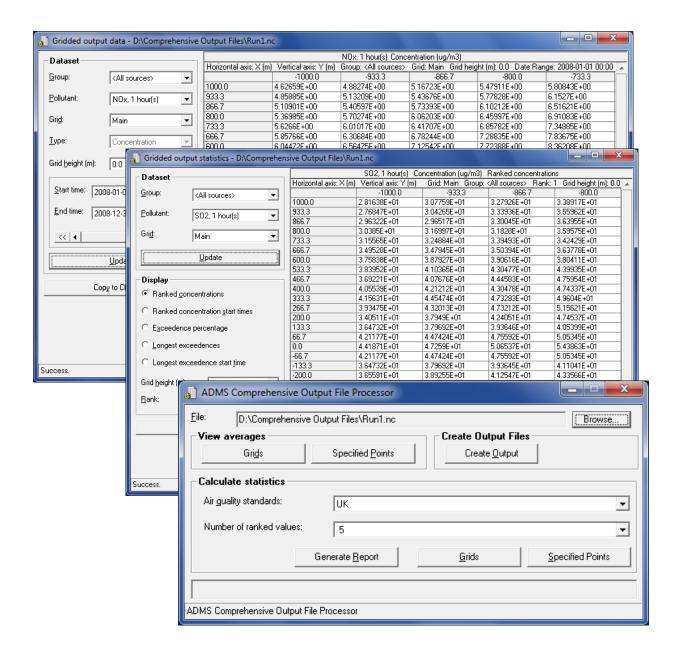


# **ADMS Comprehensive Output File Processor**



User Guide

**CERC** 

# ADMS Comprehensive Output File Processor

## **User Guide**

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# **Contents**

SECTION 1		Introduction	4
1.1	About the ADMS Comprehensive Output File Processor		
1.2	Featur	es	4
1.3	About this user guide		
SECTION 2		Using the ADMS Comprehensive Output File Processor	6
2.1	Startin	g the ADMS Comprehensive Output File Processor	6
2.2	Main Screen		
	2.2.1	File	7
	2.2.2	View averages	7
	2.2.3	Create output files	7
	2.2.4	Calculate statistics	8
2.3	View Averages		
	2.3.1	Grids	9
	2.3.2	Specified Points	12
2.4	Create Output Files		
	2.4.1	Output options	15
	2.4.2	Met. period	16
	2.4.3	Pollutant output	17
	2.4.4	Temporal subsets	23
	2.4.5	Create Files	24
	2.4.6	Saving pollutant outputs	25
2.5	Calculate Statistics		
	2.5.1	Grids	27
	2.5.2	Specified Points	30
	2.5.3	Generating Reports	32
2.6	Creatin	ng and adding new air quality standards sets	34

## **SECTION 1** Introduction

# 1.1 About the ADMS Comprehensive Output File Processor

The ADMS Comprehensive Output File Processor is a tool for viewing and analysing output from ADMS model runs. Its main purpose is to enable easy comparison of model output to air quality standards. Average concentration and deposition values can be viewed as can details of any exceedences of air quality standards.

The ADMS Comprehensive Output File Processor can be used with the comprehensive output files generated by ADMS, ADMS-Urban, ADMS-EIA, ADMS-Roads, ADMS-Airport, and the ADMS-Urban RML system. Comprehensive output files can only be processed if the meteorological data used in the model contains year/day/hour.

#### 1.2 Features

The ADMS Comprehensive Output File Processor can be used to:

- calculate average pollutant concentrations for any averaging period;
- calculate average pollutant deposition;
- output the average pollutant concentrations and depositions to ADMS format output files:
- calculate percentiles of average pollutant concentrations and depositions;
- display maximum concentrations at each grid point or specified point;
- display the time at which the maximum concentrations occurred;
- calculate average, minimum and maximum concentrations for temporal subsets, e.g. the 'working day';
- provide details of any exceedences of air quality standards including:
  - the time of occurrence of the initial exceedence, and
  - the length of time of the longest continuous exceedence;
- determine what percentage of meteorological conditions lead to an exceedence of an air quality standard;
- generate a summary report including details of:
  - the highest concentrations recorded at each specified point,
  - the location and time of the highest concentration across the entire grid,
  - the number of exceedences of the air quality standard.

Note also that:

- various air quality standards are already included in the processor;
- it is possible to create and enter new air quality standard files;
- the concentrations can be ranked into the first, second, third highest concentrations etc. and these can be displayed in the grid viewer.

### 1.3 About this user guide

This *ADMS Comprehensive Output File Processor User Guide* is a manual describing how to use the ADMS Comprehensive Output File Processor, including a section on how to create new files of air quality standards.

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

- ADMS Comprehensive Output File Processor interface controls are shown in **Arial** font, e.g. click on **Generate Report**.
- Keyboard inputs are shown in **bold**, e.g. press **Enter**.
- Directory and file names are shown in *italics*, e.g. \*.nc.
- Table and figure references are shown in **bold**, e.g. see **Figure 3.1**
- The term 'ADMS model' is used to refer to any one of the following: ADMS, ADMS-Urban, ADMS-EIA, ADMS-Roads, ADMS-Airport and ADMS-Urban RML

# SECTION 2 Using the ADMS Comprehensive Output File Processor

There are four main sections of the ADMS Comprehensive Output File Processor: the main screen which appears on starting the processor, the View Averages screen, the Create Output Files screen and the Calculate Statistics screen. Each of these is discussed in full below. Section 2.2 explains the features of the main screen of the processor. Then in Section 2.3 the View Averages part of the processor is described including details of how to view the average pollutant concentrations and deposition values at output grid points or specified output points. Then in Section 2.4 the Create output files part of the processor, where averages can be calculated and output to files, is explained. Next in Section 2.5 the Calculate Statistics feature and its use in comparing pollutant concentrations to particular air quality standards is discussed. In Section 2.5.3 the Generate Report feature of the processor is presented in which the method of generating reports and the report contents are described.

# 2.1 Starting the ADMS Comprehensive Output File Processor

To start the ADMS Comprehensive Output File Processor first click on the **Results** menu in ADMS, ADMS-Urban, ADMS-EIA, ADMS-Roads or ADMS-Airport. Then click on **Process comprehensive output**. The ADMS Comprehensive Output File Processor will then load and the main screen will be displayed, see **Figure 2.1**. If using ADMS-Urban RML, the ADMS Comprehensive Output File Processor is launched by first clicking on the **Results** menu, then clicking **Extract statistics...**.

#### 2.2 Main Screen

The main screen, shown in **Figure 2.1**, appears on starting the processor. Each of the features and buttons are described below.

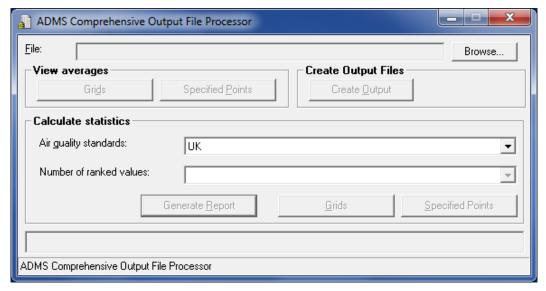


Figure 2.1 - The main screen

#### 2.2.1 File

The first step is to select the netCDF output file that is to be analysed using the processor. Click **Browse**..., navigate to the required file and click **Open**. The netCDF file is the .nc comprehensive output file that has been created by running the ADMS model with the **Comprehensive output file** option selected. After a file has been selected, the available processing options, e.g. the **Grids**, **Specified Points** and **Generate Report** buttons, are enabled.

#### 2.2.2 View averages

Click on either **Grids** or **Specified Points** in the **View Averages** box to display a table showing the average values of concentration, dry deposition or wet deposition at either grid points or specified output points respectively. The length of the averaging period can be changed as required. This is discussed further in Section 2.3.

#### 2.2.3 Create output files

Click **Create Output** to open up a screen that allows average values and statistics of concentration, dry deposition, wet deposition or total deposition data to be output to ADMS format output files. Data from multiple pollutants, different short- and long-term averaging times, and statistics such as percentiles and counts of exceedences may be output. Temporal subsets can also be used to only calculate statistics over certain hours of the day, days of the week and/or months of the year. The creation of these output files is discussed further in Section 2.4.

#### 2.2.4 Calculate statistics

In order to calculate pollutant statistics or compare the pollutant concentrations to a set of air quality standards, an option from each of the following drop-down lists must be selected.

#### Air quality standards

It is possible to use the processor to calculate statistics and compare concentrations to specific air quality standards. To do this the **Air quality standards** must be chosen using the drop-down list. User-defined air quality standards can be included; these will then appear alongside the default standards in the **Air quality standards** list. See Section 2.6 for further details on adding new air quality standards sets.

Default air quality standards sets are provided for a variety of national air quality objectives.

#### Number of ranked values

After the air quality standard has been selected, the **Number of ranked values** must be specified. This is the total number of ranked concentrations (i.e. first-highest concentrations, second-highest concentrations, etc.) that will be available for display in the viewer and used in the report. The minimum **Number of ranked values** is 1 and the maximum is 10.

Once the comprehensive output file has been specified and the air quality standard has been selected, then **Grids**, **Specified Points**, or **Generate Report** may be clicked – these options are described in Section 2.5.

#### 2.3 View Averages

Once a comprehensive output file has been selected in the main screen, a table can be displayed showing the average values of concentration, dry deposition or wet deposition at each grid point or at each specified point. The former is generated by clicking on **Grids** in the **View Averages** box and the latter is generated by clicking on **Specified Points** in the same box. Each option leads to a new screen where there are further options; these are described in Sections 2.3.1 and 2.3.2 respectively.

#### 2.3.1 Grids

After clicking on the **Grids** option under the **View Averages** section of the output processor, a new screen appears as shown in **Figure 2.2**.

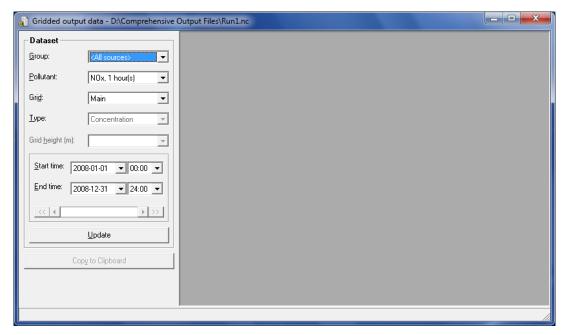


Figure 2.2 – The initial grids screen.

There are several options available on the left hand side of the screen.

#### Group

Select the particular **Group** of sources which should be included when calculating the averages. The options available depend on the groups defined in the ADMS model run that was used to create the comprehensive output file.

#### **Pollutant**

Select the pollutant and averaging time for which the averages should be calculated. The options available depend on the pollutants and averaging times selected in the output tab of the ADMS model run. Only pollutants and averaging time combinations for which long term output is selected in the ADMS model run are available for analysis in the Comprehensive Output File Processor.

#### Grid

Select the **Grid** on which the average concentrations should be calculated:

- The **Main** grid is the regular or variable grid that has been used in the ADMS model run this is always available as an option in the list.
- The Nested (Source Name) grid is a finer grid than the main grid. It is placed around each source or cluster of sources if the Source-oriented grids option for Point, Area, Volume sources has been used in the ADMS model run. If this option has been selected then there may be only one or there may be several nested grids available to choose from. For further details on nested grids please refer to your ADMS model user guide. The (Source Name) part of the grid name is the name of a source associated with each nested grid. For example, if there is a nested grid placed around a source called "Refinery Stack" then in the menu the nested grid option will state Nested (Refinery Stack).

#### Type

Select one of the following options from the **Type** drop-down list:

- **Concentration** the table will then display average concentrations.
- **Dry Deposition** the table will then display average dry deposition flux.
- Wet Deposition the table will then display average wet deposition flux.

The options available from the drop-down list will vary depending on the data in the comprehensive output file.

#### Grid height (m)

This option is disabled until **Update** (see below) has been clicked. It provides a choice of heights at which the average concentrations can be calculated, the options being the different height levels specified for the z-coordinates in the grids section of the ADMS model run. The table will automatically update when the grid height changes.

This option is only available if concentrations are being viewed on the main grid.

#### Start time and End time

These allow the date and time of the beginning and the end of the averaging period to be specified. Clicking on the drop-down arrow next to the start date displays a calendar. The start date can be changed by clicking on another date (provided that date falls within the time period covered by the comprehensive output data), using the arrows to navigate from month to month if necessary. The start hour can also be changed using the drop-down list next to the displayed time. Similarly, the date and time of the last hour may also be changed.

The start time refers to the beginning time of the first hour to be included in the averaging period. The end time refers to the end of the last hour to be included in the averaging period. Therefore to average the first hour of a day, a start time of 00:00 and an end time of 01:00 would be required.

Underneath the **End** date-time there is a scroll bar with two types of forward arrows (a ► symbol and a >> symbol) and two types of backward arrows (a ► symbol and a << symbol). Clicking the single arrows will cause the start and end times to change by one hour, while keeping the length of the averaging period constant; this gives a rolling average. Clicking the double arrows will cause the start and end times to jump by the length of time in the selected averaging period, while keeping the length of the averaging period constant; this gives a non-rolling average. The forward arrows move forwards through time, while the backward arrows move backwards through time.

For example, suppose a comprehensive output file covers the period from January 1<sup>st</sup> at 00:00 to December 31<sup>st</sup> at 24:00 (i.e. a year of data). If a start time of January 1<sup>st</sup> at 00:00 and an end time of January 1<sup>st</sup> at 24:00 is selected (i.e. a length of 1 day), then clicking on >> will change the averaging period to be from January 2<sup>nd</sup> at 00:00 to January 2<sup>nd</sup> at 24:00 (i.e. a discrete jump of length one day in the start and end times). On the other hand clicking ▶ instead will change the averaging period to be from January 1<sup>st</sup> 01:00 to January 2<sup>nd</sup> at 01:00, i.e. the start and end times jump forward by one hour.

Clicking the arrows will only change the times if the new averaging period fits within the date/time range of the data in the comprehensive output file.

#### **Update**

Click **Update** to display the average values in the table to the right of the screen as shown in **Figure 2.3**. Use the scroll bars to navigate around the table of results.

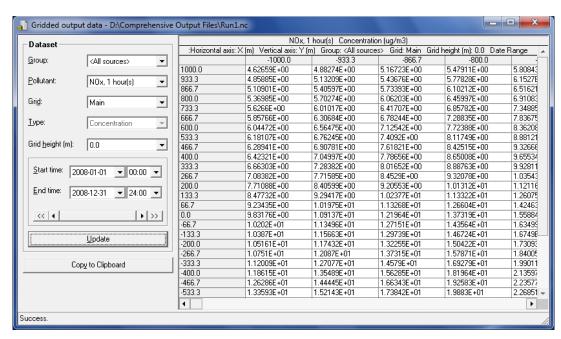


Figure 2.3 – Table of results showing average NO<sub>x</sub> concentrations on the main grid.

**Copy to Clipboard** copies the table so that it can be pasted into another application.

Click the cross in the top right hand corner to close the screen and return to the main screen of the ADMS Comprehensive Output File Processor.

#### 2.3.2 Specified Points

After clicking on **Specified Points** under the **View Averages** section of the main screen, the screen shown in **Figure 2.4** appears.

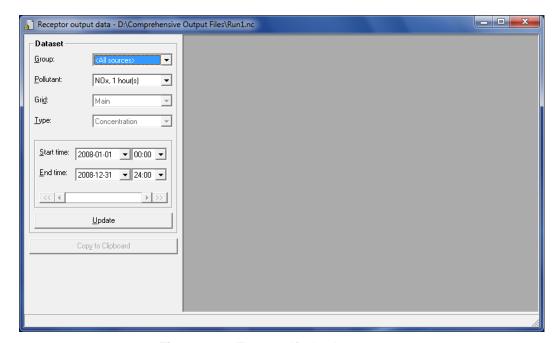


Figure 2.4 – The specified points screen.

The buttons and menus available are as follows.

#### Group

Select the particular **Group** of sources which should be included when calculating the averages. The options available depend on the groups defined in the ADMS model run that was used to create the comprehensive output file.

#### **Pollutant**

Select the pollutant and averaging time for which the averages should be calculated. The options available depend on the pollutants and averaging times selected in the output tab of the ADMS model run. Only pollutants and averaging time combinations for which long term output is selected in the ADMS model run are available for analysis in the Comprehensive Output File Processor.

#### Grid

This option is not available for specified output points and is disabled.

#### Type

From the **Type** drop-down list one of the following options can be selected:

- **Concentration** the table will then display average concentrations.
- **Dry Deposition** the table will then display average dry deposition flux.
- Wet Deposition the table will then display average wet deposition flux.

The options available from the drop-down list will vary depending on the data in the comprehensive output file.

#### Start time and End time

These allow the date and time of the beginning and the end of the averaging period to be specified. Clicking on the drop-down arrow next to the start date displays a calendar. The start date can be changed by clicking on another date (provided that date falls within the time period covered by the comprehensive output data), using the arrows to navigate from month to month if necessary. The start hour can also be changed using the drop-down list next to the displayed time. Similarly, the date and time of the last hour may also be changed.

The start time refers to the beginning time of the first hour to be included in the averaging period. The end time refers to the end time of the last hour to be included in the averaging period. Therefore to average the first hour of a day, a start time of 00:00 and an end time of 01:00 would be required.

Underneath the **End** date-time there is a scroll bar with two types of forward arrows (a ► symbol and a >> symbol) and two types of backward arrows (a ► symbol and a << symbol). Clicking the single arrows will cause the start and end times to change by one hour, while keeping the length of the averaging period constant; this gives a rolling average. Clicking the double arrows will cause the start and end times to jump by the length of time in the selected averaging period, while keeping the length of the averaging period constant; this gives a non-rolling average. The forward arrows move forwards through time, while the backward arrows move backwards through time.

For example, suppose a comprehensive output file covers the period from January 1<sup>st</sup> at 00:00 to December 31<sup>st</sup> at 24:00 (i.e. a year of data). If a start time of January 1<sup>st</sup> at 00:00 and an end time of January 1<sup>st</sup> at 24:00 is selected (i.e. a length of 1 day), then clicking on >> will change the averaging period to be from January 2<sup>nd</sup> at 00:00 to January 2<sup>nd</sup> at 24:00 (i.e. a discrete jump of length one day in the start and end times). On the other hand clicking ▶ instead will change the averaging period to be from January 1<sup>st</sup> 01:00 to January 2<sup>nd</sup> at 01:00, i.e. the start and end times jump forward by one hour.

Clicking the arrows will only change the times if the new averaging period fits within the date/time range of the data in the comprehensive output file.

#### **Update**

Click **Update** to display the average values at each specified point in the table to the right of the screen, as shown in **Figure 2.5**. Use the scroll bars to navigate around the table of results.

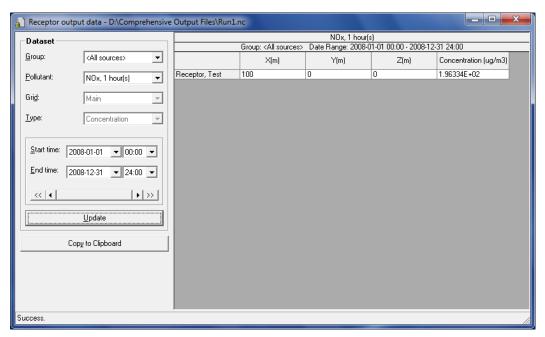


Figure 2.5 – Table of results showing average NO<sub>x</sub> concentrations at the specified points.

**Copy to Clipboard** copies the table so that it can be pasted into another application.

Click the cross in the top right hand corner to close the screen and return to the main screen of the ADMS Comprehensive Output File Processor.

### 2.4 Create Output Files

In addition to being able to view averages, the ADMS Comprehensive Output File Processor includes the option to output average values of concentration or deposition to ADMS format output files. Clicking **Create Output** opens the **Create Output Files** screen, shown in **Figure 2.6**, where the output options are defined. These options are explained below. The output files are text files in the same format as used for output by the ADMS models, i.e. separate specified points files, gridded files and gridded files split up by vertical grid level, for short term and long term outputs.

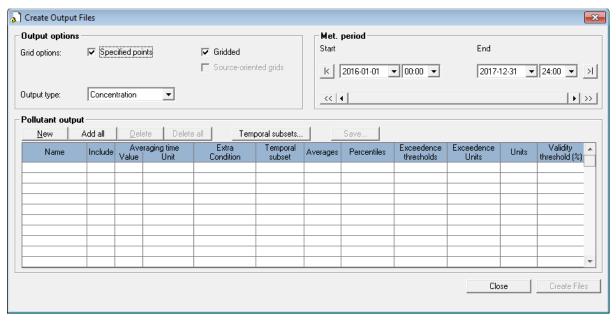


Figure 2.6 - The initial Create Output Files screen.

#### 2.4.1 Output options

The **Output options** section is where the type of data to output is selected. The options available depend on what was included in the ADMS model run.

It is possible to output multiple **Grid options** to files at once, or to output them separately. The **Grid options** to choose between are **Specified points**, **Gridded** points and **Source-oriented grids**. The only restrictions placed on the selection of grid options are that at least one option must be selected to create output files, and that the **Source-oriented grids** option can only be output if the **Gridded** option has also been selected.

Only one **Output type** can be selected for output. The options to choose between can include **Concentration**, **Dry deposition**, **Wet deposition** and **Total deposition**, as shown in **Figure 2.7**, depending on what was included in the original model run. **Total deposition** gives the average of the total (dry plus wet) deposition and as such the comprehensive output file must contain both dry and wet deposition values in order to use this option.

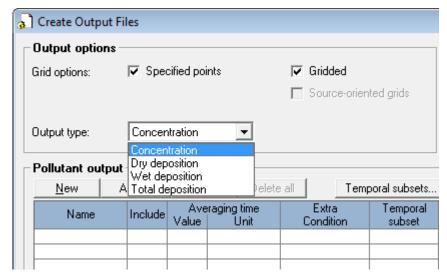


Figure 2.7 – The available Output type options in the Create Output Files screen.

#### 2.4.2 Met. period

The date and time of the beginning and the end of the averaging period can be specified. This allows averages to be calculated over any subset of times in the comprehensive output file.

Clicking on the drop-down arrow next to the **Start** date displays a calendar. The start date can be changed by clicking on another date (provided that date falls within the time period covered by the comprehensive output data), using the arrows to navigate from month to month if necessary. The start hour can also be changed using the drop-down list next to the displayed time. Similarly, the date and time of the **End** hour may also be changed.

The start time refers to the beginning time of the first hour to be included in the averaging period. The end time refers to the end time of the last hour to be included in the averaging period. Therefore to average the first hour of a day, a start time of 00:00 and an end time of 01:00 would be required.

Next to the **Start** time drop-down list there is a button with a |< symbol on it that automatically selects the first date and time in the comprehensive output data as the start date-time for the average calculations. Similarly, there is a button next to the **End** time drop down list, with a > | symbol on it, that automatically selects the last date and time in the comprehensive output data as the end date-time for the averaging period.

Underneath the **End** date-time there is a scroll bar with two types of forward arrows (a ► symbol and a >> symbol) and two types of backward arrows (a ► symbol and a << symbol). Clicking the single arrows will cause the start and end times to change by one hour, while keeping the length of the **Met. period** constant. Clicking the double arrows will cause the start and end times to jump by the length of time in the **Met. period** selected, while keeping the length of the **Met. period** constant. The forward arrows move forwards through time, while the backward arrows move backwards through time.

For example, suppose a comprehensive output file covers the two-year period from January 1<sup>st</sup> 2012 at 00:00 to December 31<sup>st</sup> 2013 at 24:00. If a start time of January 1<sup>st</sup> 2012 at 00:00 and an end time of December 31<sup>st</sup> 2012 at 24:00 is selected (i.e. a length of 1 year), then clicking on >> will change the averaging period to be from January 1<sup>st</sup> 2013 at 00:00 to December 31<sup>st</sup> 2013 at 24:00 (i.e. a discrete jump of length one year in the start and end times). On the other hand clicking ▶ instead will change the averaging period to be from January 1<sup>st</sup> 2012 01:00 to January 1<sup>st</sup> 2013 at 01:00, i.e. the start and end times jump forward by one hour.

Clicking the arrows will only change the times if the new Met. period fits within the date/time range of the data in the comprehensive output file.

#### 2.4.3 Pollutant output

The **Pollutant output** table is where the pollutants and averaging statistics to output can be specified. Each row in the **Pollutant output** table defines a separate pollutant dataset to be output, with their own set of averaging characteristics and statistics, as demonstrated in **Figure 2.8**, for example for comparison with a set of air quality objectives. Up to 30 individual pollutant output datasets may be output at once to the same set of files. Output files can only be created for pollutant datasets with an averaging time of 1 hour in the comprehensive output file (i.e. where an averaging time of 1 hour was selected in the ADMS model interface).

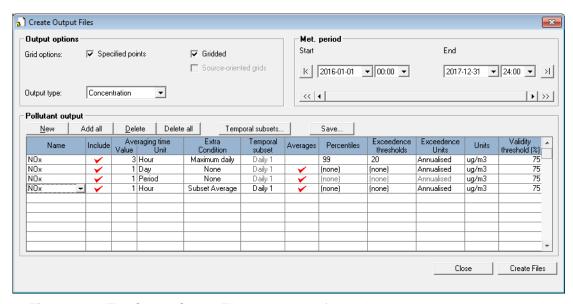


Figure 2.8 – The Create Output Files screen with four pollutant output datasets entered.

Pollutant output datasets can be added to and deleted from the **Pollutant output** table by clicking on the **New** and **Add all**, **Delete** and **Delete all** buttons respectively. Click **Add all** to add a new row for each of the pollutants with a dataset with an averaging time of 1 hour in the comprehensive output file. Click **Delete** to delete the currently selected row. Click **Delete all** to delete all of the rows in the Pollutant output table at once.

Each column in the **Pollutant output** table is described below:

#### Name

Select one of the pollutant names from the drop-down list. Only pollutants that are in the comprehensive output file with an averaging time of 1 hour are available to be selected. For pollutants with multiple datasets with different averaging times, outputs will be taken from the dataset with 1 hour averaging time. It is possible to enter the same pollutant name into multiple rows, in order to be able to calculate output with different averaging times.

#### Include

By default, a new pollutant output dataset will have a tick in this column and be included in calculated output. Un-tick this column to exclude this pollutant output dataset from output. Click in the cell to toggle between a tick and no tick, or type  $\mathbf{Y}$  in the box to add a tick,  $\mathbf{N}$  to remove it. It is possible to set the value for all pollutant rows by right clicking in this column to display a pop-up menu, and clicking **Select all** or **Deselect all**.

#### Averaging time (Value, unit)

Select the appropriate time over which to calculate averages. A variety of averaging time units are available to choose from, as shown in **Figure 2.9**, from hours to years to the full **Met. period**.

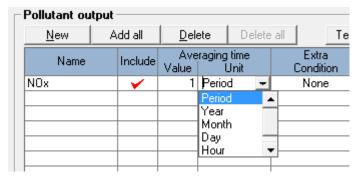


Figure 2.9 - The Averaging time Unit drop-down list

Common averaging times may include 1 Hour averages for  $NO_2$ , 8 Hour rolling averages for ozone and 1 Day averages for  $PM_{10}$  and  $PM_{2.5}$ . Pressing Alt+ $\downarrow$  while in the Value column will drop down a list of preset values such as 24 Hours. Table 2.1 describes each of the averaging time units.

As comprehensive output files contain output concentration and/or deposition data every hour, 1 hour is the shortest averaging time that can be calculated.

Averaging time Unit	Description	Allowed with non- hourly sequential data?	Allowed Values
Period	An average over all times in the selected met. period. There will only ever be one average per output point.  Percentiles and Exceedence thresholds cannot be calculated for Period averages.	Yes	1
Year	An average over an integer number of full calendar years (1st January-31st December).	No	1-99,999
Month	An average over an integer number of full calendar months.	No	1-99,999
Day	An average over an integer number of full calendar days (hour 1 to hour 24).	No	1-99,999
Hour	An average over a discreet, integer number of hours starting at the first hour in the <b>Met. period</b> . E.g. an 8-hour average might have averaging periods of hours 1-8, then hours 9-16, then hours 17-24 and so on.	Yes (1 hour averages only)	1-99,999
Hour rolling	An average over an integer number of hours, that rolls over such that the start and end times of subsequent averaging periods only differ by an hour. E.g. an 8-hour rolling average might have averaging periods of hours 1-8, then hours 2-9, then hours 3-10 and so on.	No	1-99,999

Table 2.1 – Description of the averaging time units

Averages are only ever output at the end of an averaging period. Therefore, averaging units for which there are no period ends in the selected comprehensive output file are not available. For example, using a file that covers the **Met. period** 01/01/2014 00:00 – 02/01/2014 24:00, **Year** and **Month** averaging units would not be available because the data does not cover the last hour in a year or the last hour in a month, but **Day** averaging units would be available because the data covers two last hours in a day. **Hour** and **Hour rolling** averaging time units are always available for hourly-sequential comprehensive output files.

#### Default = 1 Period

#### **Extra Condition**

The options for Extra Condition are None, Maximum daily, Subset average, Subset Minimum and Subset Maximum. If None is selected, then no Extra Condition is applied. If the averaging time is either less than 24 hours or is an Hour rolling averaging time, then Maximum daily may be selected; for each day this will give the maximum average

value over all averaging periods that end on that day. The **Maximum daily** condition cannot be used with **Period** averages, but it can be used in conjunction with **Percentiles** and **Exceedence thresholds**. If the averaging time is 1 hour, then **Subset Average**, **Subset Minimum** or **Subset Maximum** may be selected; this then allows a **Temporal subset** to be selected, as described next. These conditions can also be used in conjunction with **Percentiles** and **Exceedence thresholds**.

Default = None

#### **Temporal subset**

Select the temporal subset to be used with the **Subset average**, **Subset Minimum** or **Subset Maximum Extra Condition**. The temporal subsets themselves are defined via the **Temporal subsets**... button; see Section 2.4.4 for further details. There are three types of temporal subset; daily, weekly and yearly. If a daily subset is chosen, one value per day will be output (each hour 24), giving the average, minimum or maximum over the hours included in that subset. If a weekly subset is chosen, one value per week will be output (each Sunday, hour 24), giving the average, minimum or maximum over the days of the week included in that subset. If a yearly subset is chosen, one value per year will be output (each 31<sup>st</sup> December, hour 24), giving the average, minimum or maximum over the months of the year included in that subset. Each weekly subset can also reference a daily subset, allowing you to define .e.g. a 'working week' subset that only includes the hours 9am–5pm for Monday through to Friday. Similarly, each yearly subset can also reference a weekly subset.

#### **Averages**

A tick in this column means that **Averages** will be output for this pollutant. If there is no tick in the box then **Percentiles** and **Exceedence thresholds** can be calculated and output, but no average values will be output. If no percentiles or exceedences have been specified, then this column acts in the same way as the **Include** column. Click in the cell to toggle between a tick and no tick, or type **Y** in the box to add a tick, **N** to remove it. This column is always ticked for period averages, because percentiles and exceedences cannot be calculated with period averages.

Default =  $\mathbf{Y}$ 

#### Percentiles (non-Period averages only)

Up to 20 **Percentiles** may be calculated for each set of non-period pollutant averages. The  $N^{th}$  percentile is the average value for which N% of all the (valid) average values calculated lie below it. For example, with a **Met. period** of 24 hours (all of which contain valid data) and a 1-hour averaging time, the  $50^{th}$  percentile would be the  $12^{th}$ -highest average, because 50% of the averages (12 values) lie below it.

Multiple **Percentiles** can be entered for each pollutant average and output to the same set of files. Worst case averages can be found by calculating the 100<sup>th</sup> percentile (i.e. the maximum averages).

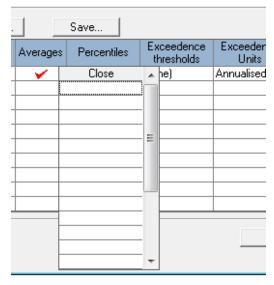


Figure 2.10 – The table for entering percentiles after clicking the drop-down arrow.

**Percentiles** are entered via a table, shown in **Figure 2.10**, which is accessed as a drop-down list by clicking or pressing **Space** in the **Percentiles** column. New values are entered by clicking in an empty row in the table and typing the percentile. Values are deleted by highlighting a filled cell and pressing the **Delete** key. The list is automatically sorted into descending order (with any duplicate values removed) when it is closed. A separate percentile output will be calculated for each percentile value entered.

#### Exceedence thresholds (non-Period averages only)

Up to 20 **Exceedence thresholds** may be entered for each set of non-period pollutant averages. An exceedence threshold is a value for which the occurrence of a pollutant average being larger than it must be found. Enter the **Exceedence thresholds** in the same units as the averages are to be calculated in (see the **Units** column). The number of values that exceed the threshold will then be output as either: an **Annualised** count, a **Percent** or a **Count** depending on the **Exceedence Units** chosen (see below).

As with percentiles, multiple exceedence thresholds can be output for each pollutant average. Exceedence values are entered in a drop-down table, as with percentiles.

#### **Exceedence Units**

The Exceedence Units must be set for each pollutant average that has Exceedence thresholds. Choose between three Exceedence Units options, as shown in Figure 2.11:

- **Annualised** the result will be the count of the number of averages that exceeded the threshold value, but scaled to be the count of the number of averages that would have exceeded the threshold value in a year (if the rate of exceedences remained the same as in the processed met. Period). A year is taken to be 365 days.
- **Percent** the result will be the percentage of averages that were calculated that exceeded the threshold value.

• **Count** – the result will be the count of the number of averages that were calculated that exceeded the threshold value.

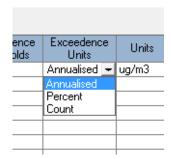


Figure 2.11 – The Exceedence Units options.

For example, for a **Met. period** of 24 hours (all of which contain valid data) and an averaging time of 1 hour, if there are 3 values that exceed a certain threshold, then the **Count** unit will output the value 3, the **Percent** unit will output the value  $3 / 24 \times 100 = 12.5\%$ , and the **Annualised** unit will output the value  $(3 / 24) \times (365 \times 24) = 1095$ .

#### Default = **Annualised**

#### **Units**

These are the concentration/deposition **Units** that will be used for average and percentiles output. They will be the same as the units used in the comprehensive output file.

#### Validity threshold (%)

The **Validity threshold** is a criterion that sets the percentage of values that must be valid before any average is valid. For example, with a 1 day average, if the **Validity threshold** is set to 50%, then at least 12 hours in any one day must be valid before the average itself is considered valid (assuming no temporal subset is used). If less than 12 hours are valid then the average output for that day will be the invalid value indicator -999. If a temporal subset is used, the **Validity threshold** applies only to those hours that are part of the chosen subset. The **Validity threshold** is applied to all averaging types, including period averages and **Maximum daily** averages. For example, for an 8 hour maximum daily average, at a 50% **Validity threshold**, at least two of the 8 hour averages must be valid before the **Maximum daily** average is considered valid. This would mean that, in any one day, at least two 8-hour periods would need to each contain at least 4 hours of valid data to average before a valid **Maximum daily** average would be output.

The **Validity threshold** is not applied to percentiles or exceedences. That is to say, that as long as there is at least one valid average value, there will be percentile and exceedence output. It should be noted, however, that percentile calculations only take valid averages into account, and **Exceedence Units** other than **Count** use the number of valid averages to convert the count into **Annualised** or **Percent** units.

Default = 75%

#### 2.4.4 Temporal subsets

Clicking on the **Temporal subsets**... button brings up the **Define Temporal Subsets** screen, as shown in **Figure 2.12**. This screen consists of three tabs, in which **Daily**, **Weekly** and **Yearly** subsets are defined respectively.

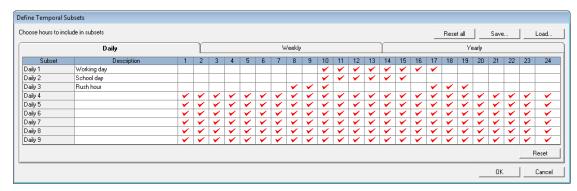


Figure 2.12 - The Define Temporal Subsets screen, with three Daily subsets defined.

Each tab contains a table with the following columns:

#### Subset

A non-editable label given to each subset (row). These labels appear in the drop-down list in the **Temporal subset** column of the **Pollutant output** table. Up to nine separate subsets can be defined for each subset type.

#### Description

An editable description given to each subset. This description appears as a tooltip in the **Temporal subset** column of the **Pollutant output** table.

**Subset used** (Weekly and Yearly subsets only)

Each Weekly subset can either be set to use [All hours] or reference one of the Daily subsets. In this way, it is possible to define e.g. a 'working week' subset that only includes the hours 9am-5pm for Monday through to Friday. Similarly, each Yearly subset can either be set to use [All days] or reference one of the Weekly subsets.

#### 1–24 / Monday–Friday / January–December

Use the tick matrix to define which hours of the day (for **Daily** subsets), days of the week (for **Weekly** subsets) or months of the year (for **Yearly** subsets) are to be included in each subset. There are right-click options that allow you to **Select all**, **Deselect all** or **Invert selection**. For the **Daily** subsets, note that the ADMS models use an hour-ending convention. Thus, if you wanted to define a 'working day' subset that includes just the hours between 9am–5pm, you would tick boxes 10 through 17.

There are also buttons to **Reset** the data in the visible tab, **Reset all** data in all the tabs, **Save**... the current set of data (in all three tabs) to a text-based file with the extension .sub, or **Load**... a previously saved set of data from a .sub file into the tabs.

It is also possible to save the current set of temporal subsets along with the current set of pollutant outputs in the **Pollutant output** table in one step; see Section 2.4.6 for further details.

Pressing **OK** or **Cancel** returns you to the **Create Output Files** screen, retaining or discarding the changes made, respectively.

#### 2.4.5 Create Files

Once the averages, percentiles and exceedences to be calculated have all been defined, then either click **Cancel** to forget the set-up and return to the main screen, or click **Create Files**. Upon clicking **Create Files**, the **Save output files to...** dialog opens as shown in **Figure 2.13**. Only one filename is required; it is not possible to name each type of output file with a different name in the same run. Output filenames will differ only by their file extension if they are created in the same **Create Files** calculation. If the names of existing files are picked, then the existing files will be overwritten without warning.

The files created by the Comprehensive Output File Processor's **Create Output Files** feature can be very large, so make sure the output location chosen has plenty of memory available. If the ADMS Comprehensive Output File Processor determines that there may not be enough space to output the files, then a warning message will be displayed showing approximately how much disk space will be required. The processing will also be stopped. It is recommended that other applications are closed before attempting to create output files.

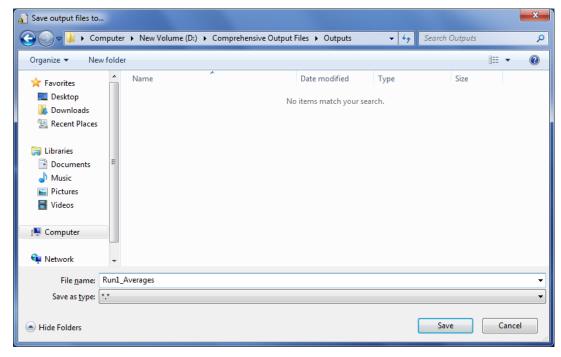
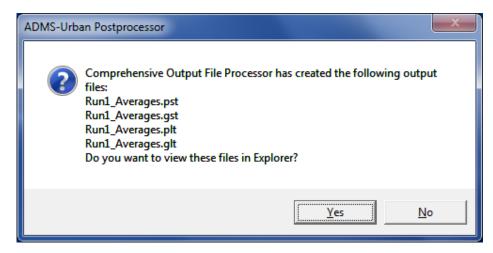


Figure 2.13 – The Save output files to... screen.

Once the output file location has been chosen and a suitable file name entered, click

**Save** to begin the calculations. The length of time taken to finish the calculations can be anywhere between a fraction of a second and several hours, depending on the length of the **Met. period**, the number of output points, the length of the averaging periods, and the number of averages, percentiles and exceedences to be calculated. There is no progress bar and the program will not respond while the calculations are running, so please allow sufficient time for it to complete the output processing.

When the calculations have completed a message is displayed, similar to that shown in **Figure 2.14**, which shows the names of all of the output files that have been created. The message also gives the option of viewing the output files in a Windows Explorer browser.



**Figure 2.14** – An example of a message that is displayed after the output files have been created.

#### 2.4.6 Saving pollutant outputs

It is possible to save a set of pollutant outputs, which can then be used again when processing subsequent comprehensive output files. Firstly, the required outputs should be entered into the **Pollutant output** table. Click **Save...** to bring up the **Save pollutant outputs to file** screen, as shown in **Figure 2.15**. In this screen:

- enter the Name; this will appear in the Air quality objectives list,
- enter a **Description**, and
- choose whether to save the currently defined temporal subsets using the **Save** temporal subsets checkbox,

then click **OK**. This saves the file(s) in the application directory, using the **Name** as the file stem.

These files must be kept in the application directory in order to be recognised by the ADMS Comprehensive Output File Processor.

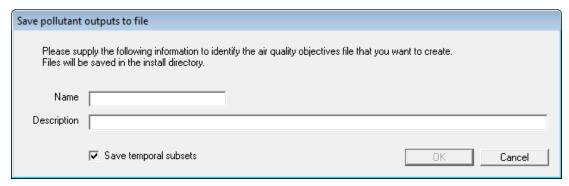


Figure 2.15 - The Save pollutant outputs to file screen.

The Air quality objectives drop-down list will now appear above the pollutant table, as shown in Figure 2.16.

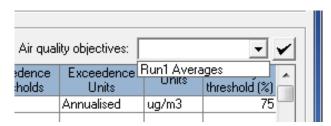


Figure 2.16 - The Air quality objectives drop-down list.

To select a set of saved pollutant outputs, click on the **Air quality objectives** drop-down list to view the available pollutant output sets. Select the required set of objectives and then click on the tick next to the list to populate the table. If the **Save temporal subsets** checkbox was ticked when the pollutant outputs were originally saved, the **Load pollutant outputs from file** screen will first be displayed, as shown in **Figure 2.17**. This includes a **Load temporal subsets** checkbox, which allows you to choose whether or not to overwrite the currently defined temporal subsets with those associated with the saved pollutant outputs.

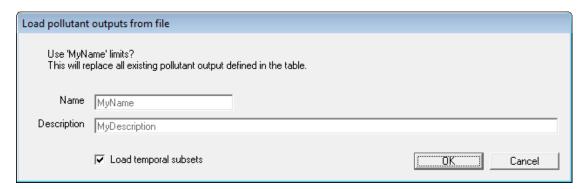


Figure 2.17 – The Load pollutant outputs from file screen.

Selecting a pollutant output set from the Air quality objectives drop-down list and clicking on the tick will delete all existing entries in the Pollutant output table.

Only pollutants that are in the comprehensive output file can be loaded into the **Pollutant output** table. If there are any pollutants in the selected **Air quality objectives** that are not in the comprehensive output file then a warning message will be displayed and those pollutants will not be loaded into the table.

#### 2.5 Calculate Statistics

As well as viewing averages or creating output files, tables of statistics can also be viewed for comparison with air quality standards.

The first step is to choose the set of **Air quality standards** to apply to the input data. This can either be one of the default options available or a user-created air quality standards set. See Section 2.6 for further details on adding new **Air quality standards** sets.

The second step is to choose the **Number of ranked values**. This is the total number of ranked concentrations (i.e. first-highest concentrations, second-highest concentrations, etc.) that will be available for display in the grid viewer and used in the report. The minimum **Number of ranked values** is 1 and the maximum is 10.

#### 2.5.1 Grids

Click **Grids** in the **Calculate statistics** section to open the screen shown in **Figure 2.18**. The options under the heading **Display** become available only after the **Update** button has been clicked. Each option is described below.

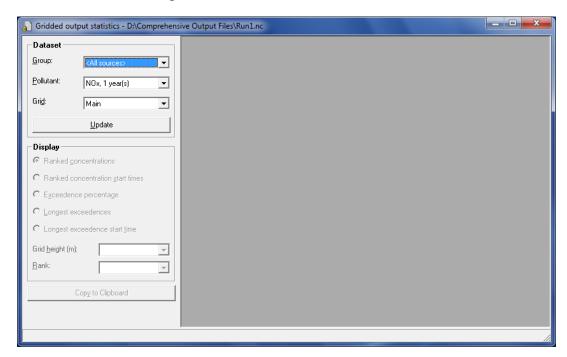


Figure 2.18 – The initial grids screen in the Calculate Statistics section of the processor.

#### Group

Select the particular **Group** of sources which should be included when calculating the statistics. The options available depend on the groups defined in the ADMS model run that was used to create the comprehensive output file.

#### **Pollutant**

Select the pollutant for which to calculate statistics. Several choices will be available depending on the output specified in the ADMS model and on the pollutants listed in

the **Air quality standards** set that is being used. There will be a choice for each pollutant that has been selected as long term output in the ADMS model that also is listed in the **Air quality standards** set, and for each pollutant in turn there will be a choice of averaging times available. These may be **year(s)**, **week(s)**, **day(s)** or **hour(s)** depending on the data in the output file and on the **Air quality standards** set that has been chosen.

For example, if the data contained sulphate concentrations for 14 days then it would be possible to create tables with averaging times of 1 week, 1 day or 1 hour, say, but it would be impossible to create a table with an averaging time of 1 year because there would be insufficient data.

#### Grid

Select the **Grid** on which the statistics should be calculated:

- The **Main** grid is the regular or variable grid that has been used in the ADMS model run this is always available as an option in the list.
- The Nested (Source Name) grid is a finer grid than the main grid. It is placed around each source or cluster of sources if the Source-oriented grids option for Point, Area, Volume sources has been used in the ADMS model run. If this option has been selected then there may be only one or there may be several nested grids available to choose from. For further details on nested grids please refer to your ADMS model user guide. The (Source Name) part of the grid name is the name of a source associated with each nested grid. For example, if there is a nested grid placed around a source called "Refinery Stack" then in the menu the nested grid option will state Nested (Refinery Stack).

#### Update

Click the **Update** button to populate the table with calculated statistics, which will initially be the maximum average concentrations of the selected pollutant at each output grid point. The options available under the heading **Display** will now be enabled. An example of this is shown in **Figure 2.19**.

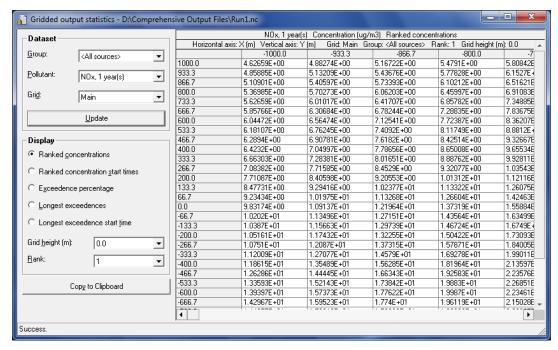


Figure 2.19 – The Grid Viewer just after Update has been clicked

#### Initial display options

Initially the radio button next to **Ranked concentrations** is selected, the **Grid height (m)** is set to a default level and the **Rank** is set to 1. This means that the table is currently showing the highest concentrations (**Rank=1**) at the default height level at each grid point. Other selections can be made using the features explained below.

#### Ranked concentrations

Select this option to display the concentrations of the current **Rank** (see below).

#### Ranked concentration start times

Select this option to display the time of occurrence of the selected ranked (e.g. highest, second-highest etc.) concentration at each grid point for the selected height. The time of occurrence given is the first hour of the averaging period for which this concentration occurs.

#### Exceedence percentage

Select this option to display the percentage of the meteorological conditions that result in an exceedence of the threshold value defined in the selected air quality standards set. If this option is selected then the **Rank** drop-down list is disabled because the **Rank** does not apply to exceedence statistics.

#### Longest exceedences

Select this option to display the length of time of the longest continuous exceedence of the given air quality standard. The units of time are the same as that chosen for the averaging time in the **Pollutant** menu. For example, if the averaging time is 8 hours and the value of the longest exceedence at a particular grid point is 6 then this means

the length of time of the longest continuous exceedence is  $6\times8$  hours, i.e. 48 hours. If this option is selected then the **Rank** drop-down list is disabled because the **Rank** does not apply to exceedence statistics.

#### Longest exceedence start time

Select this option to display the initial time of occurrence of the longest exceedence period. The time of occurrence given is the first hour of the first averaging period in this series of exceedences. If this option is selected then the **Rank** drop-down list is disabled because the **Rank** does not apply to exceedence statistics.

#### **Grid height**

If multiple height levels have been specified within the **Grids** tab of the ADMS model then use this drop-down list to select a particular height level at which to analyse the gridded data.

#### Rank

The drop-down list here contains numbers 1 to N where N is the **Number of ranked values** selected in the main screen (see Section 2.2.4). Selecting 1 produces a table showing the highest concentrations at each grid point, selecting 2 produces a table showing the second-highest concentrations and so on down to N which produces a table showing the N-th highest concentrations. This option is only enabled when either **Ranked concentrations** or **Ranked concentration start times** is selected.

**Copy to Clipboard** copies the table so that it can be pasted into another application.

The screen can be closed by clicking on the cross in the top right hand corner to return to the main screen of the ADMS Comprehensive Output File Processor.

#### 2.5.2 Specified Points

Click on **Specified Points** in the **Calculate Statistics** section of the processor to display the screen shown in **Figure 2.20**.

#### Group

Select the particular **Group** of sources which should be included when calculating the statistics. The options available depend on the groups defined in the ADMS model run that was used to create the comprehensive output file.

#### **Pollutant**

Select the pollutant for which to view statistics. Several choices will be available depending on the output specified in the ADMS model and on the pollutants listed in the Air quality standards set that is being used. There will be a choice for each pollutant that has been selected as long term output in the ADMS model that also is listed in the Air quality standards set, and for each pollutant in turn there will be a choice of averaging times available. These may be year(s), week(s), day(s) or hour(s) depending on the data in the output file and on the Air quality standards set that has

been chosen.

For example, if the data contained sulphate concentrations for 14 days then it would be possible to create tables with averaging times of **1 week**, **1 day** or **1 hour**, say, but it would be impossible to create a table with an averaging time of **1 year** because there would be insufficient data.

#### Grid

This option is not available for specified output points and is disabled.

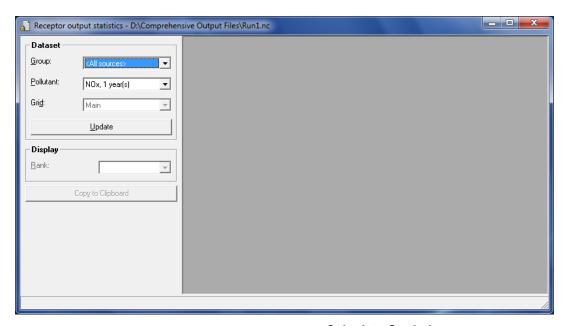


Figure 2.20 – The specified points screen in the **Calculate Statistics** section of the processor.

#### **Update**

Click on the **Update** button to populate the table with the following for each specified point (assuming that the default **Rank 1** is selected): name, location, maximum concentration, the start time of the maximum concentration, the exceedence percentage, the maximum number of consecutive exceedences and the start time of the longest exceedence. An example is shown in **Figure 2.21**.

If the **Rank** is a number other than 1 then the exceedence statistics are not given; only the concentrations of the appropriate **Rank** are displayed.

#### Rank

This determines which concentration values are displayed. The drop-down list contains numbers 1 to N where N is the **Number of ranked values** selected in the main screen (see Section 2.2.4). Select 1 to display the maximum concentration values, select 2 to display the second-highest concentrations and so on down to N to display the N-th highest concentrations.

**Copy to Clipboard** copies the table so that it can be pasted into another application.

Receptor output statistics - D:\Comprehensive Output Files\Run1.nc NOx, 1 year(s) Dataset Exceedence level: 30 ug/m3 Group: <All sources> Rank: Group: <All sources> Concentration (ug/m3) •  $\times$  (m) Y (m) Start time Excee Z(m)196 3344 2008-01-01 01:00 100.00 Receptor, Test 100 Pollutant NOx, 1 year(s) ▾ Grid: Main <u>U</u>pdate Display Rank: 1 • Copy to Clipboard

The screen can be closed by clicking on the cross in the top right hand corner to return to the main screen of the ADMS Comprehensive Output File Processor.

**Figure 2.21** – An example of the specified points screen showing the calculation statistics.

#### 2.5.3 Generating Reports

Success.

From the main screen of the ADMS Comprehensive Output File Processor, clicking **Generate Report** initially opens a **Save As** dialogue box. Here you should navigate to the desired folder, type in an appropriate file name in the **File name** box and click on **Save**. The **Save as type** box should be left as the default *CSV*. Thus a *Report.CSV* file, for example, is created which can then be viewed and examined in a spreadsheet package such as Microsoft Excel.

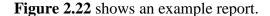
If specified points have been modelled then the report file will contain *tables* of data containing information about the concentrations and any exceedences recorded at those points. Similarly, if grid points have been modelled then the report file will contain *summary* sections of data containing information about the concentrations and any exceedences recorded at gridded output points.

The first table for each pollutant shows the average concentration at the specified points. The average is taken over the entire period of the model run.

The subsequent tables are for each objective within the **Air quality standards** set and show the ranked highest concentrations at the specified points; i.e. if in the processor main screen the **Number of ranked values** is 5 then the tables show the highest 5 concentrations at each specified point. Next to the concentration values the initial date, day and hour of occurrence are also shown. The tables also show the threshold concentration for each pollutant for the chosen **Air quality standards** set. If the threshold is exceeded then the percentage of times it is exceeded, the maximum number of consecutive exceedences and the start date, day and hour of the exceedence are also shown in the table. Note that if there is not enough data for averaging time in an **Air quality standards** set to be calculated then the table for that particular objective will be omitted.

Similarly, the first summary for each pollutant shows the highest average concentration and the location of its occurrence. This is shown for all of the grids considered together, for the main grid on its own and individually for any nested grids which may have been included in the ADMS model run. The average is taken over the entire period of the model run.

The subsequent summaries are for each objective within the **Air quality standards** set and show the ranked highest concentrations for all of the grids considered together, for the main grid on its own, and individually for any nested grid which may have been included in the ADMS model run. Next to the concentration values the initial date, day and time of occurrence are also shown.



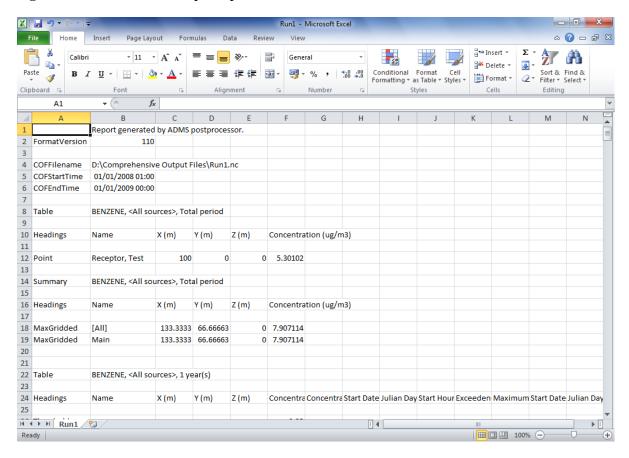


Figure 2.22 – An example report.

### 2.6 Creating and adding new air quality standards sets

It is possible to create and add new **Air quality standards** sets to the ADMS Comprehensive Output File Processor. This is required, for example, if data needs to be compared with an air quality standard that is not already listed within the default standards included with the ADMS Comprehensive Output File Processor. Recall that all the default air quality standards are listed in the **Air quality standards** drop down menu in the main screen of the processor (see Section 2.2).

The **Air quality standards** sets used in the processor are each defined in an .aqs file (where aqs stands for Air Quality Standards). The .aqs files can be viewed in a text editor such as Notepad. To create a new **Air quality standards** set simply create a new .aqs file following the file structure and conventions described here. An example .aqs file is shown in **Figure 2.23**.

The first line of the file must be ADMS-AQS indicating that the file is an .aqs file. The second line must be 120, which is the current version number. The third line is then the number of air quality objectives in the file, and the fourth line is a descriptive name. The name you choose is the name that appears in the **Air quality standards** list in the main screen of the processor. Thus the first four lines of an .aqs file file might be as shown in **Figure 2.23**, which defines an **Air quality standards** set called 'Class 1' containing 3 air quality objectives.

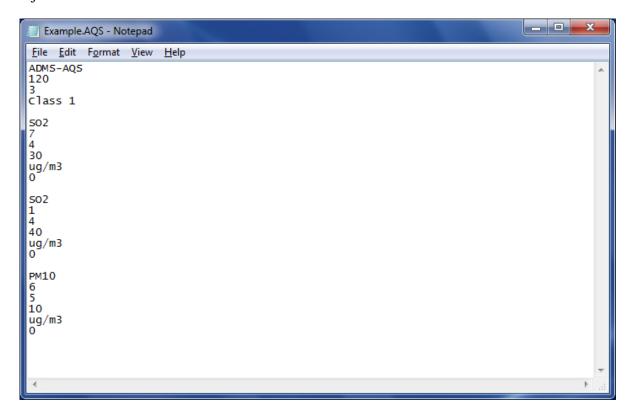


Figure 2.23 – An example .aqs file with 3 records

The first four lines must be followed by a blank line and then each of the air quality objectives must be entered with a blank line separating each one.

Each air quality objective is defined by 6 lines of data, with the following format:

Name of pollutant Averaging time Units of averaging time Exceedence threshold value Units of exceedence threshold Type

The following conventions must be used.

- The Units of averaging time must be an integer from 0 to 7 inclusive; 0 signifies the total period covered in the \*.nc file, 1 and 2 are not currently supported, 3 signifies hours, 4 signifies days, 5 signifies months, 6 signifies quarters and 7 signifies years.
- The Units of exceedence threshold must be one of mg/m3, ug/m3 or ng/m3. The first of these is milligrams per metre cubed, the second is micrograms per metre cubed and the third is nanograms per metre cubed.
- Finally the Type must be 0 which signifies that pollutant concentration is being used in the record.

Currently, running averages are not supported in .aqs files. All averaging periods are therefore distinct. Additionally, air quality standards that specify daily maximum averages or percentile exceedences are not supported.

The example file shown in **Figure 2.23** contains 3 air quality objectives. The first air quality objective is for  $SO_2$  and states that the 7 day average concentration must not exceed 30 ug/m<sup>3</sup> more than a given number of times; the second air quality objective is also for  $SO_2$  and states that the 1 day average concentration must not exceed 40 ug/m<sup>3</sup> more than a given number of times; and the third air quality objective is for  $PM_{10}$  and states that the 6 month average concentration must not exceed 10 ug/m<sup>3</sup> more than a given number of times. Note that the number of times the air quality objectives allow the exceedence threshold values to be exceeded is not specified in the *.aqs* file.

All .aqs files must be saved to the application directory in order to be automatically detected and loaded by the ADMS Comprehensive Output File Processor.



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