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Executive Summary

Prepared for
CO_2 Capture Mongstad Project
Statoil Petroleum AS

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CERC

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1. Introduction

The CO_2 capture Mongstad (CCM) project involves the planning and construction of a large-scale post-combustion carbon capture plant downstream the combined heat and power (CHP) plant at the Mongstad refinery in Norway.

Under Contract 4502451276: Atmospheric Chemistry Modelling, Cambridge Environmental Research Consultants Ltd (CERC) was commissioned by CCM Project to carry out development of the ADMS 4 model code to incorporate amine chemistry and to use the resulting model to investigate the dispersion of the amines and their degradation products, specifically nitrosamines and nitramines.

Four Activities were originally identified for consideration:

1. Hydroxyl ($^{\bullet}OH$) radical-initiated gaseous chemistry
2. Aqueous partitioning;
3. Nitrate ($NO_3^{\bullet}$) radical-initiated gaseous chemistry during hours of darkness; and
4. Chlorine ($Cl^{\bullet}$) radical-initiated gaseous chemistry.

Details of the model development and dispersion modelling carried out for Activity 1 are given in the Activity 1 report.[1] Activities 2 and 3, along with further modelling of $^{\bullet}OH$ chemistry are described in a further report.[2] The findings of recent research suggested that the gaseous reactions of amines with chlorine were not significant,[3] so this Activity was not carried out.

This Executive Summary gives an overview of the work carried out as part of these Activities, as well as supplementary work,[4,5] including some examples of the main results and findings.

2. Amine scheme development in ADMS 4 - overview

The ADMS 4 model was developed, under Activity 1 of this project, to include the effects of hydroxyl-initiated amine chemistry in the gaseous phase. This model code was further developed, under Activities 2 and 3, to include nitrate radical chemistry and aqueous partitioning.

The chemical scheme was implemented in such a way that a single model code would generally cover the reactions of different amines. To this end, the amine chemistry scheme code was set up using generic names for the various species: ‘AMINE’, ‘NITROSAMINE’ and ‘NITRAMINE’. The amino radical species is denoted ‘RADICAL’, and can also be output by the model. The reaction scheme also involves NO_x emissions and background concentrations, and ozone background concentrations. It uses information from the meteorological data to determine photolysis rates on an hourly basis.

Kinetic parameters for the various species are specified by the model user, and each can be varied independently, as can other parameters.

Any combination of $^{\bullet}OH$ chemistry, $NO_3^{\bullet}$ chemistry and aqueous partitioning can be considered in a single model run, to investigate combined effects.

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[1] Activity 1: Gaseous Phase Chemistry Modelling (initiated by hydroxyl radical). CERC. November, 2011

[2] Activity 2: Gaseous reactions of nitrate radical during hours of darkness; and Activity 3: Aqueous partitioning. CERC, April, 2012

[3] Nielsen, C.J. Atmospheric chemistry – Chlorine chemistry: Final report. Tel-Tek report no. 2211030-CC07 v2. November, 2011.

[4] Variation Order: Dispersion modelling of additional scenarios using ADMS 4. CERC, July, 2011.

[5] Variation Order 2: Dispersion sensitivity analysis. CERC, December, 2011

3. Hydroxyl radical-initiated reactions

3.1. Secondary amines

Hydroxyl radicals in the atmosphere act to abstract (remove) hydrogen atoms from amines. The site of initial attack determines the type of species formed, through two separate branches of reactions. For amines in general, the $^{\bullet}OH$ can attack (a) the hydrogen on the N atom (N—**H**) or (b) one of the hydrogen atoms in the methyl groups (C—**H**). Only abstraction of an N—**H** hydrogen atom results in the formation of nitrosamines and nitramines. The ratio between the rate of attack on the C—**H** hydrogen and an N—**H** hydrogen is known as a *branching ratio*.

Once the H atom has been removed from the nitrogen atom of the amine, the product is an amino radical species, which can react with any nitric oxide (NO) or nitrogen dioxide (NO_2) present in the atmosphere to form the nitrosamine or nitramine, respectively. The amount of nitrosamine and nitramine formed depends on the concentrations of NO and NO_2.

The reaction scheme for the reaction of dimethylamine (a secondary amine) with the hydroxyl radical is as follows, based on the $^{\bullet}OH$ scheme given in the 2011 ADA report from the Climit project.[6] Red and pink text denotes nitrosamines and nitramines, respectively.

$$(CH_3)_2NH + {}^{\bullet}OH \rightarrow (CH_3)_2N^{\bullet} + H_2O \tag{1a}$$

$$\rightarrow (CH_3)_2N(H)C^{\bullet}H_2 + H_2O \tag{1b}$$

$$(CH_3)_2N^{\bullet} + O_2 \rightarrow CH_2{=}N\text{-}CH_3 + HO_2 \tag{2}$$

$$(CH_3)_2N^{\bullet} + NO \rightarrow (CH_3)_2N\text{-}NO \tag{3}$$

$$(CH_3)_2N^{\bullet} + NO_2 \rightarrow (CH_3)_2N\text{-}NO_2 \tag{4a}$$

$$\rightarrow CH_2{=}N\text{-}CH_3 + HONO \tag{4b}$$

$$(CH_3)_2N\text{-}NO \xrightarrow{hv} (CH_3)_2N^{\bullet} \tag{5}$$

3.2. Primary amines

The reaction scheme for primary amines is different to that of secondary amines after the initial attack step, in that, immediately after formation, the nitrosamine isomerises. The product of this very fast isomerisation step then reacts very quickly with O_2 to form an imine. That is, a stable nitrosamine is not formed. The reaction scheme for methylamine, a primary amine, is shown below, as given in the 2011 ADA report:

$$CH_3NH_2 + {}^{\bullet}OH \rightarrow C^{\bullet}H_2NH_2 + H_2O \tag{17a}$$

$$\rightarrow CH_3N^{\bullet}H + H_2O \tag{17b}$$

$$CH_3NH + O_2 \rightarrow CH_2{=}NH + HO_2 \tag{18}$$

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[6] Nielson *et al*. "Atmospheric Degradation of Amines (ADA). Summary Report: Photo-oxidation of Methylamine, Dimethylamine and Trimethylamine". Climit project no. 201604. Norwegian Institute for Air Research. January, 2011.

$$CH_3N^{\bullet}H + NO \rightarrow CH_3NHNO \quad (19)$$

$$CH_3NHNO \leftrightarrows CH_2NHNOH \quad (20)$$

$$CH_2NHNOH + O_2 \rightarrow CH_2{=}NH + NO + HO_2 \quad (21)$$

$$CH_3N^{\bullet}H + NO_2 \rightarrow CH_2{=}NH + HONO \quad (22)$$

$$\rightarrow CH_3NHNO_2 \quad (23)$$

4. Nitrate radical-initiated reactions

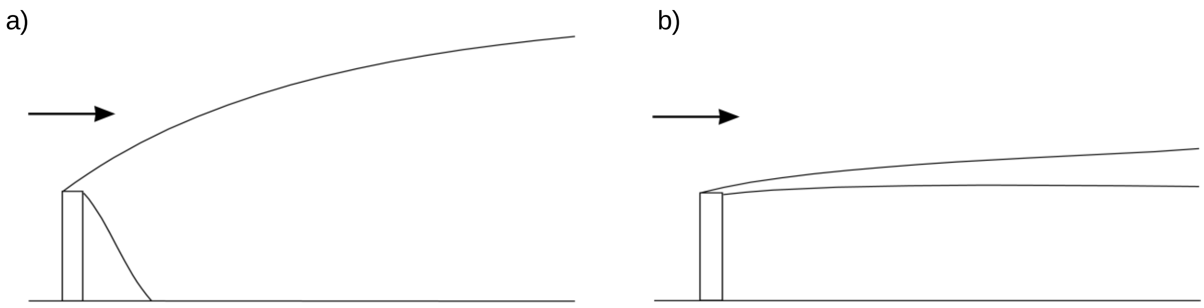
Studies have shown that the nitrate radical ($NO_3^{\bullet}$) could form nitrosamines and nitramines by reacting with amines during hours of darkness. The nitrate radical is only present during dark conditions, as it is photolysed during daylight hours.

In a similar way to hydroxyl radicals, nitrate radicals in the atmosphere act to abstract (remove) a hydrogen atom from the amine, to form an amino radical species. Once the amino radical has formed, the $NO_3\bullet$ reaction scheme proceeds in the same way as in the $^{\bullet}OH$-initiated reaction scheme; the radical species reacts with nitric oxide (NO) or nitrogen dioxide (NO_2) present in the atmosphere, to form the nitrosamine or nitramine, respectively. The rate coefficients for these subsequent reactions are the same irrespective of whether the amino radical was formed through reaction with $\bullet OH$ or with $NO_3^{\bullet}$.

Although $NO_3^{\bullet}$ rate coefficients are lower than the corresponding values for $^{\bullet}OH$ reactions, the concentrations of $NO_3^{\bullet}$ at night are generally higher than daytime $^{\bullet}OH$ radical concentrations. In kinetic terms, after balancing these two factors, it has been suggested that the reaction of amines with $NO_3^{\bullet}$ would be a minor pathway for the formation of nitrosamines and nitramines, relative to the $^{\bullet}OH$ reactions. Factoring in dispersion conditions, however, has the potential to change this picture; atmospheric conditions, and hence dispersion patterns, tend to be very different during hours of darkness.

Figure 4.1 illustrates typical dispersion conditions that occur during hours of strong solar radiation (when $^{\bullet}OH$ concentrations are highest) and those that tend to occur during hours of darkness (when $NO_3^{\bullet}$ concentrations are highest). The strong heating at the ground that occurs during the former leads to high convective turbulence, and hence promotes vigorous mixing of the plume with ambient air. In addition, this turbulence acts to bring material to the ground quickly, and hence at locations close to the stack. At night, there is no heating of the ground surface, so the air is stable; if wind speeds are low during this time, there is very little turbulence, which means that plumes can travel great distances from the stack without much mixing and dilution of the plume with ambient air.

Figure 4.1 Typical dispersion patterns during a) daytime hours with strong solar radiation and b) hours of darkness



5. Hydroxyl and nitrate chemistry scheme in ADMS 4

The rate expressions incorporated in ADMS 4 are as shown below. The expressions in blue represent those corresponding to $NO_3^\bullet$ chemistry. The numbering system for the kinetic parameters is based on that of the DMA reaction scheme. Values are required for the rate coefficients k_1, k_{1a}/k_1, k_3, k_{4a}, k_2, k_4 and j_5/j_{NO2}. For the k_1 and k_{1a}/k_1 parameters, values are specified for the attack of both the $^\bullet OH$ and the $NO_3^\bullet$ radicals.

1. Loss of the AMINE

$$\frac{d[AMINE]}{dt} = -k_{1OH}[AMINE][OH] - k_{1NO_3}[AMINE][NO_3]$$

2. Production of the amino RADICAL

$$\frac{d[RADICAL]}{dt} = k_{1aOH}[AMINE][OH] + k_{1aNO_3}[AMINE][NO_3] + j_5[NITROSAMINE] - k_2[RADICAL][O_2] - k_3[RADICAL][NO] - k_4[RADICAL][NO_2]$$

Note that $[O_2]$ is assumed to be constant.

3. Production of NITRAMINE

$$\frac{d[NITRAMINE]}{dt} = k_{4a}[NO_2][RADICAL]$$

4. Production of NITROSAMINE

$$\frac{d[NITROSAMINE]}{dt} = k_3[RADICAL][NO] - j_5[NITROSAMINE]$$

The hydroxyl radical concentration [OH] is modelled by the equation

$$[OH] = c[O_3]j_{NO_2}$$

where:

- c is a constant that is specified by the user
  A value for c can be estimated from the known typical average values of $[O_3]$, [OH] and j_{NO2}.
- $[O_3]$ is the ambient ozone concentration
- j_{NO2} is the photochemical rate constant for NO_2 photolysis
  The modelled value for j_{NO2} varies hourly according to the time of day and the time of year.

The nitrate chemistry scheme also requires a value for the night-time nitrate radical concentration, and the value of j_{NO_2} that signifies the onset of daytime/night-time.

Although the chemistry schemes are based on DMA, the model user can apply them to other amines by changing relevant parameters. An example pertinent to this project is the modelling of primary amines by setting the value of j_5 /j_{NO2} to zero and ignoring any nitrosamine output.

6. Aqueous partitioning

6.1. Overview

The chemical reaction schemes described previously consider the fate of the amines in the gaseous phase. In the atmosphere, interactions between the gaseous phase and the aqueous phase are likely; a gaseous plume can co-exist with a 'cloud droplet' or 'condensed water' or 'wet' plume. The wet plume is likely to form almost immediately after release of the gases from the stack, since these gases include significant quantities of water vapour. As the plume moves downstream it is diluted by entrainment of ambient air. This will change the water content of the plume, depending on the humidity of the ambient air; it is most likely that the water content of the plume will reduce.

In most cases, the relative humidity of the plume may fall below 100% and the droplets evaporate. Small amounts of water will be retained within Cloud Condensation Nuclei (CCN), due to the deliquescent nature of salts (ammonium sulphate, sodium chloride and possibly aminium salts). Alternatively, the 'wet' plume may persist for some kilometres downstream.

In either case, the plume may encounter higher humidity air and cloud further downstream, which may have a significant impact on the liquid water in the plume. By this time, however, the plume will be very dilute; therefore for the purpose of this project the focus is on the impact of the formation of a wet plume soon after the gases are released.

The rate of formation of nitrosamines and nitramines in the aqueous phase has been shown to be unimportant. The 'wet' plume is therefore assumed for the purpose of this project to act as a sink for the amines, thereby reducing the amount of nitrosamine and nitramine formed.

6.2. The aqueous partitioning schemes in ADMS

The aqueous partitioning schemes in ADMS quantify the transfer of the amines between the gas phase and the aqueous phase. The aqueous phase is treated as a sink for the gaseous amines, and the production of nitrosamine and nitramine in the gaseous phase chemistry schemes is limited as a result.

At each time-step, as the plume spreads and dilutes, the model calculates the *total* water content of the plume, from the initial water content plus the impact of entrainment. It then calculates the *liquid* water content of the plume, and partitions the amines between gaseous and aqueous phase according to the Henry's Law constant. The $^{\bullet}OH$ and $NO_3^{\bullet}$ gas-phase reactions are then carried out for the gaseous amines.

The model user can select either the standard aqueous partitioning, or an advanced scheme, where the latter includes the nucleation of water drops by CCN (airborne salts).

The standard scheme requires a Henry's Law constant for the amine and a value for the initial water content of the emitted plume. The advanced scheme also requires these parameters, plus:

- the number of ions in dissociation for the salt;
- the concentration of salt particles;
- the molecular mass of the salt particles; and
- the number of salt particles per cm^3.

The scheme was designed to allow for the future inclusion of wet deposition of these cloud droplets by raindrops through a washout coefficient formulation. Advanced treatment of the washout of cloud droplets and gaseous phase by rain (e.g. taking account of cloud droplet distribution and rate of uptake of amines into cloud drops by falling drop method etc.) could be implemented in the ADMS model in the future.

7. Guideline value for the protection of human health

No official limit values for nitrosamines and nitramines have been set for Norway. For the purposes of this project, CCM Project provided a value for the guideline limit of 0.3 ng/m^3, representing the total concentration of nitrosamines and nitramines in air. This guideline value is assumed to apply to annual average concentrations.

The value of 0.3 ng/m^3 has been recommended as a maximum acceptable level to ensure minimal or negligible risk of cancer for the public from exposure to nitrosamines and nitramines by the Norwegian Institute of Public Health (NIPH), following their review of existing international risk evaluations and toxicological information in the scientific literature.[7]

8. Dispersion modelling

8.1. Modelling studies - overview

For this project, several stages of model development and dispersion modelling were carried out. Prior to this, CERC carried out a project, under Call Off 1, in which the proposed method for incorporating amine chemistry was outlined, along with the first round of sensitivity tests for dispersion modelling in the Mongstad area. The reports associated with these stages are listed below.

Call-Off 1:

- *Call-Off 1 report*:[8] Plans and recommendations for model development, and a dispersion modelling Case Study

Call-off 2: (This project):

- *Activity 1 report*[1]: Description of the $^{\bullet}$OH chemistry scheme implemented in ADMS, and modelling studies
- *Dispersion modelling of additional scenarios*[4]
- *Dispersion sensitivity analysis report*[5]
- *Activities 2 to 4 report*[2]: Description of the $NO_3^{\bullet}$ chemistry scheme and aqueous partitioning schemes.

The *Activity 1 report* included extensive sensitivity tests of many model parameters and input data, building on those covering the general model setup described in the *Call-Off 1 report*. The sensitivity tests included the following:

- Amine-specific reaction parameters;
- Other reaction parameters;
- Alternative emission scenarios (Scenarios 2 to 4);
- Other meteorological data;
- With terrain and variable roughness; and
- Building effects.

The *Dispersion modelling of additional scenarios report* included calculations carried out to find the emission leading to a maximum predicted concentration equal to the guideline value for the protection of human health. The report also included calculations of atmospheric transformation of amines to nitrosamines and nitramines using a fixed percentage method rather than the amine chemistry scheme.

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[7] Låg *et al*. "Health effects of amines and derivatives associated with CO_2 capture". Norwegian Institute of Public Health. April, 2011. http://www.klif.no/no/Publikasjoner/Publikasjoner/2011/Mai/Health-effects-of-amines-and-derivatives-associated-withCO2-capture-/

[8] Contract number 257430113. H&ETQPAmine2: Modelling Atmospheric Dispersion for Components from Post-Combustion Amine-based CO_2 Capture. CERC, October, 2010.

The *Dispersion sensitivity analysis report i*ncluded dispersion modelling runs carried out using both the fixed atmospheric transformation method and the ADMS hydroxyl chemistry scheme. Sensitivity tests were carried out to investigate the effects of varying the CHP stack height and location. Also modelled were runs with emissions based on the lowest detection limits that were obtainable for each of the emitted species, and calculations to estimate concentrations in water bodies.

The *Scenarios 2 to 4 report* included runs investigating various combinations of the hydroxyl and nitrate chemistry, and aqueous partitioning schemes. The runs included two hypothetical cases representing best and worst case parameters (in terms of nitrosamines and nitramine formation), and cases that revisited the main cases considered in the Activity 1.

8.2. Model inputs common to all modelling studies

This section describes the main inputs that are common to all of the modelling studies. There have been sensitivity studies that have involved changing some of these parameters, but the values and assumptions used for the main model runs are shown here. Other modelled elements, such as building and terrain effects, were included in many of the modelling studies; descriptions of these are not given here, but full details are given in the relevant reports.

Further data, specific to certain of the model runs are given in Section 9.

8.2.1. Stack parameters, emissions and background data

The modelled CHP stack parameters are shown in Table 8.1.

Four emissions profiles, named Scenarios 1 to 4, were modelled throughout the project and are outlined in Table 8.2.

Background values for NO, NO_2 and O_3 were input as hourly sequential background data files. Background NO_x concentrations incorporated contributions from other refinery stacks.

Table 8.1: Modelled source parameters

Parameters					
Emission velocity (m/s)	**Volume flow rate (m^3/s) at 30°C**	**Source height (m)**	**Source diameter (m)**	**Emission temperature (°C)**	**Location (m)**
20	670	65	6.53	30	284412, 6747913

Table 8.2: Emissions data for each of the emissions scenarios 1 to 4

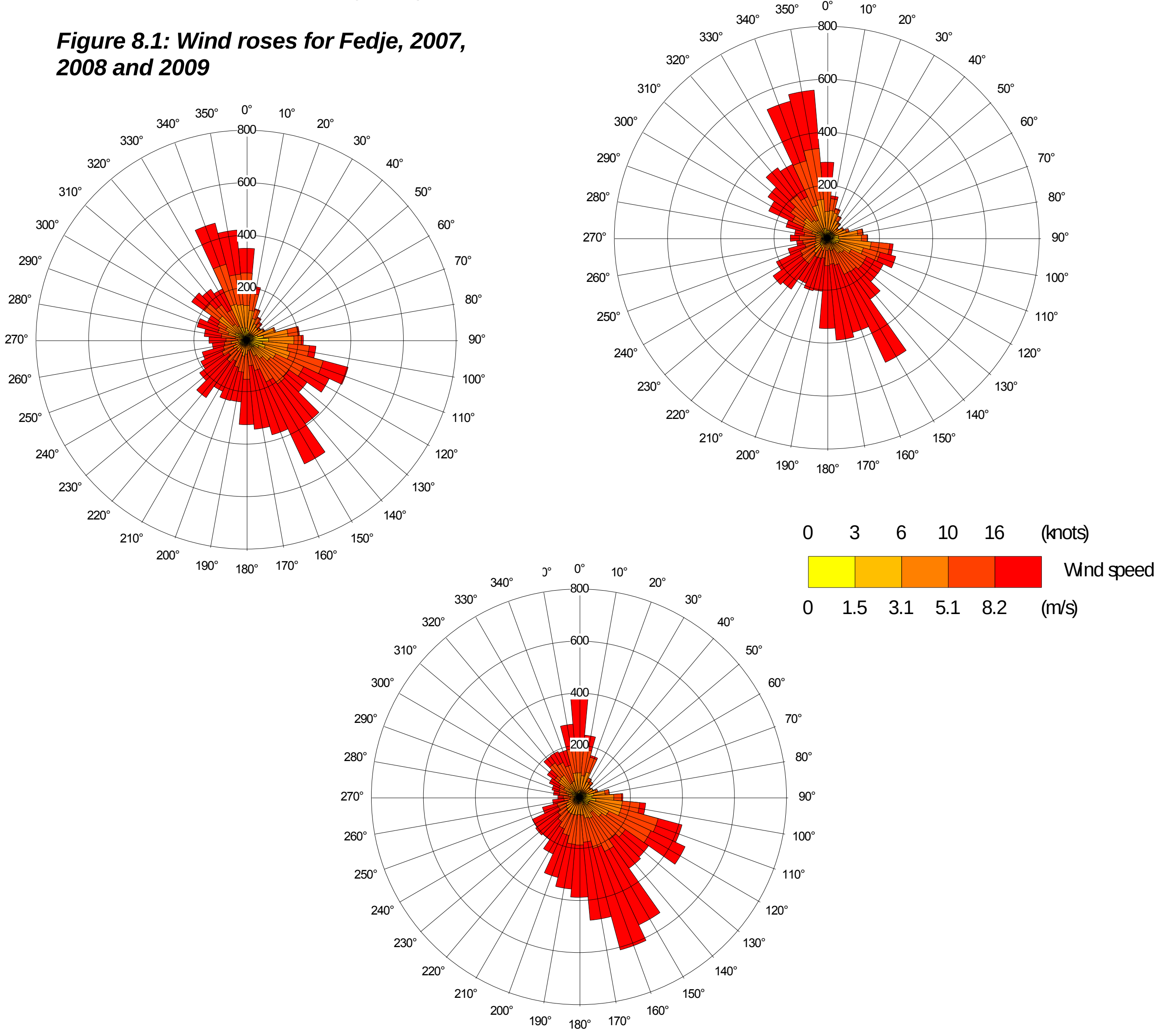
Species	**Units**	**Composition**			
		Scenario 1	**Scenario 2**	**Scenario 3**	**Scenario 4***
Amines:					
Monomethylamine	ppmv	0.1	0.2	0.05	0.1
Dimethylamine	ppmv	0.05	0.1	0.025	0.05
Monoethanolamine	ppmv	1.0	1.0	0.1	1.0
Nitrosamines (assume NDMA)	ppbv	0.25	0.5	0.1	0.25
Nitramines	ppbv	0	0	0	0

*Note that Scenario 4 has the same emission concentration profile as Scenario 1, but has an emission velocity of 6m/s and volume flow rate of 201m^3/s.

8.2.2. Meteorological data

The meteorological data used for all of the modelling studies are a combination of data from Takle, Fedje and Bergen Fresland sites, for the years 2007, 2008 and 2009. Figure 8.1 shows wind roses wind data taken from the Fedje site).

Figure 8.1: Wind roses for Fedje, 2007, 2008 and 2009



9. Selected dispersion modelling runs

This section gives examples of the main findings of the dispersion modelling runs. Note that, because the dispersion modelling evolved steadily over the course of the project, to reflect the frequent update of available input data, comparing results of runs carried out at different stages of the project is not useful. The modelling results in different sections of this report should not be directly compared with one another.

No example results from the *Activity 1 report* are given explicitly, as the main runs have been improved and then repeated in the *Activities 2 to 4 report*, using updated kinetic data and including the $NO_3^{\bullet}$ chemistry and aqueous partitioning schemes; the extensive sensitivity tests carried out for Activity 1 are too numerous to reproduce here.

9.1. Activities 2 to 4 Report examples

9.1.1. $^{\bullet}OH$, $NO_3^{\bullet}$ and aqueous scheme comparisons

This section presents results from the model runs carried out as part of Activities 2 and 3, to investigate different combinations of the hydroxyl and nitrate chemistry, and aqueous partitioning schemes.

Two 'hypothetical' cases were proposed by CCM Project, to represent 'best' and 'worst' cases respectively, in terms of the formation of nitrosamines and nitramines. These cases were proposed in order to approximately cover the range of parameters for the $^{\bullet}OH$ and $NO_3^{\bullet}$ chemistry schemes, and the aqueous partitioning scheme, that might be expected from mixtures of solvents. These two cases have been referred to nominally as 'MEA' and 'DMA', respectively.

Runs were also carried out to model emissions of Monoethanolamine (MEA), Methylamine (MMA), Dimethylamine (DMA) and NDMA. These runs were based on the main model runs carried out in Activity 1, but with slightly revised parameters, and including nitrate chemistry and aqueous partitioning effects. Emission data for all of the aforementioned cases are shown in Table 9.1; note that the emission rate is 1ppmv for all of the emitted amines.

Parameters common to all of the cases are shown in Table 9.2, and those specific to each case are given in Table 9.3. The k_{1NO3} values were calculated using a correlation derived by Wayne *et al* [9] based on the k_{OH} values.

For all the runs, a value of 0.027 kg of water per kg of dry air was input for the water mixing ratio of the emissions, which represents air that is completely saturated at the emission temperature, 30°C. All emitted amine was assumed to be in the gas phase at the emission point.

The standard aqueous scheme was applied; the advanced aqueous scheme (to include the nucleation effects of aerosol salts) was not modelled for these cases. An example run incorporating the advanced aqueous scheme is described in Section 9.1.2.

Results were output as annual average ground level concentrations, in units of ng/m^3, calculated over a 100m resolution output grid with an extent of 10km by 10km. All concentrations were calculated using 2008 meteorological data. No building or terrain effects were included for these model runs.

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[9] Wayne, R. P.; Barnes, I.; Biggs, P.; Burrows, J. P.; Canosamas, C. E.; Hjorth, J.; Lebras, G.; Moortgat, G. K.; Perner, D.; Poulet, G.; Restelli, G.; Sidebottom, H., The nitrate radical - physics, chemistry, and the atmosphere. *Atmospheric Environment Part a- General Topics* **1991,** *25* (1), 1-203.

Table 9.1: Emission parameters for each emitted amine

Case	Amine type	Molecular mass	Emission concentration (ppmv)	Emission concentration (g/m^3)	Emission rate (g/s)
Hypothetical	‘MEA’	50	1	0.0020	1.35
	‘DMA’	100		0.0040	2.70
Real	MEA	61		0.0025	1.644
	MMA	31		0.0012	0.835
	DMA	45		0.0018	1.213
	NDMA	74		0.0030	1.994

Table 9.2: Parameter values common to all cases

Parameter	Description	Value	Units
k_2	Rate coefficients	9.54×10^{-20}	cm^3/molecule/s
k_3		1.91×10^{-13}	cm^3/molecule/s
k_{4a}		3.18×10^{-13}	cm^3/molecule/s
k_4		3.88×10^{-13}	cm^3/molecule/s
c	Constant that determines the hourly-varying $^{\bullet}$OH concentration	3.92×10^{-3}	s
d	constant ambient concentration of $NO_3^{\bullet}$	3.2×10^{7}	radicals cm^{-3}
x	value of j_{NO2} used to define hours of darkness	1×10^{-4}	s^{-1}

Table 9.3: Parameter values specific to each case

Case	Amine type	k_1 (cm^3/molecule/s)		k_{1a}/k_1 (both OH and NO_3)	j_5/j_{NO2}	Henry’s Law constant (moles/(litre.atm))
		OH	NO_3			
Hypothetical	‘MEA’	3×10^{-11}	4.6×10^{-14}	0.2	0	6×10^{6}
	‘DMA’	9×10^{-11}	1.8×10^{-12}	0.5	0.32	50
Real	MEA	3.10×10^{-11}	5.14×10^{-14}	0.08	0	6×10^{6}
	MMA	1.73×10^{-11}	6.01×10^{-13}	0.75	0	50
	DMA	6.50×10^{-11}	7.42×10^{-15}	0.42	0.32	100

Tables 9.4 to 9.6 show the maximum annual average concentrations of nitrosamine, nitramine and the sum of nitrosamine and nitramine, respectively, predicted over the output grid for each of the modelled amine cases.

For these modelled scenarios, there is very little difference in the maximum predicted concentrations of nitrosamines and nitramines when the effects of $NO_3^{\bullet}$-initiated reactions are included alongside $^{\bullet}$OH-initiated reactions. There is no discernable difference in these results for both the ‘hypothetical’ and ‘real’ MEA, and for MMA, and a very small difference is seen for both the ‘hypothetical’ and ‘real’ DMA.

There is no difference in the maximum predicted concentrations of nitrosamines and nitramines when the effects of aqueous partitioning are included for these scenarios.

Table 9.4: Maximum predicted nitramine concentrations

OH	NO_3	Aq	Maximum annual average nitramine concentrations (ng/m^3)					
			Hypothetical amine cases		'Real' amine cases			
			'MEA'	'DMA'	MEA	MMA	DMA	NDMA
✓	✓	✓	0.105	1.096	0.047	0.181	0.430	1.874
✓	✓	×	0.105	1.096	0.047	0.181	0.430	1.874
✓	×	×	0.105	1.090	0.047	0.181	0.429	1.874
×	×	×	n/a	n/a	n/a	n/a	n/a	n/a

Table 9.5: Maximum predicted nitrosamine concentrations

OH	NO_3	Aq	Maximum annual average nitrosamine concentrations (ng/m^3)					
			Hypothetical amine cases		'Real' amine cases			
			'MEA'	'DMA'	MEA	MMA	DMA	NDMA
✓	✓	✓	n/a	0.500	n/a	n/a	0.182	121.0
✓	✓	×	n/a	0.500	n/a	n/a	0.182	121.0
✓	×	×	n/a	0.497	n/a	n/a	0.181	121.0
×	×	×	n/a	n/a	n/a	n/a	n/a	124.6

Table 9.6: Maximum predicted sum of nitrosamine and nitramine concentrations

OH	NO_3	Aq	Maximum annual average sum of nitrosamine and nitramine concentrations (ng/m^3)					
			Hypothetical amine cases		'Real' amine cases			
			'MEA'	'DMA'	MEA	MMA	DMA	NDMA
✓	✓	✓	0.105	1.583	0.047	0.181	0.606	121.3
✓	✓	×	0.105	1.583	0.047	0.181	0.606	121.3
✓	×	×	0.105	1.575	0.047	0.181	0.605	121.3
×	×	×	n/a	n/a	n/a	n/a	n/a	124.6

Tables 9.7 and 9.8 show the maximum annual average concentrations of amine partitioned into the gaseous and aqueous phases, respectively, for each of the modelled amine cases.

The results show that, for these modelled scenarios, the aqueous partitioning scheme leads to amines being present in the aqueous phase at ground level for the 'MEA' case only.

Table 9.7: Maximum predicted gaseous amine concentrations

OH	NO_3	Aq	Maximum annual average gaseous amine concentrations (ng/m^3)					
			Hypothetical amine cases		'Real' amine cases			
			'MEA'	'DMA'	MEA	MMA	DMA	NDMA
✓	✓	✓	78.1	164.0	95.2	51.9	74.4	n/a
✓	✓	×	83.5	164.0	101.8	51.9	74.4	n/a
✓	×	×	83.5	164.3	101.8	51.9	74.4	n/a
×	×	×	84.2	168.4	102.7	75.8	75.8	n/a

Table 9.8: Maximum predicted aqueous amine concentrations

OH	NO$_3$	Aq	Maximum annual average aqueous amine concentrations (ng/m^3)					
			Hypothetical amine cases		'Real' amine cases			
			'MEA'	'DMA'	MEA	MMA	DMA	NDMA
✓	✓	✓	5.421	0.0015	6.6118	0.0009	0.0007	n/a
✓	✓	✗	n/a	n/a	n/a	n/a	n/a	n/a
✓	✗	✗	n/a	n/a	n/a	n/a	n/a	n/a
✗	✗	✗	n/a	n/a	n/a	n/a	n/a	n/a

9.1.2. Temporal and spatial aspects of the modelled plumes

The distance of the locations of the maximum annual average ground level concentrations from the modelled stack were calculated from the hypothetical 'DMA' runs, for the $^{\bullet}$OH and NO$_3^{\bullet}$ reaction scheme cases; these values are given in Table 9.9.

The general effect of the atmospheric conditions is clearly illustrated by comparing the locations of the maximum concentrations from the $^{\bullet}$OH and the NO$_3^{\bullet}$ chemistry scheme results, respectively. These differences in location are due to marked differences in the prevailing meteorological conditions under which each of these radicals is available for reaction with the amine. The $^{\bullet}$OH radical is at its highest levels during the daytime, particularly during the middle of sunny summer days, whereas the NO$_3^{\bullet}$ radical is only present during hours of darkness. The difference in location is much more pronounced for nitramine concentrations, which is likely to be due, at least in part, to the added complexity of photolysis effects for nitrosamine.

Table 9.10 shows a temporal breakdown for a selected day, 16th June, showing the hourly concentrations, changes in travel distance and time alongside relevant meteorological parameters. This highlights the variation that typically occurs, even over a single day.

Figure 9.1 shows contour plots of the sum of nitrosamine and nitramines, for the hypothetical 'DMA' case. These are shown for a run with the $^{\bullet}$OH and NO$_3^{\bullet}$ schemes respectively. Note the difference in magnitude between the two plots, for both the concentration and the distance scales.

Table 9.9: Distances from the stack to the maximum ground level concentrations

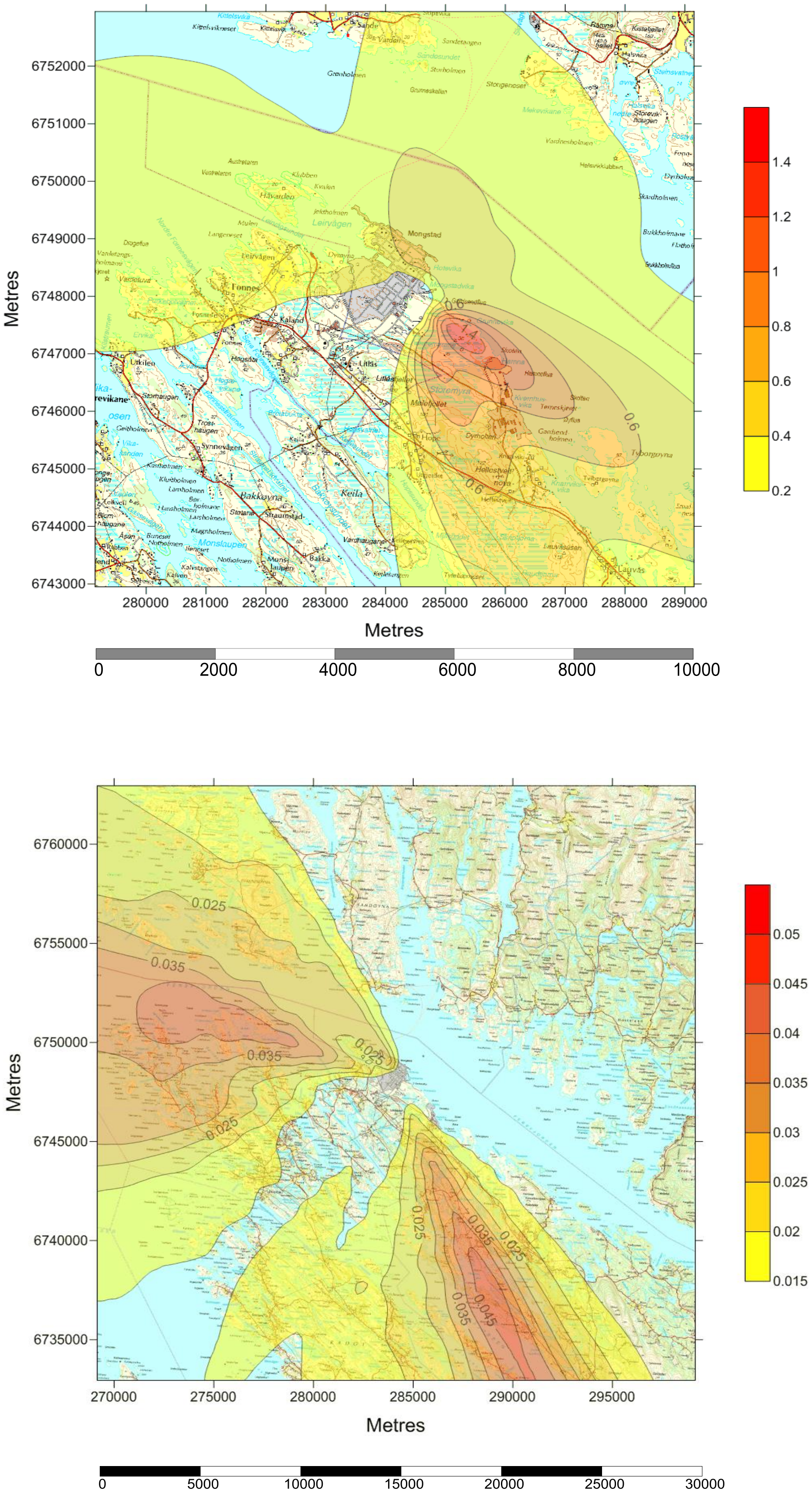
Reaction scheme (case)	Distance of the maximum concentration from the modelled stack (m)		
	Nitrosamine	Nitramine	Sum of nitrosamine and nitramine
$^{\bullet}$OH	928	1149	1012
NO$_3^{\bullet}$	1508	11681	11681

Table 9.10: Plume information for 16th June

Hour	Cloud cover (oktas)	Wind speed (m/s)	Distance* (m)	Approx travel time* (minutes)	Hourly-average concentration (ng/m^3)		
					Nitrosamine	Nitramine	Amine
3	7	5.2	5570	18	0.0	0.1	556
4	7	4.1	5670	23	0.8	6.4	407
5	7	4.2	6210	25	0.7	6.1	181
6	7	3.2	6790	35	1.5	16.1	180
7	7	3.0	5020	28	3.0	23.6	321
8	7	3.3	3870	20	5.1	28.0	468
9	3	2.4	2940	20	8.2	54.2	289
10	3	4.5	1150	4	23.4	46.1	1737
11	3	5.5	970	3	23.6	35.5	2121
12	5	6.0	1190	3	17.3	28.1	1714
13	5	5.5	970	3	19.9	30.7	2083
14	5	4.9	960	3	20.5	34.5	2087
15	4	4.4	1010	4	20.8	39.2	1898
16	4	5.3	1150	4	15.0	28.9	1777
17	4	4.2	1230	5	12.8	28.9	1570
18	5	4.2	1540	6	7.3	18.5	1245
19	5	3.8	2290	10	3.3	11.9	716
20	5	5.9	2940	8	1.4	5.1	753
21	6	5.4	4860	15	0.0	0.1	620

*to maximum ground-level nitrosamine concentration

Figure 9.1 Predicted sum of annual average nitramine and nitrosamine concentrations (ng/m^3) for the 'DMA' Case for a) $^{\cdot}$OH only and b) $NO_3^{\cdot}$ only.



9.1.3. Results scaled to Scenario 1 emissions

The preceding sections present results relating to emission concentrations of 1ppmv for all modelled amines, and the output concentrations and the input emission concentration show a linear relationship (doubling the emission concentration doubles the output concentrations), so the results can be scaled *pro-rata* to account for different emission profiles. In order to demonstrate this, and allow comparison with the guideline values, the results were scaled to represent the Scenario 1 emission profile (as shown in Table 8.2), and are given in Tables 9.11 to 9.13.

Table 9.11: Maximum predicted nitramine concentrations (if emissions were Scenario 1 emissions)

OH	NO_3	Aq	Maximum annual average concentrations (ng/m^3)			
			'Real' amine cases			
			MEA	MMA	DMA	NDMA
✓	✓	✓	0.047	0.018	0.021	0.0005
✓	✓	×	0.047	0.018	0.021	0.0005
✓	×	×	0.047	0.018	0.021	0.0005
×	×	×	n/a	n/a	n/a	n/a

Table 9.12: Maximum predicted nitrosamine concentrations (if emissions were Scenario 1 emissions)

OH	NO_3	Aq	Maximum annual average concentrations (ng/m^3)			
			'Real' amine cases			
			MEA	MMA	DMA	NDMA
✓	✓	✓	n/a	n/a	0.009	0.030
✓	✓	×	n/a	n/a	0.009	0.030
✓	×	×	n/a	n/a	0.009	0.030
×	×	×	n/a	n/a	n/a	0.031

Table 9.13: Maximum predicted sum of nitrosamine and nitramine concentrations (if emissions were Scenario 1 emissions)

OH	NO_3	Aq	Maximum annual average concentrations (ng/m^3)				
			'Real' amine cases				
			MEA	MMA	DMA	NDMA	Total
✓	✓	✓	0.047	0.018	0.030	0.030	**0.111**
✓	✓	×	0.047	0.018	0.030	0.030	**0.112**
✓	×	×	0.047	0.018	0.030	0.030	**0.111**
×	×	×	n/a	n/a	n/a	0.031	**0.031**

9.1.4. Tel-Tek comparisons

A 2011 Tel-Tek report on photolysis rates at Mongstad outlined results of simulations using the COSMO-MUSCAT model for the Mongstad area, to characterise the ambient conditions at the site.[10] Table 9.14, which is based on Table 3.1 of that report, shows some of these results. The values shown represent the average values for a selection of months, for the year 2006.

Table 9.15 shows values for the same parameters, as used in the standard ADMS modelling runs, for comparison purposes.

A model run was set up in ADMS to broadly replicate the ambient concentrations and parameters given in Table 9.14. This setup was based on the 'hypothetical' case model setup described in Section 9.1, (run with the OH scheme only), but with changes to key parameters, as shown in Table 9.16. This run was carried out for both the 'MEA' and 'DMA' scenarios; the results are given in Table 9.17.

The values of j_{NO2} are calculated by the meteorological pre-processor within ADMS, so these were kept the same as in the original runs. The ambient $^{\bullet}OH$ radical concentration is calculated by ADMS on an hourly basis, using the following relationship:

$$[OH] = c[O_3]j_{NO_2}$$

The modelled hourly values of $^{\bullet}OH$ are therefore highly dependent on the value assumed for the constant c, which in turn, is estimated by the model user, based on typical values of $^{\bullet}OH$, O_3 and j_{NO2}. The value of c input into ADMS was changed to 0.0016, calculated by approximately fitting the typical monthly concentrations of $^{\bullet}OH$ to the Tel-Tek data.

The NO and NO_2 volume mixing ratios shown in Table 9.16 are a factor of five lower than those used for the standard ADMS runs, shown in Table 9.15; a new .bgd input file was created whereby each hourly value of NO_2 and NO was reduced by a factor of five. This factor was determined by comparing the NO_x concentrations of the original ADMS runs with those given in Table 9.14.

Table 9.14: Average values of NO_2 photolysis rate, $^{\bullet}OH$ radical concentration, and NO and NO_2 volume mixing ratios in the Mongstad region (From Tel-Tek report)

Parameter	Units	March	June	September	December
j_{NO2}	s^{-1}	1.22×10^{-3}	2.76×10^{-3}	1.32×10^{-3}	2.82×10^{-5}
$^{\bullet}OH$	molecules cm^{-3}	3.90×10^{5}	2.57×10^{6}	8.88×10^{5}	6.77×10^{4}
NO	ppbv	0.228	0.212	0.106	0.268
NO_2	ppbv	1.70	1.95	1.83	1.43

Table 9.15: Average values of NO_2 photolysis rate, $^{\bullet}OH$ radical concentration, and NO and NO_2 volume mixing ratios used for the main ADMS dispersion modelling

Parameter	Units	March	June	September	December
j_{NO2}	s^{-1}	8.62×10^{-4}	2.10×10^{-3}	1.09×10^{-3}	1.29×10^{-4}
$^{\bullet}OH$	molecules cm^{-3}	2.45×10^{6}	5.86×10^{6}	3.09×10^{6}	3.62×10^{5}
NO	ppbv	1.94	2.39	1.56	1.74
NO_2	ppbv	4.50	5.23	4.59	4.30

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[10] Data from Table 3.1 of Wolke, R. *Atmospheric Chemistry – Dark Chemistry. Nighttime Chemistry in the Mongstad Area: Literature Study and Model Simulations ("Dark chemistry")*; Report no. 2211030-DC02; Tel-Tek: 2011

Table 9.16 Average values of NO_2 photolysis rate, $^{\bullet}OH$ radical concentration, and NO and NO_2 volume mixing ratios used in the Tel-Tek comparison ADMS run

Parameter	Units	March	June	September	December
j_{NO2}	s^{-1}	8.62×10^{-4}	2.10×10^{-3}	1.09×10^{-3}	1.29×10^{-4}
$^{\bullet}OH$	molecules cm^{-3}	9.81×10^{5}	2.34×10^{6}	1.24×10^{6}	1.45×10^{4}
NO	ppbv	0.39	0.48	0.31	0.35
NO_2	ppbv	0.90	1.05	0.92	0.86

Table 9.17: Predicted concentrations from Tel-Tek ambient conditions runs (OH scheme only)

Run	Assumed ambient conditions	Maximum annual average concentrations (ng/m^3)		
		Nitrosamine	Nitramine	Sum of nitrosamine and nitramine
'MEA' case	Original	n/a	0.11	0.11
	Replication of Tel-Tek report values	n/a	0.02	0.02
'DMA' case	Original	0.50	1.09	1.58
	Replication of Tel-Tek report values	0.16	0.20	0.36

9.1.5. Demonstration of the advanced aqueous scheme

The advanced aqueous partitioning scheme incorporates nucleation of water drops from airborne salts. An example calculation was carried out to demonstrate the effects of this scheme on the amine partitioning and the gaseous chemistry.

Ammonium sulphate, $(NH_4)_2SO_4$, was selected as the salt for the example calculation. Therefore, the number of ions in dissociation was set to a value of 3, and the molecular mass of the salt was input as 132.

For the first run, the concentration of $(NH_4)_2SO_4$ was set to 1 $\mu g/m^3$ and the number of salt particles per cubic centimetre was set to 100. A second run was carried out, in which the concentration was set to 5$\mu g/m^3$ and the number of salt particles per cubic centimetre was set to 500.

Table 9.17 shows the maximum annual average concentrations of amine partitioned into the gaseous and aqueous phase predicted over the output grid, at ground level for the 'MEA' and 'DMA' cases, respectively.

The results show that applying the advanced aqueous scheme makes no difference to these values for the 'DMA' case; this hypothetical species has been assigned a low solubility (low Henry's Law constant), so the formation of further water droplets by the advanced aqueous scheme has no effect on the partitioning.

The advanced scheme does, however, have a small effect for the 'MEA' case, for these parameters. Note that there is very little information available about the concentration and nature of any CCN present in the emission from the stack, so there is significant uncertainty inherent in these results.

Note that the amine concentrations shown in Table 9.18 are those output at ground level only. Note also, that the purpose of the results described in this section is to demonstrate the effect of the advanced aqueous scheme on the partitioning of the amine. The main aim of the aqueous partitioning scheme in this project is to quantify its effect on the formation of nitrosamines and nitramines; results that demonstrate this effect are given in Section 9.1.1.

Table 9.18: Maximum predicted concentrations for the 'MEA' case

Run	Maximum annual average amine concentrations (ng/m^3)			
	Gaseous		Aqueous	
	'MEA' case	'DMA' case	'MEA' case	'DMA' case
Standard aqueous scheme	78.80	168.38	5.42	0.0018
Concentration = 1 µg/m^3 Number of particles/cm^3 = 100	78.71	168.38	5.51	0.0018
Concentration = 5 µg/m^3 Number of particles/cm^3 = 500	78.39	168.38	5.83	0.0018

9.2. Other dispersion calculation examples

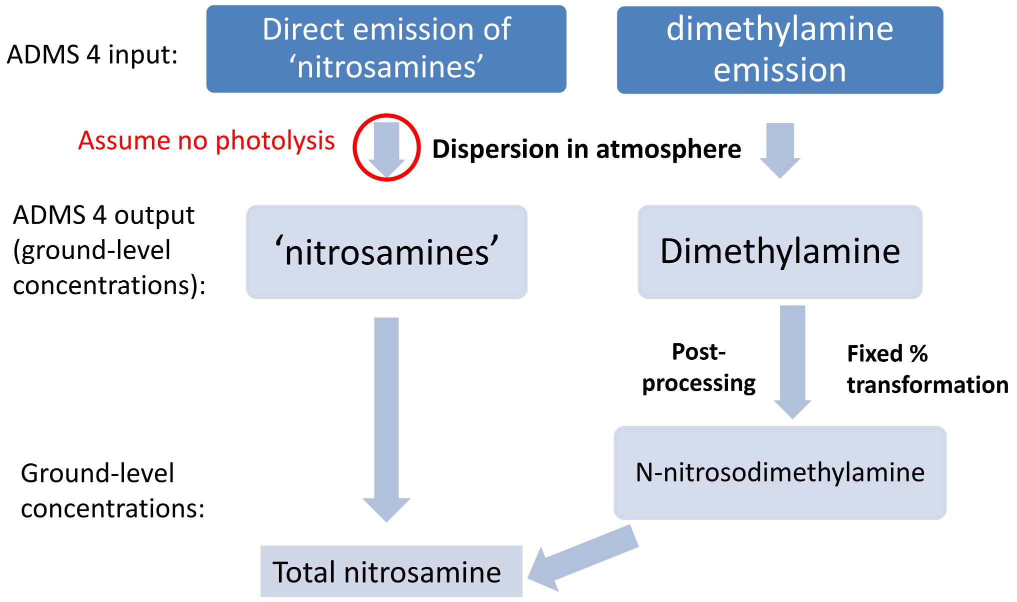
9.2.1. Fixed transformation calculations

The 'Dispersion modelling of additional scenarios using ADMS 4' report included calculations that used a fixed percentage method for atmospheric transformation of amines to nitrosamines and nitramines (as opposed to the amine chemistry scheme, which had not been incorporated into ADMS 4 at this stage of the project). The method used for these calculations is outlined in Figure 9.2, and transformation percentages are given in Table 9.18.

Some results are given in Table 9.19, which shows the sum of nitrosamine and nitramine concentrations. The concentrations are ground level concentrations, calculated over a 50m resolution output grid with an extent of 5km by 5km.

Figure 9.2: Fixed transformation calculation process for a) nitrosamines and b) nitramines

a)



b)

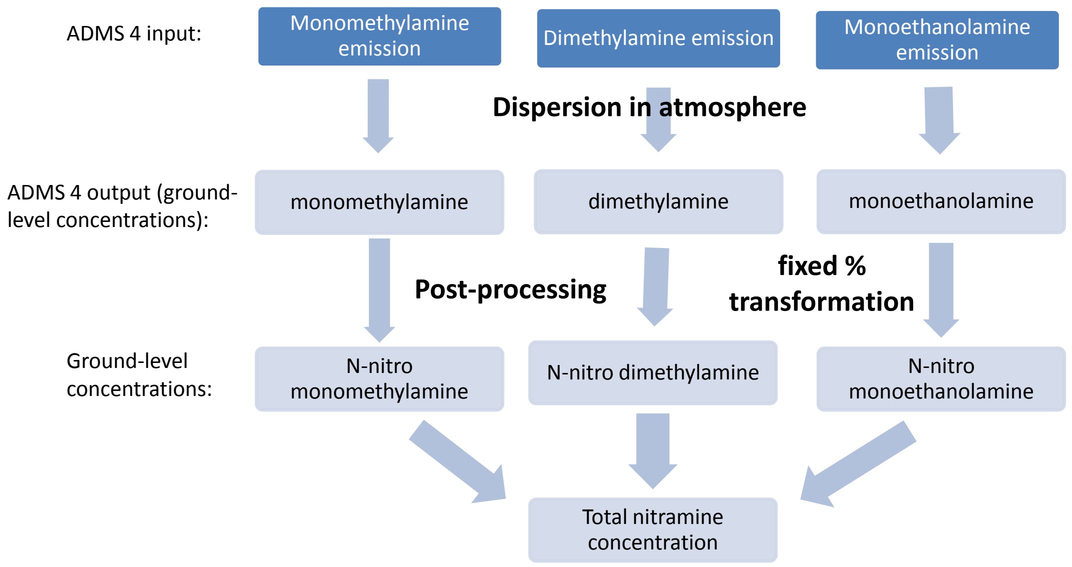


Table 9.19: Percentage transformations applied to each amine

Amine	Transformation in the atmosphere (%) to:	
	Nitramine	Nitrosamine
Monomethylamine	0.4	0
Dimethylamine	2.5	0.4
Monoethanolamine	0.3	0

Table 9.20: Maximum annual average concentrations of total (nitramines + nitrosamines)

Scenario	**Concentration (ng/m^3)**		
	2007	**2008**	**2009**
1	3.9	4.2	4.2
2	5.3	5.7	5.7
3	0.9	1.0	1.0
4	5.4	5.6	6.1

9.2.2. Reverse calculations

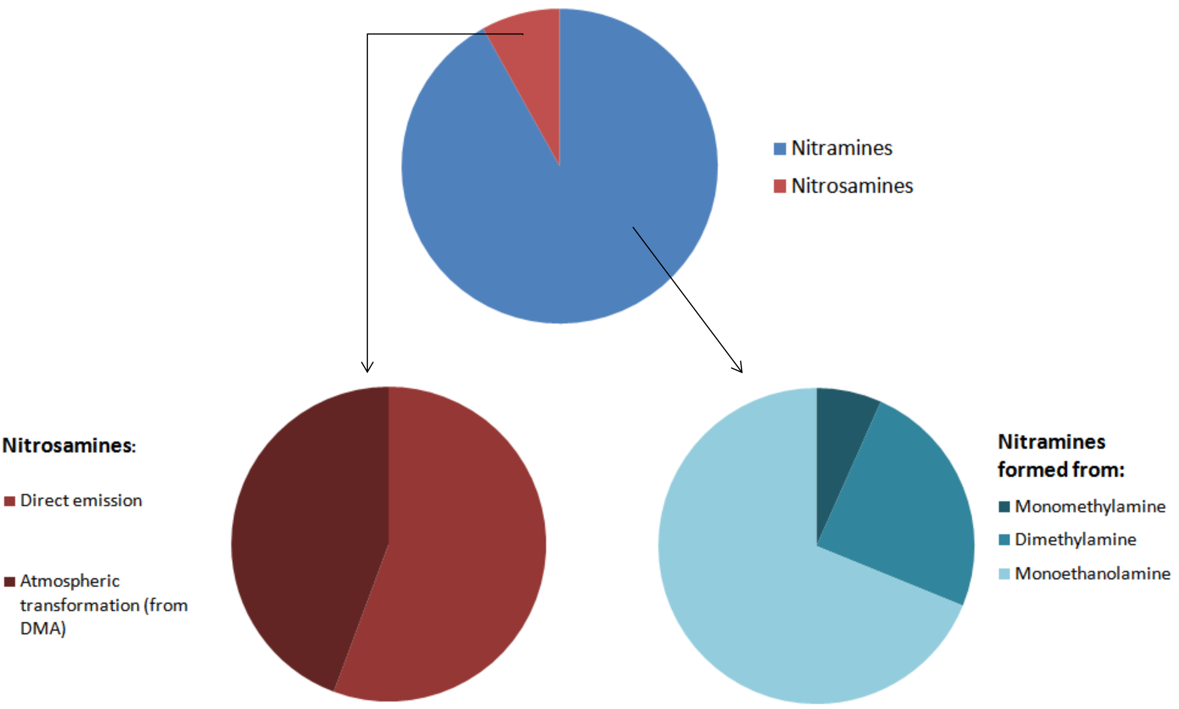
Calculations were carried out to find the emissions leading to a maximum predicted concentration equal to: (a) the guideline value. The reverse calculations incorporated the dilution effects in the atmosphere, the fixed percentage transformation rates described in the previous section, and the differences in relative molecular mass between the various species.

Table 9.20 shows the overall results for each of the emissions scenarios (previously outlined in Table 8.2). The results are based on modelling for the 2007 meteorological year. Figure 9.3 shows pie charts depicting the breakdown of the contribution from each emitted species, for emission scenario 1.

Table 9.21: Summary of reverse calculations, based on the guideline value (0.3ng/m^3)

Scenario	Emissions required to give guideline value (ppmv)			
	MMA	**DMA**	**MEA**	**NDMA**
1	0.01	0.004	0.08	0.00002
2	0.01	0.01	0.06	0.00003
3	0.02	0.01	0.03	0.00003
4	0.01	0.003	0.06	0.000004

Figure 9.3: Relative contributions of each species for Scenario 1



9.2.3. Emissions at detection limits

Task 2 of this report considered emissions based on the lowest detection limits that were obtainable for each of the emitted species, which are presented in Table 9.21. Nitra-MEA is N-nitromonoethanolamine, a directly emitted nitramine.

Table 9.22 shows some results of these runs. The ADMS $^{\bullet}$OH chemistry scheme was used to generate concentrations over a 10km by 10km output grid, at a resolution of 100m. These runs included building effects (the multiple-building scenario, which is described in the Activity 1 report).

Table 9.22: Detection limits and emission rates

Emitted species	Detection limit (µg/m^3)	Equivalent emission rate (g/s)
MMA	0.80	5.36 x10^{-4}
MEA	8.00	5.36 x10^{-3}
NDMA	0.008*	5.36 x10^{-6}
nitra-MEA	0.60	4.02 x10^{-4}

* Note that this detection limit for NDMA was increased by a factor of 10 (to 0.008 µg/m^3), for these model runs, due to the lower threshold limit specified within the ADMS amine chemistry scheme (the actual limit of detection provided was ten times lower than this).

Table 9.23: Maximum annual average concentrations (ng/m^3)

Emitted species	Nitrosamine	Nitramine	Sum (nitrosamine plus nitramine)
MMA	-	2.25×10^{-5}	2.25×10^{-5}
MEA	-	0.0002	0.0002
NDMA	0.0003	3.56×10^{-5}	0.0003
nitra-MEA	-	0.031	0.031
Total	0.0003	0.031	**0.031**

9.2.4. Calculation to estimate concentrations in water bodies

Task 4 of the *Dispersion sensitivity analysis* report involved using the ADMS amine chemistry scheme to predict concentrations in air and deposition of nitrosamines and nitramines, at a selection of locations representing freshwater bodies around Mongstad, and then using a highly simplified approach to calculate the resulting levels in the water bodies.

The deposition fluxes of the nitrosamines and nitramines were calculated by post-processing the air concentrations, based on ratios of concentrations to deposition fluxes, determined in a second model run. This second run involved an identical model set-up, but with a nominal pollutant emitted, the amine chemistry module switched off and the deposition module switched on.

Deposition parameters are extremely important for modelling dry and wet deposition but specific parameters are not available for nitrosamines and nitramines. For the dry deposition model run, the pollutant was run as the ‘reactive gas’ option in ADMS. For the wet deposition run, ADMS default values were applied. The precipitation rates were derived from the meteorological data.

Following the calculation of the deposition fluxes in air, a rough approximation of the resulting concentration of nitrosamines and nitramines in each water body was made, by post-processing the deposition results described above. This calculation assumes that the nitrosamines and nitramines in the aqueous phase are well-mixed to a depth of 1m below the surface of the water.

Table 9.23 shows a summary of the results for each of the water bodies.

Table 9.24: Concentrations in air, deposition rates and resulting approximate concentrations in water

Water body	Location (m)		Sum of nitrosamines and nitramines		
	x	y	Modelled concentration in air (ng/m^3)	Total (dry plus wet) deposition rate (ng/m²/s)	Annual average concentrations in water (ng/dm^3)
Dingevatnet	288600	6772500	0.004	2.85×10^{-4}	9.0
Langevatnet	287900	6755900	0.010	6.76×10^{-4}	21.3
Svardalsvatnet	287600	6759300	0.008	5.63×10^{-4}	17.7
Sliersvatnet	295000	6755400	0.007	5.26×10^{-4}	16.6
Kvamsdalsvatnet	298600	6755700	0.005	4.19×10^{-4}	13.2
Mollandsvatnet	299100	6755900	0.005	4.07×10^{-4}	12.9
Hallandsvatnet	284800	6730800	0.007	2.98×10^{-4}	9.4
Sorkingevatnet	304200	6739800	0.011	6.57×10^{-4}	20.7

10. Discussion

10.1. Nitrate radical chemistry

The model results from the *Activities 2 to 4 report* show that the nitrate radical chemistry produces much lower maximum annual average ground level concentrations of both nitrosamines and nitramines than the hydroxyl radical chemistry. For the hypothetical 'DMA' case, the maximum nitramine concentration resulting from the nitrate chemistry is 4% of that resulting from the hydroxyl chemistry, and the corresponding value for nitrosamine concentrations is 2%. The equivalent value for the 'MEA' case, for nitramine concentrations, is 0.3%.

The results also show that the model runs carried out using the nitrate radical chemistry scheme give maximum nitramine concentrations at a much larger distance from the stack than the equivalent hydroxyl radical chemistry runs. The two sets of concentrations will, therefore, tend not to be additive.

The very low relative concentrations, coupled with the fact that maximum concentrations tend to occur much further from the stack than for the hydroxyl chemistry, raises the question of whether or not nitrate chemistry should be included in future dispersion modelling studies.

In answering this question, one factor to take into consideration is the uncertainty in the input values for ambient conditions at Mongstad. The sensitivity tests suggest that the modelled concentrations are not sensitive to the cut-off point for darkness/nighttime, which dictates the time during which nitrate radicals are assumed to be present in the atmosphere. The concentrations are, however, inherently sensitive to the concentration of the nitrate radical; a doubled nitrate radical concentration would double the concentrations.

Therefore, a precautionary approach would be to include nitrate chemistry in the dispersion modelling. This is particularly important where any information arises that suggests that ambient nitrate conditions at Mongstad are higher (or that any of the reaction kinetic parameters are more conservative) than the values used in this modelling. It should be stressed, however, that the nitrate chemistry modelling does not need to form a major part of future dispersion modelling studies; attention should be focused primarily on the effects of hydroxyl chemistry.

10.2. Aqueous partitioning

For this project, the focus was to treat the aqueous partitioning as a sink for the gaseous amines, with the production of nitrosamine and nitramine being reduced as a result. The results of the modelling with and without the aqueous partitioning scheme show that there is very little effect on the maximum ground level concentrations of nitrosamines and nitramines when the aqueous partitioning is included.

Further runs were carried out to test the differences between the partitioning of different amine species and the sensitivity of the aqueous partitioning schemes to various inputs. The results show that the aqueous partitioning scheme leads to amines being present in the aqueous phase *at ground level* for the highly soluble amines only (the 'hypothetical' and 'real' MEA cases). The calculated amounts of the less soluble amines (both MMA and DMA) in the aqueous phase at ground level are negligible.

The recommendation of whether or not aqueous partitioning should be used as a sink for the amines in future dispersion modelling is similar to that given for the nitrate chemistry scheme. If the assumed input parameters are shown to be significantly different to those used in these model runs, then further sensitivity tests should be carried out. This is particularly true of the parameters for the advanced aqueous scheme, where very little information is known about the possible concentration and nature of any CCN present in the emission from the stack. Sensitivity tests would also be advisable if a more soluble amine than MEA was to be considered.

Although the application of the aqueous partitioning scheme as a *sink* for the amines might not be an important factor in future dispersion modelling studies, there is, however, the important question of ‘rain out’ of droplets; this effect has not been assessed in the current project. The aqueous partitioning schemes were instead designed to allow for the future inclusion of deposition from the aqueous phase and hence the assessment of this deposition onto sensitive areas such as drinking water reservoirs.

10.3. Sensitivity to ambient conditions assumptions

The difference between the concentrations of nitrosamines and nitramines from the majority of the runs given in this report, and those generated by approximating the modelled ambient conditions reported by Tel-Tek, demonstrate the importance of understanding the ambient conditions at the Mongstad site. There is significant difference between the two sets of values.

The fact that the nitrosamine and nitramine concentrations are so sensitive to the ambient conditions is not surprising, as the reactions are inherently dependent on values such as the hydroxyl radical and NO_x concentrations. This issue highlights the importance of understanding and quantifying, through measurement and/or modelling, the conditions at Mongstad: both the general ambient background conditions in the surrounding area, and the effects of local refinery sources.

10.4. Comparison with guideline limits when all schemes are included

The hypothetical ‘MEA’ and ‘DMA’ model runs represent unit emission rates of the hypothetical amines ‘MEA’ and ‘DMA’, so absolute values for comparison with the guideline value for the protection of human health are not appropriate for these runs.

Although the re-modelled Activity 1 runs also involve unit emission rates, it is possible to relate these values to the Scenario 1 emissions profile modelled in Activity 1, by linearly scaling the output concentrations to the emission rates, thus enabling a comparison with the guideline value of 0.3ng/m^3.

For this Scenario 1 comparison, for the run incorporating the full combination of hydroxyl, nitrate and aqueous schemes, the total of the maximum annual average ground level concentrations of the sum of nitramines and nitrosamines, from the three amines and directly emitted NDMA, is 0.11ng/m^3.