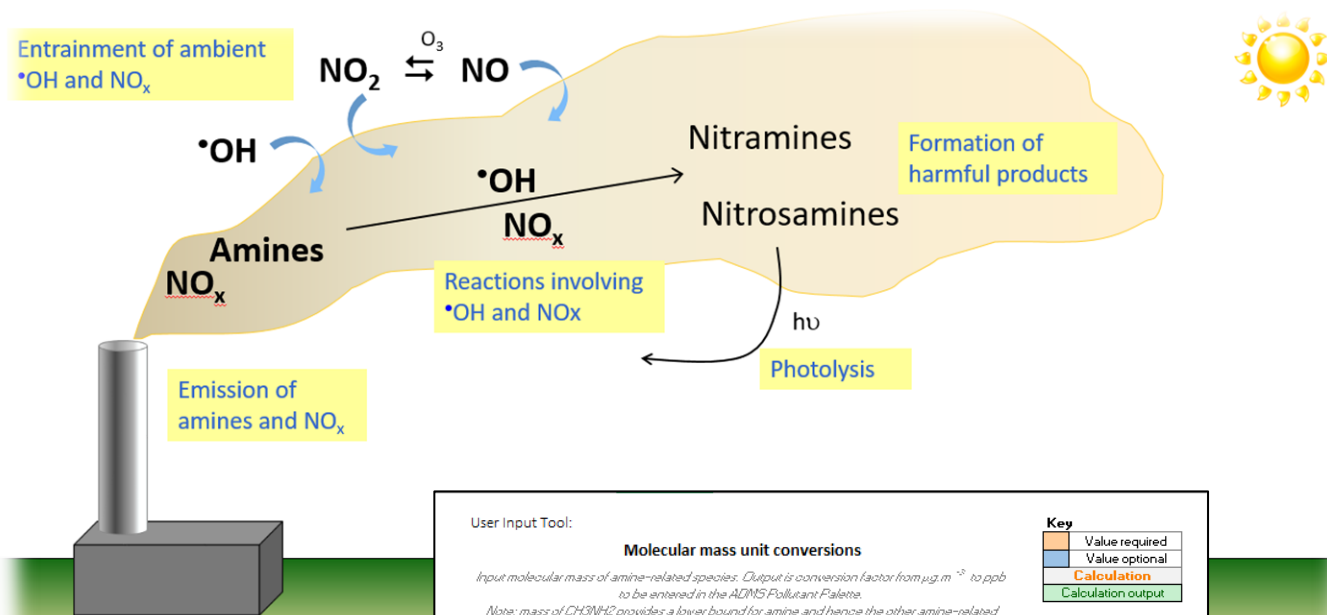


Amine Chemistry User Input Tool



User Input Tool:

Molecular mass unit conversions

Input molecular mass of amine-related species. Output is conversion factor from $\mu\text{g}\cdot\text{m}^{-3}$ to ppb to be entered in the ADMS Pollutant Palette.

Note: mass of CH_3NH_2 provides a lower bound for amine and hence the other amine-related

Amine-related species	Relative molecular mass INPUT	Relative molecular mass calculated from amine	Conversion factor $\mu\text{g}\cdot\text{m}^{-3}$ to ppb
Amine	31	31.0	0.776
Nitramine	90	76.0	0.267
Nitrosamine		60.0	0.401
Radical		30.0	0.802

Constants

Molar volume at 293.15 K and 101.3 kPa (L)	24.06	Relative molecular mass simplest amine (CH_3NH_2)	31.0
--	-------	---	------

Key

- Value required
- Value optional
- Calculation
- Calculation output

CERC

New Pollutants Palette Sheet Delete additional Pollutants Palette Sheet Clear Contents

User Guide

CERC

ADMS

Amine Chemistry User Input Tool

User Guide

Version 1.1

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SECTION 1 Introduction

ADMS 6 contains an amine chemistry module which models the resulting emissions from amine-based carbon capture. The amines released during the carbon capture process may undergo a series of reactions with other species in the exhaust gas and atmosphere which result in the formation of potentially harmful products, such as nitramines and nitrosamines.

The Amine Chemistry User Input Tool, henceforth referred to as the User Input Tool or simply the Tool for brevity, can be used to calculate various input parameters to the amine chemistry module.

In this section, the main features of the User Input Tool are given and computational requirements are provided. Section 2 describes how to use the User Input Tool. Section 3 provides technical details. References are given in Section 4.

Details of the amine reaction scheme and using the ADMS amine chemistry module can be found in the ADMS 6 Amine Chemistry Supplement.

1.1 About User Input Tool

The User Input Tool generates amine chemistry parameters for use with the ADMS amine chemistry module, including $\mu\text{g}/\text{m}^3$ to ppb conversion factors and reaction rate constants. The User Input Tool runs within Microsoft Excel.

One of the parameters the Tool calculates is derived from hourly time series data, specifically ADMS O_3 background concentration data and ADMS processed incoming solar radiation (K) values.

1.2 Features

The User Input Tool can be used to calculate:

- Amine, nitramine, nitrosamine and radical $\mu\text{g}/\text{m}^3$ to ppb conversion factors for input into the **ADMS Palette of Pollutants**
- Reaction rate constants and other parameters for input into the **Amine species** screen of the **Additional Input file editor**
- The **Constant for OH concentration calculations** for input into the **Amine chemistry** screen of the **Additional Input file editor**

Values are calculated within the spreadsheet tool, and require copying across to the appropriate sections of the ADMS interface/ **Additional Input file editor**.

1.3 Requirements

The User Input Tool is supported on:

- Microsoft Excel 2016 or 2019,

but may work with older or newer versions. Microsoft Excel macros included within the tool may require enabling prior to running the tool depending on your security settings. Within Excel select **File**, then **Options**, then **Trust Center** and open **Trust Center Settings**. From there, select **Macro Settings** and choose either **Disable all macros with notification** or **Enable all macros**, click **OK**. Then close and reopen the Tool. If you selected **Disable all macros with notification**, you should see a security warning – click **Enable Content**.

1.4 About this user guide

This *User Input Tool User Guide* is a manual describing how to use the User Input Tool.

To make this manual simpler to use, certain conventions have been followed with regard to layout and style.

- Non-editable text on the worksheets are shown in **Arial** font, e.g. ‘enter values in the **Molecular mass INPUT column**’
- Buttons that initiate macros are shown in **bold**, e.g. press **Calculate**
- Directory and file names are shown in *italics*, e.g. *.*bgd*.
- Table and figure references are shown in **bold**, e.g. see **Figure 1**
- Notes are shown *italics* with lines and above and below:

e.g. Here is a Note.

SECTION 2 Using the User Input Tool

This section describes the inputs required and steps needed to use the User Input Tool to obtain outputs ready for entering in the ADMS amine chemistry module. The key outputs are conversion factors, reaction constants converted to necessary units and the OH concentration constant.

The Tool is colour coded to highlight inputs, outputs and non-editable sections, described at the beginning of Section 2.1.

From input molecular mass for amine related species, the Tool outputs conversion factors, this is described in Section 2.2.1.

From input reaction constants in units of $\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$, the Tool outputs reaction constants in units of $\text{ppb}^{-1} \cdot \text{s}^{-1}$, this is described in Section 2.2.2.

From input files containing hourly O₃ concentrations and hourly incoming solar radiation data, with a value for annual average hydroxyl radical concentration, the Tool outputs the OH concentration constant, this is described in Section 2.3.

In the process of calculating the OH concentration constant a data table is generated with all of the valid data used. After calculating the OH concentration constant a second data table is generated using this value to predict hourly OH concentration. These data tables are described in Section 2.4.

2.1 Getting started

Make a copy of the Amine Chemistry User Input Tool and save it in a working directory e.g. alongside the current working ADMS amine chemistry *.apl file. Open the spreadsheet.

Refer to the **Cover** page, this contains version details and a **Summary of Tool**.

The Tool is colour coded for sheet tabs and cells, as shown in **Figure 1** (a) and (b), respectively, below. Sheet tabs are coloured:

- Yellow for **Cover** sheet
- Green for active sheets (**Pollutants_palette**, **Kinetics-AMINE** and **c_calculation**) which require input and contain the output values
- Blue for data tables (**Data_table1** and **Data_table2**) which display the data used in the calculations and should not be changed.

Cells are coloured:

- Orange flag for cells which require input values for calculations
- Blue flag for cells where an input value may be entered if known, else it will be calculated by the Tool

- Orange text on grey for intermediate values calculated by the tool
- Green for calculation output values for input into the ADMS amine chemistry module
- Grey for constant values used in the calculations

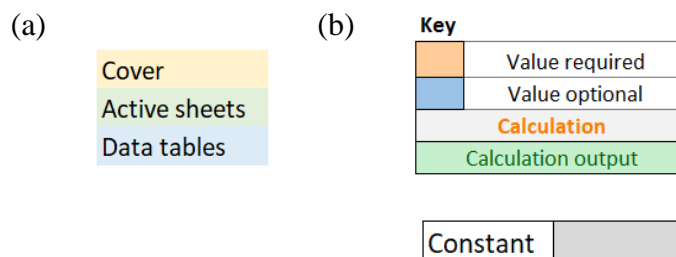


Figure 1 Colour codes used for (a) sheet tabs and (b) cells within the sheets.

2.2 Molecular mass and kinetics unit conversions

Sheet **Pollutants_palette** calculates $\mu\text{g.m}^{-3}$ to ppb conversion factors and requires inputs of relative molecular mass of amine and (if known) of the related species. Sheet **Kinetics-AMINE** calculates reaction constants in units of $\text{ppb}^{-1}.\text{s}^{-1}$ and requires inputs of reaction constants in units of $\text{cm}^3.\text{molecule}^{-1}.\text{s}^{-1}$.

These two sheets have three buttons, an example is shown in Figure 2: to create a copy of the sheet, to delete the sheet and to clear the contents of the sheet. To repeat the process for additional amine species, a copy of each of these sheets can be created by clicking the **New Pollutants Palette/Kinetics-AMINE Sheet** button, a pop-up will appear requiring a unique identifier for the new sheet tab. If the new sheet is no longer required click **Delete additional Pollutants Palette/Kinetics-AMINE Sheet** button, note that the original sheet cannot be deleted. To clear all user in inputs in the active sheet, click the **Clear Contents** button.

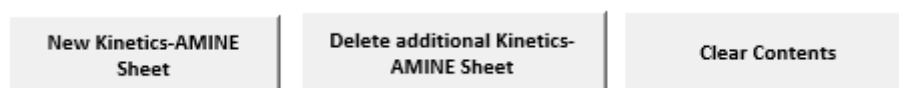


Figure 2 Screenshot of the buttons available on sheet **Kinetics-AMINE**, to make a copy or delete the sheet and to clear the user input data from that sheet.

2.2.1 Conversion factors

As can be seen in **Figure 3**, in the **Relative molecular mass INPUT** column, the value for the **Amine** is required. From this value, the **Relative molecular mass calculated from amine** of the amine-related species (**Nitramine**, **Nitrosamine** and **Radical**) are calculated by the Tool. **Conversion factor** is then calculated for each. However, the molecular mass for each of the amine-related species may also be input if known. These input mass values will take precedence over the automatically calculated mass and will be used to calculate the **Conversion factor**, indicated by a strikethrough and greying out of the calculated value. Calculation output values (green cells) are ready for input into the ADMS **Palette of Pollutants**.

Amine-related species	Relative molecular mass INPUT	Relative molecular mass calculated from amine	Conversion factor $\mu\text{g}\cdot\text{m}^{-3}$ to ppb
Amine			
Nitramine			
Nitrosamine			
Radical			

Constants

Molar volume at 293.15 K and 101.3 kPa (L)	24.06	Relative molecular mass simplest amine (CH ₃ NH ₂)	31.0
--	-------	---	------

Figure 3 Screenshot of sheet **Pollutants_palette**, required and optional molecular mass inputs, calculation of molecular mass from amine input mass and output conversion factors.

The calculations performed by the Tool for **Relative molecular mass calculated from amine** and **Conversion factor** are described in Section 3.1.

2.2.2 Reaction constants

As can be seen in **Figure 4**, in the **INPUT** column, values are required for the reaction rate parameters, in units of $\text{cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$, and ratio parameters, which are dimensionless.

*Input values must be plain numbers, scientific format or entered as a formula e.g. 3.88×10^{-13} may be entered as “3.88E-13”, “=3.88*10^-13” or “0.000000000000388”*

Amine chemistry parameters	Symbol	INPUT	Input Units	Output	Output Units
Amine/OH reaction rate	k1		$\text{cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$		$\text{ppb}^2\cdot\text{s}^{-1}$
Amino radical/O ₂ reaction rate	k2		$\text{cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$		$\text{ppb}^2\cdot\text{s}^{-1}$
Rate of formation of nitrosamine	k3		$\text{cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$		$\text{ppb}^2\cdot\text{s}^{-1}$
Rate of formation of nitramine	k4a	3.18E-13	$\text{cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$	7.95E-03	$\text{ppb}^2\cdot\text{s}^{-1}$
Amino radical/NO ₂ reaction rate	k4	3.88E-13	$\text{cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$	9.70E-03	$\text{ppb}^2\cdot\text{s}^{-1}$
Branching ratio for amine/OH	Branching		dimensionless		dimensionless
Ratio of J(nitrosamine) to J(NO ₂)	$J_{\text{J}}/J_{\text{NO}_2}$		dimensionless		dimensionless

Constants

Units conversion factor	2.50E+10
-------------------------	----------

Other parameters:

Symbol	INPUT	Input Units
k4b		$\text{cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$

Figure 4 Screenshot of sheet **Kinetics-AMINE**, required and optional Amine chemistry parameters inputs (orange and blue flags, respectively) and outputs (green).

The exception is that only two of the parameters **k4**, **k4a** and **k4b** are required, as the third can be calculated by the Tool. If all three values are entered, the Tool will check that they are consistent. The tool converts the reaction rate parameters to units of $\text{ppb}^{-1}\cdot\text{s}^{-1}$ or

leaves ratios as dimensionless in the **Output** column. Calculation output values are ready for input into the **Amine species** screen of the **Additional Input file editor**.

The conversion calculations performed by the tool are described in Section 3.2.

2.3 Constant for OH concentration calculations

Sheet **c_calculation** requires four inputs, as shown in **Figure 5**:

- Step 1** **Browse** to ADMS background **.bgd* file path which contains hourly O₃ concentrations.
- Step 2** **Browse** to ADMS meteorological **.mop* file path which contains hourly values of incoming solar radiation (K) in W.m⁻².
- Step 3** Input annual average hydroxyl radical concentration, **[OH] value**.
- Step 4** Select **[OH] units** from the dropdown list.

*Details on the format of *.bgd and *.mop files can be found in the main ADMS 6 User Guide*

The screenshot shows a window titled "Inputs" with the following elements:

- Two text input fields for ".bgd path:" and ".mop path:", each with a "Browse" button to its right.
- A text input field for "[OH] value:".
- A dropdown menu for "[OH] units:" with "molecules.cm-3" selected. The dropdown list shows "molecules.cm-3", "µg.m-3", and "ppb".
- A "Calculate" button centered at the bottom of the input area.

Figure 5 Screenshot of sheet **c_calculation (Inputs)**, requires input file paths to a **.bgd* file, a **.mop* file, an annual average value of [OH] and selection of the units of [OH].

When all four inputs are ready, click the **Calculate** button, this will populate the **Outputs** section, shown in **Figure 6**. The **Constant for OH concentration calculations, c** is ready for input into the **Amine chemistry** screen of the **Additional Input file editor**. Displayed above this are additional intermediate calculations, such as time data and the parameter used to calculate **c**.

Outputs		
Start date		
End date		
Num hours included		
Parameter	Symbol	
Average of ozone concentration (ppb) × photochemical rate constant for NO ₂ photolysis	O ₃ × J(NO ₂) (ppb.s ⁻¹)	
Constant for OH concentration calculations	c (s)	
Constants		
J(NO ₂) constant 1	8.00E-04	J(NO ₂) constant 2
Conversion factor	2.50E+10	Relative molecular mass OH
Molar volume at 293.15 K and 101.3 kPa (L)	24.06	7.40E-06

Figure 6 Screenshot of sheet **c_calculation** (Outputs).

The **Calculate** button will also populate sheet **Data_table1** and **Data_table2**. The **Clear Contents** button will clear user inputs on this sheet and data in the data tables. Details on the inputs are given in Sections 2.3.1, 2.3.2 and 2.3.3 and on the outputs in Section 2.3.4.

2.3.1 O₃ hourly concentration file

The file should be in *.bgd format as described in ADMS 6 User Guide. An example is shown in **Figure 7**. The file should contain hourly O₃ concentration in .csv format, missing data should be identified with the value '-999'. Key features are: version on line one, number of pollutants on line two followed by the pollutant names, "UNITS:" followed by the units for each pollutant listed and "DATA:" followed by the hourly background data.

```

background.bgd - Notepad
File Edit Format View Help
BACKGROUNDVERSION2
3
NOx
NO2
O3

UNITS:
ug/m3
ppb
ug/m3

*****
Comments may be added here.
*****

DATA:
2019,1,1,8.26719,7.09445,61.99975
2019,1,2,-999,-999,59.871
2019,1,3,8.74534,7.77319,58.77337
2019,1,4,11.29027,9.53115,55.03143
2019,1,5,11.61418,9.39212,52.38713
2019,1,6,14.57556,12.16834,47.74712
2019,1,7,21.42376,19.8961,38.26755
2019,1,8,24.2926,21.0984,33.32819
2019,1,9,25.35684,16.56123,43.10712
2019,1,10,20.17442,14.98964,44.70368
2019,1,11,20.20427,16.77703,42.17703

```

Figure 7 ADMS format *.bgd file containing O₃ concentration data.

The extraction of the hourly O₃ data and calculations involving the O₃ values are described in Section 3.3.2.

2.3.2 Hourly solar irradiance file

The file should be in ADMS processed *.*mop* format as described in the ADMS 6 User Guide. This file should contain processed hourly solar irradiance K (W.m⁻²) data in column 43, missing data will be identified with the value '-999'.

The extraction of the hourly K data and calculations involving the K values are described in Section 3.3.2.

2.3.3 [OH] value: annual average hydroxyl radical concentration

[OH] value can be taken from local data or a regional average from the literature. [OH] units are required to be selected from the dropdown list: molecules.cm⁻³, µg/m³, ppb. Typically, literature values are given in molecules.cm⁻³.

Conversion from molecules.cm⁻³ or µg/m³ to ppb and calculations involving the [OH] value are described in Section 3.3.2.

2.3.4 Outputs

As shown in Figure 6, the associated time data, **Start date**, **End date** and the **Num hours included** in the calculation are displayed in **Outputs**. Below these, the **Average of ozone concentration × photochemical rate constant for NO₂ photolysis** is displayed, from which the **Constant for OH concentration calculations, c** is calculated and output. **c** is ready for input into the **Amine chemistry** screen of the **Additional Input file editor**

Calculations performed to obtain the time data, averages and **c** value are described in Sections 3.3.1 and 3.3.2.

2.4 Data tables

Sheets **Data_table1** and **Data_table2** contain tables which display calculated output data, so that the data can be extracted and analysed outside of the Tool. Sheet **Data_table1** contains the time calculations to obtain **Average O₃ × J(NO₂)** alongside time data. Sheet **Data_table2** contains calculated hourly OH concentrations, **OH_calc**.

An example of a populated sheet **Data_table1** is shown in **Figure 8**. **Data_table1** contains all valid hourly data for K and O₃, provided in the input *.bgd and *.mop files, conversion of O₃ to ppb is performed, if required. The Tool calculates **J(NO₂)** and **O₃ × J(NO₂)**. Beside the main data table are the **Average O₃ × J(NO₂)** and **Time data**.

OUTPUT DATA										Average O ₃ (ppb) ×		Time data			Number of hours of data:		
All hours of valid data for K and O ₃										O ₃ × J(NO ₂) average		Start time:			End time:		Hours recorded
TYEAR	TDAY	THOUR	K	O ₃	O ₃ _unit	O ₃ _ppb	J(NO ₂)	O ₃ _ppb × J(NO ₂)	O ₃ _ppb × J(NO ₂) average	TYEAR	TDAY	THOUR	TYEAR	TDAY	THOUR	Hours recorded	
2019	1	1	0	62.13279	ugm3	31.14406099	0	0	0.037862815	2019	1	1	2019	364	17	707	
2019	1	2	0	59.34096	ugm3	29.2434062	0	0									
2019	1	13	219.748	63.81251	ugm3	31.98602064	0.002390546	0.076464047									
2019	1	14	96.0097	61.2181	ugm3	30.68557263	0.004313339	0.043321471									

Figure 8 Example of populated sheet **Data_table1**.

An example of a populated sheet **Data_table2** is shown in **Figure 9**. **Data_table2** is populated from sheet **Data_table1** and the calculated **c** value on sheet **c_calculation**. It displays the **O₃_ppb** data and **OH_calc** values, also in ppb.

TYEAR	TDAY	THOUR	O ₃ _ppb	OH_calc
2019	1	1	31.14406099	0
2019	1	2	29.2434062	0
2019	1	13	31.98602064	6.05851E-05
2019	1	14	30.68557263	3.48005E-05
2019	1	15	28.65987601	2.92925E-05
2019	1	16	25.73386423	4.36035E-06

Figure 9 Example of populated sheet **Data_table2**.

Calculations performed to convert O₃ units, calculate **J(NO₂)**, **c** and **OH_calc** are described in 3.3.2.

SECTION 3 Technical Summary

This section contains the formulas used and technical details of how calculations are performed.

Calculations performed on sheet **Pollutants_palette** are described in Section 3.1, detailing conversion factors and molecular mass calculations of amine-related species.

Calculations performed on sheet **Kinetics-AMINE** are described in Section 3.2, detailing calculation of reaction constants.

Calculations performed involving sheet **c_calculation** are described in Section 3.3. This section describes the relationships between the outputs on sheet **c_calculation**, which are calculated from the data in **Data_table1**, and the output of **c_calculation**, which is used to populate **Data_table2**.

3.1 Calculation of conversion factors

The ADMS amine chemistry module has been developed to follow a general reaction scheme for a variety of different amines, this includes primary, secondary and tertiary amines. This may also include amines with other functional groups, if the general reaction scheme is similar. To achieve this, the new pollutants must be added to the **Palette of Pollutants** which requires entering the relevant generic **Pollutant name** of the amine-related species name and the **Conversion factor $\mu\text{g}/\text{m}^3 \rightarrow \text{ppb}$** . This step calculates each of the necessary conversion factors from the **Molecular mass INPUT, M**, of the amine-related species. It also provides generic **Relative molecular mass calculated from amine** values for each of the amine-related species.

Details on the general reaction scheme and amine chemistry involved can be found in the ADMS Amine Chemistry Supplement.

The Tool calculates the conversion factor from $\mu\text{g}/\text{m}^3$ to ppb using the equation:

$$1 \text{ ppb} = \frac{(1 \mu\text{g}/\text{m}^3 \times 24.06)}{M} \quad (1)$$

where the constant 24.06 is the volume constant (L) derived from the Ideal Gas equation for 1 mole at temperature $T = 20 \text{ }^\circ\text{C}$ ($= 293.15 \text{ K}$) and pressure $P = 1013 \text{ mb}$ ($= 101.3 \text{ kPa}$).

From the molecular mass of **Amine**, suitable values for the molecular mass of **Nitramine**, **Nitrosamine** and **Radical** can be calculated.

$$\begin{aligned} M_{\text{nitramine}} &= M_{\text{amine}} + 45, \\ M_{\text{nitrosamine}} &= M_{\text{amine}} + 29, \\ M_{\text{radical}} &= M_{\text{amine}} - 1. \end{aligned} \quad (2)$$

These values are obtained based on the assumption that the starting **Amine** substitutes a hydrogen atom for NO_2 to produce the nitramine, $\text{N}=\text{O}$ to produce nitrosamine or is lost to produce the radical. An example, using the simplest amine, methylamine, is shown in **Figure 10**.

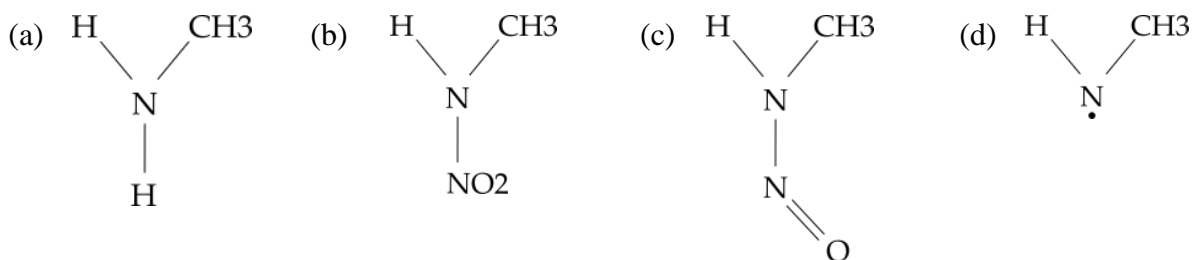


Figure 10 Chemical structures for (a) methylamine ($M = 31$), (b) methylnitramine ($M = 76$) (c) methylnitrosamine ($M = 60$) and (d) methylamine radical ($M = 30$).

As methylamine is the simplest amine, this sets the minimum allowed **Molecular mass INPUT** of **Amine** as the **Molecular mass methylamine** (CH_3NH_2), 31.0. Hence, this also sets the minimum allowed **Molecular mass INPUT** for the other amine-related species using Equation (2).

3.2 Calculation of reaction constants

The reaction rates and kinetic parameters involved in the steps of the generic amine reaction scheme must be defined. These values in literature are typically provided in units of $\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$, however, the ADMS amine chemistry module requires units of $\text{ppb}^{-1} \cdot \text{s}^{-1}$. The Tool converts from $\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ to $\text{ppb}^{-1} \cdot \text{s}^{-1}$ using equation:

$$k_x (\text{ppb}^{-1} \cdot \text{s}^{-1}) = k_x (\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}) \times 2.5 \times 10^{10}, \quad (3)$$

where the constant 2.5×10^{10} is defined as the **Units conversion factor**.

The reaction constants **k4**, **k4a** and **k4b** are related by:

$$k4 = k4a + k4b, \quad (4)$$

hence, **INPUT** requires only two of the three **k4** values to be entered and the third is calculated by the Tool and blue flagged as an optional input, as shown in Section 2.2.2, **Figure 4**. If the third value is also known and is entered the Tool checks whether Equation (4) is satisfied.

The dimensionless values for **Branching ratio for amine/OH** and **Ratio of J(nitrosamine) to J(NO₂)** do not require conversion and are simply copied across to the **Output** column.

3.3 Calculation of constant for OH concentration calculations

The ADMS amine chemistry module requires input of **Constant for OH concentration calculations** (c). On sheet **c_calculation**, the result **Average O₃ ppb × J(NO₂)** is displayed and used alongside the input **[OH] value** to calculate **c**. A table containing the calculation steps is displayed in sheet **Data_table1**, the main table is populated from the provided O₃ and K data and the intermediate calculations to find **Average O₃ ppb × J(NO₂)**. The extracted time data is also displayed in **Data_table1**. An example was shown in Section 2.4, **Figure 8**. From **c**, **J(NO₂)** and **O₃ ppb**, hourly predicted values for OH can be calculated (**OH_calc**), these are displayed in sheet **Data_table2**.

3.3.1 Equations used in calculations

The NO₂ photolysis rate coefficient, **J(NO2)**, is calculated using the hourly solar irradiance from the *.mop file, using the equation [1]:

$$J(NO_2) = 8 \times 10^{-4} \exp\left(\frac{-10}{K}\right) + 7.4 \times 10^{-6} K, \quad (5)$$

where the constants are labelled **J(NO2) constant 1** = 8×10^{-4} and **(JNO2) constant 2** = 7.4×10^{-6} .

The **Constant for OH concentration calculations** is calculated using the equation [2]:

$$c = [OH] / \overline{[O_3] \times J(NO_2)} \quad (6)$$

where, [OH] is **[OH] value** and $\overline{[O_3] \times J(NO_2)}$ is the calculation output **Average O3_ppb** × **J(NO2)**. The Tool reads in the selected **[OH] units** and **[OH] value** is converted from molecules.cm⁻³ to ppb using the conversion factor in Equation (3) or from μg/m³ to ppb using Equation (1), or remains unchanged if ppb is selected.

3.3.2 Calculations performed in Data_table1

From the input *.bgd and *.mop files, only hours which contain both valid data for O₃ and valid data for K are kept. The remaining valid data is used to calculate the **Start time** from taking the first line of data and **End time** from taking the last line of data. **Number of hours of data** is calculated by counting the number of rows of data.

For the valid data set, the Tool extracts **O3_units** from the *.bgd file and converts from input ng.m⁻³/μg.m⁻³/mg.m⁻³/g.m⁻³ to ppb using appropriate powers of 10 with Equation (1), where $M_{O_3} = 48.0$, or if units are ppb or ppm, copies data across with appropriate powers of 10, this yields column **O3_ppb**.

From the valid data set, **J(NO2)** is calculated using Equation (5) for each hour of column **K** data. Column **O3_ppb*J(NO2)** (ppb.s⁻¹) is obtained from the multiplication at each hour of the columns **O3_ppb** and **J(NO2)**. **Average O3 (ppb) × J(NO2)** is then obtained by taking the mean of this column, this value is used in Equation (6) to calculate **c**.

3.3.3 Calculations performed in Data_table2

From the calculated **Constant for OH concentration calculations, c** and rearranging Equation (6) for **[OH]**, the expected value for OH, **OH_calc**, at each hour can be calculated. The results of this calculation are displayed in **Data_table2** alongside the **O3_ppb** column used to calculate it. The daily expected value for [OH] can be plotted.

SECTION 4 References

- [1] CERC, “NO_x Chemistry Model in ADMS 5,” [Online]. Available: https://www.cerc.co.uk/environmental-software/assets/data/doc_techspeg/P18_02.pdf.
- [2] CERC, “ADMS 5 Amine chemistry User Guide Supplement,” [Online]. Available: http://www.cerc.co.uk/environmental-software/assets/data/doc_userguides/CERC_ADMS_5_2_Amine_chemistry_supplement.pdf.

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