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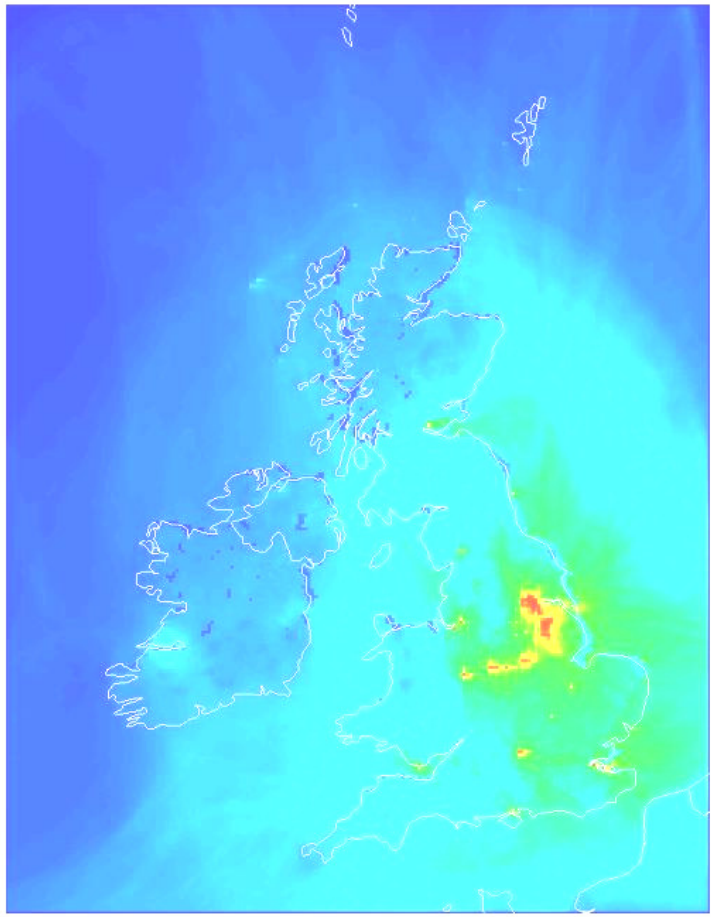
Report of Working Group 4

Status of regional modelling of atmospheric ammonia

Addo van Pul
Eiko Nemitz
Tony Dore
Liu Xuejun
Hilde Fagerli
Camilla Geels
Ole Hertel
Roy van Kruijt
Maciej Kryza
Robert Bergström
Massimo Vieno
Rognvald Smith
Stefan Reis



Objectives for modeling atmospheric ammonia

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- To assess local contributions vs. long-range transport.
- To provide spatial coverage (beyond what can be achieved with measurements).
- To establish link between emissions, concentrations and deposition.
- To provide deposition estimates for comparison with critical loads.
- To provide prediction of concentrations and deposition in response to emission abatement measure and scenarios.
- To improve and assess our understanding of processes.
- To quantify the role of ammonia in the formation of particulate matter.
- To establish source-receptor relationships.
- To establish national budgets and country-to-country transport matrices.

Key conclusions and recommendations

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- Assessment of model uncertainties
- Emissions
- Spatial scales and model resolution
- Vertical resolution
- Parameterisation of the surface/atmosphere exchange
- Chemical schemes
- Model intercomparison
- Measurement database
- Effects of uncertainties on integrated assessment modelling

Assessment of model uncertainties

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1. Spread of parameter spaces are poorly defined.
2. Ranking of uncertainties:
   - National scale models:

     Emissions (depending on country)
     ⇨ deposition (dry & wet)
     ⇨ diffusion

   - Regional scale models:

     Emissions
     ⇨ dry deposition/vertical resolution *(coupled problem)*
     ⇨ boundary layer height

In general, models are performing reasonably well for the purposes they have been developed for.

Emissions

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1. Quality of emissions varies greatly across the member states to the Convention.
2. Detailed emission inventories exist in some countries with an ammonia problem (*NL: 1 km; DK: farm level; UK: 1 km*).
3. Confidentiality issues prevent data availability at finer resolution.
4. Improvement in model performance is achieved using temporal variation in emissions in relation to meteorology and agricultural activity, which is not available in the same detail for all countries.
5. National gridded emissions should be submitted to EMEP every year, where available.
6. Emissions for NH_3 are estimated to be less accurate than for CO, CO_2, SO_2, NO_x, of similar quality as primary PM, but more accurate than those of heavy metals, POPs and N_2O.

Spatial scales and model resolution

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1. The spatial scale currently reasonably achievable in national and regional Chemical Transport Models is limited by a combination of
    a) the resolution of the input data *(in particular emissions),*
    b) computing power *(particularly true for regional modeling)* and
    c) the resolution for which the model parameterizations are formulated
2. Improvement of the spatial resolution clearly improved the ability of e.g the EMEP unified model to predict Critical Loads exceedances to forests *(but: even most high resolution models still underestimate Critical Loads exceedances by spatially averaging concentrations and deposition)*
3. High resolution modeling is desirable
    a) for comparison of model performance with measurement data,
    b) to demonstrate that processes are correctly represented and
    c) to provide plot-scale inputs of N and acidity to specific ecosystems, *(e.g. with regard to the Habitats Directive)*.

    However, at present, in most cases the latter still needs to be achieved in targeted local scale modeling studies

Vertical resolution

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1. Modeling ammonia emissions is complex due to the low emission height and the fast deposition rate of atmospheric ammonia, making it very important to model the surface layer accurately.
2. To reduce the influence of the currently implemented vertical resolution, the validation of long-range transport models should concentrate on remote sites and exclude source areas.
3. Improved sub-grid parameterizations for the lowest layers should be explored.

Parameterisation of the surface/atmosphere exchange

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1. Current parameterizations are suspected to over-estimate dry deposition (and underestimate the lifetime and transport distance of atmospheric ammonia).
2. Bi-directional surface / atmosphere exchange (compensation point models) should eventually be included in the models. To achieve this, generalized parameterizations need to be developed, together with strategies to deal with the additional emissions and landuse dependent surface concentration in larger scale models.
3. Initially, sensitivity studies should explore the effects of compensation points on predicted concentrations.
4. In the long term, emission from vegetation (agricultural and semi-natural) should be calculated in an atmospheric transport model.
5. More measurements of dry deposition are required to validate the dry deposition schemes, especially over semi-natural vegetation, and to improve mechanistic parameterizations (Γ *values*).

Chemical schemes

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1. Are not considered to be the major uncertainty for modeling NH_3 deposition
2. Chemical schemes differ greatly in complexity between models.
3. Currently implemented schemes are deemed fit for the purpose for which the individual models were developed, with models predicting PM using more advanced schemes.
4. Real progress would require modeling of the total aerosol size-distributions (including organics).
5. More measurements of gas / aerosol partitioning are required to assess model performance.

Model intercomparison

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1. A model intercomparison is required at both the national scale (over one or two countries) and at the European scale to assess model performance and to assess what processes lead to uncertainties.
2. The objectives would be
   a) to validate the model response to emission changes,
   b) to compare model predictions against robust measurement databases,
   c) to assess the impact of model resolution,
   d) to explore which differences in the models causes which differences in the results,
   e) to provide a model ensemble approach for uncertainty assessment.
3. A model intercomparison requires resources and hence backing by national funding agencies. It should be explored whether the interaction of the groups (meetings, compilation of results) could be further supported through ACCENT or ESF-NINE.

Measurement database

1. The EMEP database contains few measurements of NH_3 and NH_4^+.
2. More measurements are held in national databases.
3. It is recommended that EMEP/TFMM develops an approach to maximize the use of available data and, at a minimum, compile a meta database.

Integrated assessment modeling results cannot be better than the source-receptor relationships that come from the chemical transport models; in particular, non-linearities are expected arising from e.g.:

- change in oxidation capacity and oxidation rate with time, affecting bulk reaction schemes not coupled to a photochemical scheme
- change in the NO_x/SO_x ratio
- change in SO_2/NH_3, changing the deposition rate of NH_3
- increase in free available NH_3
  (lower acid concentrations means less incorporation into aerosol)
- increase in the relative importance of import from outside the EMEP domain and from shipping
- increase of compensation points with increase of temperature

Summary of model performance

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	European scale				National scale			
Model name	**NH_3 conc**	**NH_4^+ conc**	**NH_4^+ wet dep**	**Precip**	**NH_3 conc**	**NH_4^+ conc**	**NH_4^+ in precip**	**Precip**
EMEP unified	-- ***(scale, dry dep)***	o	o	*Location?*				
EMEP4UK (UK)								
DAMOS (DK)	-- ***(scale, dry dep)***	+ (conversion rate)	o	**-**	+ (siting)			
FRAME (UK, PL)					o	-- (chemistry, import?)	o	*prescribed*
LOTUS/EUROS (NL)	- ***(scale) (polluted sites: --)***	o	o	*prescribed*	- (polluted sites: --)	o	o	*prescribed*
MATCH (SE)	-- ***(dry dep, scale)***	**-** (N Europe) + (Spain) (dep)	o		?	-	o	
OPS (NL)					- (emission, dry dep)	- (emission, dry dep)	- (emission, dry dep)	*prescribed*

modelled vs. measured: o = within 10% -/+ 10-30% ++/-- > 30%

Notes:

- this is a rough representation; the measurement database differs between studies
- general tendency to do better in background regions than in source regions;
- bias in gas/aerosol measurements
- scavenging ratio derived from the measurements!

Model applicability [1)]

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Objective	OPS	MATCH	DAMOS	LOTUS/ EUROS	FRAME	EMEP unified	EMEP4UK
To establish national budgets	+	+	+	+	+	+	+
To provide spatial coverage (beyond what can be achieved with measurements).	+	+	+	+	+	+	+
To assess local contributions vs. long-range transport.	+/-	+/-	+	+/-	+/-	+/-	+
To establish link between current emissions, concentrations and deposition.	+	+	+	+/-	+	+	+
To provide landuse dependent deposition estimates for comparison with critical loads.	+ (1 km)	+ (20-40 km)	+ (400 m)	+ (25 km)	+ (5 km)	+ (50 km)	+ (5 km)
To provide prediction of concentrations and deposition in response to emission abatement measure and scenarios.	-	+	+	+	+	+	+
To improve and assess our understanding of processes.	+/-	+/-	+/-	+/-	+/-	+/-	+/-
To quantify the role of ammonia in the formation of particulate matter.	+	+/-	+/-	+	+/-	+/-	+/-
To provide source / receptor relationships for IAMs	+	+/-	+/-	-	+	+	-

[1)] combination of operationality & quality, based on current model versions

Recommendation: nested models can address a large number of objectives (DAMOS/DEHM & EMEP4UK)