

# Application of CMAQ to Regulatory Issues in the UK Power Sector

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# Overview

## **JEP Mesoscale Modelling Capability (Paul Sutton)**

- > The Joint Environment Programme (JEP).
- > JEP requirements & selection of mesoscale model.
- > Current JEP Models-3 set-up.
- > JEP validation of Models-3 simulation.

## **Regulatory Applications (Steve Griffiths)**

- > Source impact approach – Power station footprints.
- > Habitats Directive – Acid and Nitrogen deposition.
- > Ambient Air Quality Directive – PM<sub>2.5</sub> concentrations.
- > NECD and Gothenburg protocol – Sensitivities to particulate toxicity assumptions.



# Joint Environmental Programme (JEP)

- > Future environmental regulation is among the most significant source of risk factors affecting plant operation and asset strategy.
- > Key factors include air quality, health effects & ecosystems effects.
- > Research programme jointly funded by eight companies – cover majority of the UK coal and oil-fired generation.
- > Investigate environmental issues of relevance to the power industry.
- > Sector level discussions with the Environment Agency & DEFRA.



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# JEP Has Developed an In-house Mesoscale Modelling Capability

> This allows JEP:

- To produce its own independent view of the environmental impact of JEP power stations.
- To assess the consequences of developing UK, EU & UN/ECE regulation on JEP power stations.
- To participate in discussions of the developing regulation.

> Regulatory issues addressed by JEP mesoscale modelling:  
Air Quality, Acid Deposition, Eutrophication, Ozone & Particulates



# Selection of Mesoscale Model

## > Key JEP requirements of mesoscale model:

- **Multi-issue:** Air quality, acidification, eutrophication, ozone, particulates in a single 'one atmosphere' model - consistency.
- **Multi-timescale:** Range of timescales to enable simulation of air quality episodes through to annual depositions – dynamic model.
- **Flexibility of spatial scales:** To enable simulation of single power stations through to transboundary calculations – via grid nesting.
- **Treatment of point sources:** Plume rise.
- **'Future proof' science:** Software modularity of science treatment.  
Active research & development of science.
- **Transparent:** Open source-code, widely available.

## > JEP selected Models-3/CMAQ as best-fit to its requirements.



# JEP Models-3 Timeline

1999

## ◆ Model Selection and Review

### ◆ Build European & UK version

- 1<sup>st</sup> CMAQ Users in UK
- Initial evaluation of Models-3

## ◆ Maintain Models-3 capability

- Upgrade Models-3 versions
- Upgrade computer hardware
- Validation studies

## ◆ Application to regulatory issues

- Power station footprints
- Population exposure studies
- Habitats assessment

## ◆ JEP organised Models-3 workshops

## ◆ Currently:

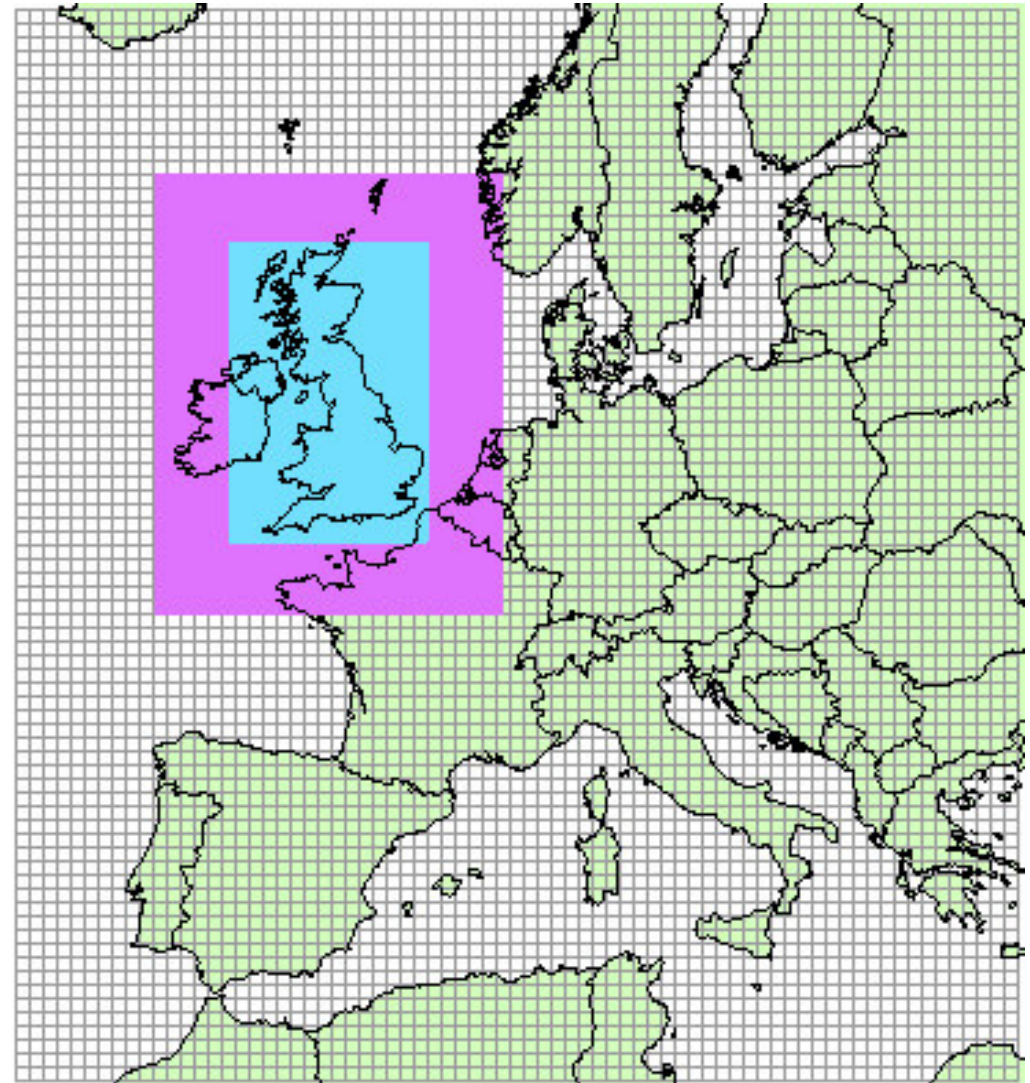
- JEP is using CMAQv4.7, MCIPv3.4.1 & SMOKEv2.5
- Participating in CREMO & DEFRA Air Quality Model Intercomparison

Now



# Current JEP Models-3 Set-up (1)

- > Using CMAQv4.7.
- > Have modelled whole calendar years.
- > Nested horizontal grids (45km/15km/5km).
- > 15 vertical layers (0 to 15km). (Ground layer depth ~35-40m.)
- > CB05CL chemical scheme with coupling to aqueous and cloud processes.



# Current JEP Models-3 Set-up (2)

- > Emissions input data obtained from:
  - Public domain sources: EMEP, GEIA and NAEI.
  - Actual hourly emissions data for JEP power stations.
- > Models-3 pre-processing of emissions data done using SMOKEv2.5.
- > Outer grid boundary conditions were taken from STOCHEM dataset.
- > Initial conditions were obtained using a ‘spin-up’ process:
  - Runs started on 25<sup>th</sup> Dec of previous year to allow one week of spin-up.
  - Initial conditions for 25<sup>th</sup> Dec generated using the same approach as for the boundary conditions for the outer grid.

# Current JEP Models-3 Set-up (3)

- > Meteorological input data produced using WRFv3.0.1.  
Models-3 pre-processing done using MCIPv3.4.1.
- > HP XW6400 workstation.
  - 2x quad-core Xeon processors (2.33GHz speed).
  - 8GB RAM.



# Validation of Ground Level Air Concentrations Simulation (1)

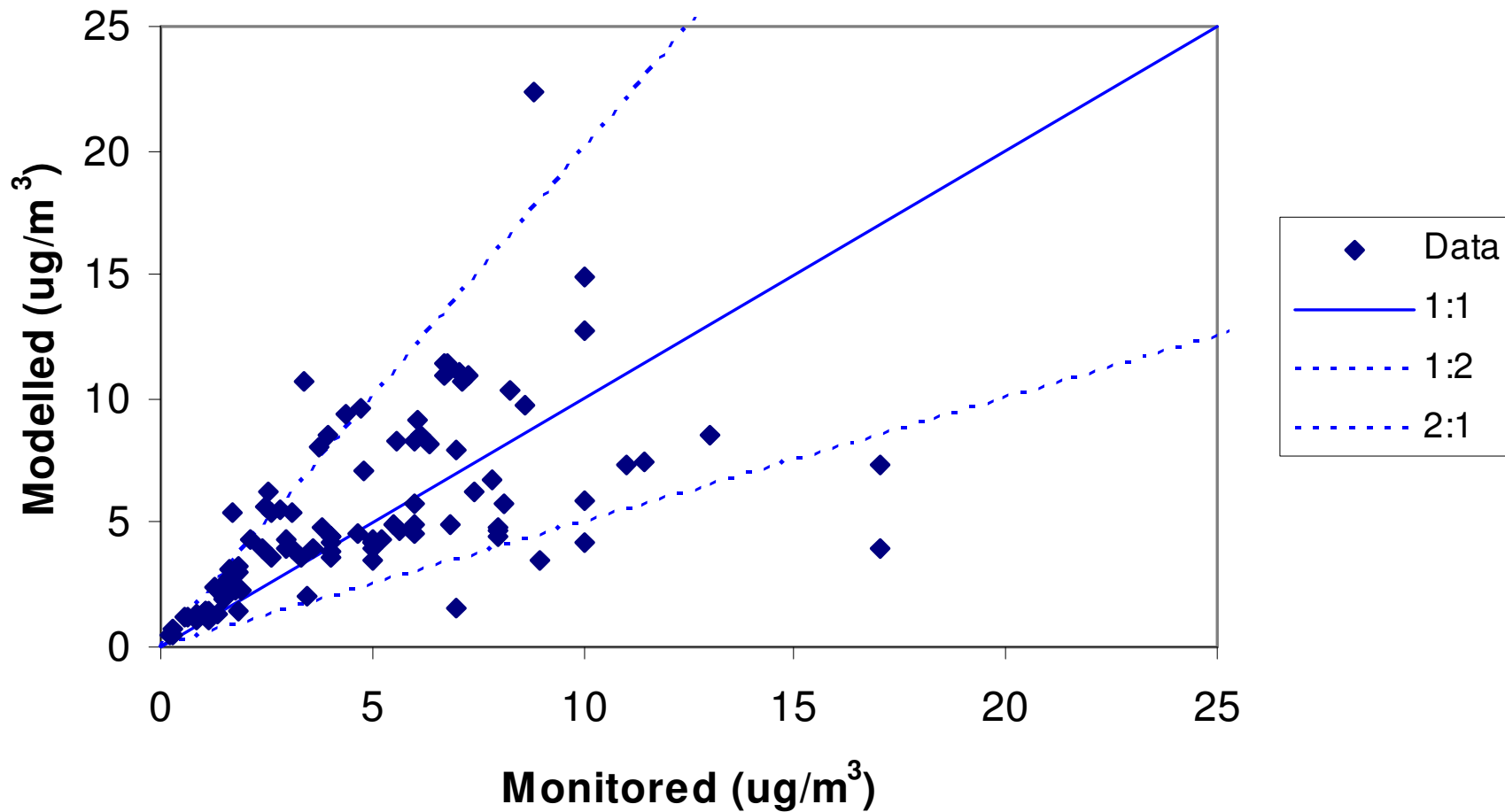
- > Compared 2003 annual mean ground level air concentrations measured at monitoring sites with values modelled by Models-3 on 5km grid.
- > The following chemical species and corresponding monitoring sites were used:

Measured Species	Monitoring Sites
SO <sub>2</sub>	AURN+JEP+ADMN
NO <sub>x</sub>	AURN+JEP
NH <sub>3</sub>	NAWN
NH <sub>4</sub> <sup>+</sup>	NAWN
HNO <sub>3</sub>	ADMN
SO <sub>4</sub> <sup>2-</sup>	ADMN
nss-SO <sub>4</sub> <sup>2-</sup>	ADMN
NO <sub>3</sub> <sup>-</sup>	ADMN

- ‘Urban centre’, ‘urban industrial’, ‘roadside’ and ‘kerbside’ sites were excluded from the AURN dataset.
- Appropriate combinations of modelled species are summed to correspond to measured species.

# Validation of Ground Level Air Concentrations Simulation (2)

**SO2 annual mean ground level air concentration**



# Validation of Ground Level Air Concentrations Simulation (3)

> Model performance assessed using two standard quantities:

– *FAC2 = Fraction of simulated values where  $2.0 \geq S_i / O_i \geq 0.5$ .*

– 
$$NMB = \frac{\sum_{i=1}^N (S_i - O_i)}{\sum_{i=1}^N O_i}$$

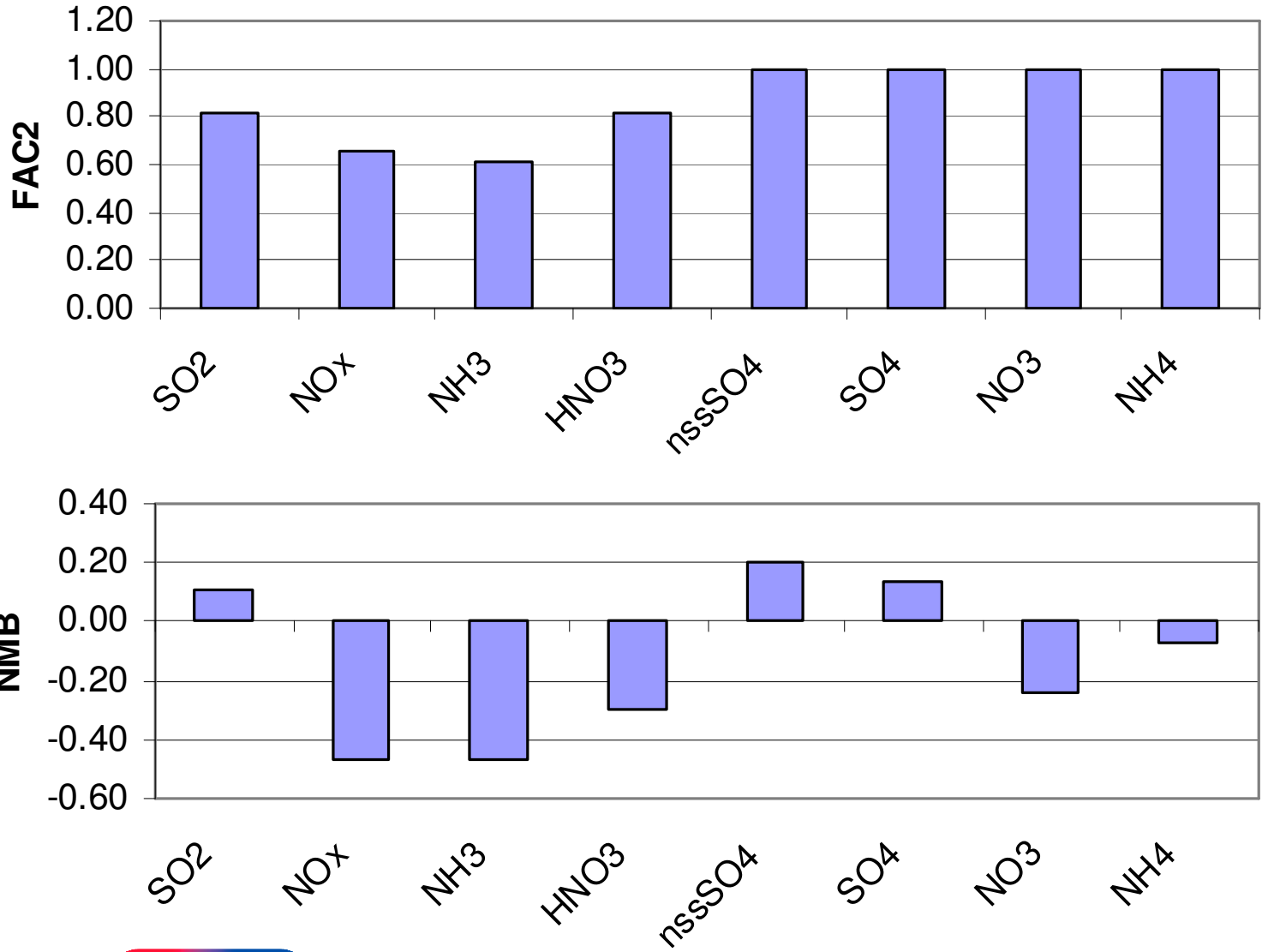
where

$N$  is the number of data points

$S_i$  is the simulated value for a data point

$O_i$  is the observed value for a data point

# Validation of Ground Level Air Concentrations Simulation (4)



- The precision with which these quantities can be determined needs to be considered. For example, if the conversion from ppbV → ug/m<sup>3</sup> is done at 10°C rather than 20°C, this would reduce the NMB values by 0.04.



# Validation of Wet Deposition Simulation (1)

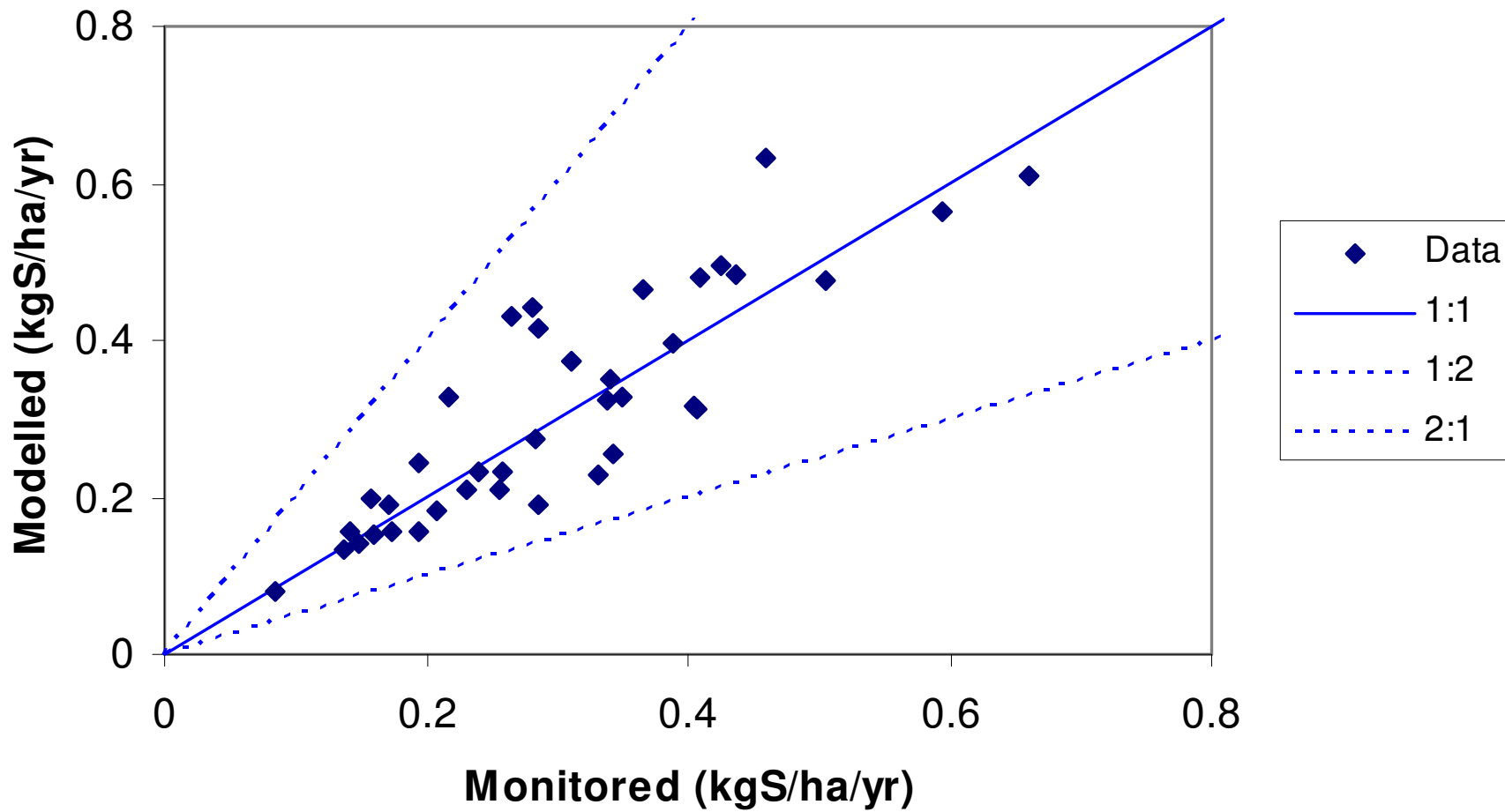
- > Compared 2003 annual total wet deposition measured at monitoring sites with values modelled by Models-3 on 5km grid.
- > The following chemical species and corresponding monitoring sites were used:

Measured Species	Monitoring Sites
Oxidised S (wss)	ADMN
Oxidised S (nss)	ADMN
Oxidised N	ADMN
Reduced N	ADMN

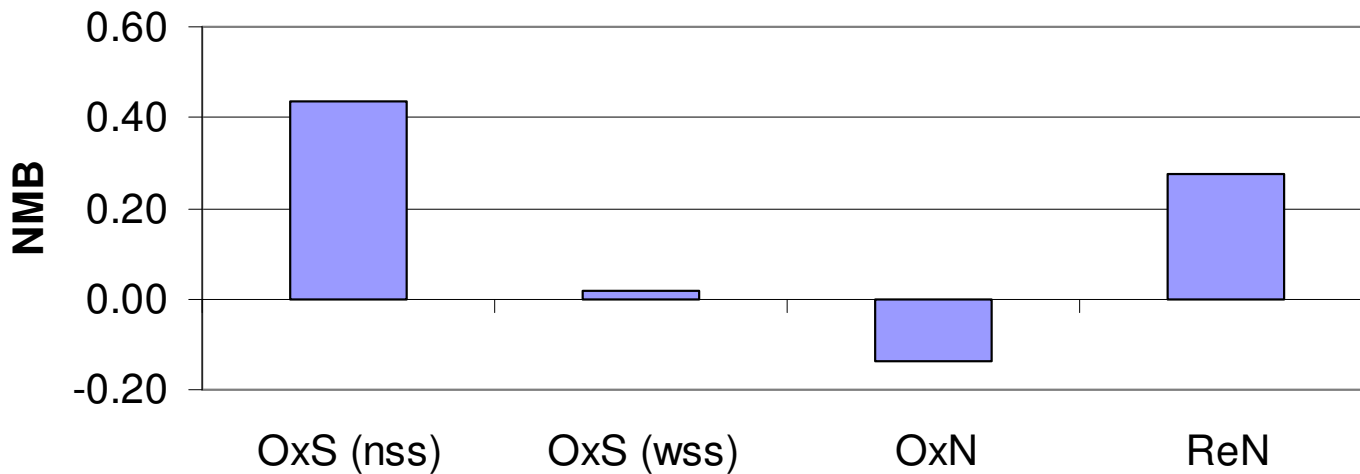
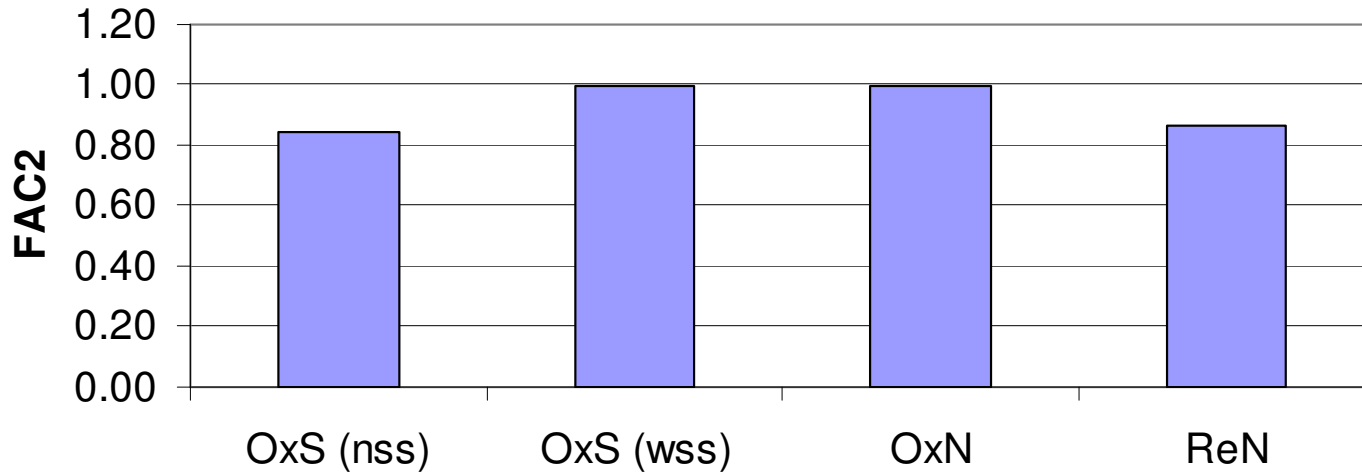
- Appropriate combinations of modelled species are summed to correspond to measured species.

# Validation of Wet Deposition Simulation (2)

Oxidised S (wss) annual total wet deposition

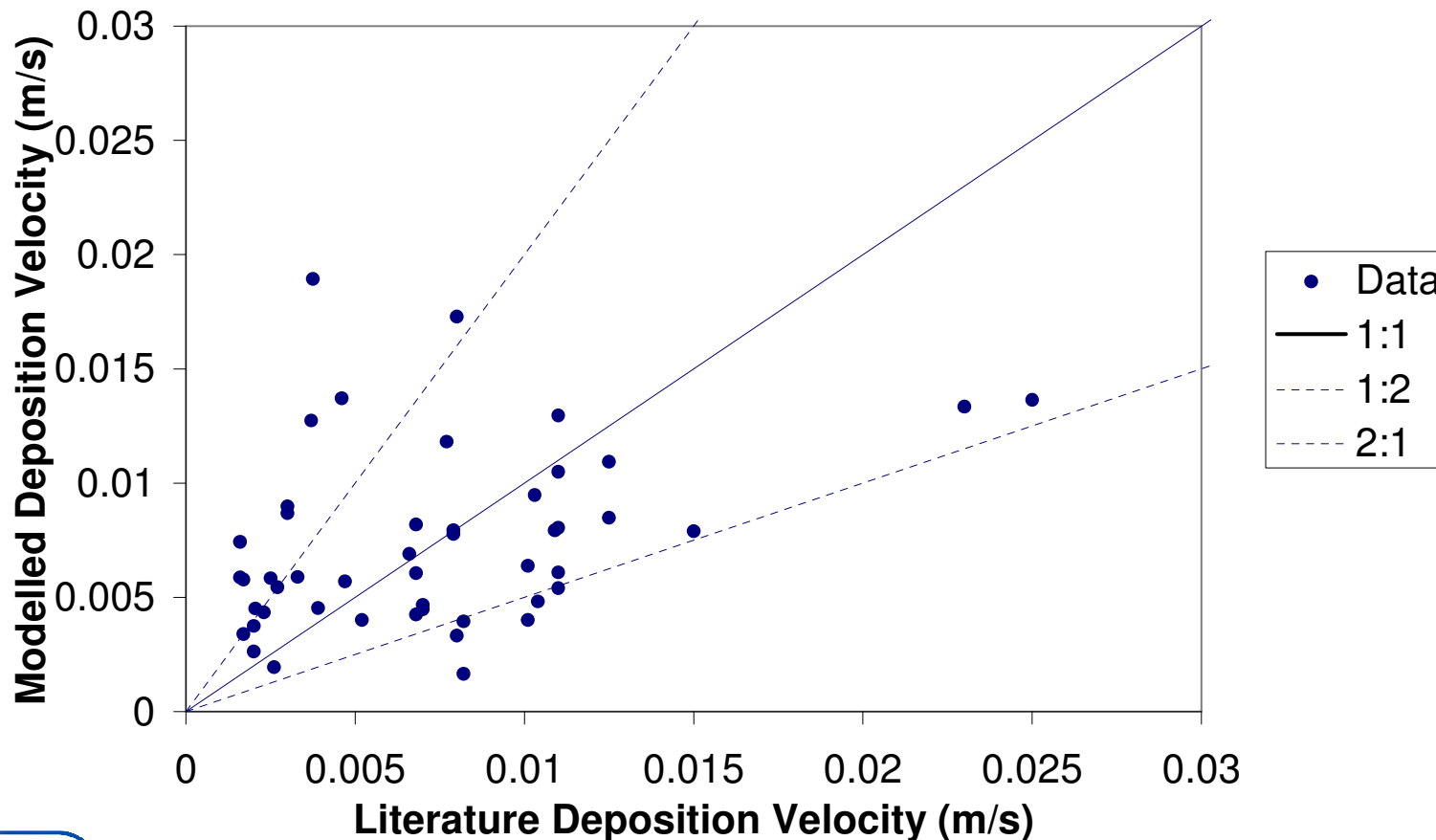


# Validation of Wet Deposition Simulation (3)



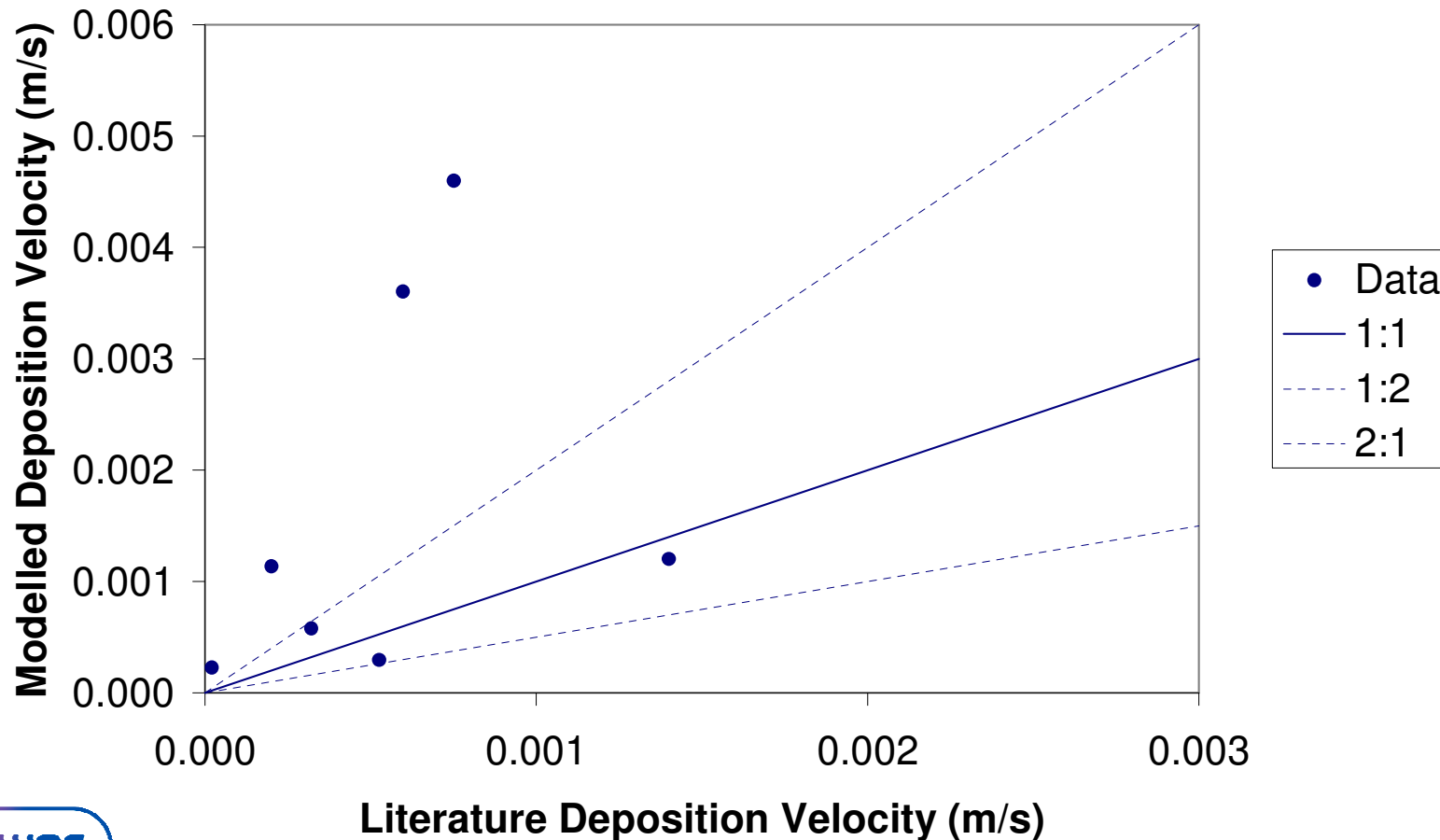
# Validation of Dry Deposition Simulation (1)

- > Compared SO<sub>2</sub> dry deposition velocities obtained from literature for a variety of cases (e.g. land use, season, dry/wet, day/night) with values modelled by MCIPv2.2 ('Models-3' scheme).



# Validation of Dry Deposition Simulation (2)

- > Compared NO<sub>2</sub> dry deposition velocities obtained from literature for a variety of cases (e.g. land use, season, day/night) with values modelled by MCIPv2.2 ('Models-3' scheme).



# Conclusions

- > CMAQ selected as mesoscale model providing best-fit to JEP requirements.
- > JEP has invested significant resources into building UK CMAQ capability.
- > JEP has extensive experience with CMAQ over the last 10 years.
- > Validation studies show, in general, good agreement between CMAQ modelled data & observed data.
- > Validation confirms the CMAQ model is suitable for addressing regulatory issues.