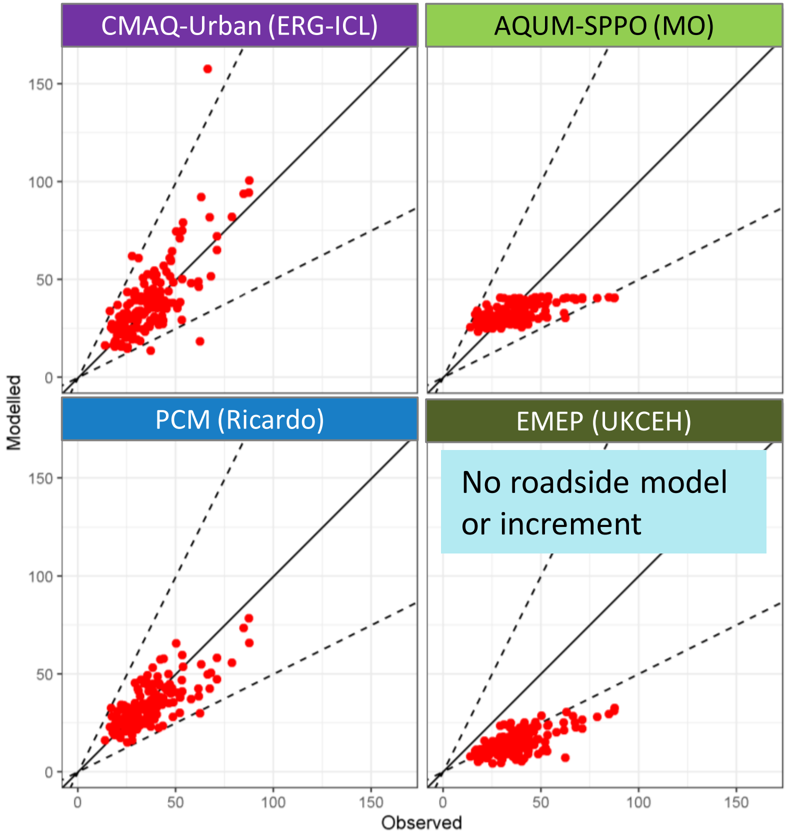
Annual mean at 122 background sites



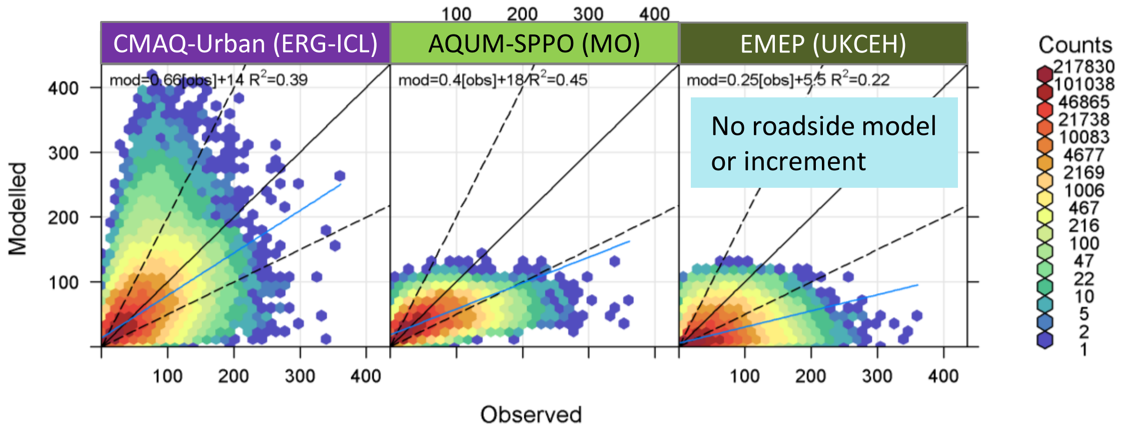
Average weekend diurnal variation at 122 background sites



Annual mean at 160 roadside sites



Hourly mean at 160 roadside sites



Model evaluation statistics for NO_2

Evaluation of **annual** mean concentrations in µg/m³

Site type	Modelling group	Model	Mean	RMSE	NMB	NMSD	$MQI_{annual\ 90}$
Background		Observed	19.8				
	ERG-ICL	CMAQ-Urban	21.6	5.8	0.09	0.32	1.06
	MO	AQUM-SPPO	18.3	6.0	-0.08	-0.46	0.96
	Ricardo	PCM	**18.5**	**4.7**	**-0.07**	**0.04**	0.73
	UKCEH	EMEP	15.0	6.9	-0.25	-0.18	1.10
		Ensemble	*17.8*	***4.7***	*-0.10*	*-0.11*	***0.71***
Roadside		Observed	36.6				
	ERG-ICL	CMAQ-Urban	38.8	13.1	0.06	0.36	1.43
	MO	AQUM-SPPO	33.0	12.4	-0.10	-0.67	1.45
	Ricardo	PCM	**34.6**	**9.6**	**-0.06**	**-0.20**	**1.27**
	UKCEH	EMEP	14.9	24.3	-0.59	-0.57	2.70

Evaluation of **hourly** concentrations in µg/m³

Site Type	Organisation	Model	Mean	RMSE	R	NMB	NMSD	CoE	Fac2
Background		Observed	19.9						
	ERG-ICL	CMAQ-Urban	21.8	13.3	0.74	0.09	**0.11**	0.32	0.73
	MO	AQUM-SPPO	**18.4**	**11.1**	**0.77**	**-0.08**	-0.30	**0.43**	**0.77**
	UKCEH	EMEP	15.0	13.8	0.68	-0.25	-0.14	0.31	0.66
		Ensemble	*17.5*	*11.1*	*0.77*	*-0.12*	*-0.17*	*0.45*	*0.79*
Roadside		Observed	35.9						
	ERG-ICL	CMAQ-Urban	**37.3**	23.4	0.62	**0.04**	**0.05**	0.20	0.73
	MO	AQUM-SPPO	32.7	**19.8**	**0.67**	-0.09	-0.40	**0.33**	**0.79**
	UKCEH	EMEP	14.5	31.6	0.47	-0.60	-0.47	-0.14	0.36

RMSE: root mean square error
NMB: Normalised mean bias
NMSD: Normalised mean standard deviation
MQI: Model Quality Index
R: correlation coefficient
CoE: Coefficient of Efficiency
Fac2: Fraction of modelled hours within factor of 2 of observed

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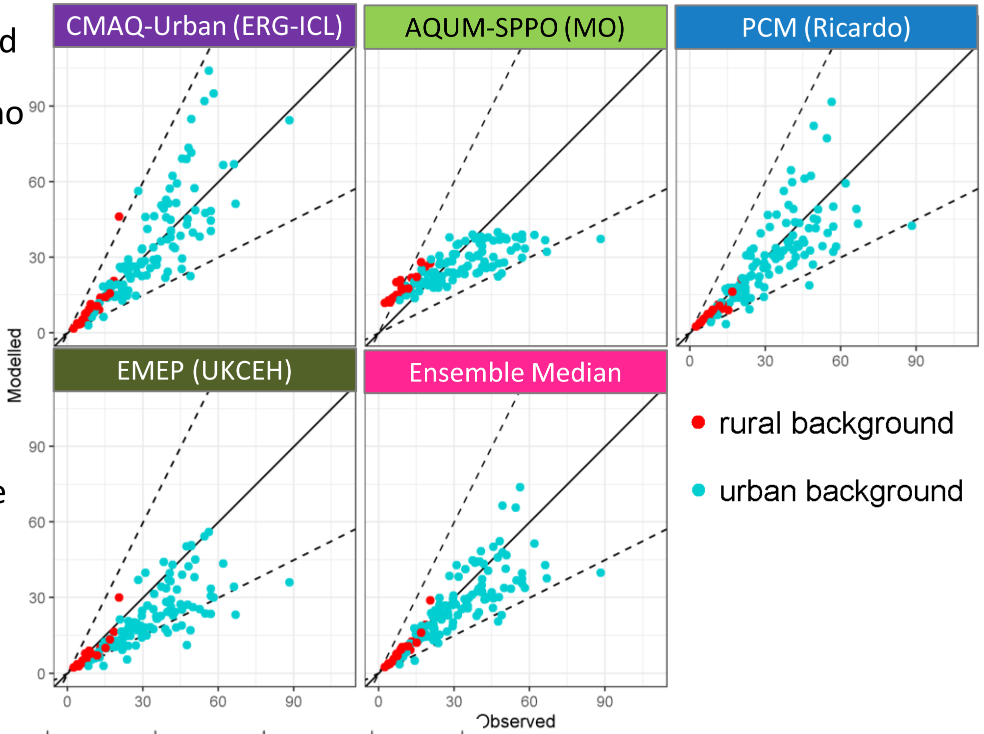
Summary of model evaluation results for NO_X

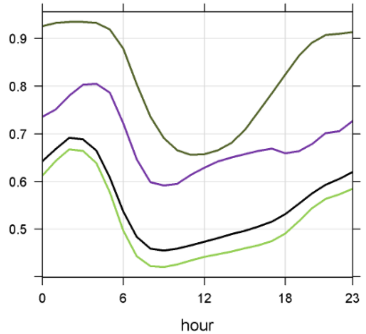
Concentrations in μg/m³

- Good overall agreement for **PCM**
- **EMEP** slightly underestimates at background sites and underestimates at roadside sites; overestimates NO_2/NO_X at roadside sites (no roadside model or increment)
- **AQUM-SPPO** overestimates at rural sites
- **AQUM-SPPO** and **EMEP** underestimate variability
- **CMAQ-Urban** overestimates variability in annual mean between background sites
- **CMAQ-Urban** and **AQUM-SPPO** capture the diurnal variation at roadside sites
- **CMAQ-Urban** overestimates NO_2/NO_X at roadside sites

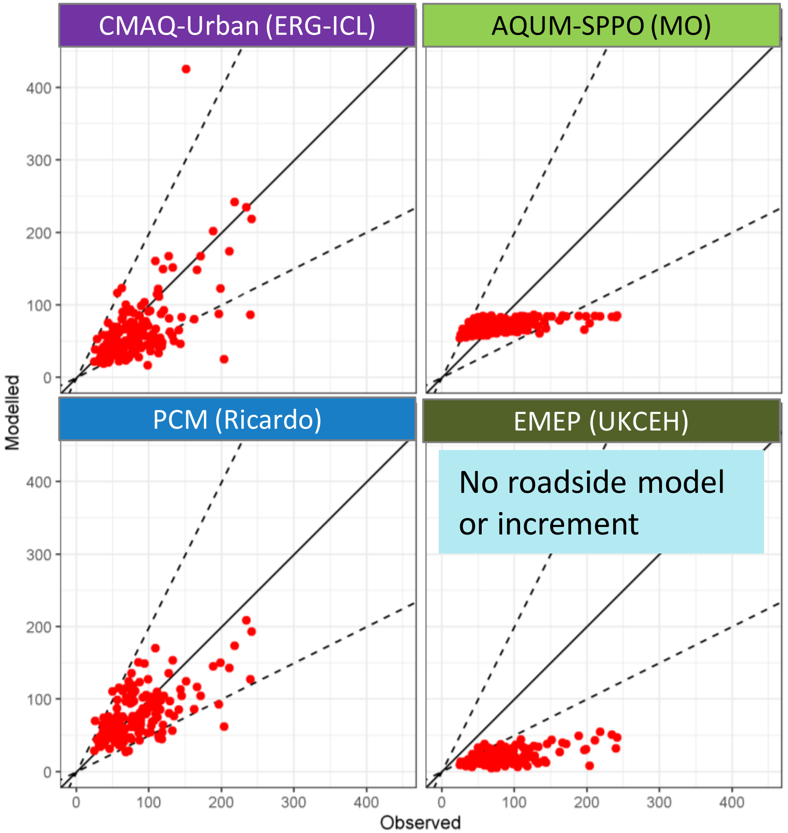
Annual mean at 122 background sites



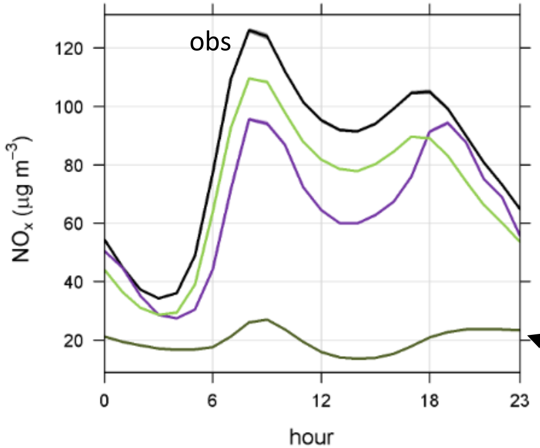
Average diurnal variation of NO_2/NO_X over 160 roadside sites



Annual mean at 160 roadside sites



Average diurnal variation over 160 roadside sites



CMAQ-Urban (ERG-ICL)

AQUM-SPPO (MO)

EMEP (UKCEH)

EMEP has no roadside model or increment

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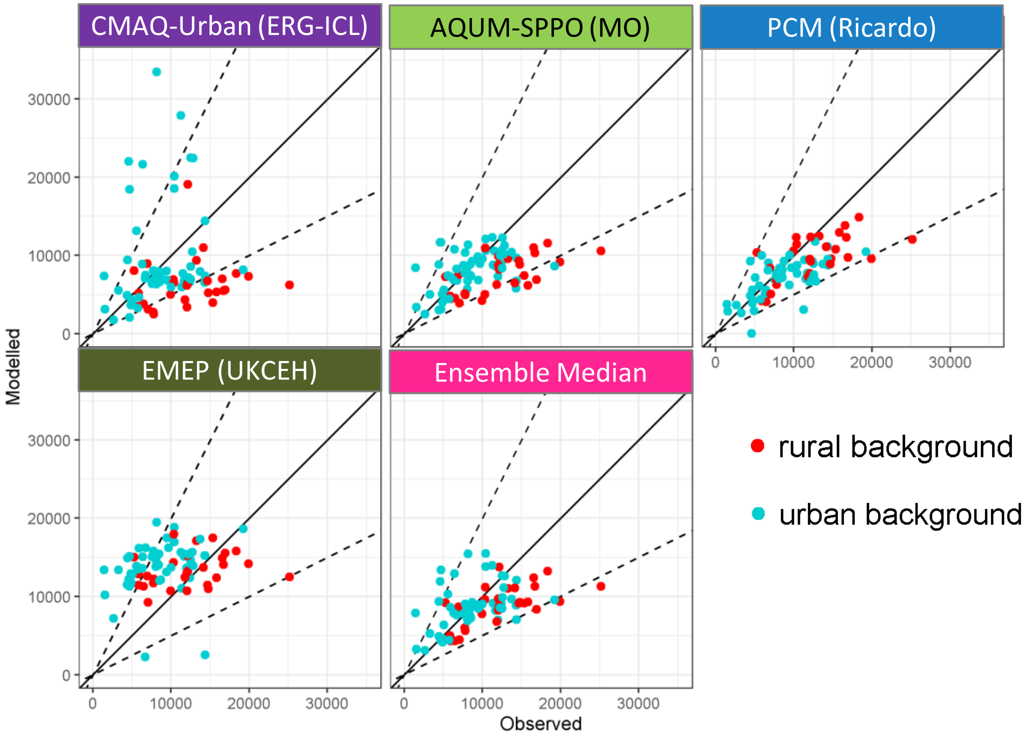
Summary of model evaluation results for O_3

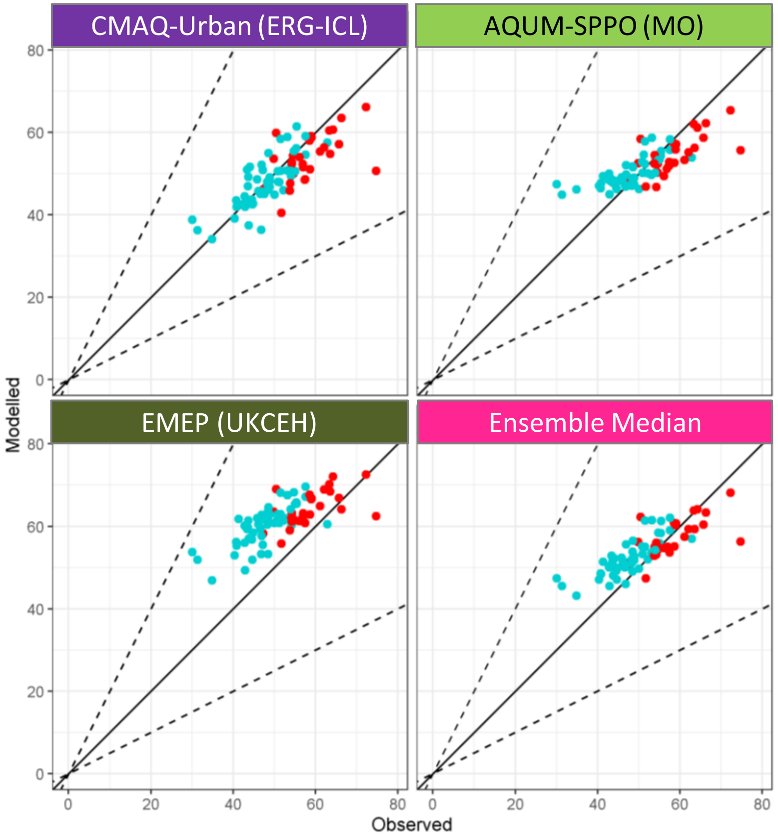
- Good annual mean agreement for **CMAQ-Urban** and **AQUM-SPPO**
- Good AOT40 agreement for **AQUM-SPPO** and **PCM**
- **EMEP** overestimates annual mean and AOT40 at urban background sites
- **CMAQ-Urban** underestimates summertime ozone at rural sites
- **PCM**, **AQUM-SPPO** and **EMEP** underestimate AOT40 variability
- **CMAQ-Urban** overestimates AOT40 variability
- **AQUM-SPPO** captures best the daily maximum of 8-hour rolling mean metric, as used in forecasting

AOT40 at 81 background sites

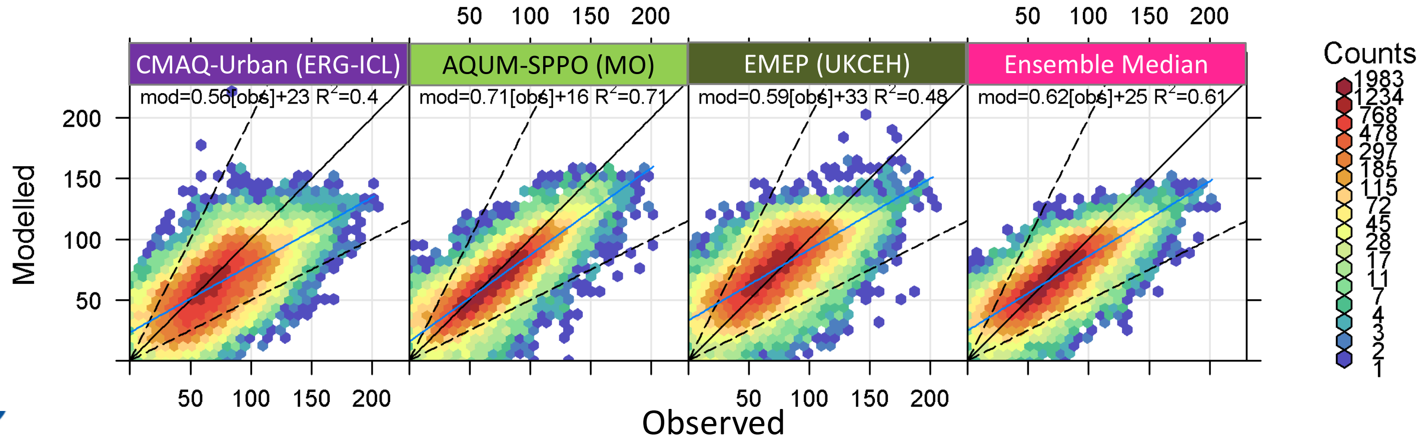


Concentrations in µg/m³

Annual mean at 81 background sites



Hourly mean at 27 rural background sites, May to July only



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Summary of model evaluation results for O_3

- Good annual mean agreement for **CMAQ-Urban** and **AQUM-SPPO**
- Good AOT40 agreement for **AQUM-SPPO** and **PCM**
- **EMEP** overestimates annual mean and AOT40 at urban background sites
- **CMAQ-Urban** underestimates summertime ozone at rural sites
- **PCM**, **AQUM-SPPO** and **EMEP** underestimate AOT40 variability
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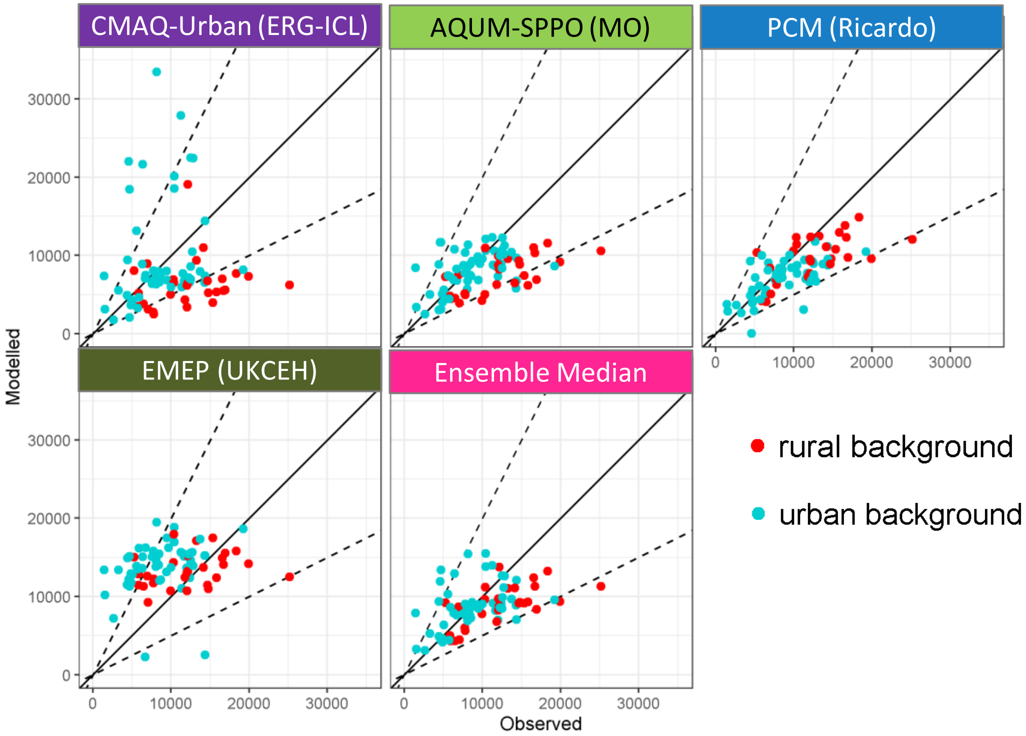
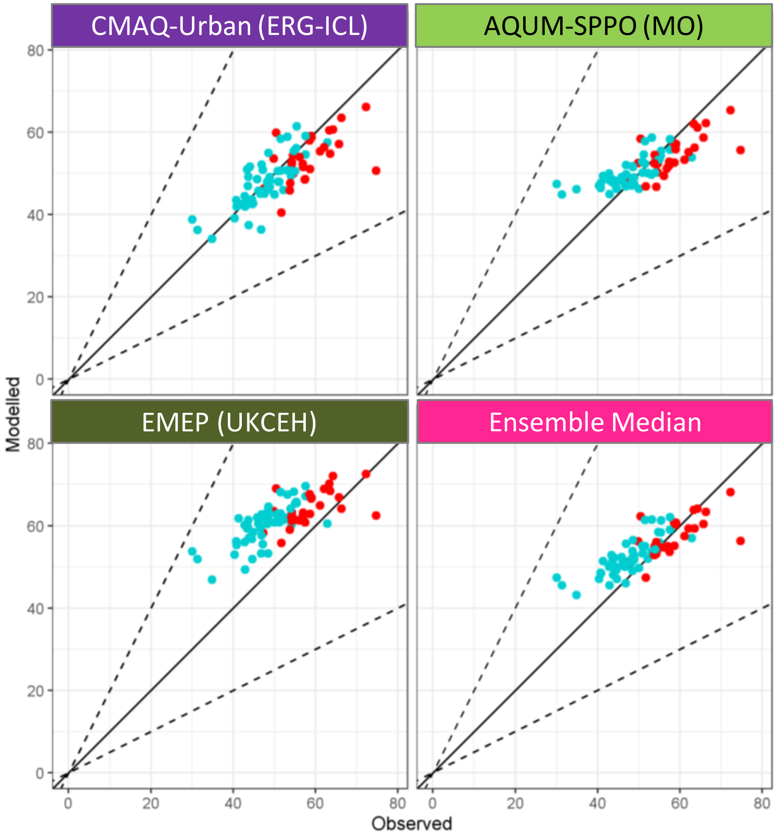
AOT40 at 81 background sites

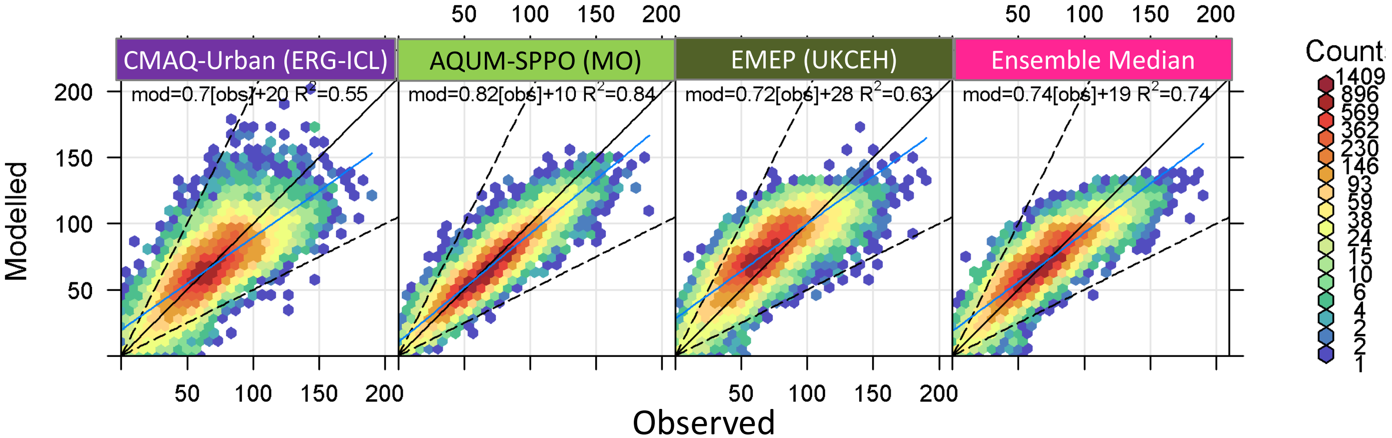


Concentrations in µg/m³

Annual mean at 81 background sites



Daily maximum 8-hour rolling mean at 81 background sites



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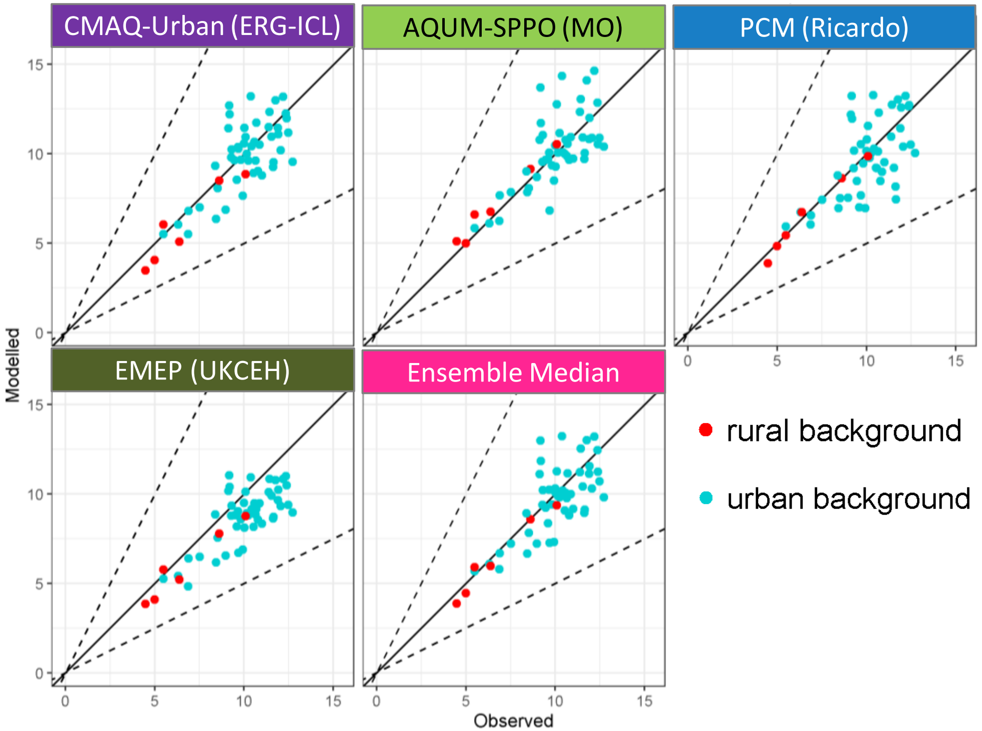
Summary of model evaluation results for $PM_{2.5}$

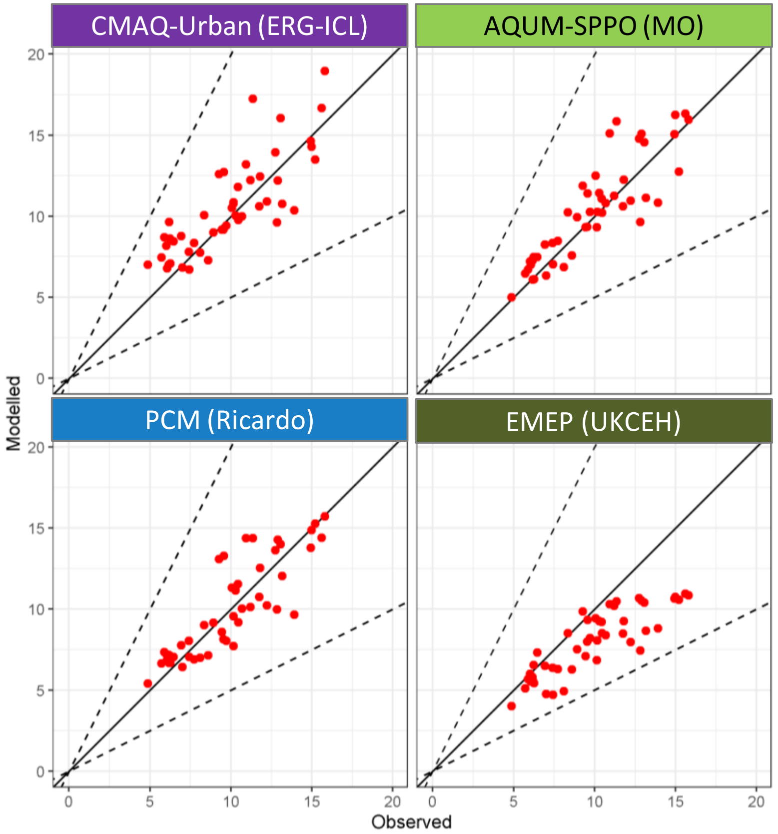
- Good overall agreement for all models
- **AQUM-SPPO**, **CMAQ-Urban** and **EMEP** reproduce the monthly variation
- **EMEP** and **CMAQ-Urban** show too much diurnal variation
- **AQUM-SPPO** overestimates levels and variability sites

Annual mean at 54 background sites



Concentrations in µg/m³

Annual mean at 48 roadside sites



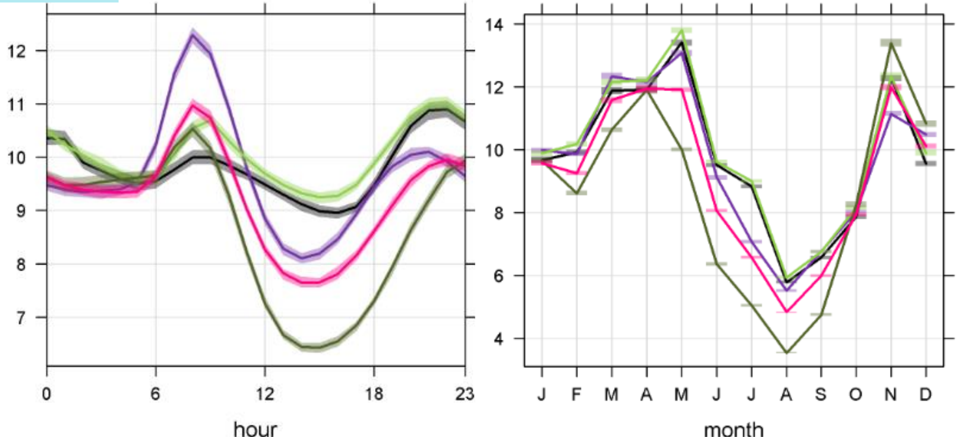
Average diurnal and monthly variation over 54 background sites

CMAQ-Urban (ERG-ICL)

AQUM-SPPO (MO)

EMEP (UKCEH)

Ensemble Median



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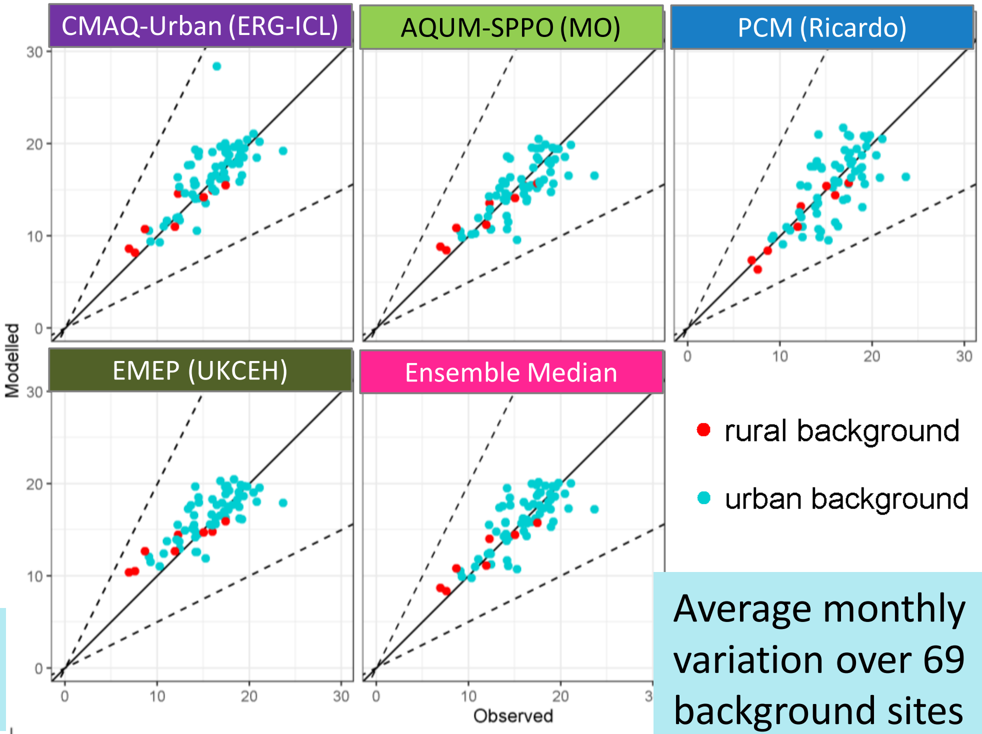
Summary of model evaluation results for PM_{10}

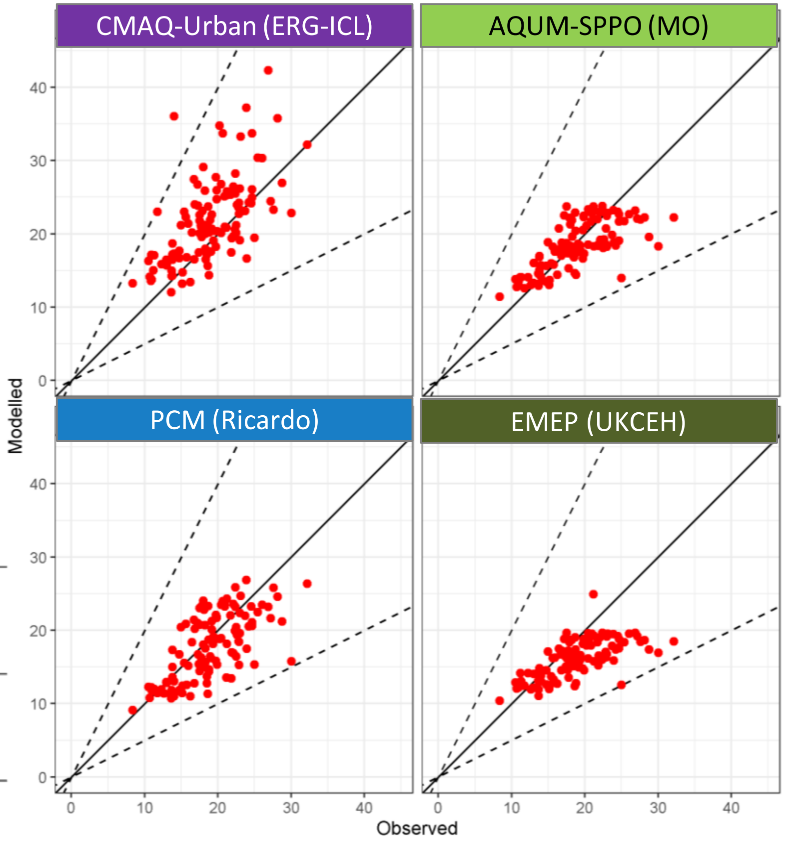
- Good overall agreement for all models
- **AQUM-SPPO**, **CMAQ-Urban** and **EMEP** reproduce the monthly variation
- **EMEP** slightly underestimates the variability between sites
- **CMAQ-Urban** slightly overestimates at roadside sites
- **CMAQ-Urban** overestimates diurnal variation at roadside sites

Annual mean at 69 background sites

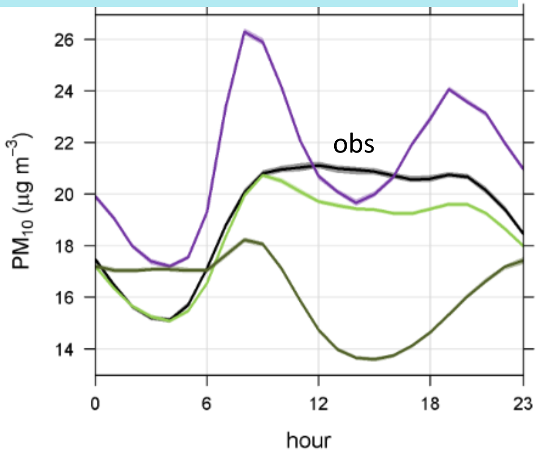


Concentrations in µg/m³

Annual mean at 115 roadside sites

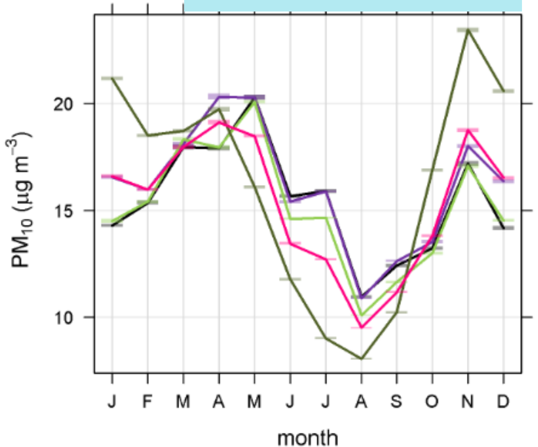


Average diurnal variation over 115 roadside sites

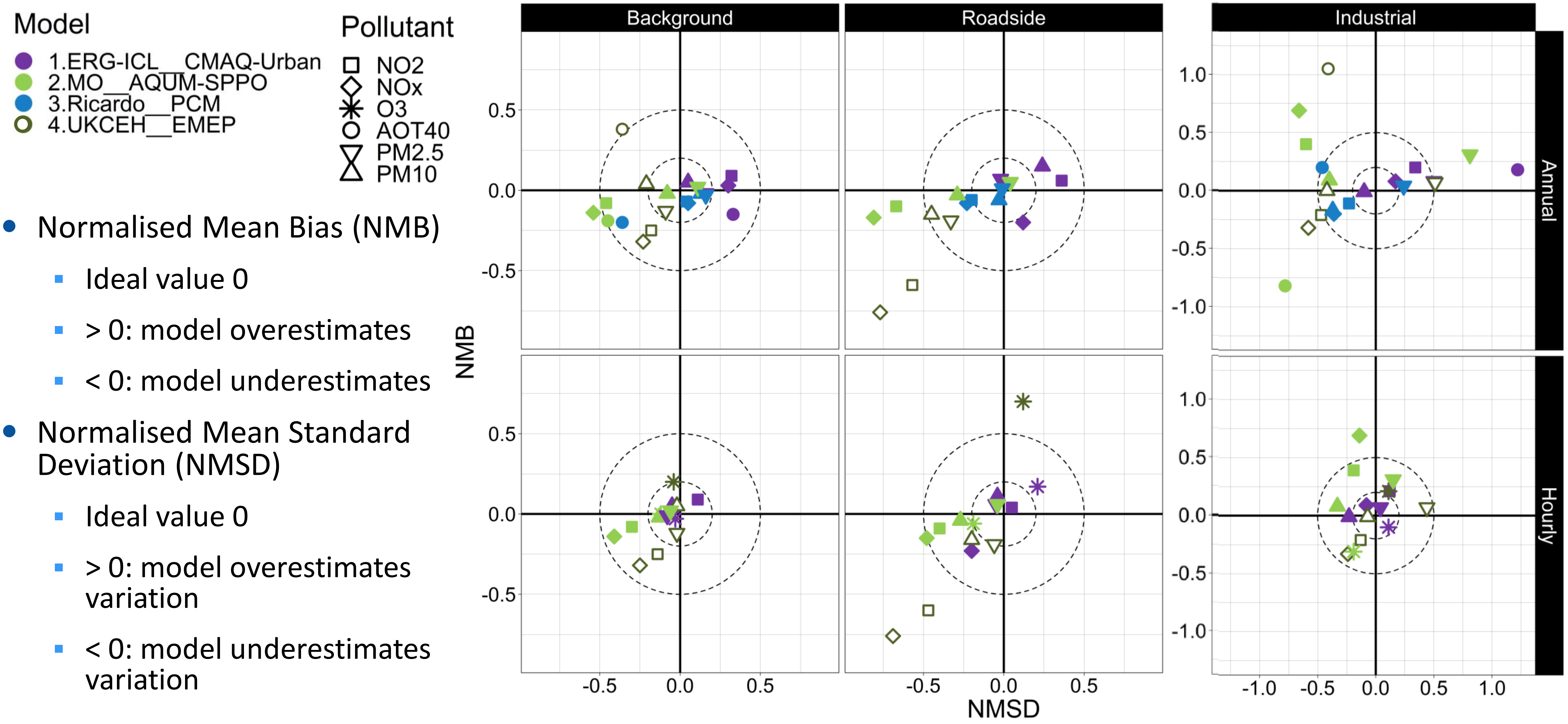


CMAQ-Urban (ERG-ICL)
AQUM-SPPO (MO)
EMEP (UKCEH)
Ensemble Median

Average monthly variation over 69 background sites



Summary of model evaluation



- Normalised Mean Bias (NMB)
  - Ideal value 0
  - > 0: model overestimates
  - < 0: model underestimates
- Normalised Mean Standard Deviation (NMSD)
  - Ideal value 0
  - > 0: model overestimates variation
  - < 0: model underestimates variation

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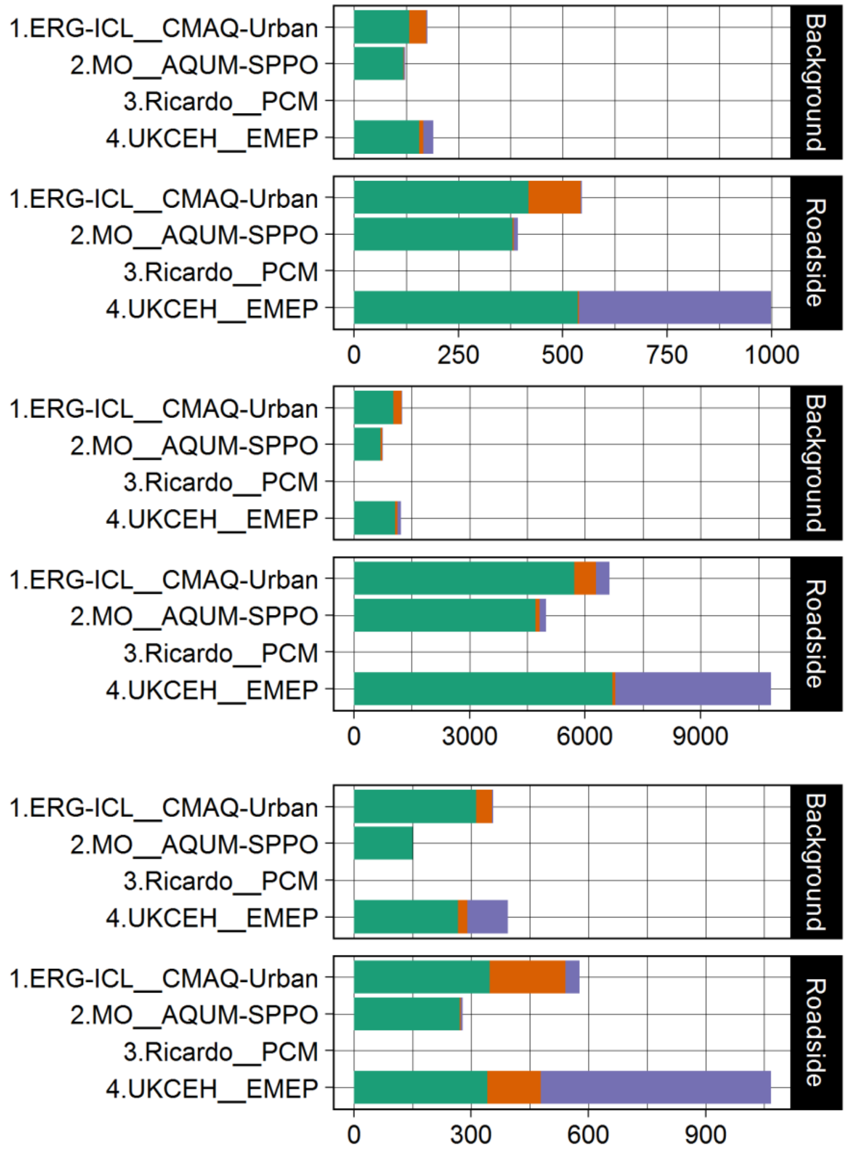
Uncertainties assessment: gaseous pollutants

Hourly

NO_2

NO_X

O_3

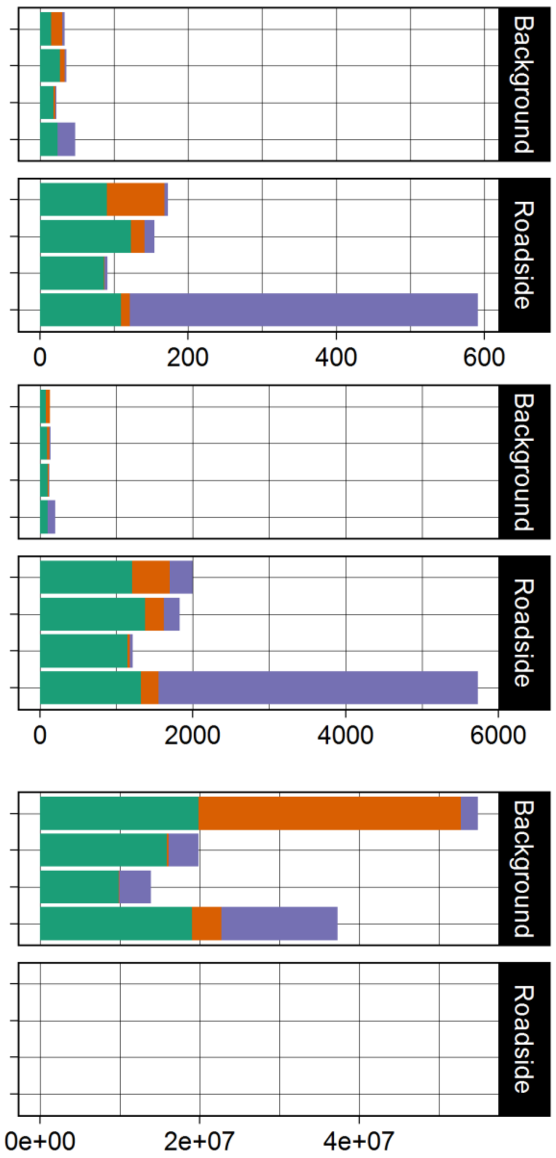


Annual

NO_2

NO_X

O_3 AOT40



Hourly data are not available from PCM (Ricardo)

- MSE.uncor — Proportion of observed variance unexplained by the model
- MSE.cor — Error in model variance correlated with observed variance
- MSE.bias — Mean bias element of model error

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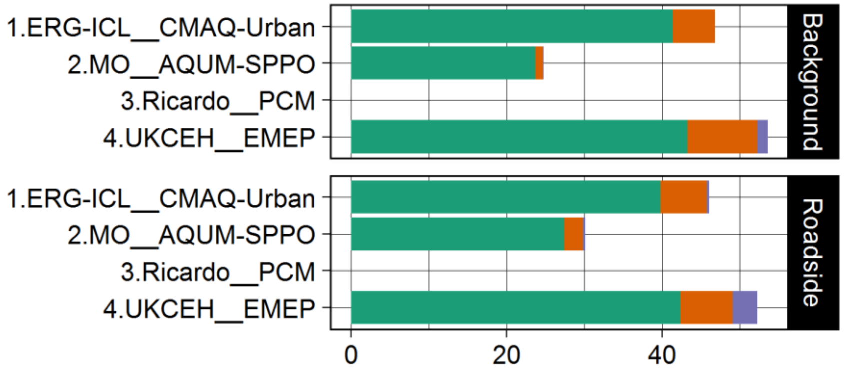
Uncertainties assessment: particulate pollutants

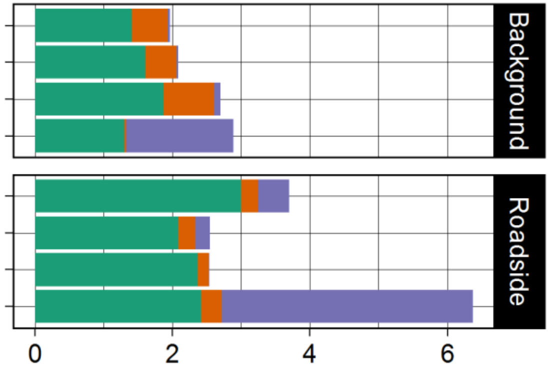
Hourly	Annual

**Hourly data are not available from PCM (Ricardo)*

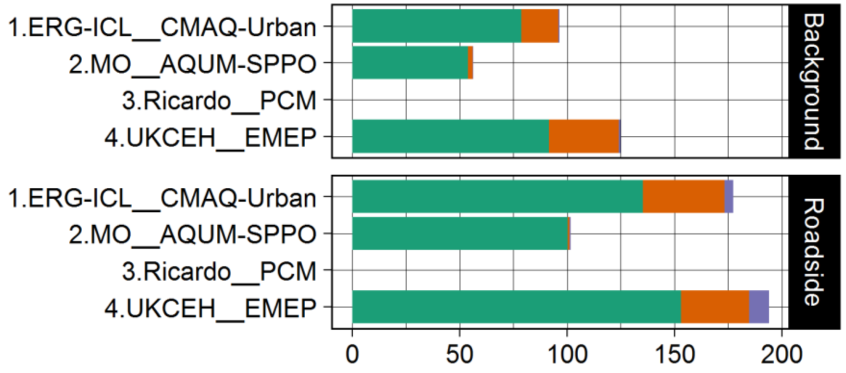
$PM_{2.5}$



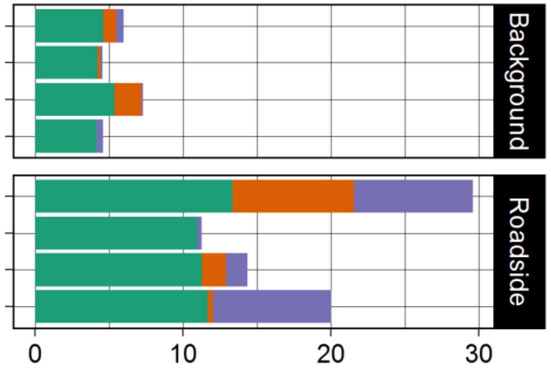
$PM_{2.5}$



PM_{10}



PM_{10}



MSE.uncor — Proportion of observed variance unexplained by the model

MSE.cor — Error in model variance correlated with observed variance

MSE.bias — Mean bias element of model error

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Common themes: data

- Land use inputs: some UK-specific land use categories not included in US developed WRF (meteorological) and MEGAN (biogenic emissions) models
- Emissions
  - NAEI sub-sector data not widely available: hard to assign appropriate properties for lumped sectors eg. ‘other transport’
  - Point source properties not available from NAEI eg. release height and temperature needed for explicit modelling
  - NAEI includes NO_x emissions, assumptions required to define proportion released as NO_2 for modelling
  - NAEI traffic NO_x emissions may be too low due to emissions factors and fleet estimates
  - Individual road emissions not available from NAEI (required for specific road modelling)
  - Individual major road emissions based on DfT count points do not cover all roads with adjacent monitoring sites
- Urban morphology data for defining street canyons not freely available

SNAP sector 8:
Other transport

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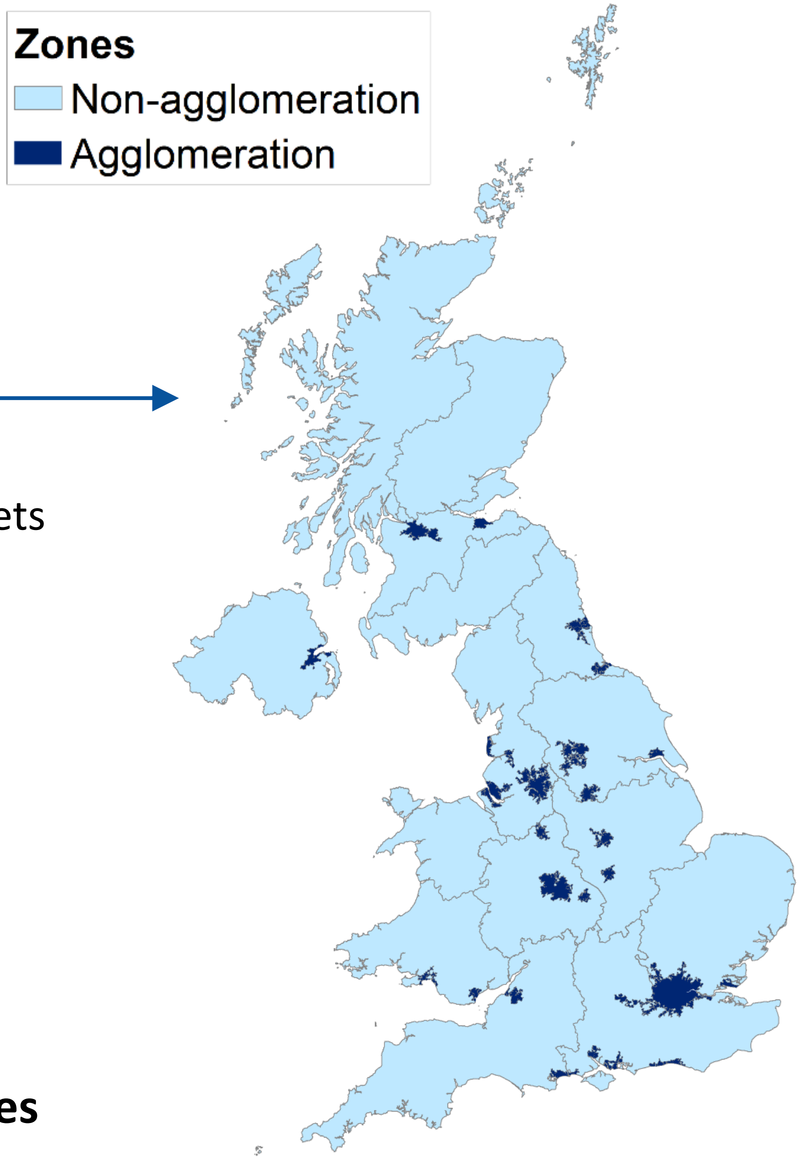
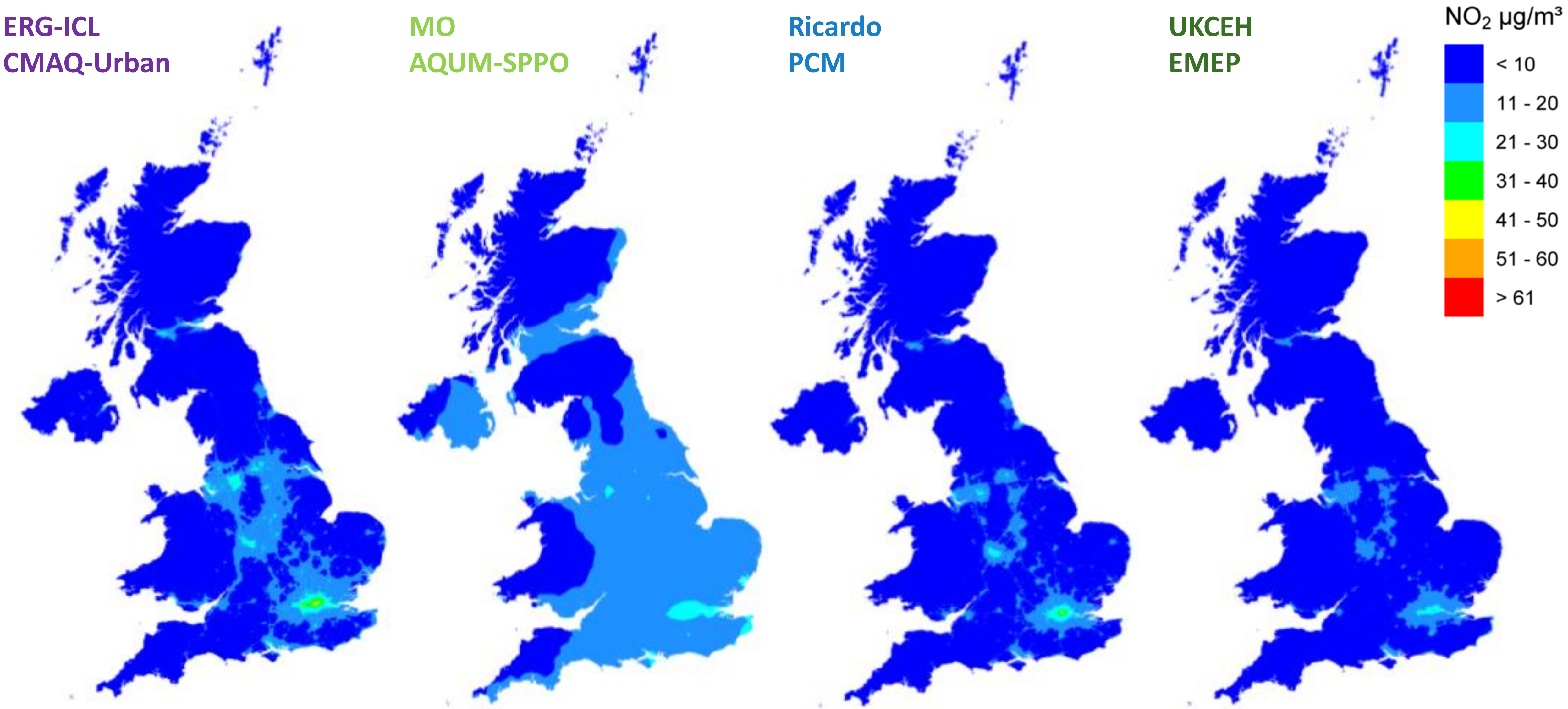
Compliance comparison: Overview

- **Metrics considered**
  - Annual metrics, to allow direct comparison with PCM
  - *Hourly resolution models could evaluate short-term metrics explicitly (PCM derives short-term metrics from annual values)*
- **Approach methodology**
  - Calculations for 43 zones: agglomeration (28) and non-agglomeration (15)
  - Separate grid and roadside datasets, to allow direct comparison with PCM – zonal exceedances are calculated as the maximum concentration over grid and road datasets
  - PCM roadside concentrations: single link value, with no variation with side of road, road on 'CENSUS ID' network
  - *Use of continuous, multi-scale models e.g. ERG-ICL (CMAQ-Urban) would motivate a single-dataset assessment approach (excluding road carriageways etc), with along- and across-road variability*
- **Mapped domains**: UK, Greater London, Greater Manchester
  - Grid: NO_2, NO_x, $PM_{2.5}$, PM_{10} and O_3
  - Road network : NO_2, $PM_{2.5}$, PM_{10}
- **Ricardo assisted with ensuring consistency with AQD processing methodologies**



NO_2 gridded data

Annual average limit value 40 µg/m³



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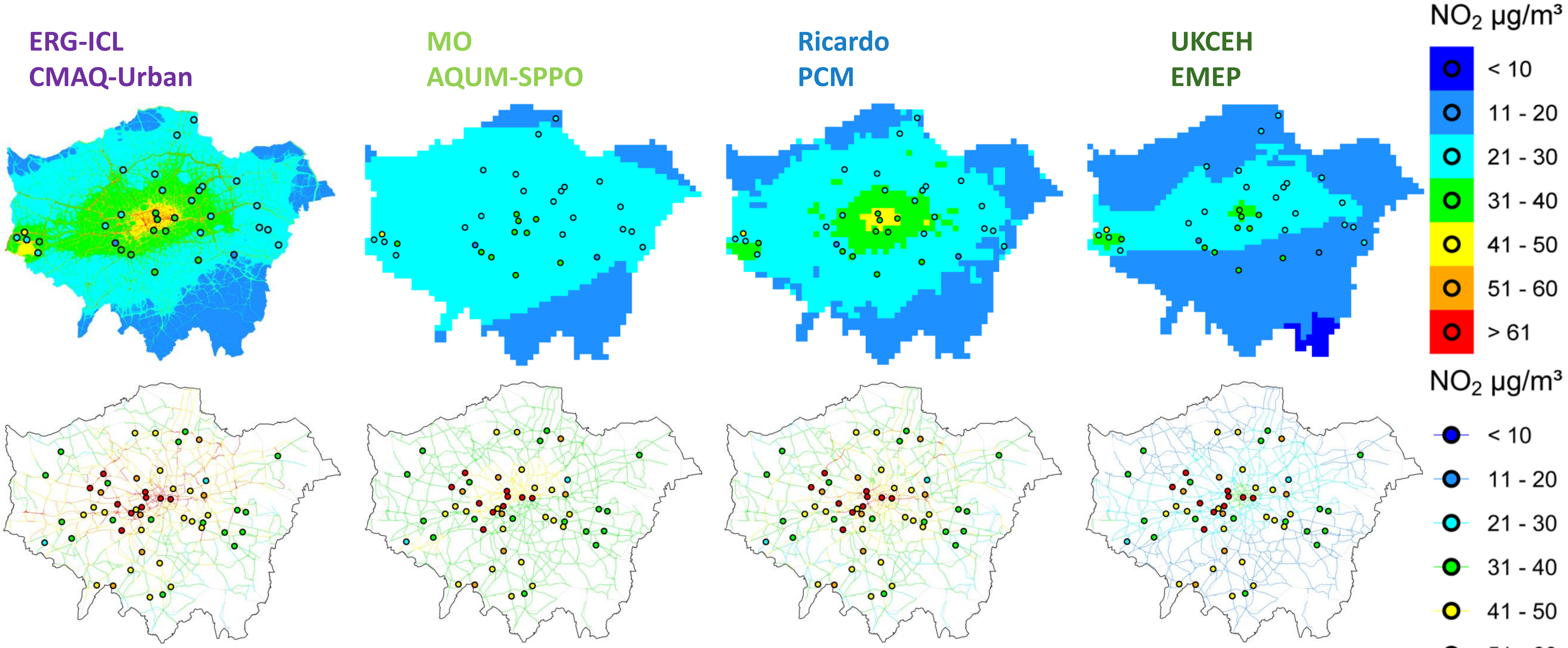
Urban comparison: gridded and roadside NO_2



Annual average NO_2 concentrations in London, 2018

Coloured circles show measurement locations and concentrations
Background sites on gridded plots, near-road sites on roadside

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Conclusions

- Conclusions:
  - The detailed model validation has revealed strengths and limitations of the four models considered
  - An examination of the model uncertainties shows that the proportion of observed variance unexplained by the models is broadly similar for each of the models. It is not straightforward to determine the specific causes of these errors
  - The proportion of the observed variance correlated with the models and the mean bias element of the model error is easier to explain (e.g. related to emissions or lack of resolution). These errors tend to be higher for the uncalibrated models, but can be reduced.
- Implications for future model intercomparison work:
  - Consider additional PM component analyses
  - Examination of detailed concentration variation near roads
  - Comparison of metrics, e.g. exceedances of short-term limits, population-weighted means, exposure reduction
  - Use of consistent emissions inputs to allow sensitivity testing between models

Questions?

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