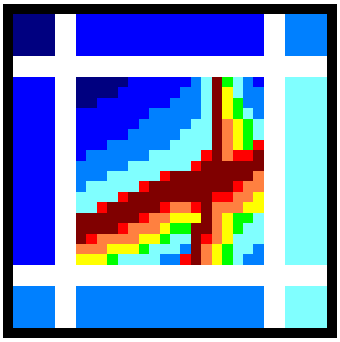


MAQS

Automated Coupled System for Nesting Street-scale Dispersion Modelling in a Regional Air Quality Model

User Guide **CERC**

MAQS

Automated Coupled System for Nesting Street-scale Dispersion Modelling in a Regional Air Quality Model

User Guide

Version 1.2

November 2023

Cambridge Environmental Research Consultants
3, King's Parade
Cambridge
CB2 1SJ
UK

Telephone: +44 (0)1223 357773
Email: help@cerc.co.uk
Website: www.cerc.co.uk

Copyright © Cambridge Environmental Research Consultants Limited, 2023

Contents

SECTION 1 Introduction

1.1 About the MAQS coupled system

The Multi-Model Air Quality System (MAQS) coupled system is an automated system for coupling the high resolution air quality models ADMS-Local (Seaton *et al.*, 2022) or ADMS-Urban (McHugh *et al.*, 1997) to a regional air quality model with hourly concentration output such as CMAQ (Byun and Schere, 2006), CAMx (ENVIRON, 2016), EMEP4UK (Vieno *et al.*, 2010, Simpson *et al.*, 2012), CHIMERE (Schmidt *et al.*, 2001) or WRF-Chem (Grell *et al.*, 2005). Additional 'generic' regional model file formats allow output from other models to be reformatted and used in the system. In addition, annual average background concentration maps generated by PCM (Brookes *et al.*, 2020) can be used as the regional model data for UK annual average runs. The output from the coupled system comprises predictions of pollutant concentrations for an output area, which take into account both regional and local pollutant transport and chemistry effects.

The aim of the MAQS coupled system is to combine the complementary advantages of regional and local models to improve the prediction of concentration values for all types of receptors. Regional (usually Eulerian) models contain complex chemistry mechanisms, which can operate over long spatial and temporal scales, and can model the accumulation of concentrations in very low wind speed conditions. The gridded nature of their emissions data and dispersion calculations, however, does not allow them to resolve the high gradients of concentration found in the immediate vicinity of an individual source such as a road. Local (usually Gaussian-type plume) models can represent the fine-scale concentration gradients from explicitly defined sources in detail, but generally only include simplified chemical mechanisms and spatially homogeneous meteorological data, limiting their applicability for receptors far from the source (typically defined as more than 50 km). They are also of limited applicability in very low wind speed conditions.

Coupling a local model to a regional model can allow both the resolution of high concentration gradients close to a source, and the accurate representation of transport and chemistry over larger spatial and temporal scales. The MAQS coupled system combines the regional and local concentrations in such a way as to minimise double-counting of emissions, while remaining computationally efficient and user-friendly. It is an off-line system, meaning that the regional models can be run separately from the local modelling, which allows the use of archived regional model data. Meteorological data either from the WRF meso-scale model (Dudhia *et al.*, 2005) or another model with output converted to 'generic' format is used for both the regional modelling and the local modelling. An overview of the MAQS coupled system is given in Section 1.3 while a technical summary of the concept and implementation of the coupled system can be found in Section 8.

At present the MAQS system is directly compatible with hourly outputs from the WRF meso-scale meteorological model and the CMAQ, CAMx, EMEP4UK, CHIMERE and WRF-Chem regional air quality models. Annual average background maps from the PCM model are also supported. Additional 'generic' meteorological and concentration data file formats have been defined, which can allow outputs from other meteorological and/or chemical-transport models to be reformatted for use in the system, including annual or period-average concentration data.

1.2 MAQS coupled system features

The principal features of the MAQS coupled system are:

- An automated control system with logging of progress to file and screen;
- Compatibility with the widely-used regional air pollution models CMAQ, CAMx, WRF-Chem and CHIMERE;
- Option to use regional air pollution and/or meteorological model data from models not directly supported via a 'generic' format;
- Option to run with annual average background regional concentration data, for example the Defra background maps (Brookes *et al.*, 2020);
- Flexibility regarding the size and shape of the modelling domain;
- No requirement to re-run the regional air quality or meteorological models;
- Automatic division of a large nesting domain into separate runs for each regional model grid cell, with appropriate local meteorology from a meso-scale model and background concentrations;
- Option for automatic conversion of regional model emissions into ADMS-Urban 3D grid file format (CMAQ and WRF-Chem only);
- Inclusion of advanced modelling techniques for urban areas through the use of ADMS-Local or ADMS-Urban, such as street canyon and urban canopy flowfield calculations;
- Output files in portable netCDF format, which can then be used in the MAQS post-processing tools and verification system;
- Built in parallelisation; and
- Possibility of linking to scheduling systems, for example for use in forecasting.

1.3 Overview of the MAQS coupled system

The MAQS coupled system uses output meteorological and concentration data from regional modelling to provide inputs to ADMS-Local or ADMS-Urban model runs, and calculates output concentrations from a combination of the regional and local output concentrations.

1.3.1 MAQS coupled system components

The main components of the coupled system are as follows:

- the ADMS-Local (Seaton *et al.*, 2022) or ADMS-Urban (McHugh *et al.*, 1997) local dispersion model; and
- the MAQS coupled system Controller, which consists of a package of control scripts and seven utility programs.

The main inputs to the MAQS coupled system are:

- meteorological data output files from the WRF meso-scale model or in 'generic' netCDF format;
- concentration data output files from the CMAQ, CAMx, EMEP4UK, WRF-Chem or CHIMERE regional models, or in 'generic' hourly or annual average format;
- if using ADMS-Urban as local model, one or two ADMS-Urban model parameter files (*.upl*) containing local emissions data and definitions of output locations and species; and
- MAQS system parameters saved in five configuration files, separated into: regional model and domain options; input data locations; modelling time period; local model input data and options; and (optionally) details of remote machines to use for parallel runs.

If using output from the WRF-Chem regional model, the same files may include both meteorological and concentration data. These files are considered equivalent to WRF output files for meteorological data.

There is an option for automatic conversion of CMAQ or WRF-Chem regional model emissions for use in ADMS-Local or ADMS-Urban via 3D gridded emissions files.

The regional meteorological and concentration data can be created by the user of the MAQS coupled system or obtained from a third party.

1.3.2 User methodology

The tasks which the user must carry out for a complete run of the MAQS coupled system are as follows:

Step 1 Compile an emissions inventory appropriate for use in both local and regional dispersion modelling, including both gridded and explicit source data;

Step 2 Set up and run the a meso-scale meteorological model;

Step 3 Set up and run a regional dispersion model such as CMAQ, CAMx, EMEP4UK, WRF-Chem or CHIMERE;

Note that if either the WRF-Chem regional model or coupled WRF-CMAQ system is in use, Steps 2 and 3 will be a single procedure.

Step 4 Set up local model inputs, including the highest available resolution emissions data for the modelling area with explicit definitions of road sources and the desired final output locations;

Step 5 Set up MAQS coupled system input configuration files for validation at monitor locations; run the coupled system initially using the verification option; check for and correct any input errors;

Step 6 Run the full modelling period and compare outputs to monitor data; and

Step 7 Set up and run MAQS coupled system input configuration files for contours of concentration (air quality maps).

Guidance for setting up the MAQS coupled system input files can be found in Section 4. Details of how to set up the local model input file(s) are given in Section 4.4.6.

Instructions for installing and configuring the components of the MAQS coupled system, which should be carried out before setting up the local model input files, are given in Section 2.2.

Note that if the regional model output data are obtained from a third party, information about the regional model emissions and some other inputs must also be obtained, as described in Section 3.

1.4 Overview of the MAQS coupled system User Guide

This *MAQS Coupled System User Guide* is both a manual and a technical summary of the MAQS coupled system. The contents are discussed briefly below.

Familiarity with ADMS-Local or ADMS-Urban is assumed throughout this user guide, please refer to the ADMS-Urban User Guide (CERC, 2020b) for details of standard ADMS-Urban installation, inputs and runs. MAQS-Health project reports and publications (Seaton *et al*., 2022) describe ADMS-Local. Training in the use of ADMS-Urban and the MAQS system is available from CERC.

Section 2 describes the computational resource requirements for running the MAQS coupled system and gives instructions for installing the coupled system, including configuration instructions.

Running the MAQS coupled system requires various sources of data in addition to those needed for a stand-alone local model run. The additional requirements, in particular those relating to consistency with the chosen regional model, are described in Section 3.

All the user options are covered in Section 4, with details of the corresponding configuration (*.cfg*) files. This section also includes details of how to set up local model input data file(s) used in the MAQS coupled system.

Section 5 describes the output files from the MAQS coupled system and methods for processing the concentration outputs from the system.

Some guidance on how to investigate and solve common errors is given in Section 6 .

Three worked examples showing how to use the MAQS coupled system to obtain concentrations at receptor locations or for contours are given in Section 7. The files required to run these worked examples are supplied as part of the MAQS coupled system installation.

A technical summary of the concept and implementation of the MAQS coupled system is given in Section 8. Each procedure required to generate output concentrations for receptor and gridded output locations is described. The limits of the MAQS coupled system are also described.

References are given in Section 9.

Each of the utility programs used in the MAQS system is described in an appendix. The utility for reading the regional model grid definition and writing it to a standard text file is described in Appendix A. The optional conversion of regional model emissions data into ADMS-Urban 3D grid file format uses the utility described in Appendix B. Appendix C gives details of the utility used to generate output calculation locations along the sides of roads. The utility used to extract ADMS-format meteorological data from gridded regional meteorological data files is covered in Appendix D. The core system utility used both for extracting background concentrations from the regional air quality model files and for calculating nesting output concentrations is described in Appendix E. Appendix F describes the utility for re-combining results from multiple spatial domains. The final utility in the MAQS coupled system, used for adding interpolated source-oriented grid points to output files for contour runs, is described in Appendix G. The format of the primary input file for stand-alone ADMS-Local runs is defined in Appendix H. Some features of ADMS-Urban only used within the coupled system are described in Appendix I.

1.5 Conventions

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

- Script variables and samples are shown in Courier New font, e.g. `MODEL_DIR` and

```
find . -type f -name '*.log'
```

- Directory and file names are shown in *italics*, e.g. *WRFtoMet.out*, *<install_path>/Data*.
- Tips and other notes are shown thus:

Think about the area you want to include in the calculation before specifying the output grid.

- Table and figure references are shown in **bold**, e.g. refer to **Table 3.2**, **Figure 2.1**.

SECTION 2 Getting started

2.1 System requirements

The operating systems on which each major component of the MAQS coupled system is currently supported are listed in **Table 2.1**.

Program	Version used in MAQS coupled system	Supported operating systems
ADMS-Urban MAQS control scripts	1.2	CentOS 6, 7
ADMS-Urban model	5.0	CentOS 6, 7 (64-bit)
ADMS-Local model	1.0	CentOS 7 (64-bit)

Table 2.1 List of software components of the MAQS coupled system with current version numbers and supported operating systems.

The MAQS coupled system may work on other "flavours" of Linux, but these are neither tested nor supported. The operating system must be 64-bit.

The MAQS coupled system control scripts have been developed using Bash 4.1 and also depend on the bc package. In order to use the parallelisation option, the GNU parallel package must be installed on each machine which will be used to run the system, this may also require the perl package.

2.2 Installing the MAQS coupled system

Unzip *maqs_v1.2.0.zip* in the desired install location and set read, write and execute permission for this folder and its subdirectories. The ADMS-Urban or ADMS-Local model and MAQS coupled system utilities will be stored in *model* and *utils* subdirectories respectively, and the worker scripts in *scripts*.

The top-level installation directory that contains the main executable script (*run-maqs*) will be referred to as <*install_path*> throughout this guide.

The MAQS licence file will be supplied separately by email. In order to run the coupled system, the MAQS licence file needs to be saved in the <*install_path*>*/utils* subdirectory with the filename *MAQS.lic*.

The ADMS-Urban model file *ADMSUrbanModel.out* will be supplied and licensed separately and should be copied to the MAQS coupled system <*install_path*>*/model* subdirectory.

2.2.1 Configuring the MAQS coupled system: folders

The location of the key directories can be changed in *folders.cfg*. An example directory structure suitable for running the MAQS coupled system on Linux is shown in **Figure 2.1**. The *scripts*, *model*, *utils* and *Data* directories must remain with these names within the installation directory.

The ADMS-Urban model file *ADMSUrbanModel.out* and ADMS-Urban licence file *ADMS-Urban.lic* should be copied to the *<install_path>/model* directory.

Users are advised to create additional directories to store their own system inputs and outputs, for example *maqsinputs* and *maqsoutputs*. The `DEF_INPUT_DIR` and `ARCH_DIR` environment variables should be set to these directory paths using the *folders.cfg* file.

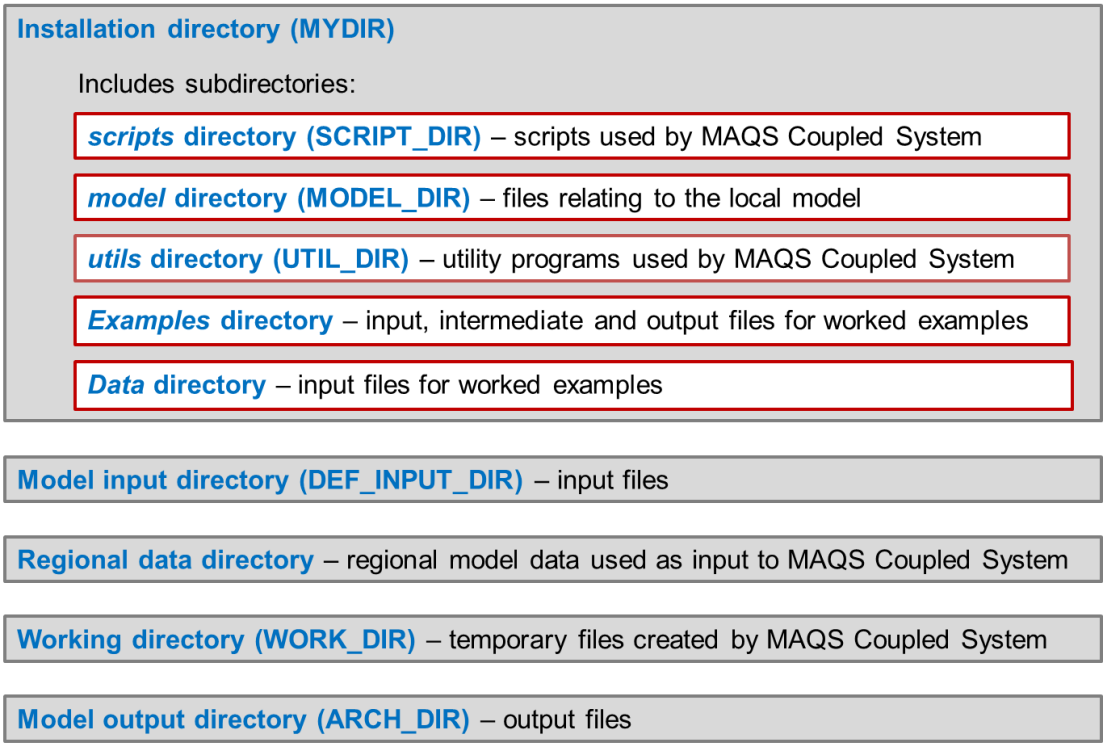


Figure 2.1 Example directory structure for the MAQS coupled system on Linux, where fixed directories within the installation directory are outlined in red. Environment variable names referring to directories are given in blue upper case letters.

folders.cfg is a user-editable configuration file that contains the following variables relating to directory paths:

- `SCRIPT_DIR` – contains all worker scripts, and should only be changed if customisation to a specific queue submission system is required.
- `MODEL_DIR` – should contain at least one of:
  - the desired version of *ADMSUrbanModel.out*, along with a valid ADMS-Urban licence (required to use ADMS-Urban as the local model within the coupled system); and/or
  - *ADMSLocal.out* (to use ADMS-Local as the local model within the coupled system).

- UTIL_DIR – should contain all utilities required by the system.
- WORK_DIR – is the active working location and should be a new and fully accessible folder, preferably somewhere with at least 20GB+ of space that can support a high read/write frequency.

  *Note that in order to avoid conflicts with automatic cell folder names, the working directory path must not follow the pattern C*C*C, ie. starting with a C and including two further C characters.*

- ARCH_DIR – is the designated output storage location, and should have read/write permissions and sufficient space for all your output.

  Note that a large volume of files can be generated in ARCH_DIR by the MAQS coupled system, particularly if the PreserveWorkingFiles option is in use.

- DEF_INPUT_DIR – is the location where *run-maqs* expects the *inputdata.cfg*, *options.cfg, localmodel.cfg, run.cfg* and *sshlogin.cfg* control files to be stored, unless overridden by the `--inputs` command line flag.

The ARCH_DIR, DEF_INPUT_DIR and WORK_DIR directories are sub-directories of MYDIR (same as <*install_path*>) by default, but the user is advised to change them to other locations, as shown in Figure 2.1. For example, we would expect WORK_DIR to be set to a location with sufficient space for all of the intermediary files.

DEF_INPUT_DIR requires read permissions and ARCH_DIR requires read and write permissions. WORK_DIR can be created at run time by the control system and should have read, write and execute permissions.

If running the system with the parallelisation option for distributing tasks between different machines, users are advised to make the regional model data files accessible to all running machines using a single file path, for example via a shared file system. The MAQS coupled system can copy files to the remote machines but this will increase run times for large data files. More information about this system option is given in Section 4.1.12.

2.2.2 Configuring the MAQS coupled system: parallelisation

The code used within the control scripts for submitting and retrieving run files may need to be customised for a specific HPC system. In particular, the run_script_all_cells function in the *process.sh* file submits scripts as local background processes by default, which typically allows up to one process per core of the controlling node. This function would need to be altered to use appropriate commands for submitting runs to and retrieving runs from a queuing system. Alternatively, it is usually possible to submit the top-level MAQS coupled system process to the queuing system.

An option for using the GNU parallel package to distribute runs between a host machine and remote machines is also provided within the scripts. This option is enabled using a flag in the *options.cfg* input file and requires an additional input file, *sshlogin.cfg*, with details of the machines which should be used, as described in Section 4.8. A template *sshlogin.cfg* file can be created using the *make_def_inputs.sh* script, as described in

Section 2.3.1.

When the GNU parallel option is in use, the user can also choose an additional option for whether to copy the MAQS coupled system installation and input files from default directories to the remote machines. More details of how to set up this option are given in Section 4.1.12.

In order to use the GNU parallel option in the MAQS coupled system, the user is required to set up passwordless ssh access from the current user on the local machine to all remote machine(s), for example using ssh keypairs. If using the option to transfer files to remote machines, the run working directory (`WORK_DIR`) must be located under the user's */home* directory and the folder settings in *folders.cfg* should be kept as default values wherever possible. This may not be necessary if the MAQS coupled system is installed under identical file paths on each remote machine and input files are available via identical shared file paths.

Contact CERC for further advice on customisation for your system.

2.3 Editing control files and running the MAQS coupled system

Section 1.3.2 summarises the full user methodology for modelling using the MAQS coupled system. If the regional model data are already available and all components of the system are correctly installed and configured, the following steps must be taken to generate results from the coupled system:

- create a new set of MAQS coupled system control files (*options.cfg, inputdata.cfg, run.cfg, localmodel.cfg, sshlogin.cfg*);
- enter data to define the problem;
- save the MAQS coupled system control files;
- run the MAQS coupled system; and
- display the output generated by the MAQS coupled system.

The first four of these steps are described in Sections 2.3.1 to 2.3.4. Entering model data is described in general terms here, and in full detail in Section 4. The post-processing utilities developed for analysing and visualising MAQS coupled system output are described in separate user guide documents.

2.3.1 Creating control files

To create a new set of control files (*options.cfg, inputdata.cfg, run.cfg, localmodel.cfg, sshlogin.cfg*) in the *<install_path>/default inputs* directory, run the script *<install_path>/default inputs/make_def_inputs.sh* using the `bash` command. For example, if MAQS is installed in the directory */disk/maqs*, the required command is

```
bash /disk/maqs/default\ inputs/make_def_inputs.sh
```

The five *.cfg* files can then be copied to a new directory of your choice, opened and altered in your preferred text editor. Keep the files together in a single directory and do not rename them.

For existing files, just open them in your preferred text editor.

2.3.2 Entering information

Control file format

The MAQS coupled system control files contain sets of environment variables that are used in the main scripts, along with descriptions of their purpose, units, and range of allowed values.

Changing values in the control files

Load files into a suitable text editor, edit the required values and save the files.

Numerical values can be entered in scientific format, for example `1.00E+1, 1.00E-1`, or floating point decimal format, for example `10.00`.

Non-numeric values, such as paths and dates, should be enclosed in quotes. In most cases, we would recommend single quotes (') for literal interpretation of strings. However, for path variables, you may want to use an environment variable as defined in *folders.cfg*, such as `${DEF_INPUT_DIR}`, in which case double quotes (") should be used as the enclosing character (text delimiter).

Refer to https://www.gnu.org/software/bash/manual/html_node/Quoting.html#Quoting for more information about text delimiter characters and quoting mechanisms in bash scripts.

Nesting period dates in *run.cfg* should be formatted as `'yyyy-mm-dd hh'`, where the hour (`hh`) value is in the range of 0-23.

Data validity and integrity checking

If the user-entered data is not consistent with the model's logic or is outside the range of allowed values, the run will usually fail to execute the model or one of the utilities. These mistakes can be identified by running the system in verification mode, as described in Section 2.3.4.

2.3.3 Saving input data to a control file

Remember to save any edited control files in your editor before running the system. You can set the folder that contains your control files as your default input folder using the `DEF_INPUT_DIR` variable in *folders.cfg*. Alternatively, it can be loaded using a command line argument, as explained in the following section.

2.3.4 Running the MAQS coupled system

Having saved the current scenario as a set of control files, the MAQS coupled system can be run from the terminal or another script. Further options and overrides can be set using the following command line arguments. All arguments are optional and the order is flexible, except for the attached values of `--date` and `--inputs`.

- `-d, --date START_DATE END_DATE`

  Specify the start and end dates of the coupled system nesting run, using the same date format as *run.cfg* (see formatting rules in Section 2.3.2 above). Using this command line option overrides the values from *run.cfg*.

- `-i, --inputs NEW_INPUT_DIR`

  Specify directory containing *options.cfg*, *inputdata.cfg*, *run.cfg*, *localmodel.cfg* and *sshlogin.cfg* (if using the GNU parallel option). Using this command line option overwrites the setting of `INPUT_DIR`.

- `-p, --preserve`

  Archive all intermediary files, overriding the setting of `PreserveWorkingFiles` in *options.cfg* and equivalent to setting `PreserveWorkingFiles=$ALL_FILES`. This option is only recommended for debugging, as it generates a large volume of input and output files. By default all *.log* files are archived by the system.

- `-v, --verify`

  Run in verification mode, changing the end date to be a few hours after the start date. Use to check whether the current configuration can complete a nesting run.

The following is an example command line to run the main *run-maqs* script for a set of control files in */disk/working/Example 1/* with verification and preserve options set to make it run for a brief met period, keeping all intermediary files. This is a standard way to test a new configuration or set of input files.

```
/disk/maqs/run-maqs –v -p –-inputs '/disk/working/Example 1/'
```

When setting up a large run of the MAQS coupled system, it is recommended to test the system inputs by initially running in verification mode. This will allow you to verify your inputs and to estimate the disk space required to store the complete run. To run the system in verification mode with the current set of control files, use the `–v` or `–-verify` arguments given above.

Note that neither the duration nor the disk space requirement of the complete run is linearly related to the duration of the verification run, due to overheads of initial processing task time and file structure, however an upper estimate for the disk space required for the complete run will be proportional to the increase in the number of modelled hours when compared to the verification run.

While the MAQS coupled system is running, the status of the various tasks performed by the system is reported via the terminal (`stdout`).

Cancelling a run

It is possible to cancel a MAQS coupled system run which is in progress, for example in order to alter an input parameter, by closing the controlling terminal.

2.3.5 Displaying model output

Suggestions for netCDF processing approaches are given for the Worked Example runs in Sections 7.2.2 and 7.3.2. The post-processing utilities developed to analyse and visualise MAQS coupled system outputs are described in separate User Guide documents.

SECTION 3 Data requirements

The ADMS-Urban model User Guide describes the general input data required to run local modelling for stand-alone simulations, typically using measured meteorology and background concentrations. Additional requirements for the MAQS coupled system are described in this section, with specific information about meteorology, emissions, regional model output concentrations and other requirements. Further information about the ADMS-Local model has been published (Seaton *et al.*, 2022). It is important for the validity of the final nested concentration output that consistent data is used for the different components of the modelling system, in particular for the time-variation of gridded emissions.

If you are obtaining regional model output data from a third-party provider, please note that related information about the regional model inputs is also required.

3.1 Coordinate system

All spatially-varying inputs to the MAQS coupled system must be defined in the same projected coordinate system with units of metres. This coordinate system should be consistent with the regional model grid definition, so that the regional model grid is rectilinear in the chosen coordinate system. If WRF output files are used for meteorological data, the model coordinate system is required to use either the Lambert Conformal Conic or Polar Stereographic projection with no false easting or false northing, or the Universal Transverse Mercator coordinate system.

Note that the regional model horizontal grid must be regular but is not required to be isotropic (equal spacing in x and y directions).

For models where output file coordinates are specified in latitude-longitude values, including WRF, it is also important to specify the underlying coordinate system datum. The MAQS coupled system has pre-set defaults of a spherical datum as used in WRF, EMEP and CMAQ or the WGS84 ellipsoid datum. Users may also define a custom sphere or ellipsoid datum. When using annual average UK concentration maps, the Airy 1830 datum associated with OSGB (UK national grid) coordinates can also be selected. More details of the coordinate system datum setting options are given in Section A.2.

The vertical grid definition requirements for the regional model data are model-specific. More details are given in Section A.1.

3.2 Meteorology

The MAQS coupled system extracts meteorological data either from the meso-scale model WRF or a ‘generic’ format of hourly meteorological data netCDF files. Each model grid cell which is included in the nesting domain uses meteorology from the corresponding regional grid cell.

The regional meteorological data used in the MAQS coupled system should be the same as that

used to run the regional photochemical model, with a consistent grid definition. Each WRF output file should contain at least the following variables:

- Wind speed components in the x and y directions (U and V), either at 10 m or at each vertical grid level – in the latter case, height variables must also be available; and
- Incoming solar radiation or surface sensible heat flux.

Other variables which can be extracted for use as input to the local model run include boundary layer height and precipitation. The most suitable combination of variables may depend on any meteorological pre-processor used for the regional photochemical model. The extraction of both incoming solar radiation and surface sensible heat flux is recommended for use in ADMS-Urban if available in the input files.

Meteorological model data supplied to the coupled system in the 'generic' gridded file format must contain data for wind at 10 m above ground, near surface air temperature (screen height or 2 m above ground) and surface sensible heat flux. Generic format meteorological data files may optionally also include boundary layer height data. Full details of this data format are described in Section 4.2.3.

WRF output files may contain values of roughness length or dominant land use category values which are each associated with a value of roughness length. If using ADMS-Local, spatially varying roughness values can be entered in the 'site properties' file, described in Section 4.7.6, in addition to urban canopy flow parameters.

When using ADMS-Urban, a value of roughness length consistent with that used by the regional meteorological model within the nesting domain should be entered into the ADMS-Urban interface. The roughness length chosen for use in ADMS-Urban should reflect the value used by WRF for the areas with highest emissions within the nesting domain. For the main ADMS-Urban run with explicit sources in the MAQS coupled system, the integrated urban canopy flow field module can be used to calculate local values of roughness based on building parameters, which may be more appropriate for local modelling than the dominant land use values in WRF.

The file paths and names of the meteorological data files should follow a pattern which indicates the date and time of the first hour of valid data contained within the file.

For full details of the utility which is used to extract ADMS format met data from WRF or generic meteorological data output files in the MAQS coupled system, which can also be used as a stand-alone program, please refer to Appendix C.

3.3 Emissions

In addition to the standard emissions data which is required to model an urban area using ADMS-Local or ADMS-Urban, for the MAQS coupled system, gridded emissions data consistent with that used in the regional model must be processed in order to obtain valid nesting background concentrations, as described in Section 8.2. Both the total emissions and the time-variation of emissions should be matched as closely as possible to the regional model equivalents.

There is a MAQS coupled system user option for automatic conversion of regional model

emissions files from the CMAQ and WRF-Chem regional models, as described in Section 4.3.7. This option creates an ADMS format 3D grid source file for the nesting domain and applies it to all of the local model runs in the system, which allows very close matching between the local and regional model emissions. ADMS format 3D grid source files could also be created from 2D gridded emissions and associated profiles in EMIT (CERC, 2022) or manually from other regional model emissions data. The ADMS 3D gridded emission file format definition can be found in the ADMS-Urban User Guide.

WRF-Chem emissions files for use in the MAQS coupled system must contain: the coordinate variables 'XLAT' and 'XLONG'; and the simulation time variable 'Times'. In addition, the attributes required to define the projected coordinate system in which the grid is regular and orthogonal must be defined, including 'MAP_PROJ' and 'STAND_LON'.

The emissions species and units used in regional models are generally different from those in local ADMS modelling so a 'species map' must be defined, which contains the factors used to convert between regional model and local model emissions species and units. In general this mapping will be different for emissions and concentration species.

Please refer to Section 4.3.1 for more details of the species mapping method used in the MAQS coupled system.

If a 3D grid source cannot be used, a 2D grid source should be created in ADMS-Urban with resolution and grid cell horizontal geometry corresponding to the relevant regional model domain. The 2D grid source depth defined in ADMS-Urban should be set to twice the depth of the regional model grid layer(s) containing the majority of ground-level emissions. Please refer to Section 4.7.13 for more details of the ADMS-Urban run inputs. This option is not available when using ADMS-Local as the local model.

3.4 Regional model concentrations

Regional air quality models usually contain more detailed chemistry schemes, with a larger number of chemical species, than are required in a local model such as ADMS-Local or ADMS-Urban. For example, regional models generally use NO and NO_2 for nitrogen chemistry rather than NO_2 and NO_x, so the regional model NO_x concentration must be calculated in the MAQS coupled system utilities by combining NO and NO_2 in order to use the ADMS-Local or ADMS-Urban NO_x chemistry module. In order for the MAQS coupled system system to take into account local chemistry effects, a 'species map' must be defined, which contains the factors used to convert between regional model and local model species and units.

It is possible to model individual particulate species in ADMS-Urban if the emissions data are defined with the same species, however it is more common to model 'lumped' particulates such as PM_{10} and $PM_{2.5}$, as these are the classifications by which concentrations are most commonly measured and for which air quality standards and objectives are specified. If the ADMS-Local or ADMS-Urban sulphate chemistry module is required, in order to include local conversion of SO_2 to $PM_{2.5}$ and PM_{10}, lumped particulate species must be used in the local model.

Please refer to Section 4.3.1 for more details of the species mapping method used in the MAQS coupled system.

The file paths and names for the regional model concentration files should follow a pattern which indicates the date and time of the first valid hour of data contained within the file.

The regional model concentration output file names must be compatible with use on the operating system being used for the MAQS coupled system control system.

The regional model output concentration files should either contain hourly average concentrations from each hour of the modelling period, with each file containing one or more hours of data, or period (usually annual) average concentrations for the whole modelling period.

WRF-Chem output files for use in the MAQS coupled system may contain meteorological data only, concentration data only or both meteorological and concentration data. Each file must also contain: the coordinate variables 'XLAT' and 'XLONG'; the geopotential variables 'PH' and 'PHB'; the terrain height variable 'HGT'; and the simulation time variable 'Times'. In addition, the attributes required to define the projected coordinate system in which the grid is regular and orthogonal must be defined, including 'MAP_PROJ' and 'STAND_LON'.

3.5 Other information

ADMS-Local and ADMS-Urban run in local solar time, whereas meso-scale meteorological and air quality models often run in UTC. The user is required to specify the time difference between the regional model data and local solar time.

SECTION 4 System inputs

Before running the MAQS coupled system, the user needs to define the system inputs, for example the file locations of regional model outputs. This section provides a guide to the available input options for the MAQS coupled system and describes how they are specified. An overview of the locations of input data is given in **Table 4.1**.

The system input data is entered into up to five configuration text files, with some additional or alternative command line options as described in Section 2.3.4.

Input	Input file	Section
Regional model meteorological data file type	options.cfg	4.1.1.1
Time difference between local time and regional model time	options.cfg	4.1.1.2
Regional model concentration and emissions data file type	options.cfg	4.1.2.1
Time difference between local time and regional model time	options.cfg	4.1.2.2
Local model type	options.cfg	4.1.3
Step size between output location matching checks	options.cfg	4.1.4
Reference sea-level temperature, model top pressure and/or surface layer heights	options.cfg	4.1.5
Coupled modelling domain extents	options.cfg	4.1.6
Whether to interpolate regional model concentrations	options.cfg	4.1.7
Choice of meteorological variables to extract and whether to adjust invalid heat flux values	option.cfg	4.1.8
File save options	options.cfg	4.1.9
Coordinate system datum settings	options.cfg	0
Permitted number of simultaneously running background processes	options.cfg	4.1.11
Parallel run settings	options.cfg	4.1.12
Location, file-name pattern and hours per file for meteorological data	inputdata.cfg	4.2.1
Path of custom configuration for WRF extraction	inputdata.cfg	4.2.2
File path for concentration species map file	inputdata.cfg	4.3.1
Location, file-name pattern and hours per file for hourly concentration data	inputdata.cfg	4.3.2
File path for the regional model grid heights file	inputdata.cfg	4.3.3
File path(s) for annual average background pollution map files	inputdata.cfg	4.3.4
File path for monthly diurnal background profile data file	inputdata.cfg	4.3.5
File path for *.cco* coordinate conversion definition file	inputdata.cfg	4.3.6
Location, file-name pattern, hours per file and file path for emissions species map files for each type of emissions file	inputdata.cfg	4.4.2
Number of emissions layers to use	inputdata.cfg	4.4.3
Custom 3D emissions data files	inputdata.cfg	4.4.4
Disaggregation options	inputdata.cfg	4.4.5

Input	Input file	Section
Whether model output is for specific receptor locations or a grid for contouring	inputdata.cfg	4.5.1
Output file name stem	inputdata.cfg	4.5.2
Start and end date and time of modelling period	run.cfg	4.6
Whether to use a static *.asp* file and file path	localmodel.cfg	4.7.1
File paths for local model inputs relating to roads: geometry, canyon properties and emissions	localmodel.cfg	4.7.2
Road traffic flow settings	localmodel.cfg	4.7.3
Time varying emission factors	localmodel.cfg	4.7.4
Daylight saving time	localmodel.cfg	4.7.5
File path for site properties file	localmodel.cfg	4.7.6
File path for receptor locations file	localmodel.cfg	4.7.7
Definition of regular grid output	localmodel.cfg	4.7.8
Source-oriented grid point settings	localmodel.cfg	4.7.9
List of output pollutants	localmodel.cfg	4.7.10
Chemistry options	localmodel.cfg	4.7.11
Conversion factors	localmodel.cfg	4.7.12
File path(s) for ADMS-Urban input *.upl* file(s)	localmodel.cfg	4.7.13
SSH login details of runs machines to use in parallel processing and the permitted runs for each	sshlogin.cfg	4.8

Table 4.1 Summary of system inputs. The Section column indicates the location of further information about each option.

4.1 Modelling options

The *options.cfg* file contains options that may need to be changed for different modelling scenarios, but are unlikely to vary between runs. Key folder configuration options, such as the working and default input directories, can be found in *folders.cfg*, described in Section 2.2.1.

4.1.1 Regional model meteorological data file type

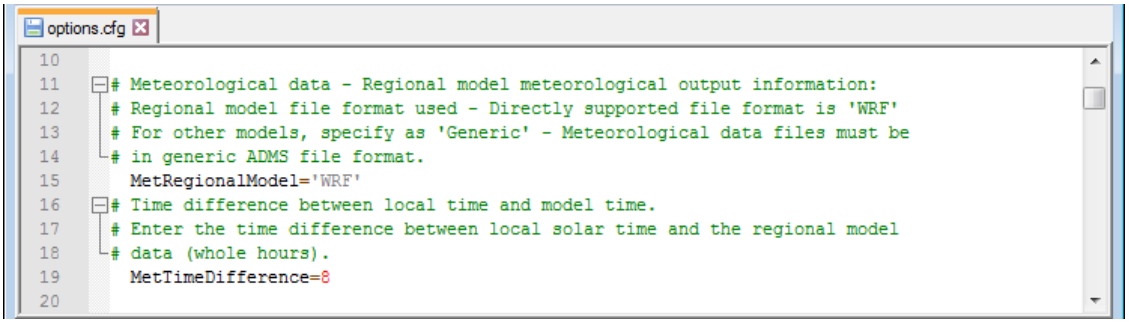


Figure 4.1 The meteorological model data variables in the *options.cfg* file

4.1.1.1 Regional model used

Specify the mesoscale meteorological model file format from which met data can be extracted by setting the variable `MetRegionalModel` in the *options.cfg* file, with available options:

- `='WRF'` for WRF;
- `='Generic'` for other data in Generic 2D grid format.

The system directly reads WRF meteorological data to drive the model. When using other mesoscale meteorological models, data must be re-gridded and re-formatted into the generic 2D grid file format (described in Section 4.2.3), then select the `Generic` option for `MetRegionalModel`.

4.1.1.2 Time difference between local time and regional meteorological model time

Enter the time difference between local solar time, as used in ADMS-Local and ADMS-Urban, and the time zone used in the meteorological model data files, in whole hours using the variable `MetTimeDifference` in *options.cfg*.

Regional models are often run in a standard time system such as UTC, whereas ADMS-Urban and ADMS-Local run in local solar time. For example, if meteorological data are obtained with UTC times and the local solar time is UTC +8, as in Hong Kong, a value of 8 should be entered. Both positive and negative values of time difference are permitted.

If the local solar time for your modelling area is a non-integer number of hours different from the time zone used in the meteorological model data files, enter the nearest whole hour value for the time difference.

4.1.2 Regional model concentration and emissions data file type

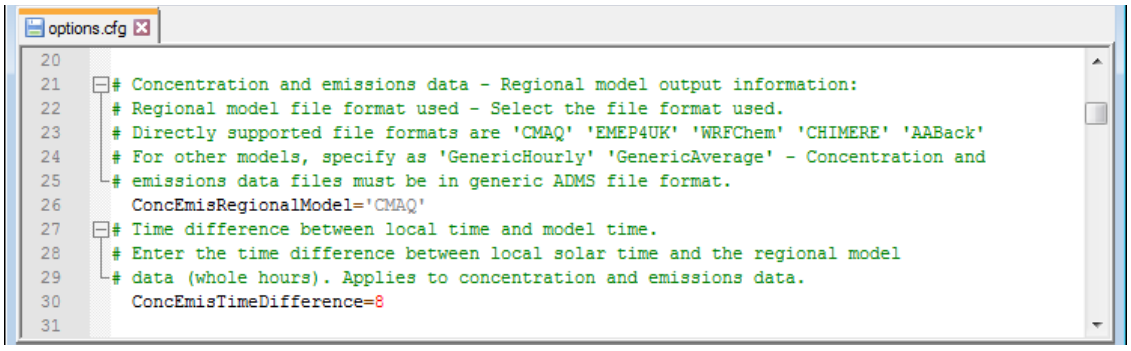


Figure 4.2 The regional model concentration data variables in the *options.cfg* file.

4.1.2.1 Regional model used

Specify the regional model from which concentration and emissions output files are available by setting the variable `ConcEmisRegionalModel` in the *options.cfg* file.

The available options for hourly regional model data are:

- `='CMAQ'` for CMAQ or CAMx in I/OAPI format;
- `='EMEP4UK'` for EMEP4UK;
- `='CHIMERE'` for CHIMERE;
- `='WRFChem'` for WRF-Chem; and
- `='GenericHourly'` for other data in Generic 3D data format.

Supported annual average regional concentration data options are:

- `='AABack'` for the Defra background maps; and
- `='GenericAverage'` for other data in Generic 2D data format.

Direct links are available for regional model outputs from CAMx, CMAQ, EMEP4UK, CHIMERE and WRF-Chem. CAMx output files must be converted into the I/OAPI format for use in the MAQS coupled system. Any other regional model data re-gridded and re-formatted into the generic file formats could be used by selecting either of the GenericHourly or GenericAverage options.

Note that, if CHIMERE is chosen as the regional model, a coordinate conversion definition file must be created. Please refer to Section 4.3.6 for further details.

4.1.2.2 Time difference between local time and hourly regional model time

Enter the time difference between local solar time, as used in ADMS-Local and ADMS-Urban, and the time zone used in the regional model data files, in whole hours using the variable `ConcEmisTimeDifference` in *options.cfg*.

If the local solar time for your modelling area is a non-integer number of hours different from the time zone used in the regional model data files, enter the nearest whole hour value for the time difference.

4.1.3 Local model

The regional model is linked to a local urban dispersion model, referred to as ADMS-Local, which is intrinsic to the MAQS coupled system. The widely used ADMS-Urban is also supported by the system as an alternative local dispersion model. Select the model to be used by the system by setting the variable `LocalModel` in the *options.cfg* file.

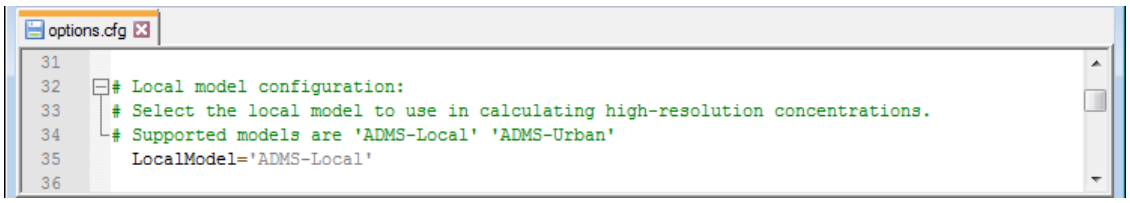


Figure 4.3 The local model option in the *options.cfg* file

Note that a valid licence is required to be able to use ADMS-Urban as the local model. The ADMS-Urban licence file should be copied to the model directory.

ADMS-Urban can only be used as the local model with hourly regional model concentration data. ADMS-Local can be used with both hourly and annual average regional model concentration data.

4.1.4 Step size between output location matching checks

The calculation of nested output concentrations requires local model output from runs with gridded and explicit emissions at exactly matching output locations. The locations are checked by the **Processor** utility to ensure that they match to within a suitable tolerance. If a MAQS coupled system run includes a large number of output points, it may be desirable to increase the step size between checks in order to reduce the **Processor** utility run times. The control scripts enforce matching output locations in the runs with gridded and explicit emissions by using the same *.asp* file in both runs, so the step size is set to a default large number value of 100000.

The step size option is enabled by `UseOptLocMatchFrequency=1` and the value specified by `OptLocMatchFrequency=value`, both in the *options.cfg* control file.

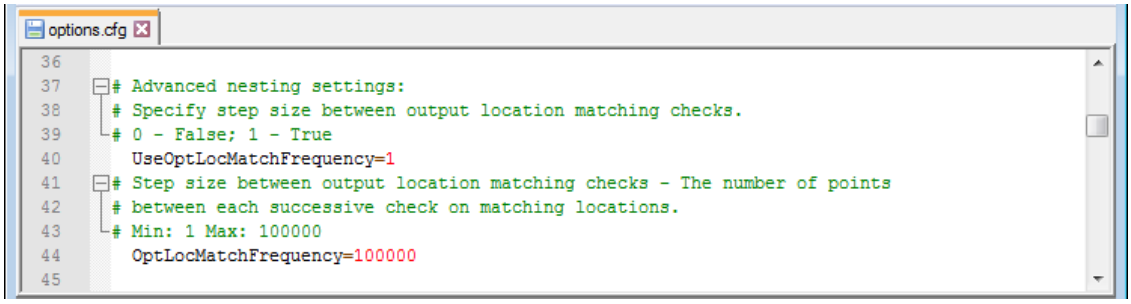


Figure 4.4 The step size option in the *options.cfg* file

If the output type option is set to Receptor (refer to Section 4.5.1 for more details) with ADMS-Urban as the chosen local model and two .upl *files are input, the user-specified output locations are retained for each run so the step size should be set to 1, to ensure that all output locations are checked for matching coordinates.*

4.1.5 Reference conditions

This section contains temperature and pressure conditions which are used to convert regional model layer sigma coordinate values into heights, in order to select the appropriate regional model vertical grid layer for output concentrations, as described in Appendix A.1. These values are not required for WRF-Chem as this model has a different type of vertical grid specification, nor for CMAQ where an additional file is used to define the vertical grid specification. This section also contains the option to set the layer depth of a single-layer regional model grid.

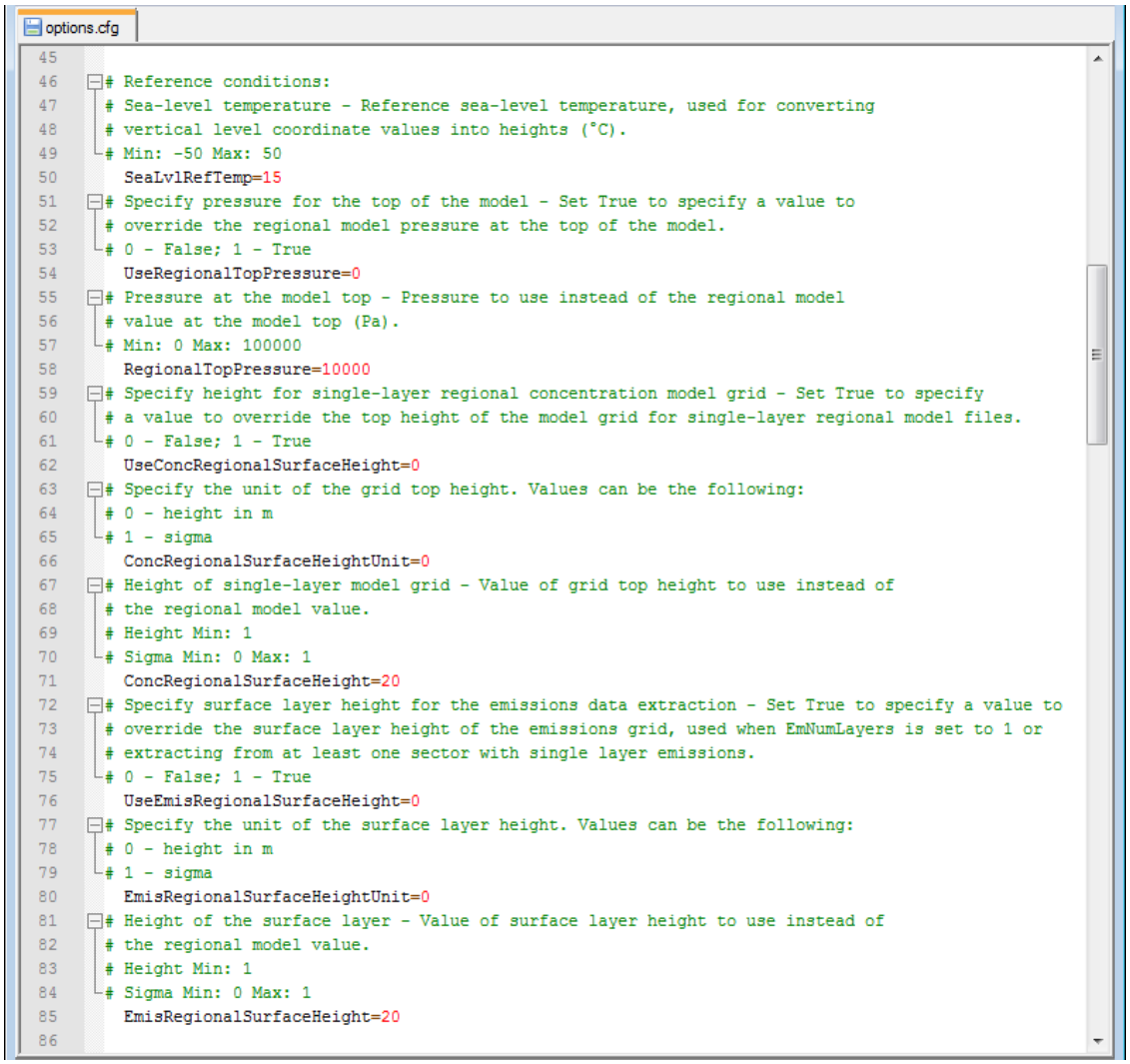


Figure 4.5 The reference conditions variables in the *options.cfg* file

- **Sea-level temperature**

  Enter a standard sea-level temperature for the modelling domain in degrees Celsius, for example an annual or period average for the modelling domain, by setting the variable `SeaLvlRefTemp` in the *options.cfg* control file.

- **Specify reference pressure for the top of the model**

  By default the MAQS coupled system control scripts and utilities will obtain the pressure at the top of the regional model grid from the concentration output files. However, this value may be incorrect if the output has been re-formatted. The user option to specify a reference pressure, overriding the model-top pressure found in the regional model concentration output files, is enabled by setting the variable `UseRegionalTopPressure=1` in the *options.cfg* control file. The reference value of model-top pressure is entered in Pascals by setting the variable `RegionalTopPressure` in the same file.

  If you are using output files from the CMAQ or CAMx regional models in IOAPI format, the model top pressure can be found from the value of the VGTOP attribute.

- **Specify the height for the single-layer grid of the regional concentration model**

  The vertical layer heights of the regional model grid are extracted from the concentration output files by default, if available. Some regional model output data are cut down to a single vertical layer. However, the layer depth may not be available or accurate within the file. To enable the user option to define the layer height, set the variable `UseConcRegionalSurfaceHeight=1` in the *options.cfg* control file and then set the variable `ConcRegionalSurfaceHeightUnit` to specify whether the value will be defined as absolute height above ground level in metres or in pressure (sigma) coordinates. The height value is entered by setting the variable `ConcRegionalSurfaceHeight` in the same file, overriding the layer height within the regional model file.

  If using annual average Defra background concentration maps and this option is not enabled, the height value will be set to 10 metres by default.

- **Specify the height of the surface layer for the extraction of single-layer emissions data**

  In the extraction of regional model emissions data, the user has the option to define the vertical layer height if extracting only a single layer of data or if processing at least one sector with a single layer of emissions. Set the variable `UseEmisRegionalSurfaceHeight=1` in the *options.cfg* control file to enable the option and then set the variable `EmisRegionalSurfaceHeightUnit` to specify whether the value will be defined as absolute height above ground level in metres or in pressure (sigma) coordinates. Enter the height value by setting the variable `EmisRegionalSurfaceHeight` in the same file.

4.1.6 Nesting domain

The geometry of the nesting domain, which is the spatial region within which nesting calculations will be performed, is defined by specifying corner coordinates as shown in **Figure 4.6**.

Note that the nesting domain must be defined to coincide with a rectangular set of regional model grid cells, to within a tolerance of 1% of the regional model grid cell size.

The nesting domain must be fully within the regional model grid, with a border of at least one unused cell in each direction, to allow the local upwind background concentrations to be calculated using the cells bordering the nesting domain for any upwind direction.

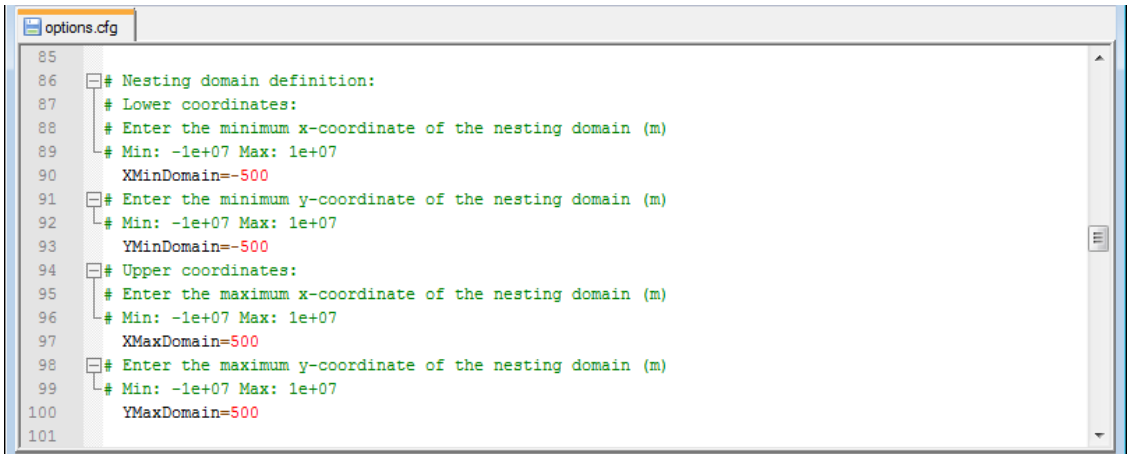


Figure 4.6 The lower left and upper right x and y coordinates of the nesting domain in the *options.cfg* file

Enter the minimum (lower left) and maximum (upper right) x and y coordinates of desired nesting domain using the variables `XMinDomain`, `YMinDomain`, `XMaxDomain` and `YMaxDomain` in the *options.cfg* file. The coordinates should be given in a projected coordinate system consistent with that used to define the regional model grid and in which the regional model grid is regular and orthogonal. As in ADMS-Local and ADMS-Urban, all coordinate values must be entered in metres.

Refer to Section 2.3.2 for more information on valid formats for numerical values in the input files.

4.1.7 Interpolate regional model concentrations

The user option to interpolate regional model concentrations will result in smoother contours across regional model cell boundaries. Set the `InterpRMConc` variable to 1 in the *options.cfg* file in order to use this option. Using this setting both applies interpolation to the regional model concentrations and changes settings for the local model runs such that the runs with gridded emissions include similar interpolation.

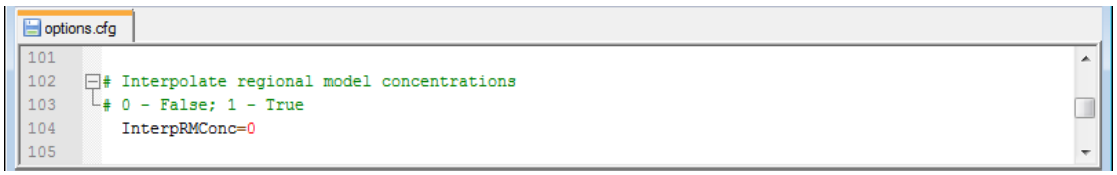


Figure 4.7 The option to interpolate regional model concentrations in the *options.cfg* file

4.1.8 Meteorological variables

This section contains the options for selecting which meteorological variables will be extracted by the **RM Met Data** utility and included in generating *.met* files for input to the local model. If selecting any variable for extraction, the attribute or variable must be available in the meteorological output files for the whole modelling period and the unit must be the same as that required by the local model, except for temperature which is converted from Kelvin to Celsius (as described in Appendix D.2).

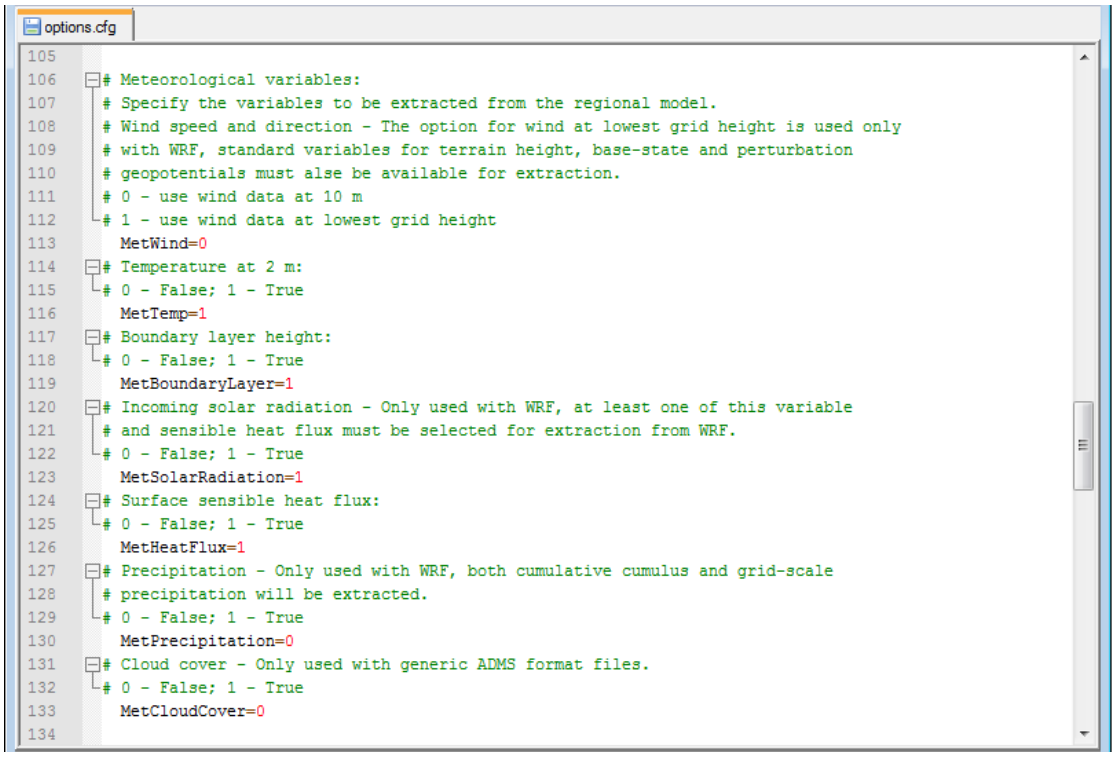


Figure 4.8 The meteorological variables to extract in the *options.cfg* file

- **Horizontal wind speed and direction**

  The wind speed conditions are always extracted and assumed to be in units of metres per second (m/s). Setting the variable `MetWind=0` in the *options.cfg* file enables extraction of wind speeds at 10 metres above ground level. An alternative option, if extracting from WRF meteorological data files, is to set the variable `MetWind=1` in the same file to extract wind speeds at the lowest grid height. If using the latter option, the terrain heights, base-state and perturbation geopotentials variables will also be extracted.

- **Near surface air temperature**

  Temperature at 2 metres can be extracted if it is available in the meteorological data. Values are assumed to be in units of Kelvin, conversion is then applied as ADMS-Local and ADMS-Urban expect degrees Celsius (°C) in input files. Setting `MetTemp=1` in the *options.cfg* file will select this variable for extraction.

- **Boundary layer height**

  Boundary layer height in metres can be extracted if it is available in the meteorological data. Setting `MetBoundaryLayer=1` in the *options.cfg* file will select this variable for extraction.

- **Incoming solar radiation**

  Incoming solar radiation in Watts per metre squared (W/m^2) is extracted only if WRF is chosen as the meteorological model and ADMS-Urban as the local model. Selecting `MetSolarRadiation=1` in the *options.cfg* file will select this

variable for extraction.

At least one of solar radiation and surface sensible heat flux must be selected for extraction from WRF in order to create valid .met *files for use in ADMS-Urban. The selection of both of these variables is recommended in order to support chemistry calculations.*

- **Surface sensible heat flux**

  Surface sensible heat flux in Watts per metre squared (W/m^2) can be extracted if it is available in the meteorological data. Setting `MetHeatFlux=1` in the *options.cfg* file will select this variable for extraction.

If ADMS-Local is the selected local model, the surface sensible heat flux must be selected for extraction. For ADMS-Urban, if the surface sensible heat flux is not selected for extraction, either solar radiation or cloud cover must be specified if available in the regional model data. That is, if extracting from WRF solar radiation must be used, otherwise if extracting from generic files cloud cover must be used.

- **Precipitation**

  Precipitation is extracted only if WRF is chosen as the meteorological model and will only be used if ADMS-Urban is selected as the local model and wet deposition calculations are implemented. As WRF output contains cumulative precipitation values in millimetres, these are converted to hourly rates by subtracting the previous hour's cumulative precipitation from the current hour. If extracting this variable, data from the hour before the specified start time must also be available. Setting `MetPrecipitation=1` in the *options.cfg* file will select this variable for extraction.

- **Cloud cover**

  Cloud cover is extracted only if extracting from generic meteorological format files and with ADMS-Urban selected as the local model. Values are expressed as a dimensionless fraction in the file and then converted to oktas for compatibility with the local model. Setting `MetCloudCover=1` in the *options.cfg* file will select this variable for extraction.

If using generic files, either cloud cover or surface sensible heat flux must be selected for extraction in order to create valid .met *files for use in ADMS-Urban. If both variables are selected, ADMS-Urban will only use the surface sensible heat flux.*

- **Adjust invalid heat flux values**

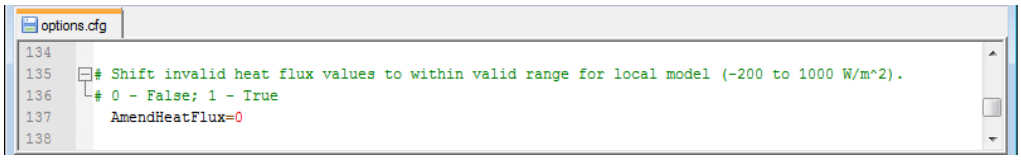


Figure 4.9 The `AmendHeatFlux` variable in the *options.cfg* file

Some modelled meteorological data files include surface sensible heat flux values outside the allowed range for ADMS-Local or ADMS-Urban. This will cause MAQS coupled system runs to stop with an error. The **RM Met Data** utility will adjust invalid values to within the valid range if the variable `AmendHeatFlux=1` is set in *options.cfg*.

4.1.9 File storage options

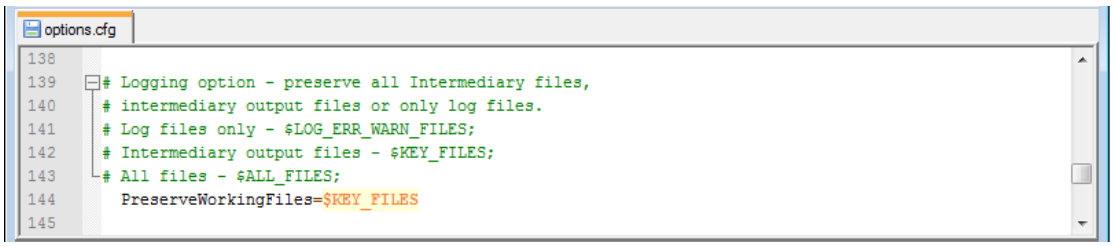


Figure 4.10 The `PreserveWorkingFiles` variable in the *options.cfg* file

The `PreserveWorkingFiles` variable gives options for the number and types of intermediate files which should be saved and returned by the MAQS coupled system, in addition to the results files:

- The default option is only to keep log files, which will include any information, warning and/or error messages issued by each component of the coupled system. This requires the least storage space and is suitable for all types of system runs. The variable setting `PreserveWorkingFiles=$LOG_ERR_WARN_FILES` should be used to specify this option.
- The intermediate option is to keep 'key files', which includes all ADMS format meteorology and background concentration files; these files may be useful for model validation and comparison purposes. A list of the files included in the 'key files' category is given in **Table 4.2**. If any component of the coupled system fails, the input and any output files for that component will also be saved. The variable setting `PreserveWorkingFiles=$KEY_FILES` should be used to specify this option.

  Note that if the nesting domain is large and the MAQS coupled system is run for an extended modelling period, this option may generate a large volume of data.

- The final option is to keep all the files used in every component of the coupled system, which may be useful for detailed investigation of the system behaviour. Due to the number and size of files involved in the MAQS coupled system, this option is not recommended for runs with large nesting domains or large numbers

of output locations.

The variable setting `PreserveWorkingFiles=$ALL_FILES` should be used to specify this option. Alternatively, the value of `PreserveWorkingFiles` can be overridden by using the `-p` command line option to select this option, as described in Section 2.3.4.

File extension	MAQS coupled system component	File description	Each cell?
.txt	Extraction of regional model grid information	**RM Grid Info** utility output grid information file	N
.asp	Extraction of regional model grid information	**RM Grid Info** utility output file defining output locations in centre of regional model surface layer grid cells	N
.nc	Extraction of regional model grid information	ADMS format 2D annual average concentrations file (only when using annual average background maps)	N
.nc	Conversion of regional model emissions data into ADMS format (optional)	ADMS 3D hourly emissions file	N
.asp	Creation of *.asp* file containing source-oriented grid points	ADMS additional specified point location input file (runs for contour output only)	N
.met	Extraction of WRF met data	ADMS format met file	Y
.bgd	Extraction of local upwind background	ADMS format background file	Y
.nc	Initial local model run for nesting background	ADMS comprehensive output file	Y
.bgd	Calculation of nesting background concentrations	ADMS format background file	Y
.nc	Main local model runs (gridded and explicit emissions)	ADMS comprehensive output file format	Y
.bgd	Local model run with explicit emissions (annual average only)	ADMS format background file containing annual average NOx/NO_2 in photo-stationary equilibrium	Y
.nc	Calculation of MAQS output concentrations	Nested output (runs for contour output only)	Y
.nc	Combination of nested output from multiple grid cells	Combined nested output prior to addition of interpolated source-oriented grid points (runs for contour output only)	N

Table 4.2 List and descriptions of files kept under the 'key files' option. The 'Each cell?' column indicates whether files are created for each regional model grid cell covered by the nesting domain.

4.1.10 Coordinate system datum

This section contains information about the datum underlying the projected coordinate system in which the regional model grid is rectilinear and orthogonal. There are two pre-set options, EMEP sphere for a spherical datum with radius 6370 000 m (as used internally in the EMEP and WRF models) or WGS84 for an ellipsoid datum. The user can also specify an alternative spherical or ellipsoid datum by setting the datum type to 'Custom' and entering appropriate values for semi-major axis and inverse flattening. There is an additional 'datum' option for use when annual average background concentration maps from Defra (which are in UK national grid, OSGB) are used in combination with WRF meteorological output. The OSGB eastings and northings are converted into longitudes and latitudes using the Airy 1830 ellipsoid. The met data extraction process then uses the EMEP sphere datum. Further details of the datum setting options are given in Appendix A.2. The input control file variables used to define the coordinate system datum are shown in **Figure 4.11**.

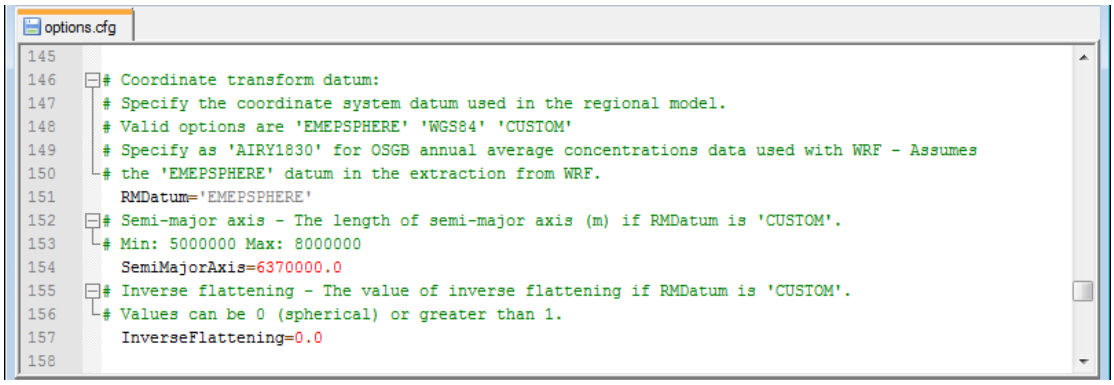


Figure 4.11 The `RMDatum` variable and associated coordinate transform parameters in the *options.cfg* file

- **Coordinate datum type**

  Select the appropriate coordinate datum type by setting the variable `RMDatum` in the *options.cfg* file, with available options:

  * `='EMEPSPHERE'` for the EMEP sphere;
  * `='WGS84'` for the WGS84 ellipsoid;
  * `='AIRY1830'` for the Airy 1830 ellipsoid (only allowed with annual average background concentration maps and WRF meteorological data); and
  * `='CUSTOM'` for a user-defined sphere or ellipsoid, requiring further parameters as described below.

- **Semi-major axis length**

  Set the value in metres of semi-major axis length for an ellipsoid custom datum or the radius for a spherical custom datum using the variable `SemiMajorAxis` in the *options.cfg* control file.

- **Inverse flattening ratio**

  Set the variable `InverseFlattening` in the *options.cfg* control file to the inverse flattening ratio value (greater than 1) for an ellipsoid custom datum or a value of 0.0 for a spherical custom datum.

4.1.11 Permitted number of background processes

By default all utilities and ADMS-Local runs for the MAQS coupled system are run as background processes on a single computer, where the `run-maqs` main script is located. Each stage, for example the extraction of local upwind background concentrations, is carried out for all cells before the next stage is started. For runs with large nesting domains or large number of cells, the resource limits (which vary with different computers) may not allow for a sufficiently large number of 'jobs', open files or simultaneously running background processes to handle all cells. If these limits are reached, the system will not be able to run all cells and can stop unexpectedly.

Specify the maximum number of simultaneously running processes to an appropriate value for your system by setting the variable `JobLimitCount` in the *options.cfg* file.

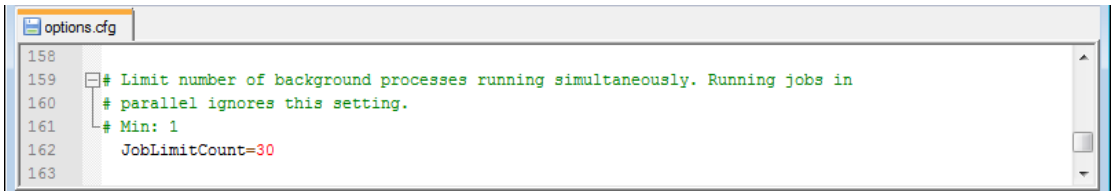


Figure 4.12 The `JobLimitCount` variable in the *options.cfg* file

4.1.12 Parallel running of system

There is a user option for using the GNU parallel library to distribute the utility and ADMS-Local runs for each cell across multiple computers in order to reduce run times. This option also changes the way that operations are grouped in the MAQS coupled system. With the parallel option selected, all processes for a single cell (from extraction of meteorological data to calculation of output concentrations) are grouped and run in sequence, independently of other cells. By default, GNU Parallel determines the number of groups to run on each computer automatically, ignoring the maximum limit set by the `JobLimitCount` variable in the same file. This can reduce the time required for file transfers and increase computational efficiency when multiple machines are in use. There is an associated option to copy system and input files from the host machine to the remote machine(s) and an option to clean up these files on the remote machine(s).

There are two user variables relating to use of the parallel option in the *options.cfg* file, described below and shown in **Figure 4.13**. In order to use the parallel run option the user must also set up the *sshlogin.cfg* file to define the machine(s) to which runs can be distributed, as described in Section 4.8.

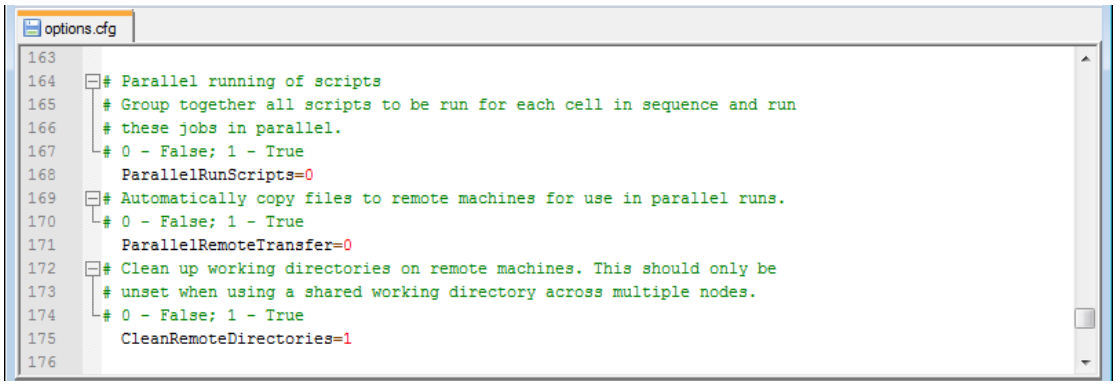


Figure 4.13 The variables used to define use of the GNU parallel library in the *options.cfg* file

- **Run system in parallel**

  Set `ParallelRunScripts=1` in order to use the GNU Parallel option for distributing runs across multiple machines.

- **Automatic file transfers**

  Set `ParallelRemoteTransfer=1` in order to use the option for the system to copy MAQS coupled system script, utility and input files from the host machine to remote machines. The system will create the MAQS coupled system top directory on each remote machine and then copy the directories *SCRIPT_DIR*, *MODEL_DIR*, *UTIL_DIR*, *INPUT_DIR* and *MYDIR/Data*. If this option is used, the working directory (*WORK_DIR*) must be defined within the user's */home* directory. This option is not required if the MAQS coupled system is installed under the same file path on the host machine and remote machine(s) and all input files are available through shared directories.

- **Clean up remote files and directories**

  Set `CleanRemoteDirectories=1` in order to use the option for the system to clean up automatically copied directories on the remote machine(s). This option should be switched off (`CleanRemoteDirectories=0`) if the MAQS coupled system is installed under the same file path on the host machine and the remote machine(s) and all input files are available through shared directories.

4.2 Regional model meteorological data files

Information must be supplied to the MAQS coupled system about the regional meteorological model data used to run the regional air quality model and which will be extracted for use in ADMS-Local or ADMS-Urban. At present, only output from the WRF model is directly supported by the system. Output files from the WRF-Chem model containing both concentration and meteorological data are equivalent to standard WRF output. If you have output data from a different meteorological model, it will need to be re-formatted into Generic 2D grid format for use in the MAQS coupled system, as defined in Section 4.2.3. If you are using regional model data files obtained from a third party provider, you may need to obtain some additional information about the runs in order to specify these inputs.

4.2.1 Meteorological data files

The file paths for regional model output files (containing meteorological, concentration or emissions data) often include date and time information. The location of the files is specified in two parts for the MAQS coupled system:

- a date-independent directory path; and
- a date and/or time-dependent file path template which may also include any date or time-dependent directory structure components.

The use of a file name template enables the MAQS coupled system to generate file paths for regional model output for a specific date and time according to the defined pattern. The template is defined using 'tags', which consist of a percent sign (%) and a single letter, to indicate particular date or time components, for example %Y is used to represent a four-digit year value. A full list of currently available tags with example values for two dates is given in **Table 4.3**.

The following example shows a typical directory and file name structure for hourly WRF output files:

/usr/WRF/run1/<year>/<month>/wrfout_<year>-<month>-<day>_<hour>0000

where the terms in angle brackets indicate a numerical value, such that the path for the file containing data for 1 am on 1st January 2014 has file path

/usr/WRF/run1/2014/01/wrfout_2014-01-01_010000

This directory and file name structure would be entered into the input file by specifying the date-independent directory

```
usr/WRF/run1/
```

and the date-dependent file name template as

```
%Y/%M/wrfout_%Y-%M-%D_%h0000
```

Note that the tag character is case-sensitive to distinguish between %M for month and %m for minute. The values for minute and second tags are always set to zero.

Tag	Description	Example values	
		1 am 1st January 2014	**2 pm 6th March 2010**
%Y	Four-digit year	2014	2010
%M	Two-digit month	01	03
%D	Two-digit day of month	01	06
%J	Three-digit Julian day	001	065
%h	Two-digit hour	01	14
%m	Two-digit minute	00	00
%s	Two-digit second	00	00

Table 4.3 Tags used to indicate date and time information in file name templates

Note that if the WRF-Chem regional model is in use, the same data files may contain both meteorological and concentration data. The file details will need to be entered in both the meteorological and concentration input data sections.

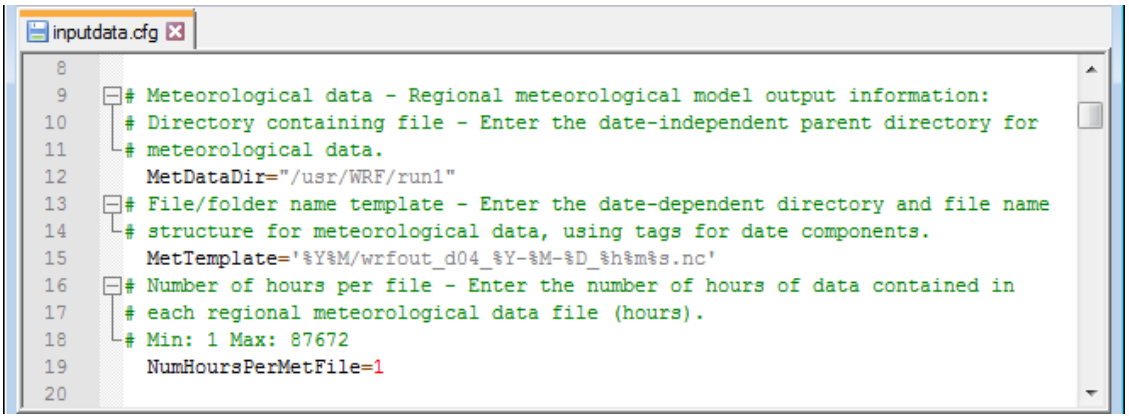


Figure 4.14 The regional model meteorological data variables in the *inputdata.cfg* file

The following items are used to define the meteorological data files for the MAQS coupled system:

- **Directory containing files**

  Specify the date-independent directory used to store the meteorological data files by setting the variable `MetDataDir='/usr/WRF/run1/'` in *inputdata.cfg*.

- **File name template**

  Enter the date-dependent directory and file name structure for the meteorological data files, using tags for date components, in the variable `MetTemplate='%Y/%M/wrfout_%Y-%M-%D_%h0000'` in *inputdata.cfg*.

- **Number of hours per file**

  Specify the number of hours of data included in each meteorological data file by setting the variable `MetHoursPerMetFile` in *inputdata.cfg*.

4.2.2 Custom WRF extraction configuration file

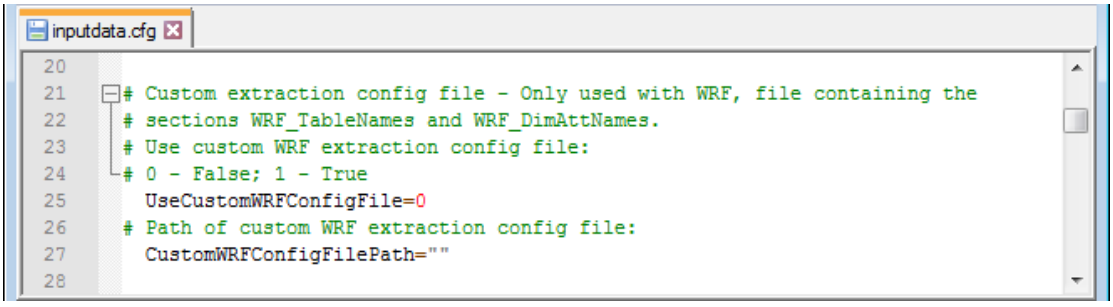


Figure 4.15 The custom WRF extraction configuration file variables in the *inputdata.cfg* file

The user may choose to specify their own configuration file with non-default settings for the utility which extracts ADMS format met data from WRF files, by setting the

variable `UseCustomWRFConfigFile=1` and the variable `CustomWRFConfigFilePath` to a suitable file path in the *inputdata.cfg* control file.

The format of the configuration file is defined in Appendix D.3. An example file can be found in a sub-directory of the MAQS coupled system install directory, by default *<install_path>/Data* (where *<install_path>* is the main script location), and may be used as a template when creating a custom configuration file.

Any user-edited input file for the met extraction utility must not be saved in the MAQS coupled system install directory.

4.2.3 Meteorological data file format

The Generic 2D meteorological data file is a netCDF file which follows CF metadata conventions, containing 2D arrays of meteorological data.

Note that CF-compliance requires that all variable, dimension and attribute names should start with a letter and include only letters, numbers and underscores. Note that the variable and attribute names are case-sensitive.

The dimensions used in the file format are described in **Table 4.4**, the variables in **Table 4.5**, global and variable attributes in **Table 4.6** and attributes associated with specific meteorological data variables in **Table 4.7**.

Name	Description
x	Number of grid cells in x horizontal coordinate direction
y	Number of grid cells in y horizontal coordinate direction
time	Number of time-steps in file (should be defined as the ‘unlimited’ dimension)

Table 4.4 Dimensions in the Generic 2D meteorological data file.

Name	Dimensions	Description
x	x	Cell centre x coordinates in projected coordinates
y	y	Cell centre y coordinates in projected coordinates
time	time	Hour-ending time in days since midnight on 1st January 1900
ADMS_grid_mapping	(none)	Dummy variable containing coordinate projection information attributes
WIND_U10	x, y, time	U-component of horizontal wind speed at 10 m above ground level in m/s
WIND_V10	x, y, time	V-component of horizontal wind speed at 10 m above ground level in m/s
TEMP_T2	x, y, time	Near surface air temperature; this could be screen height 1.22 m or 2 m
HEAT_FLUX	x, y, time	Surface sensible heat flux in W/m^2
BLAYER_HGT	*x, y, time*	*Boundary layer height in m*
CL_COVER	*x, y, time*	*Cloud cover as dimensionless fraction*

Table 4.5 Variables in the Generic 2D meteorological data file. Dimensions are listed with the fastest varying first. The variables in italics are optional.

Associated with	Name	Example value	Comment
Global	Conventions	CF-1.6	May be used by viewing utilities
Global	Title	MAQS 2D Meteorology file	
Global	File_version	ADMS_3DMF_v1.0	Checked by utility
Global	History		May be useful for QA
ADMS_grid_mapping	grid_mapping_name	lambert_conformal_conic	Projection type[1]
ADMS_grid_mapping	earth_radius	6.370e+006	
ADMS_grid_mapping	(projection parameters)		(depend on projection used)
x, y	standard_name	projection_x_coordinate	Allows viewing utilities to identify coordinates
x, y	axis	X	
x, y	units	m	
x, y	grid_mapping	ADMS_grid_mapping	
x, y	resolution_m	1000.0	Allows simple extraction of grid geometry
time	long_name	local time at end of meteorological period	
time	units	days since 1900-01-01 00:00:00	
<all data variables>	long_name		
<all data variables>	units		
<all data variables>	coordinates	x y	
<all data variables>	grid_mapping	ADMS_grid_mapping	
<all_data_variables>	_FillValue	-999.0	

Table 4.6 Global and variable attributes in the Generic 2D meteorological data file. [1]Projection types and required parameters for CF convention compliance are given in Appendix F of the CF Metadata Conventions document.

Variable	long_name attribute	units attribute	Comment
WIND_U10 (or WIND_V10)	U- (or V-) component of horizontal wind speed at 10 m above ground level	m s^-1	
TEMP_T2	Near-surface air temperature (1 - 2 m)	K	Either screen height or 2 m
HEAT_FLUX	Surface sensible heat flux	W m^-2	
BLAYER_HGT	Planetary boundary layer	m	Optional
CL_COVER	Total cloud cover	1	Optional

Table 4.7 Attributes associated with specific meteorological data variables in the Generic 2D meteorological data file.

4.3 Regional model concentration data

The MAQS coupled system links regional model output to either ADMS-Local or ADMS-Urban to allow high-resolution air dispersion modelling. The output files from a range of regional models, including CMAQ, CAMx, EMEP, WRF-Chem, and CHIMERE, are directly supported by the system. The system also links to annual average regional model output, such as Defra's 1 km resolution background map datasets. Output data from other regional models will need to be re-formatted into the appropriate Generic input file format (defined in Section 4.3.7) to allow for compatibility with the MAQS coupled system.

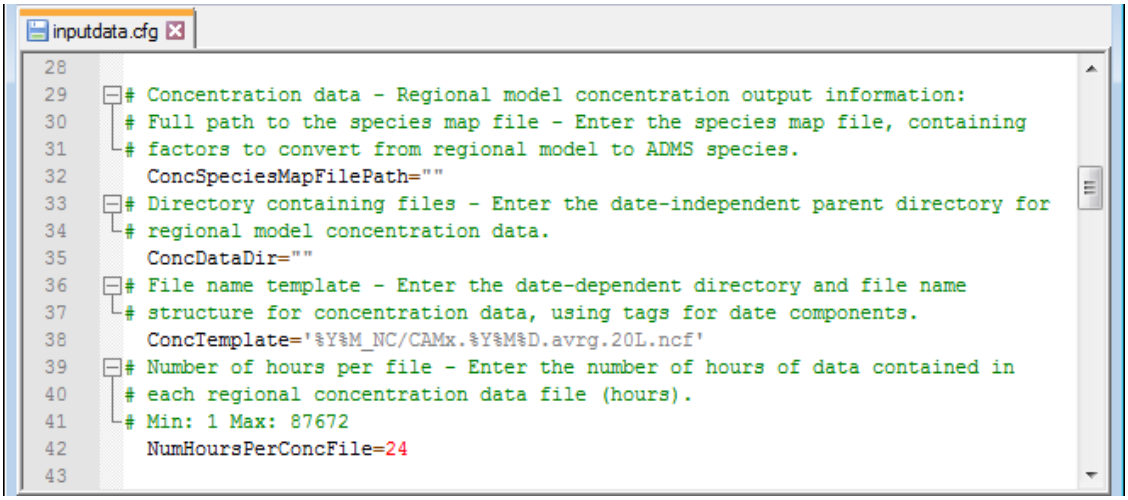


Figure 4.16 The regional model concentration data variables in the *inputdata.cfg* file.

4.3.1 Full path to the concentration species map file

The concentration species map file is used to link regional model output concentration species to local model chemical species. An example species map file is shown in **Figure 4.17** Example concentration species map file viewed in Excel. Select the desired concentration species map file by setting the variable `ConcSpeciesMapFilePath` to a suitable file path in *options.cfg.*

If the option for automatic conversion of regional model emissions files is in use, as described in Section 4.4.1, then there will be two species map files in the MAQS coupled system, one for output concentration species and one for emissions species. In general regional models have different emissions and output species, and the requirements for unit conversion factors are also different between the two files.

The columns in the species map file each represent an ADMS-Local or ADMS-Urban species, and the rows a regional model species. The values in the matrix are conversion factors, such that the value A_i for local model species i in corresponding units (µg/m^3 for concentration, g/m^2/s for emissions) is given by:

$$A_i = \sum_{j=1}^{n_{RM}} S_{ij} R_j$$

where n_{RM} is the number of regional model species, S_{ij} is the species map conversion

factor from regional model species j to local model species i, and R_j is the regional model value for species j in the associated concentration or emissions units. Most of the species map values are 0, but this approach allows:

- regional model species to be part of more than one local model lumped species, for example all $PM_{2.5}$ component species also contribute to PM_{10};
- unit conversion factors to be specific to the local model species, for example the NO contribution to NO_x as NO_2 would have a different conversion factor to NO as an explicit species; and
- local model lumped species to have an arbitrary number of components, for example ten regional model species may contribute to local model PM_{10}, but only one to O_3.

Note that the concentration species map conversion factors should include an appropriate unit conversion to µg/m^3 for all species. The emissions species map conversion factors should include a unit conversion to g/m^2/s.

Local model and regional model species names should be given exactly as used in the models, including capitalisation. In particular, the regional model species names must match the variable name in the relevant netCDF file (concentration or emissions).

Saving the species map file from Excel in .csv *format may lead to extra commas at the end of the header lines.*

The conversion direction keyword is always ROWSTOCOLUMNS within the MAQS coupled system.

Note that if using Defra's gridded annual average background concentration maps as regional model data, no species map file is required by the system.

The structure of the species map file, which should be saved as a comma-separated text file (*.csv*), is as follows:

Version string: 'SPECIESMAPVERSION2'

Conversion direction: 'ROWSTOCOLUMNS'

Number of output (local model) species

Number of input (regional model) species

Header line: 'Variables' followed by comma-separated list of names of all output concentration or emissions species (as used in ADMS-Local or ADMS-Urban)

Data lines: Name of an input species (matching the species variable name used in the regional model netCDF output or emissions files), followed by a comma-separated list of multiplying factors for how much of this input species should be added to each output species, including unit conversions to µg/m^3 (concentration) or g/m^2/s (emissions) where necessary.

	A	B	C	D	E	F	G	H	I
1	SPECIESMAPVERSION2								
2	ROWSTOCOLUMNS								
3	7								
4	19								
5	Variables	O3	NO2	NOX	SO2	CO	PM10	PM2.5	
6	O3	2000	0	0	0	0	0	0	
7	NO2	0	1900	1900	0	0	0	0	
8	NO	0	0	1900	0	0	0	0	
9	SO2	0	0	0	2700	0	0	0	
10	CO	0	0	0	0	1160	0	0	
11	PNO3	0	0	0	0	0	1	1	
12	PSO4	0	0	0	0	0	1	1	
13	PNH4	0	0	0	0	0	1	1	
14	POA	0	0	0	0	0	1	1	
15	PEC	0	0	0	0	0	1	1	
16	FPRM	0	0	0	0	0	1	1	
17	FCRS	0	0	0	0	0	1	1	
18	CPRM	0	0	0	0	0	1	0	
19	CCRS	0	0	0	0	0	1	0	
20	NA	0	0	0	0	0	1	0	
21	PCL	0	0	0	0	0	1	0	
22	PH2O	0	0	0	0	0	0	0	
23	ASOA	0	0	0	0	0	1	1	
24	BSOA	0	0	0	0	0	1	1	
25									

ADMS_CAMx_SpeciesMap

Figure 4.17 Example concentration species map file viewed in Excel

4.3.2 Concentration data files

This section contains items relating to the regional model concentration data files, similar to those for meteorological data files. Please refer to Section 4.24.2.1 for more details of the specification of date-independent directory path and date-dependent file name template, which are the same for both the meteorological and concentration data files.

Note that if the WRF-Chem regional model is in use and the WRF-Chem data files contain both meteorological and concentration data, the concentration data file inputs will be the same as the meteorological file inputs.

If using Defra's gridded annual average background concentration maps, these variables are ignored by the MAQS coupled system and the input data files are specified differently. Please refer to Section 4.3.4 for further details.

- **Directory containing files**

  Specify the date-independent directory containing the regional model concentration data files by setting the variable `ConcDataDir` to an appropriate file path in *inputdata.cfg*.

- **File name template**

  Specify the file name pattern including date and time information by setting the variable `ConcTemplate` in *inputdata.cfg*, using tags as described in **Table 4.3**. Please refer to Section 4.2.1 for more details of the file name template conventions.

- **Number of hours per file**

  Specify the number of hours of concentration data contained in each regional model concentration file by setting the variable `NumHoursPerConcFile` in *inputdata.cfg*. For example, if a separate regional model data file is created for each modelled day, a value of 24 should be entered.

4.3.3 Regional model grid height file (CMAQ only)

In general, regional model output files contain information relating to the height of each vertical layer in the regional model grid. However, newer versions of the CMAQ model (version 5.3 onwards) include the option to use hybrid vertical coordinates in modelling. In such cases, the height information is included in the CMAQ output files and an additional data file is required to define the regional model grid height(s). Set the variable `UseGridHeightsFile=1` and the variable `GridHeightsFilePath` to a suitable file path in *inputdata.cfg*. The file must be a netCDF file containing 3D gridded data and the variable `ZF`, which is the full-layer (grid top) height values in metres varying in space (dimensioned x, y, z) and time. The METCRO3D output file from the Meteorology-Chemistry Interface Processor (MCIP) component of the CMAQ modelling system (Otte and Pleim, 2010) for the same domain as the CMAQ concentration output is suitable for use as a grid heights file.

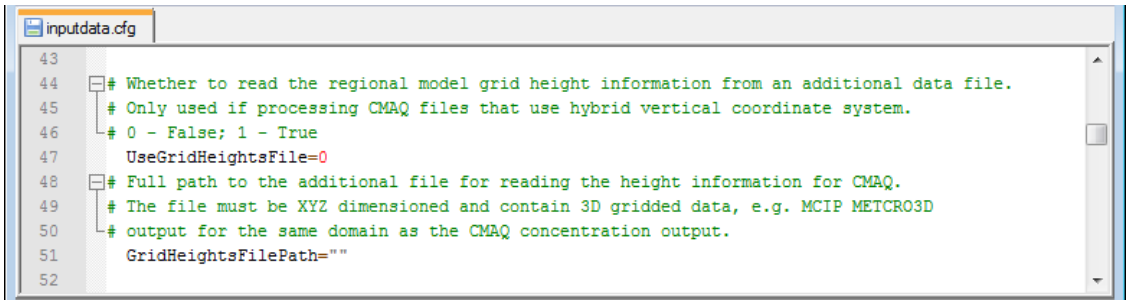


Figure 4.18 The regional model grid height data file variables in the *inputdata.cfg* file

4.3.4 Annual average background pollution map files

This section contains items relating to the input concentration data files if using Defra's 1 km resolution annual average background pollution maps. This option is only available when using ADMS-Local as the local model. Concentration data from the pollution maps are read by the **RM Grid Info** utility and written to a Generic format

intermediate file. Subsequent **Processor** utility runs within the MAQS coupled system work with the Generic format data file.

Summary information about the dataset must be defined in the first four rows of each file containing the pollutant name, modelled year, metric and units.

Annual mean concentrations must be in appropriate units. The MAQS coupled system currently supports µg/m^3 and mg/m^3. Consequently, the user is not required to specify a species map file.

The pollutant names must be consistent with those used in the local model and for which output is to be calculated by the system (refer to Section 4.7.10). There should be a corresponding file for each output pollutant.

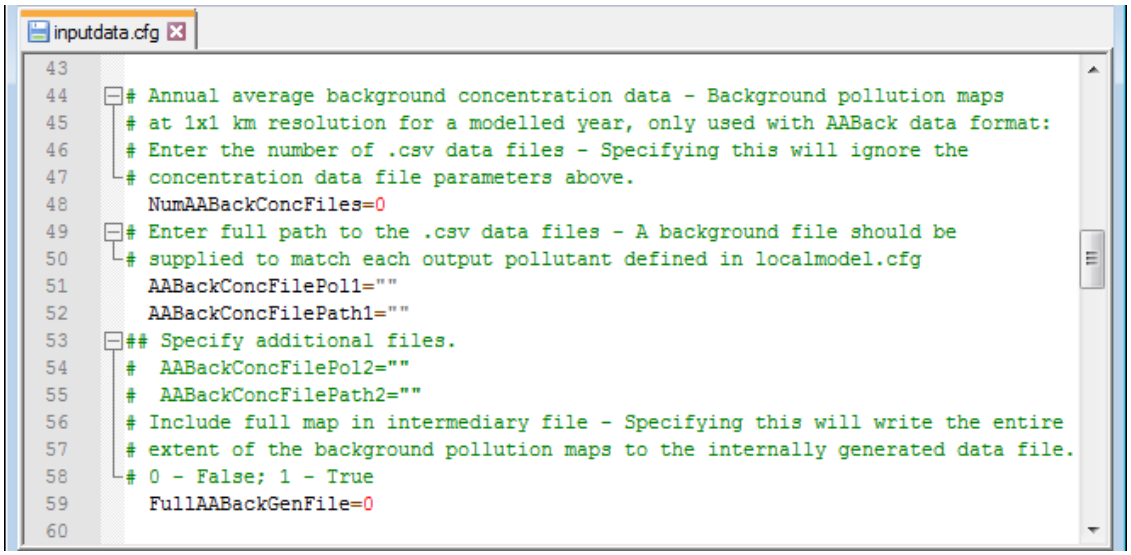


Figure 4.19 The annual average concentration data variables in the *inputdata.cfg* file

- **Number of data files**

  Specify the number of annual average background pollution map files to process by setting the variable `NumAABackConcFiles` in *inputdata.cfg*.

- **Full path to the data files per output pollutant**

  Specify the appropriate data file for each output pollutant by setting the `AABackConcFilePol<N>` and `AABackConcFilePath<N>` variables, where `<N>` is replaced by the file number, for example `AABackConcFilePol1`, `AABackConcFilePath1`. The variables for two files are defined in the default *inputdata.cfg* file but the user may define additional files as required.

- **Write full extents to intermediate file**

  By default, the intermediate file will only contain data for the nesting domain and a border of one cell on each side to minimise file size. The user may choose to include the entire domain by setting the variable `FullAABackGenFile=1` in *inputdata.cfg*.

4.3.5 Background profile data file

If modelling NO_x chemistry effects with annual average regional model concentrations, the user must supply appropriate monthly-varying diurnal profiles of rural background NO_x, NO_2 and O_3 concentrations for the nesting domain. The background data is used by ADMS-Local to adjust the primary NO_x and NO_2 values into photo-stationary equilibrium with local O_3, applying conservation of mass for NO_x as well as conservation of the total mass of NO_2 and O_3 according to the updated oxidant-partitioning model. Specify the background profile data file by setting the variable `BgdProfFile` to a suitable file path in *inputdata.cfg*.

O_3 should not be specified as an output pollutant when running with annual average regional model concentrations.

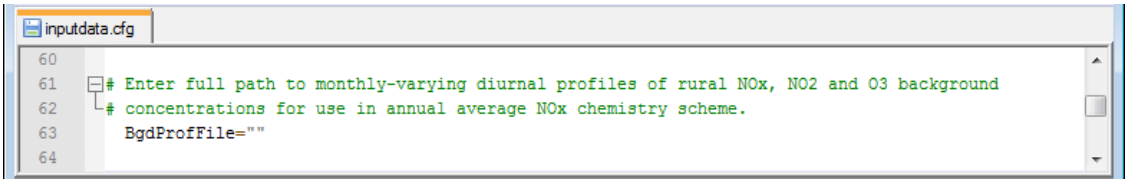


Figure 4.20 The background profile data file variable in the *inputdata.cfg* file

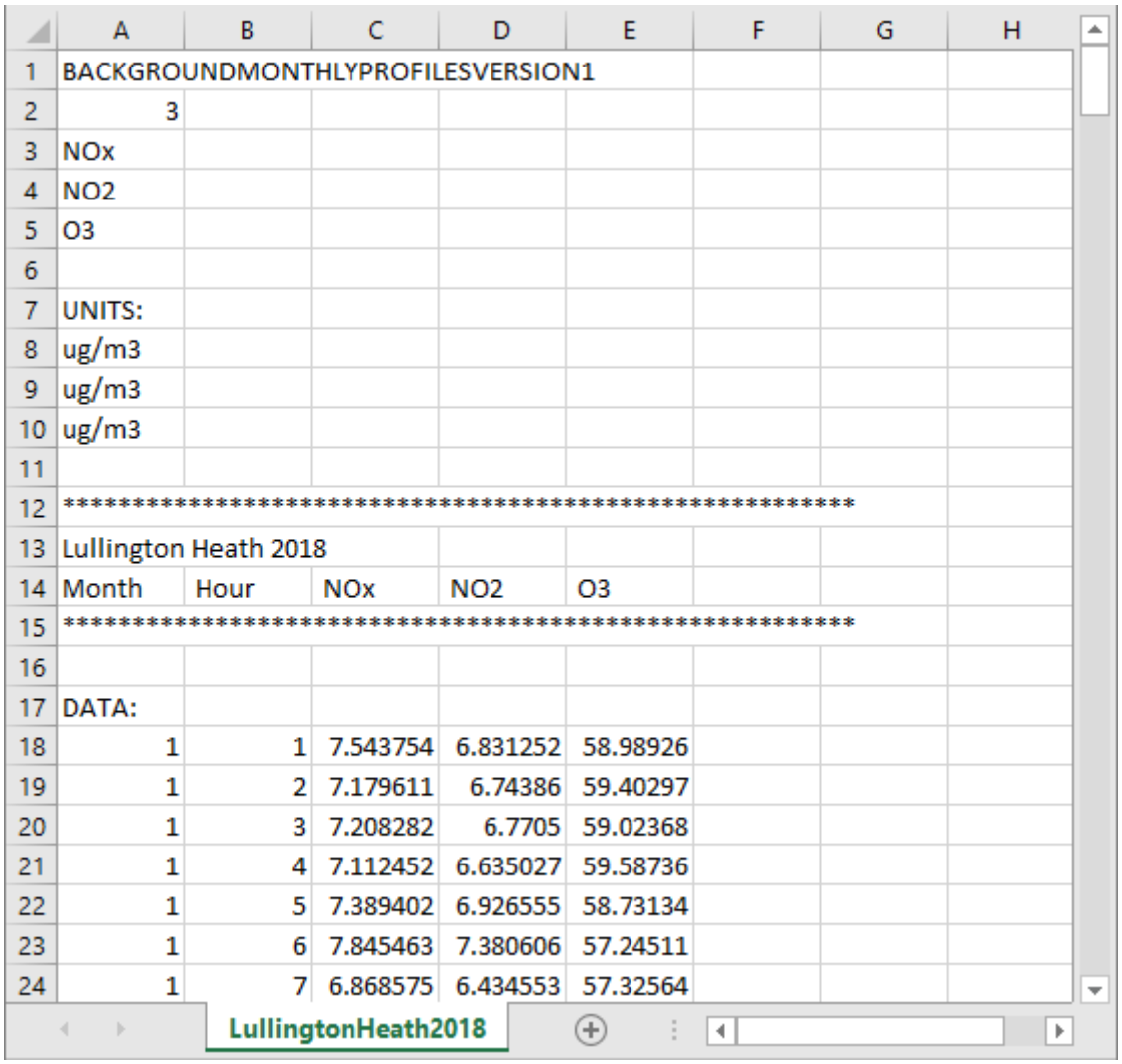
The format of the background file, which is a comma-separated text file, is as described below. An example file is shown in **Figure 4.21**.

Version string: 'BACKGROUNDMONTHLYPROFILESVERSION1'

Pollutants: The number of pollutants for which background data are contained in the file followed by a list of pollutant names (one per line). This should always be NO_x, NO_2 and O_3.

Units: The keyword 'UNITS:' followed by a list of the concentration units for each of the pollutants, in the same order as the pollutant names were listed.

Data lines: The pollutant data listed after the keyword 'DATA:' in the format Month, Hour, Pollutant data.



	A	B	C	D	E	F	G	H
1	BACKGROUNDMONTHLYPROFILESVERSION1							
2	3							
3	NOx							
4	NO2							
5	O3							
6								
7	UNITS:							
8	ug/m3							
9	ug/m3							
10	ug/m3							
11								
12	**********							
13	Lullington Heath 2018							
14	Month	Hour	NOx	NO2	O3			
15	**********							
16								
17	DATA:							
18	1	1	7.543754	6.831252	58.98926			
19	1	2	7.179611	6.74386	59.40297			
20	1	3	7.208282	6.7705	59.02368			
21	1	4	7.112452	6.635027	59.58736			
22	1	5	7.389402	6.926555	58.73134			
23	1	6	7.845463	7.380606	57.24511			
24	1	7	6.868575	6.434553	57.32564			

LullingtonHeath2018

Figure 4.21 Example background profile data file viewed in Excel

4.3.6 .cco coordinate conversion definition file path (CHIMERE only)

CHIMERE regional model output files contain slightly different data to those of other regional models, in that they do not contain any information about the coordinate system in which they are rectilinear, and the coordinates in the regional model files are latitude-longitude values. Therefore, in order to use the MAQS coupled system with CHIMERE regional model files, an additional file must be provided that defines the coordinate conversion from latitude-longitude to projected; a *.cco* file.

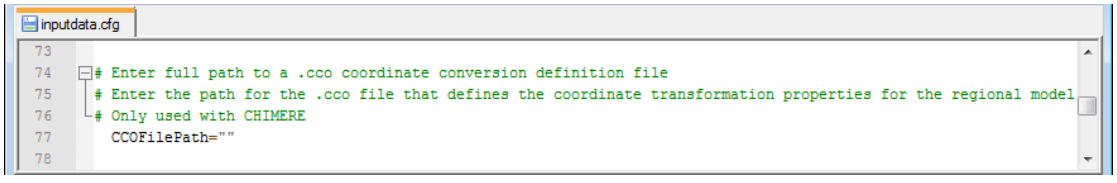


Figure 4.22 The coordinate conversion definition file variable in the *inputdata.cfg* file.

The path of the desired input *.cco* file is defined by setting the `CCOFilePath` variable in the *inputdata.cfg* file, as shown in **Figure 4.22**.

Note that .cco *files can only be used in conjunction with CHIMERE regional model files. For all other regional models the coordinate system must be defined in the regional model output files.*

Three types of projected coordinate systems can be defined through a *.cco* file: Lambert Conformal Conic (LCC), Polar Stereographic (PS) and Universal Transverse Mercator (UTM). Only one of these coordinate conversion systems should be selected and defined at any one time in a *.cco* file.

An example *.cco* file, which defines the Lambert Conformal Conic projection used in the example regional model files, is included in the MAQS coupled system installation *Data* subdirectory for reference. The full format definition for the file is as follows:

The first line of the *.cco* file is the version string `ccofileversion1`.

This is followed by a keyword indicating the type of projection which is in use:

- `LCC` for Lambert Conformal Conic;
- `PS` for Polar Stereographic; or
- `UTM` for Universal Transverse Mercator.

The detailed parameters required depend on the projection used. They should be entered on subsequent lines in the order specified, and should match the definition of projected coordinate system used for the regional model and all local model inputs. All latitude and longitude values should be given in decimal degrees.

Four parameters are required to define the Lambert Conformal Conic projection:

- Reference Longitude;
- Reference Latitude;
- First standard parallel (latitude); and
- Second standard parallel (latitude).

Two parameters are required to define the Polar Stereographic projection:

- Reference Longitude; and
- Reference Latitude – used for determining whether the projection is based on the north or south pole.

One parameter and a keyword are required to define the Universal Transverse Mercator projection:

- UTM zone number – an integer between 1 and 60; and
- Hemisphere keyword: either north or south.

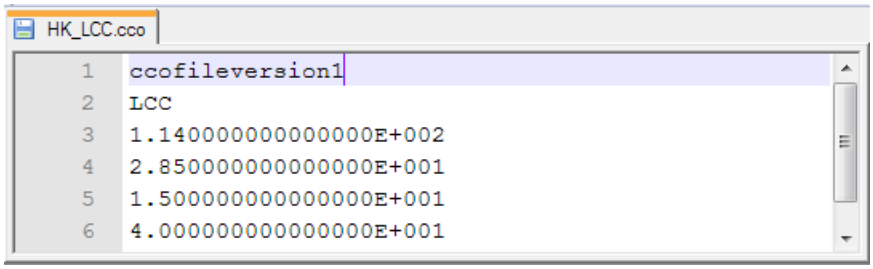


Figure 4.23 An example *.cco* file defining a coordinate system using Lambert Conformal Conic projection.

4.3.7 Concentration data file format

Generic concentration data files are netCDF format files containing 3D gridded hourly or 2D gridded period average concentration data, which follow CF metadata conventions.

Note that CF-compliance requires that all variable, dimension and attribute names should start with a letter and include only letters, numbers and underscores. Note that the variable and attribute names are case-sensitive.

The dimensions used in the file format are described in **Table 4.8**, the variables in **Table 4.9** and common global and variable attributes in **Table 4.10**. Global attributes specific for 2D average concentration files are described in **Table 4.11**.

Name	Description
x	Number of grid cells in x horizontal coordinate direction
y	Number of grid cells in y horizontal coordinate direction
z	*Number of vertical layers of grid cells*
time	*Number of time-steps in file (should be defined as the 'unlimited' dimension)*

Table 4.8 Dimensions in the Generic 2D / 3D concentration data file. The dimensions in italics are only required for 3D hourly files.

Name	Dimensions	Description
x	x	Cell centre x coordinates in projected coordinates
y	y	Cell centre y coordinates in projected coordinates
z	z	*Cell top z coordinate in m above ground level*
time	*time*	*Hour-ending time in days since midnight on 1st January 1900*
ADMS_grid_mapping	(none)	Dummy variable containing coordinate projection information attributes
<pollutant concentration>	x, y, z, time (x, y for 2D files)	One variable for each concentration species, concentration units compatible with conversion to µg/m^3 through species map factors

Table 4.9 Variables in the Generic 2D / 3D concentration data file. Dimensions are listed with the fastest varying first. The variables in italics are only required for 3D files.

Associated with	Name	Example value	Comment
Global	Conventions	CF-1.6	May be used by viewing utilities
Global	Title	MAQS 3D Hourly Concentration file	Refer to Table **4.11** for 2D files
Global	File_version	ADMS_3DCF_v1.0	Checked by model; Refer to Table **4.11** for 2D files
Global	History		May be useful for QA
ADMS_grid_mapping	grid_mapping_name	lambert_conformal_conic	Projection type[1]
ADMS_grid_mapping	earth_radius	6.370e+006	
ADMS_grid_mapping	(projection parameters)		(depend on projection used)
x, y	standard_name	projection_x_coordinate	Allows viewing utilities to identify coordinates
x, y	axis	X	
x, y	units	m	
x, y	grid_mapping	ADMS_grid_mapping	
x, y	resolution_m	1000.0	Allows simple extraction of grid geometry
Z	long_name	height of top of cell above local ground level	3D hourly files only
Z	units	m	
Z	positive	up	
Time	long_name	local time at end of emissions period	3D hourly files only
Time	units	days since 1900-01-01 00:00:00	
<pollutant concentration>, e.g. NO2	long_name	NO2 concentrations	
<pollutant concentration>	units	ug m^-3 or ppb	Unit conversions must be present in the concentration species map file
<pollutant concentration>	coordinates	x y z (x y for 2D files)	
<pollutant concentration>	grid_mapping	ADMS_grid_mapping	
<pollutant concentration>	_FillValue	-999.0	

Table 4.10 Global and variable attributes in the Generic 2D / 3D concentration data file. [1]Projection types and required parameters for CF convention compliance are given in Appendix F of the CF Metadata Conventions document.

Name	Example value	Comment
Title	MAQS 2D Average Concentration file	
File_version	ADMS_2DCF_v1.0	
Period_start_time	43099.0416666667	Days since 1900-01-01 00:00; Checked by the system
Period_end_time	43464	

Table 4.11 Global attributes specific to the Generic 2D average concentration data file.

4.4 Regional model emissions data

There is an option in the MAQS coupled system for automatic conversion of CMAQ or WRF-Chem regional model emissions into Generic 3D gridded emissions format. The converted emissions are then automatically used as gridded emissions in all ADMS-Local or ADMS-Urban runs within the system.

Consistent gridded pollutant emissions in the local and regional models are key to the MAQS coupled system concept, as local model runs with gridded emissions are used to imitate the regional model calculations within the mixing time. This approach is adopted in order to minimise the double-counting of emissions when combining the regional and local model output concentrations, as described in Section 8.1. The option to **Use regional model emissions in all local model runs** is recommended for MAQS coupled system runs with the CMAQ and WRF-Chem regional models as it ensures the required consistency of emissions data.

An equivalent conversion of regional model emissions data into Generic 3D gridded emissions file format through manual processing or EMIT (contact CERC for details) should be considered for other regional models. The resulting emissions file can be specified using the **Use custom 3D emissions data file** option.

The use of the automatic regional model emissions option requires information about the input regional model emissions files, which is specified in the *inputdata.cfg* file, shown in **Figure 4.24**.

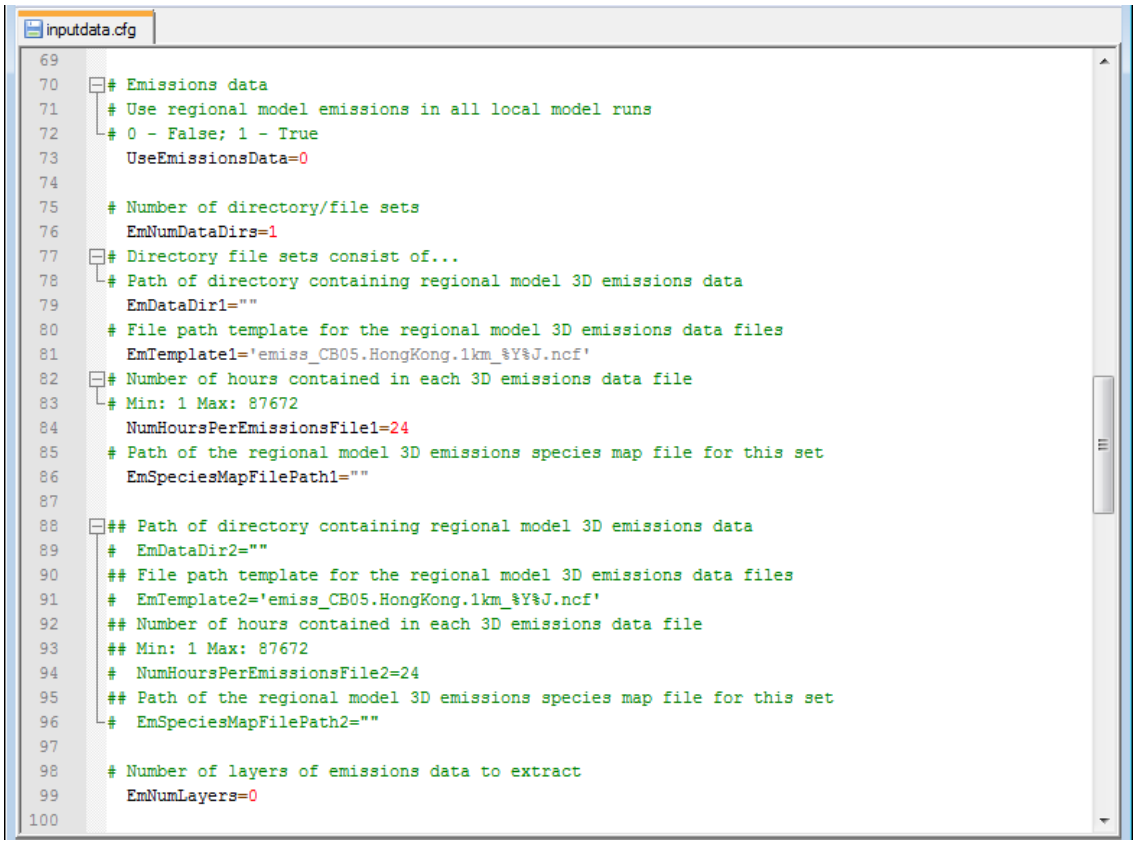


Figure 4.24 The regional model emissions data options in the *inputdata.cfg* file.

4.4.1 Use regional model emissions in all local model runs

Set `UseEmissionsData=1` in the *inputdata.cfg* file to specify that the option for automatic conversion of regional model emissions for use in all local model runs within the system should be used.

4.4.2 Emissions data files

This section contains information about the regional model emissions data files. Multiple types of emissions data can be combined during the conversion from regional model to Generic 3D gridded format, for example those from different source types such as road transport or domestic heating. The utility program used for the conversion is described in Appendix B.

Initially the number of file types must first be specified using the `EmNumDataDirs` variable. For each file type, the `EmDataDir<N>`, `EmTemplate<N>`, `NumHoursPerEmissionsFile<N>` and `EmSpeciesMapFilePath<N>` variables must be defined and set, where `<N>` is replaced by the type number, for example `EmDataDir1`, `EmTemplate1`. The variables for two types are defined in the default configuration files, but the user may define additional types as required. All of these variables are set in the *inputdata.cfg* file.

Please refer to Section 4.2.1 for more details of the specification of date-independent directory path and date-dependent file name template, which are the same for the meteorological, concentration and emissions files.

- **Directory containing files**

  Specify the date-independent directory containing the current type of regional model emissions data files by setting the variable `EmDataDir<N>` to an appropriate file path in *inputdata.cfg.*

- **File name template**

  Specify the file name pattern including date and time information by setting the variable `EmTemplate<N>` in *inputdata.cfg,* using tags as described in **Table 4.3**. Please refer to Section 4.2.1 for more details of the file name template conventions.

- **Number of hours per file**

  Enter the number of hours of emissions data contained in each regional model emissions file of the current type, by setting the variable `NumHoursPerEmissionsFile<N>` in *inputdata.cfg*. For example, if a separate regional model emissions data file is created for each modelled day, a value of 24 should be entered.

- **Full path to the emissions species map file**

  The emissions species map file is used to link regional model emissions species to ADMS chemical species. It has the same file format as the concentration species map file, described in Section 4.3.1, but in general will contain different factors due to different unit conversion requirements and different regional model emissions and output species. Different regional emission variables may be included in different file types, for example representing anthropogenic and biogenic sources. All emissions species maps should include the same ADMS emissions variables. Select the appropriate emissions species map file for the current emissions file type by setting the variable `EmSpeciesMapFilePath<N>` in *inputdata.cfg*.

4.4.3 Number of layers of emissions data to extract

Enter the number of vertical layers of emissions data to extract, up to the maximum number of vertical layers included in any of the input emissions file types, by setting the variable `EmNumLayers` in *inputdata.cfg.*

4.4.4 Use custom 3D emissions data file

If the user specifies a Generic (ADMS) 3D gridded emissions file generated through manual processing, the automatic conversion of regional model emissions will not be carried out. This is done by setting the variable `UseCustomEmissionsFile=1` and the variable `CustomEmissionsFilePath` to a suitable file path in *inputdata.cfg*. The emissions from the supplied file will be used in all local model runs by default.

Optionally, a separate Generic 3D gridded emissions file can be specified for the main nesting and background runs to match the emissions used in the regional model as closely as possible. This is done by setting the variable `UseGriddedEmissionsFile=1` and the variable `GriddedEmissionsFilePath` to a suitable file path in *inputdata.cfg*. When a second gridded emissions file path is defined through `GriddedEmissionsFilePath`, the file specified in `CustomEmissionsFilePath` will only be used in the main local model run with explicit emissions.

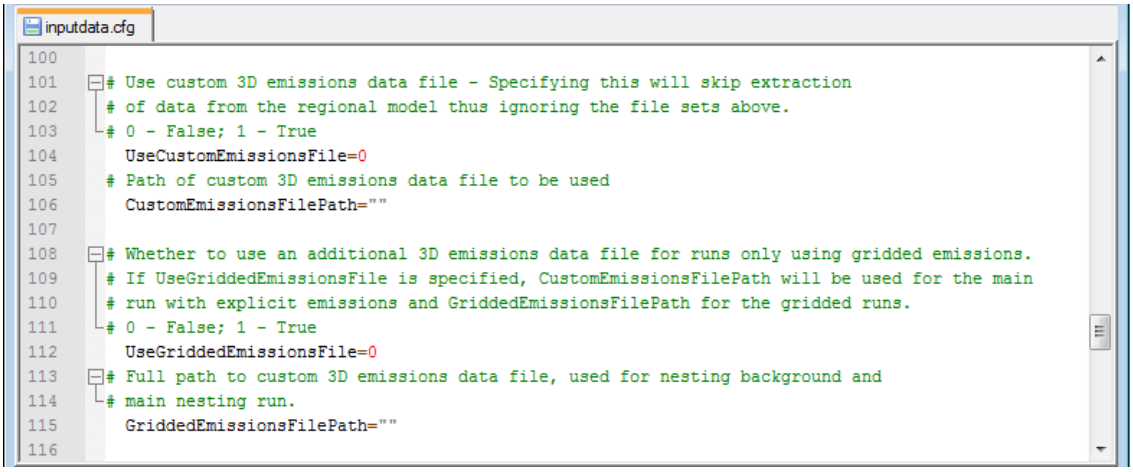


Figure 4.25 The custom 3D emissions file variables in the *inputdata.cfg* file

4.4.5 Disaggregation options

This section contains options for controlling how emissions from sources modelled explicitly in ADMS-Local or ADMS-Urban should be disaggregated from the 3D grid of regional model emissions.

If ADMS-Urban is the chosen local model, these options are identical to the options available in the .uai *file when specifying a 3D gridded emissions file directly.*

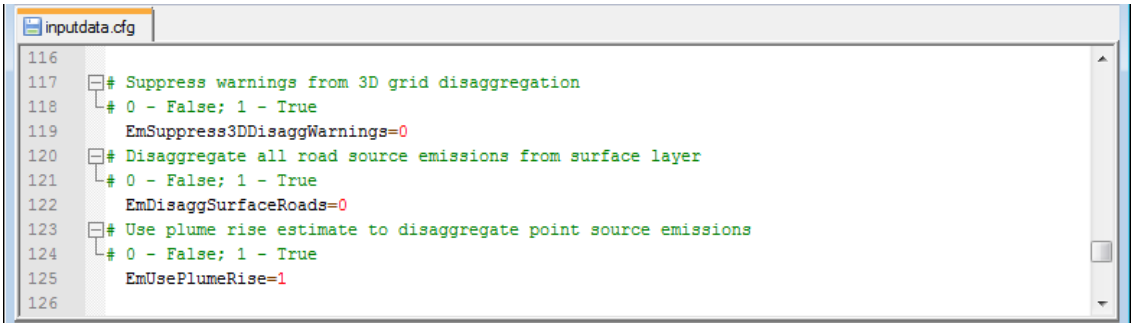


Figure 4.26 The disaggregation options in the *inputdata.cfg* file

- **Suppress warnings from 3D grid disaggregation**

  Set the variable `EmSuppress3DDisaggWarnings=1` in *inputdata.cfg* to prevent disaggregation warning messages being issued for every 3D grid cell, pollutant and time-step, which may generate a large log file if there are substantial inconsistencies between the explicit and gridded emissions.

- **Disaggregate all road source emissions from surface layer**

  Set the variable `EmDisaggSurfaceRoads=1` in *inputdata.cfg* to disaggregate all explicit road source emissions from the surface layer (regardless of source height), if this approach was used to aggregate the emissions.

- **Use plume rise estimate to disaggregate point source emissions**

  Set the variable `EmUsePlumeRise=1` in *inputdata.cfg* to disaggregate explicit point source emissions from the vertical layers of the 3D grid using an estimate of initial plume rise, if this corresponds to the aggregation approach. This option is applicable only for ADMS-Urban.

4.4.6 Emissions data file format

The generic 3D grid emissions data file is a netCDF format file containing pollutant species' emission rates for each cell of the 3D grid for each hour of the model period. The file format follows CF metadata conventions.

Note that CF-compliance requires that all variable, dimension and attribute names should start with a letter and include only letters, numbers and underscores. Note that the variable and attribute names are case-sensitive.

The dimensions used in the emissions file are described in **Table 4.12**, the variables in **Table 4.13** and global and variable attributes in **Table 4.14**.

Name	Description
x	Number of grid cells in x horizontal coordinate direction
y	Number of grid cells in y horizontal coordinate direction
z	Number of vertical layers of grid cells
time	Number of time-steps in file (should be defined as the 'unlimited' dimension)

Table 4.12 Dimensions in the Generic 3D emissions data file.

Name	Dimensions	Description
x	x	Cell centre x coordinates in projected coordinates
y	y	Cell centre y coordinates in projected coordinates
z	z	Cell top z coordinate in m above ground level
time	time	Hour-ending time in days since midnight on 1st January 1900
ADMS_grid_mapping	(none)	Dummy variable containing coordinate projection information attributes
<emitted pollutant species>	x, y, z, time	One variable for each emitted pollutant species, emissions in $g/m^2/s$ for each grid cell and each hour

Table 4.13 Variables in the Generic 3D emissions data file. Dimensions are listed with the fastest varying first.

Associated with	Name	Example value	Comment
Global	Conventions	CF-1.6	May be used by viewing utilities
Global	Title	ADMS 3D Emissions file	
Global	File_version	ADMS_3DEF_v1.0	Checked by model
Global	History		May be useful for QA
ADMS_grid_mapping	grid_mapping_name	lambert_conformal_conic	Projection type[1]
ADMS_grid_mapping	earth_radius	6.370e+006	
ADMS_grid_mapping	(projection parameters)		(depend on projection used)
x, y	standard_name	projection_x_coordinate	Allows viewing utilities to identify coordinates
x, y	axis	X	
x, y	units	m	
x, y	grid_mapping	ADMS_grid_mapping	
x, y	resolution_m	1000.0	Allows simple extraction of grid geometry
Z	long_name	height of top of cell above local ground level	
Z	units	m	
Z	positive	up	
Time	long_name	local time at end of emissions period	
Time	units	days since 1900-01-01 00:00:00	
<emitted pollutant species>, e.g. PM2_5	long_name	gridded emissions of PM2.5	
<emitted pollutant species>	ADMS_species	PM2.5	Species name as used in the local model
<emitted pollutant species>	units	g m^-2 s^-1	Emission units of $g/m^2/s$
<emitted pollutant species>	coordinates	x y z	
<emitted pollutant species>	grid_mapping	ADMS_grid_mapping	
<emitted pollutant species>	_FillValue	-999.0	

Table 4.14 Global and variable attributes in the Generic 3D emissions data file. [1]Projection types and required parameters for CF convention compliance are given in Appendix F of the CF Metadata Conventions document.

4.5 Other input data options

4.5.1 Local model output type

The user must specify whether the MAQS coupled system run output is for a small number of receptor locations, for example at monitoring sites for model validation purposes, or based on a regular grid of locations which will be used to produce contours of concentration. In the latter case, additional procedures are included in the MAQS coupled system to ensure that source-oriented grid points added along road sources are included in the final output, which allows high-resolution contour images to be produced following post-processing.

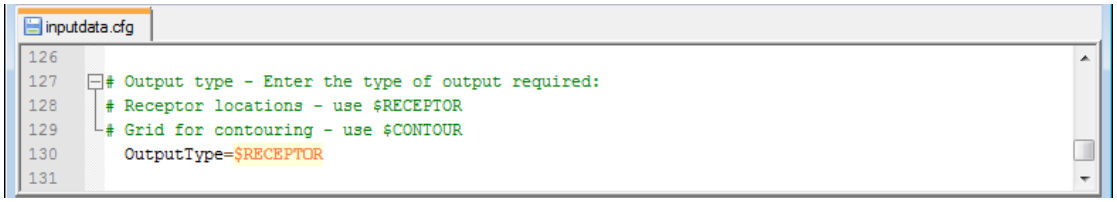


Figure 4.27 The local model output type in the *inputdata.cfg* file

Specify an appropriate value for the `OutputType` variable in the *inputdata.cfg* control file:

- Choose the **Receptor locations** option (`OutputType=$RECEPTOR`) if your local model runs contain only specified points.
- Choose the **Grid for contouring** option (`OutputType=$CONTOUR`) if you want to produce high-resolution contour plots.

Please refer to Section 8.4 for details of the additional procedures which are included in the MAQS coupled system when the **Grid for contouring** option is chosen.

4.5.2 Project name

The file name stem for the main MAQS coupled system output file and log file can be defined using the `ProjectName` variable in the *inputdata.cfg* file.

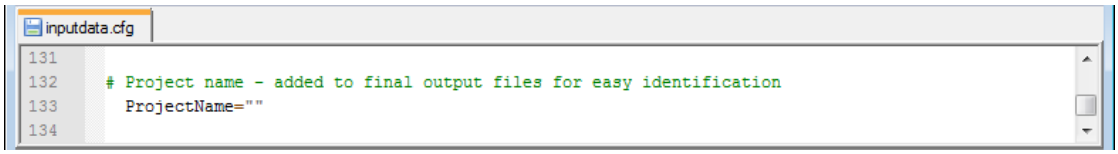


Figure 4.28 The `ProjectName` variable in the *inputdata.cfg* file

Note that the full name conventions for the MAQS coupled system output files (described in Section 5.3.1) are relatively long, so it is advisable to use a descriptive but short setting for `ProjectName`.

4.6 Nesting period

The nesting period can either be defined in the *run.cfg* file, as shown in **Figure 4.29**, or via the command line as described in Section 2.3.4. If the command line option is used, it overrides the values in *run.cfg*.

If a modelling period longer than the available regional model data is defined, the output will be restricted to the period when regional model data are available. The last hour may be equal to the first hour to run only a single hour of data.

Note that the dates and times for the start and end of the nesting period should be defined in local solar time, as used in the local model.

If a modelling period of a single hour is desired, the first and last date and time should be set to the same values.

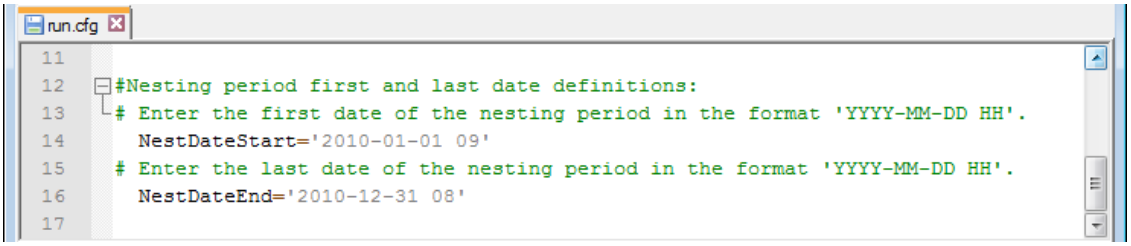


Figure 4.29 The nesting period start and end variables in the *run.cfg* file

4.6.1 Date and time of the first hour

Specify the date and time of the first hour of the nesting period using the format `YYYY-MM-DD HH`, where the two-digit hour value is in the range 0-23. The format is the same for both the variable `NestDateStart` in the *run.cfg* control file and the command line option.

4.6.2 Date and time of the last hour

Specify the date and time of the last hour of the nesting period using the format `YYYY-MM-DD HH`, where the two-digit hour value is in the range 0-23. The format is the same for both the variable `NestDateEnd` in the *run.cfg* control file and the command line option.

4.7 Local model options

The *localmodel.cfg* file contains options for setting up the local model runs within the MAQS coupled system. The parameters in the file include shared options applicable to both ADMS-Local and ADMS-Urban, and options specific to each.

If using ADMS-Urban, the *localmodel.cfg* file is primarily used to set the file path to the input *.upl* file(s) and all ADMS-Local input options (Sections 4.7.2 to 4.7.12 inclusive) are not used by the system.

4.7.1 Static .asp file

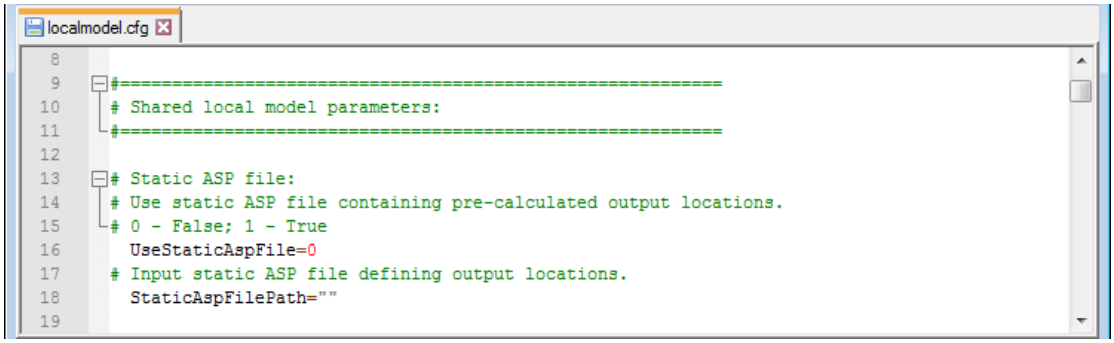


Figure 4.30 The option to use a static *.asp* file in the *localmodel.cfg* file

If the user is repeatedly running contour runs with the same output grid resolution and extent, identical explicit road sources and settings for source-oriented grid points, for example within a forecasting system, then the *.asp* file created by the system to hold all model output locations (as described in Section 8.4.1) will be identical in every run. The user may wish to use a pre-calculated *.asp* file to remove the run time requirement of re-creating the file in every run. This is specified using by setting the variable `UseStaticAspFile=1` and the variable `StaticAspFilePath` to a suitable file path in the *localmodel.cfg* control file, as shown in **Figure 4.30**.

If a static *.asp* file is specified when running in receptor mode, the static *.asp* file will be used to override any output location settings in the *localmodel.cfg* file (or *.upl* file(s), if using ADMS-Urban).

When running in contour mode (described in Section 4.5.1), any static *.asp* file supplied by the user must conform to the point naming conventions used by the **CreateASP** utility for compatibility with the **AddInterpIGP** utility, as described in Appendix G. One way of ensuring that this is the case would be to use the following steps.

Step 1 Carry out a verification run of the MAQS coupled system in contour mode with `PreserveWorkingFiles` set to `$KEY_FILES` or `$ALL_FILES` and `UseStaticAspFile=0`.

Step 2 Copy the *CreateAsp.out.asp* file from the output files directory to a suitable input location and possibly rename for clarity

Step 3 Set `UseStaticAspFile=1` and define the `StaticAspFilePath` to specify the previous *CreateAsp.out.asp* from the input location for use as a static *.asp* file.

4.7.2 Road source data files (ADMS-Local only)

The MAQS coupled system performs explicit modelling of local sources in order to represent the fine-scale concentration field due to local emissions from explicit road sources. Detailed information about each road source such as name, carriageway width, geometry, emissions and (optionally) street canyon properties are defined through a number of input text files using this option. For ADMS-Urban, the equivalent information is supplied via the input explicit *.upl* file and associated data files.

In this section, the input data files describing various aspects of each road source to be included in the modelling can be specified. If setting `UseRoadEmissionsData=1`, the user is required to specify all files i.e. road information (*.rdi*), geometry (*.rdg*) and emissions (*.rde*) files using the variables `RoadInfoFilePath`, `RoadGeometryFilePath` and `RoadEmissionsFilePath`, respectively, in the *localmodel.cfg* file.

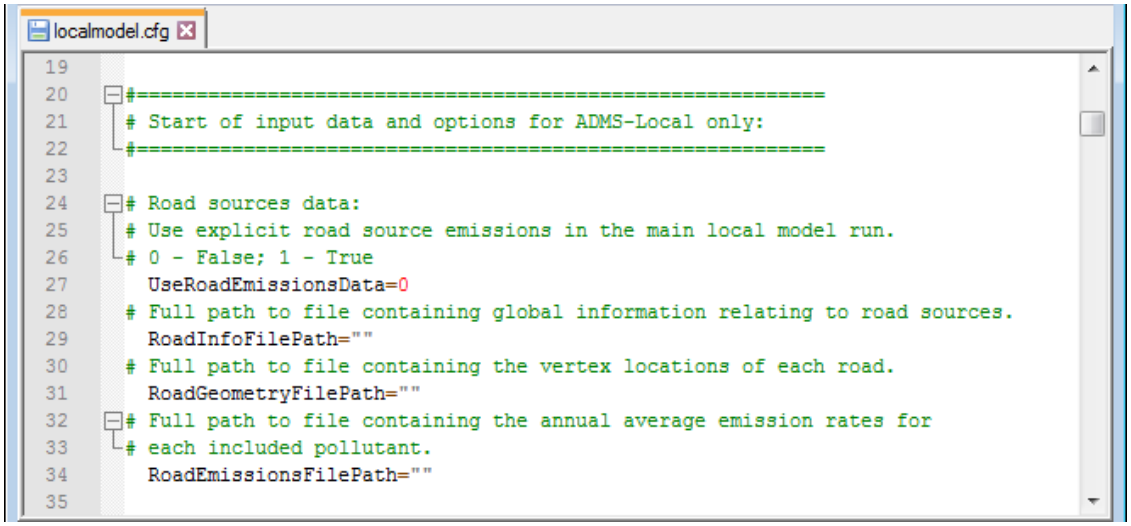


Figure 4.31 The road source data file paths in the *localmodel.cfg* file

Each file shares a similar format structure: the first line specifies a version string, followed by optional comment lines that must begin with the '!' character, followed by a comma-separated header line, and finally the comma-separated data lines. Each road input file is described below. When defining the road sources, the road names used must be consistent across all input files.

In addition to the .rd* *file formats specific to ADMS-Local, the MAQS coupled system also supports the equivalent files used by the ADMS-Urban import and export facility i.e. source properties (*.spt*) file modified to contain only road sources and the corresponding vertex information (*.vgt*) and pollutant emissions (*.eit*) file.*

- **Road information file**

  Version string: 'RDIVERSION1'

  The version string is 'rdiversion1' in uppercase. Note that the 'I' and number '1' may appear identical in some text editors. To avoid confusion, lowercase may be used as version strings in road source data files are not case-sensitive.

  Header: 'Source name, Height (m), Road width (m), Canyon width (m), Building height (m), Building coverage'

  Data: One line of data per road source. The road height can be used to represent any elevation of the road carriageway above local ground level. The road width should be the width of the road carriageway (i.e. kerb to kerb). The last three columns are required only if modelling street canyon effects. The canyon width is the average width between the canyon walls on either side of the road carriageway. The building height is the average height over both sides of the

road carriageway and should be above 2 metres to be modelled as street canyon. The building coverage is a fraction ranging from 0 (no buildings i.e. standard road) to 1 (solid canyon on both sides). Please refer to Section 8.3.4 for more details.

- **Road geometry file**

  Version string: 'RDGVERSION1'

  Header: 'Source name, X (m), Y (m)'

  Data: One line of data per vertex per road source using the same projected coordinate system used throughout the system. The road names must be consistent with those used in other road source data files. Up to 51 vertices (i.e. 50 segments) may be specified for each road source. Adjacent vertices for the same road source must be separated by at least 1 m.

- **Road emissions file**

  Version string: 'RDEVERSION1'

  Header: 'Source name, Pollutant name, Emission rate (g/km/s)'

  Data: One line of data per source per emitted pollutant, using the same road names as those used in other road source data files, and pollutant names matching ADMS conventions. The emission rates must be in units of g/km/s.

4.7.3 Road traffic flow (ADMS-Local only)

In the modelling of road sources, ADMS-Local also accounts for the extra turbulence produced by the movement of vehicles, especially on busy roads. Activity data in terms of vehicle counts per hour, average speeds and category can be used to calculate this traffic-induced turbulence. The optional parameters are specified for each road source using an input text file. Note that the road names must be consistent with those used in the road source data files. If not available, the traffic counts are back-calculated from emission rates of NO_x, PM_{10}, or VOC (in that order of preference). Further, if no emissions are defined for any of these pollutants, no traffic-induced turbulence is modelled. In ADMS-Urban this data can be specified via the *.upl* file.

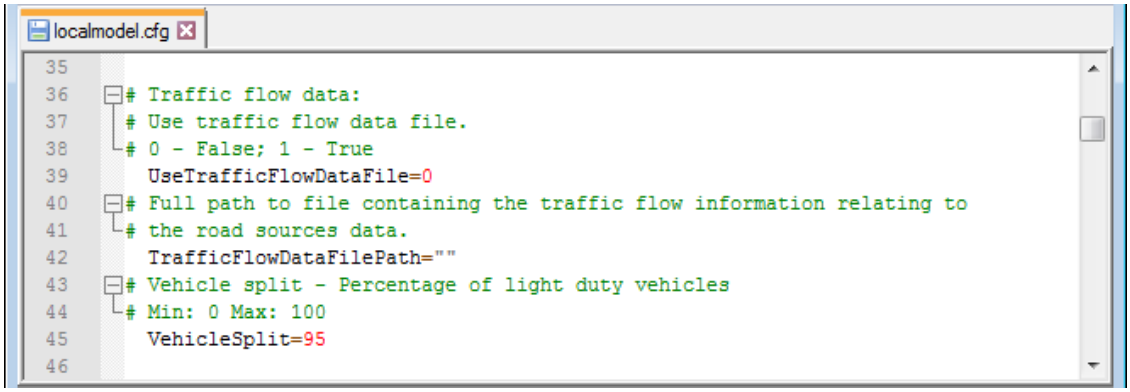


Figure 4.32 The traffic flow variables in the *localmodel.cfg* file

- **Use road traffic file in local model runs**

  Set `UseTrafficFlowDataFile=1` in the *localmodel.cfg* file to specify the traffic flow parameters to use in local model calculations.

- **Full path to the road traffic file**

  Specify the data file by setting the variable `TrafficFlowDataFilePath` to an appropriate file path in *localmodel.cfg*. The road traffic (*.rdt*) file shares the same format structure as the other road data files described in Section 4.7.2.

  Version string: 'RDTVERSION1'

  Header: 'Source name, Average speed (km/hr), Vehicle count (vehicles/hour), Vehicle area (m^2)'

  Data: One line of data per speed-vehicle area combination per road source. The road names must be consistent with those used in other road source data files.

- **Vehicle split**

  For road sources where no traffic flow data have been provided, i.e. sources not included in the road traffic data file or if no data file is supplied, a back-calculation from emissions of the standard pollutants NO_X, PM_{10} or VOC is used to determine the traffic flow, using a default split of 95% light duty vehicles and 5% heavy duty vehicles and an average vehicle speed of 30 km/hr. If this is inappropriate, the percentage of light vehicles for the calculation of traffic flow can be altered by setting the variable `VehicleSplit` in *localmodel.cfg*.

4.7.4 Time varying emission factors (ADMS-Local only)

Unless otherwise specified, emission rates are assumed to be constant. However, time variation of emissions can also be modelled by specifying emission factors using input files containing either regularly repeating profiles or hour-by-hour factors. Some roads may use profiles and others hourly factors, but any given road can only use one type. Note that the road names must be consistent with those used in the road source data files. For ADMS-Urban time-varying emissions data is specified via the *.upl* file. Please refer to the ADMS-Urban User Guide (CERC, 2020b) for details of the *.fac* time-varying profiles file and *.hfc* hourly factors file formats

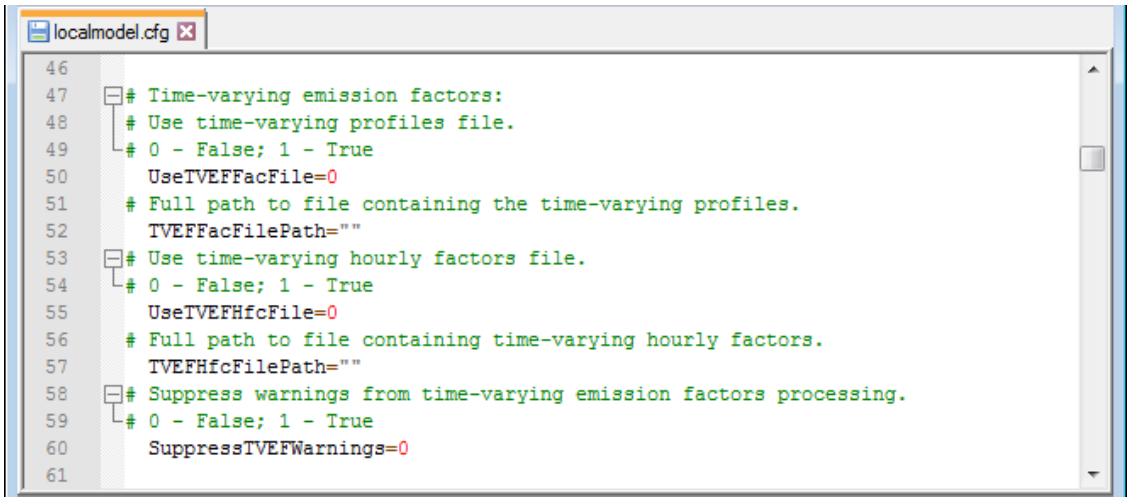


Figure 4.33 The time varying factors variables in the *localmodel.cfg* file

- **Full path to the time varying profiles file**

  If specifying a time varying profiles file (*.fac* file), set the variable `UseTVEFFacFile=1` and the variable `TVEFFacFilePath` to a suitable file path in *localmodel.cfg*.

- **Full path to the hourly factors .hfc file**

  If specifying an hourly factors file (*.hfc* file), set the variable `UseTVEFHfcFile=1` and the variable `TVEFHfcFilePath` to a suitable file path in *localmodel.cfg*.

- **Suppress warnings from time varying emission factors processing**

  Set the variable `SuppressTVEFWarnings=1` in *localmodel.cfg* to prevent time varying emission factor warning messages from being written to the log file, which may result in a large log file if there are substantial inconsistencies in the data.

4.7.5 Daylight saving time (ADMS-Local only)

Times entered into the MAQS coupled system are read as hour ending values in local solar time and should be consistent between input files including the time-varying emission factors. In many countries, daylight saving time is used during the summer to shift the times forward by one hour. This changes the relationship between local solar time and clock time during the daylight saving time periods. The system can also account for time shifts during British Summer time. Daylight saving time settings for ADMS-Urban are implemented via an *.uai* file linked to the main explicit *.upl* file.

In the *.hfc* file, where the year, day and hour are input, the times should all remain in local solar time convention. For emission factors specified using a *.fac* file however, it may be required to include effects of the one hour shift during daylight saving time.

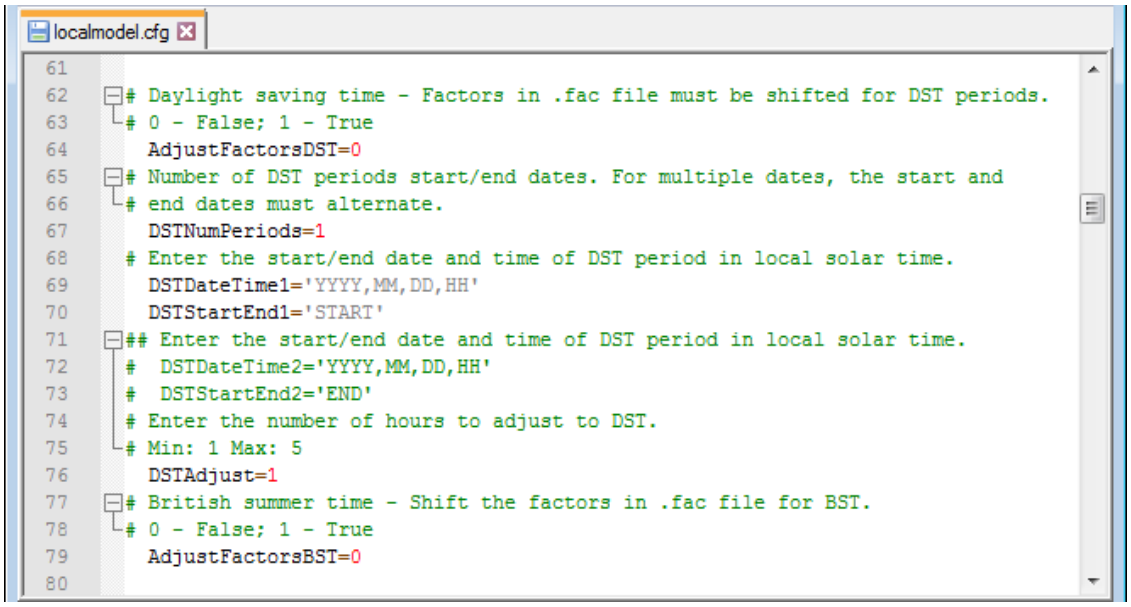


Figure 4.34 The daylight saving time options in the *localmodel.cfg* file

- **Adjust factors for daylight saving time**

  Set `AdjustFactorsDST=1` in *localmodel.cfg* to specify that the emission factors for all explicitly modelled road sources will be shifted during daylight saving time.

- **Number of daylight saving time periods**

  Specify the number of periods by setting the variable `DSTNumPeriods` in *localmodel.cfg*.

- **Start or end date and time of daylight saving time periods**

  For each period, the `DSTDateTime<N>` and `DSTStartEnd<N>` variables in *localmodel.cfg* must be defined and set, where `<N>` is replaced by the period number, for example `DSTDateTime1` and `DSTStartEnd1`. Enter the `START` and `END` times of the daylight saving periods, note that the times must be entered in the format `YYYY`, `MM`, `DD`, `HH` and the start and end date-times for all periods must be entered in sequential order.

- **Number of hours to adjust for daylight saving time**

  Enter the number of hours to shift the times forward for daylight saving time by setting the variable `DSTAdjust` in *localmodel.cfg*.

- **Adjust factors for British Summer Time**

  Set `AdjustFactorsBST=1` in *localmodel.cfg* to apply hourly shift to the emission factors automatically for British Summer Time. If using this option, the daylight saving time period date-times do not need to be manually specified by the user.

4.7.6 Site properties (ADMS-Local only)

Surface properties for meteorology are defined using several site parameters. When running the MAQS coupled system with ADMS-Urban, these parameters are entered using the main *.upl* file with explicit sources. When running with ADMS-Local, the site parameters are specified for each grid cell including spatial variation, comprising:

- `Latitude` in degrees, which is required in order to calculate the solar elevation angle (longitude is optional as it is not used directly in calculations);
- `Z0` surface roughness length in metres, used to characterise the boundary layer profiles;
- `Min_LMO` minimum Monin-Obukhov length in metres, used to prevent very stable conditions in urban areas; and
- Optional parameters relating to building morphology, used to define the urban canopy boundary layer profile that allows for changes in the upwind wind speed and turbulence profiles caused by the presence of buildings in an urban area.

This section allows details about the site surface conditions to be entered by the user. The gridded site properties data are input to the system using a text file format. An example site properties data file is shown in **Figure 4.35**. This includes the optional urban canopy flow parameters that are used if the **Use urban canopy flow field in local model runs** option is set. The additional variables used to determine the urban canopy flow parameters are as follows:

- `H` average building height within the cell in metres;
- `G` average street canyon width within the cell in metres;
- `LambdaP` ratio of plan area occupied by buildings to total plan area within the cell (must be between 0 and 1); and
- `LambdaF phi1 to phi2` ratio of total frontal area of building perpendicular to a wind direction to total plan area within the cell (may be greater than 1), for a range of wind directions phi1 to phi2 in degrees.

The LambdaF angle thresholds have the following restrictions:

- The upper ('to') threshold of one sector must be equal to the lower ('from') threshold of the next (sectors must be in order).
- The first 'from' threshold must be equal to the last 'to' threshold, to describe a complete range of wind directions. Wind directions will be considered to belong to the sector where they are greater than or equal to the 'from' threshold and less than the 'to' threshold.
- Each threshold value must be within 0 to 360 degrees.
- Exactly one sector may have a 'from' threshold greater than or equal to its 'to' threshold (crossing 0 degrees).
- There must be at least one sector up to a maximum of forty.

The structure of the site properties file, which should be saved as a comma-separated text file (*.csv*), is as follows:

Version string: 'SITEPROPERTIESVERSION1'

Grid section: 'GRID:' followed by the specification of the horizontal grid in projected coordinates i.e. the minimum, maximum coordinates and the grid cell size in each direction.

Variables section: 'VARIABLES:' followed by the number of included variables and the names in separate rows.

Data lines: 'DATA:' followed by a comma-separated list of the actual values in the same order as listed in the variables section with one line for each grid cell, with projected cell centre coordinates used to match the data to the relevant model grid cell.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	SITEPROPERTIESVERSION1															
2																
3	GRID:															
4	0	0														
5	2000	2000														
6	1000	1000														
7																
8	VARIABLES:															
9	16															
10	X															
11	Y															
12	Latitude															
13	Z0															
14	MinLMO															
15	H															
16	G															
17	LambdaP															
18	LambdaF 337 to 022															
19	LambdaF 022 to 067															
20	LambdaF 067 to 112															
21	LambdaF 112 to 157															
22	LambdaF 157 to 202															
23	LambdaF 202 to 247															
24	LambdaF 247 to 292															
25	LambdaF 292 to 337															
26																
27	DATA:															
28	500	500	52	0.8	75	11.5	10	0.006	0.008	0.008	0.006	0.007	0.008	0.008	0.006	0.007
29	500	500	52	0.7	75	14.2	9.2	0.025	0.021	0.019	0.02	0.019	0.021	0.019	0.02	0.019
30	1500	1500	52	0.7	75	7.3	7.3	0.038	0.038	0.04	0.038	0.039	0.038	0.041	0.038	0.039
31	1500	1500	52	0.8	75	5.9	7.3	0.006	0.005	0.004	0.005	0.005	0.005	0.004	0.005	0.005
32																

SiteProperties

Figure 4.35 Example site properties file viewed in Excel

Saving the file from Excel in .csv *format may lead to extra commas at the end of the non-data lines.*

Comment lines, for example to give metadata about the data source, may be included in the site properties file by using a '#' character at the beginning of the line.

The horizontal grid must be defined so that it includes the nesting domain. If they coincide, ensure that the edges are consistent within a tolerance of 1% of the regional model grid cell size. Similarly, the grid cell size must be the same as that of the regional model.

It is advisable to specify a spatial variation of the minimum Monin-Obukhov length for domain extents including multiple area types (e.g. suburban, urban, rural); however, step changes in values between neighbouring grid cells will lead to discontinuities in concentrations for the more stable atmospheric conditions and so smoothly varying values are recommended.

Suggested surface roughness length and minimum Monin-Obukhov length values for different types of land use are given in the ADMS-Urban User Guide (CERC, 2020b).

Site parameters relating to road sources i.e. road widths, canyon heights, etc., are entered alongside the road source input data.

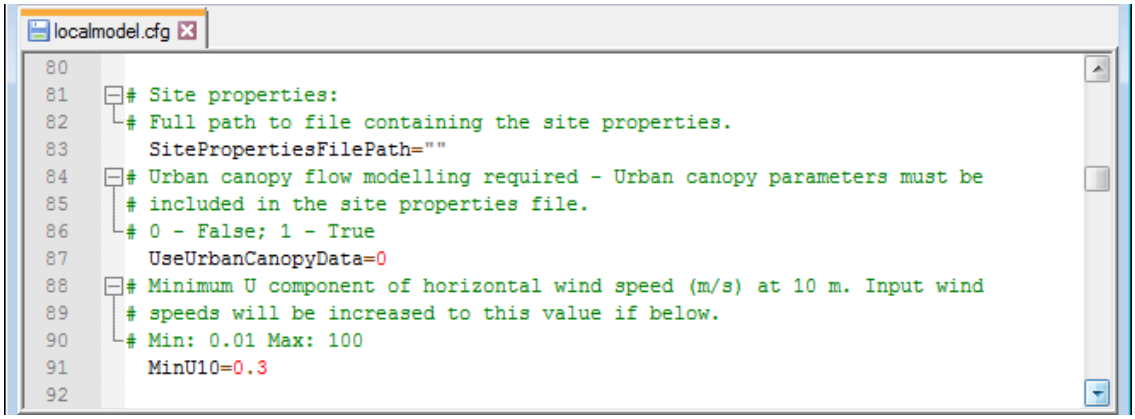


Figure 4.36 The site data variables in the *localmodel.cfg* file

- **Full path to the site properties data file**

  Specify the site properties data file by setting the variable `SitePropertiesFilePath` to an appropriate file path in *localmodel.cfg*.

- **Use urban canopy flow field in local model runs**

  Set `UseUrbanCanopyData=1` in *localmodel.cfg* to specify that the urban canopy flow option will be used in the ADMS-Local model runs and additional variables will be read in from the site properties file.

- **Minimum U component of horizontal wind speed at 10 m**

  The value of the U component of the wind speed at height 10 m is adjusted to 0.3 m/s by default if the value is below. Setting the variable `MinU10` in *localmodel.cfg* allows the user to specify the minimum value.

4.7.7 Full path to the receptor locations file (ADMS-Local only)

The output locations section allows the user to define the points at which concentration values will be output by the coupled system when running with ADMS-Local. For ADMS-Urban the equivalent inputs are included in the main explicit *.upl* file. The output points may be at specific, individual locations that are specified by the user via an input text (*.asp*) file. Select the file by setting the variable `OutputLocationsFilePath` to a suitable file path in *localmodel.cfg*. This file must be specified if the **Receptor** output type is selected in *inputdata.cfg* (Section 4.5.1).

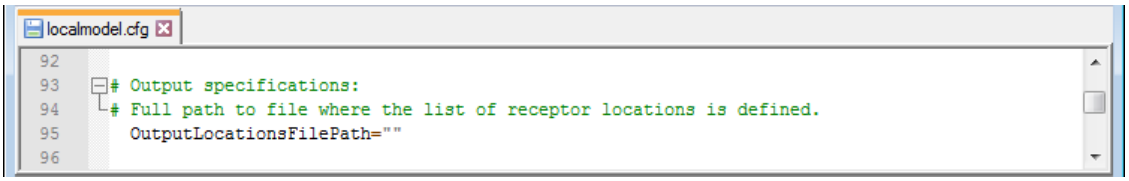


Figure 4.37 The output locations file path in the *localmodel.cfg* file

4.7.8 Regular gridded output options (ADMS-Local only)

The output points can also be a regular grid of receptors used to produce contours of concentration data covering the nesting domain. The MAQS coupled system runs a utility that creates the *.asp* file if the **Contour** output type is selected in *inputdata.cfg* (Section 4.5.1). When running with ADMS-Local, the extent of the regularly spaced output grid is defined by specifying the corner coordinates and the minimum and maximum heights in *localmodel.cfg*, shown in **Figure 4.38**. When running with ADMS-Urban, a regular grid of output points can be defined through the main explicit *.upl* file.

The grid should be fully within the nesting domain (see Section 4.1.6) but offset inwards from the domain limits in each direction, by a margin not exceeding the regional model cell size.

The projected coordinate system used to specify the extent of the regular output grid should be consistent with that used to define the nesting domain.

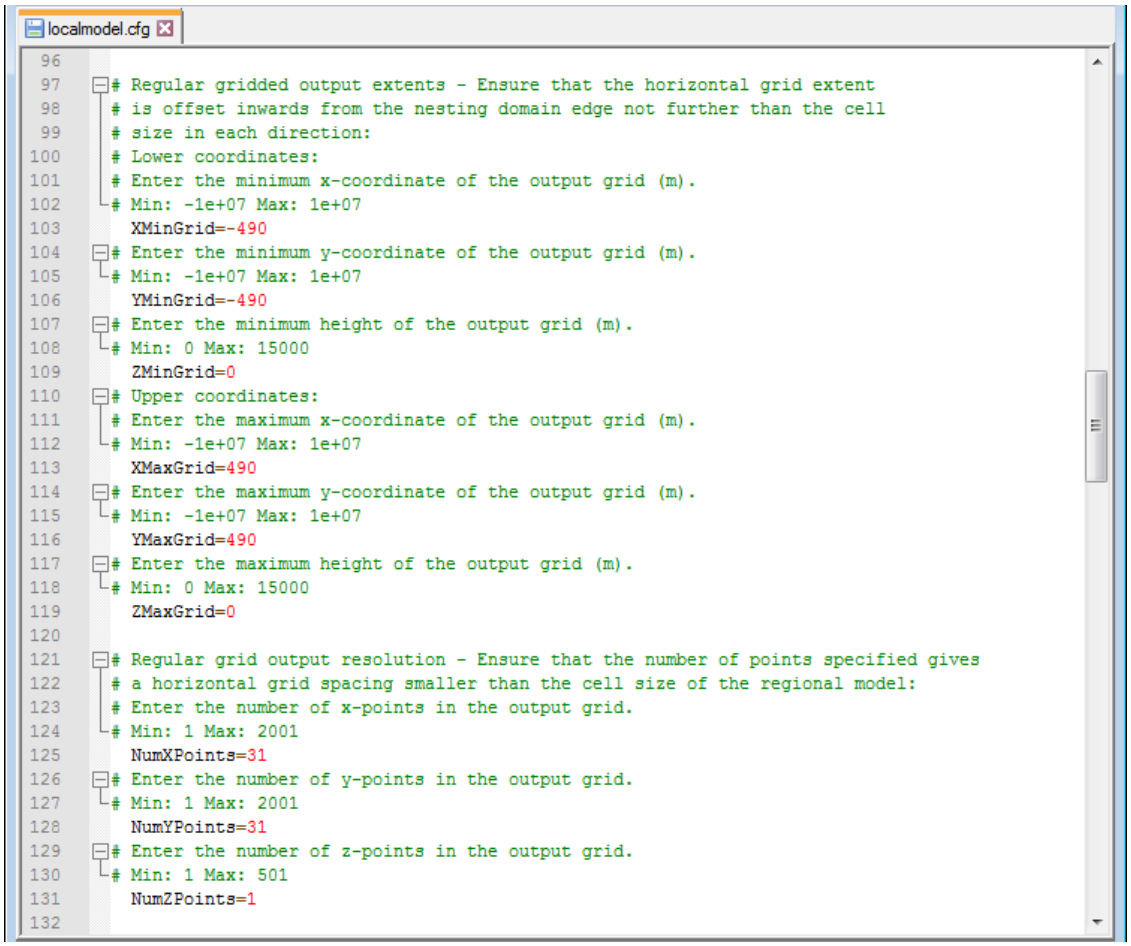


Figure 4.38 The regular grid output options in the *localmodel.cfg* file

Enter the coordinates for the minimum and maximum values of the extents of the output grid using the variables `XMinGrid`, `YMinGrid`, `ZMinGrid`, `XMaxGrid`, `YMaxGrid` and `ZMaxGrid` in *localmodel.cfg*. By default, the regular grid will include 31 by 31 by 1 receptor points. To alter these numbers in order to define a required spatial resolution, modify the values of the variables `NumXPoints`, `NumYPoints` and `NumZPoints`, taking into account the maximum permitted resolution in each direction.

4.7.9 Source-oriented grids (ADMS-Local only)

If modelling a large number of road sources, a regular grid may not capture all the features of the pollutant concentration distribution within the study area. The MAQS coupled system will add receptor points close to the roads, where the pollutant concentration gradients are often greatest. Settings relating to this process are specified via a *.uai* file for ADMS-Urban or in the *localmodel.cfg* file for ADMS-Local.

The process of adding receptor points close to explicitly modelled road sources is carried out in two stages:

1. Firstly, a number of extra receptor points will be added in and around road sources and the local model will calculate concentrations at these points in the same way as at any other specified point. These form rows of points aligned with the road segments themselves. For details on the default perpendicular distances

of these rows of points from the source centrelines and options for adjusting these distances, refer to the **Across-source locations** section below. For details on the number and spacing between points on the same row along each source, refer to the **Along-source locations** section further below. For details on which road sources receive these extra points, refer to the **Included sources** section further below.

2. Secondly, three additional interpolated points will be added between each 'pair' of points from the first stage, i.e. between neighbouring points on the same row alongside a given road segment, unless (i) only one point has been added to that segment row during the first stage, or (ii) the distance between a pair of points is large compared with the resolution of the regular grid. Concentrations at these additional points will be calculated by linearly interpolating between the values at the points from the first stage. However, if a linear interpolation between a given pair of points would be inappropriate, the interpolation points will be replaced with actual receptor points i.e. the full concentration calculations will be performed. By default, this second stage of adding interpolated points will always be carried out, but it can be disabled using the **Add interpolated points** option; refer to the **Along-source locations** section further below.

It is possible to modify how the source-oriented grid points will be added by specifying the parameters in this section. High-resolution output grids are required to generate fine-resolution output concentration contour images. However, specifying large numbers of receptor points will increase the system run time and memory requirements, so testing may be required to identify the optimum configuration of output points for a specific domain and application.

4.7.9.1 Across-source locations

By default, four rows of extra points are added along road sources, and six along street canyons. For a standard road source, the points are placed at perpendicular distances of 0.45 and 2.0 times the road width away from the road centreline on either side of the road, i.e. two points lie inside the road carriageway and two lie outside it. For a street canyon, they are placed at a perpendicular distance of 0.45 times the road width (i.e. inside the road carriageway) and 0.45 and 0.55 times the canyon width from the road centreline on either side of the road (i.e. just either side of each canyon wall). This ensures that the large concentration gradients that often exist across the canyon walls are well captured. If the two rows of points at 0.45 times the road width and 0.45 times the canyon width from the road centreline are sufficiently close (within 1 metre), the points at 0.45 times the canyon width will be discarded. As with canyon-related properties in ADMS-Local, the rows of points are all symmetric about the road centreline. It is possible to modify the default across-source locations of the source-oriented grid points for standard road sources using the options shown in **Figure 4.39**.

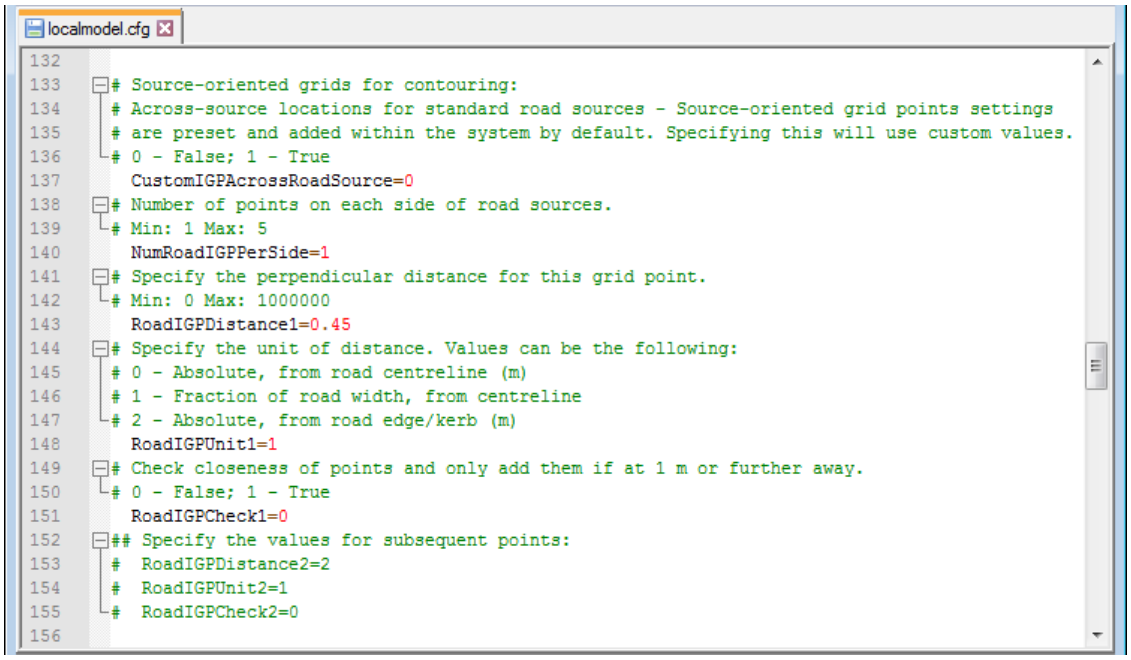


Figure 4.39 The across-source locations parameters of source-oriented grid points for road sources in *localmodel.cfg* file

- **Use custom across-source locations**

  Set `CustomIGPAcrossRoadSource=1` in the *localmodel.cfg* file to define the following parameters for standard road sources (without canyons).

- **Number of rows of points on each side**

  Set `NumRoadIGPPerSide` in *localmodel.cfg* to define how many rows of source-oriented grid points should be added on either side of the road. Points defined at any non-zero distance from the road centreline will be duplicated on each side of the road, whereas a row along the road centreline itself will not be duplicated. For each row, the `RoadIGPDistance<N>`, `RoadIGPUnit<N>` and `RoadIGPCheck<N>` variables must be defined and set, where `<N>` is replaced by the row number, for example `RoadIGPDistance1`.

- **Distance**

  Specify the perpendicular distance for this row(s) of source-oriented grid points (depending on the choice of **Units**) by setting the variable `RoadIGPDistance` in *localmodel.cfg*.

- **Units**

  Set the units and reference point for this row(s) of source oriented grid points by setting the variable `RoadIGPUnit` in *localmodel.cfg*. The following options are available:

  * **Absolute, from road centreline (m)** – the value in the **Distance** option is taken as the absolute distance in metres from the road centreline; this option must be used to specify any points that are inside the road carriageway if using absolute distances.

* **Fraction of road width, from centreline** – the value in the **Distance** option is taken as a fractional distance of the road width from the centreline, e.g. a value of 2 would mean add points on either side of the road centreline at a distance of two times the road width.
* **Absolute, from road edge (m)** – the value in the **Distance** option is taken as the absolute distance away from the road edge, i.e. the distance from each kerb.

- **Check closeness**

  By default, source-oriented grid points will be added for all rows defined regardless of point spacing. Set `IGPCheck=1` in *localmodel.cfg* so that each row will only be added if it is more than 1 m away from the row on the same side of the road associated with the previous entry.

Setting the across-source locations of source-oriented grid points for canyons is similar as for road sources without canyons, as shown in **Figure 4.40**.

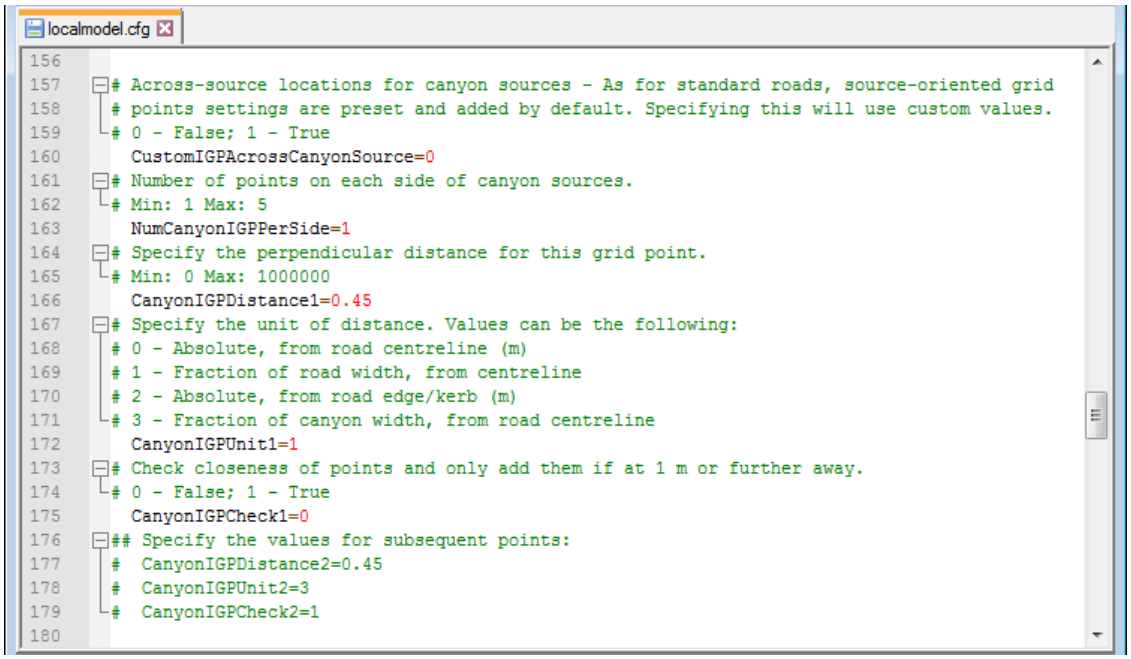


Figure 4.40 The across-source locations parameters of source-oriented grid points for canyon sources in *localmodel.cfg* file

- **Use custom across-source locations**

  Set `CustomIGPAcrossCanyonSource=1` in the *localmodel.cfg* file to define the following parameters for canyon sources.

- **Number of rows of points on each side**

  Set `NumRoadIGPPerSide` in *localmodel.cfg* to define how many rows of source-oriented grid points should be added on either side of the canyon road source. Points defined at any non-zero distance from the road (canyon) centreline will be duplicated on each side of the road, whereas a row along the road (canyon) centreline itself will not be duplicated. For each row, the variables

`CanyonIGPDistance<N>`, `CanyonIGPUnit<N>` and `CanyonIGPCheck<N>` must be defined and set, where `<N>` is replaced by the row number, for example `CanyonIGPDistance1`.

- **Distance**

  Specify the perpendicular distance for this row(s) of source-oriented grid points (depending on the choice of **Units**) by setting the variable `CanyonIGPDistance` in *localmodel.cfg*.

- **Units**

  Set the units and reference point for this row(s) of source oriented grid points by setting the variable `CanyonIGPUnit` in *localmodel.cfg*. The following options are available:

  * **Absolute, from road centreline (m)** – the value in the **Distance** option is taken as the absolute distance in metres from the road centreline; this option must be used to specify any points that are inside the road carriageway if using absolute distances.
  * **Fraction of road width, from centreline** – the value in the **Distance** option is taken as a fractional distance of the road width from the centreline, e.g. a value of 2 would mean add points on either side of the road centreline at a distance of two times the road width.
  * **Absolute, from road edge (m)** – the value in the **Distance** option is taken as the absolute distance away from the road carriageway edge, i.e. the distance from each kerb.
  * **Fraction of canyon width, from centreline** – the value in the **Distance** option is taken as a fractional distance of the canyon width from the road centreline.

- **Check closeness**

  By default, source-oriented grid points will always be added for all rows defined regardless of point spacing. Set the variable `CanyonIGPCheck=1` in *localmodel.cfg* so that each row will only be added if it is more than 1 m away from the row on the same side of the road associated with the previous entry.

4.7.9.2 Along-source locations

By default, the maximum number of source-oriented grid points (not including interpolated points) that are added to road sources is around 5000. The default average spacing between pairs of points (again, not including interpolated points) is the maximum of:

(a) The spacing that would be achieved if the maximum number of source-oriented grid points were added to all road segments that fall within the output grid

(b) 0.5% of the output grid length (defined as the geometric mean of the ouput grid length in X and Y)

(c) The source width

If modelling a large region or a large number of road sources, it is desirable to increase the number of source-oriented grid points in order to improve the resolution of contour plots. It is therefore possible to modify the defaults described using the options shown in **Figure 4.41**.

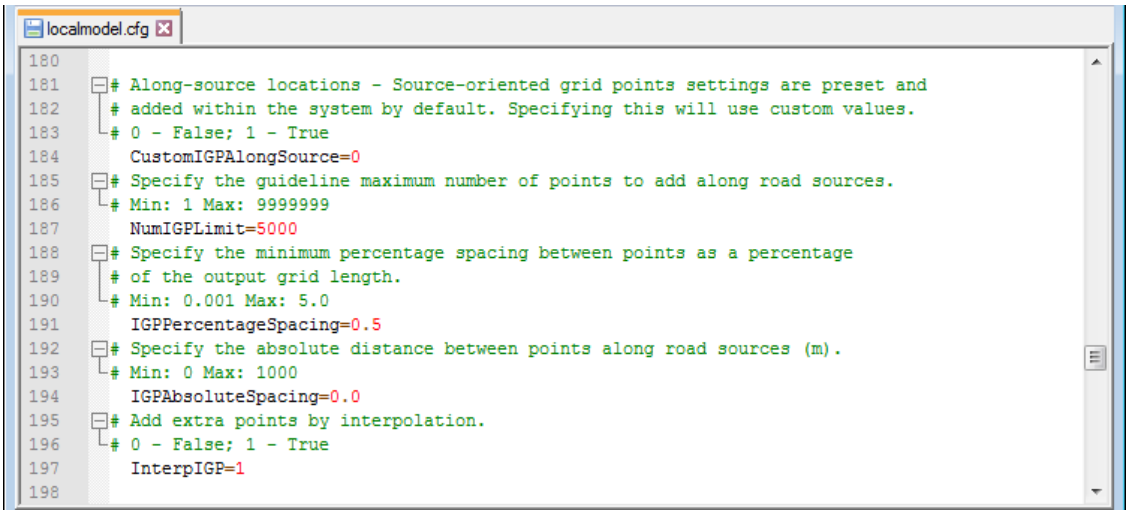


Figure 4.41 The along-source parameters of source-oriented grid points in *localmodel.cfg* file

- **Use custom along-source locations**

  Set `CustomIGPAlongSource=1` in the *localmodel.cfg* file to define the following options.

- **Guideline number of points to add**

  Specify the guideline maximum number of extra output points that can be added along road and canyon sources during the first stage of source-oriented gridding by setting the variable `NumIGPLimit` in *localmodel.cfg*.

- **Percentage spacing**

  Specify the minimum along-source spacing between the extra output points added during the first stage of source-oriented gridding, as a percentage of the output grid length by setting the variable `IGPPercentageSpacing` in *localmodel.cfg*.

- **Absolute spacing**

  Specify the actual along-road distance in metres between the extra output points added during the first stage of source-oriented gridding by setting the variable `IGPAbsoluteSpacing` in *localmodel.cfg*. This value will only be used if it is greater than (a) and (b) above, where (b) uses the specified **Percentage spacing** and not necessarily the default value of 0.5%.

- **Add interpolated points**

  Set `InterpIGP=1` in *localmodel.cfg* in order to carry out the second stage of source-oriented gridding (adding additional points by interpolation). Enabling this option is recommended to obtain the best results for contouring output.

4.7.9.3 Included sources

By default, the model will add source-oriented grid points to all the road and canyon sources that lie within the output grid. It is possible to modify this behaviour using the options shown in **Figure 4.42**. The source names must be consistent with those used in all road source data files (as described in Section 4.7.2).

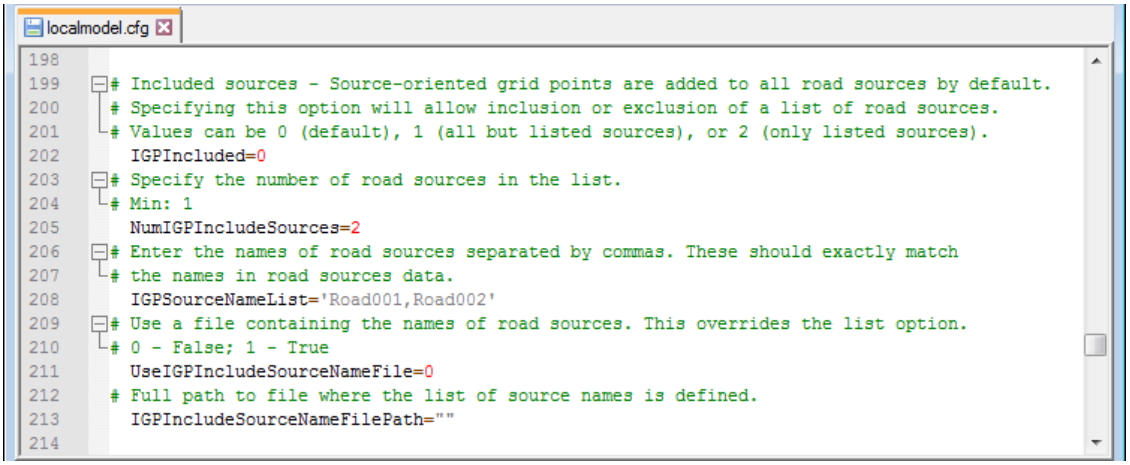


Figure 4.42 The parameters to control which sources should have source-oriented grid points in *localmodel.cfg* file

- **Sources to be used**

  By default, `IGPIncluded=0` is set in *localmodel.cfg* so that extra grid points will be added to all sources. If the variable is set to `IGPIncluded=1`, extra grid points will be added to all sources except those listed; if set to `IGPIncluded=2`, extra grid points will be added to only those sources listed.

- **Number of sources**

  Specify the number of sources in the list using the `NumIGPIncludeSources` variable in *localmodel.cfg*.

- **List of source names**

  Specify the source names in a single line separated by commas using the variable `IGPSourceNameList` in *localmodel.cfg*. This option provides a simple approach to listing source names and is only advised if including or excluding a small number of sources.

- **Use source name list file**

  If there are a large number of sources to include or exclude, the user can specify an input text file containing only the source names. Each source name should be listed on a separate line. This is done by setting the variable `UseIGPIncludeSourceNameFile=1` and the variable `IGPIncludeSourceNameFile` to a suitable file path in *localmodel.cfg*. This overrides the **List of source names** option.

4.7.10 Output pollutants (ADMS-Local only)

ADMS-Local can calculate output pollutant concentrations for any pollutant which is included as a local pollutant in the concentration species map file. Specify the pollutants for which output is to be calculated by entering the number of pollutants using the variable `NumOutputPols` and setting the variable `PolName<N>` to the appropriate species name, adding new variables as necessary replacing `<N>` with the pollutant number, for example `PolName1`. The equivalent settings for ADMS-Urban are defined in the *.upl* file(s).

The pollutant names must be consistent with the local model pollutant names in the concentration species map file (refer to Section 4.3.1).

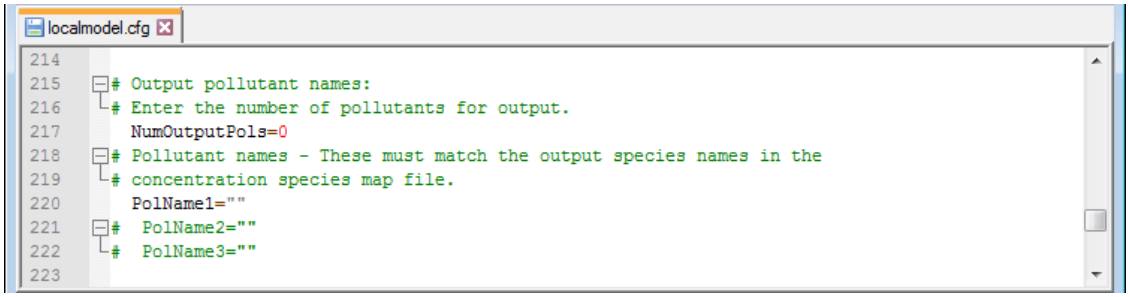


Figure 4.43 The output pollutant variables in the *localmodel.cfg* file

4.7.11 Chemistry (ADMS-Local only)

The MAQS coupled system includes the effect of chemical reactions in the concentrations obtained from the regional model, which are modelled over large temporal and spatial scales. ADMS-Urban and ADMS-Local incorporate local scale chemistry schemes. The calculations are described in more detail in Section 8.3.7. This section allows the user to specify which chemistry schemes are to be used in ADMS-Local. The equivalent settings for ADMS-Urban are defined in the *.upl* file(s).

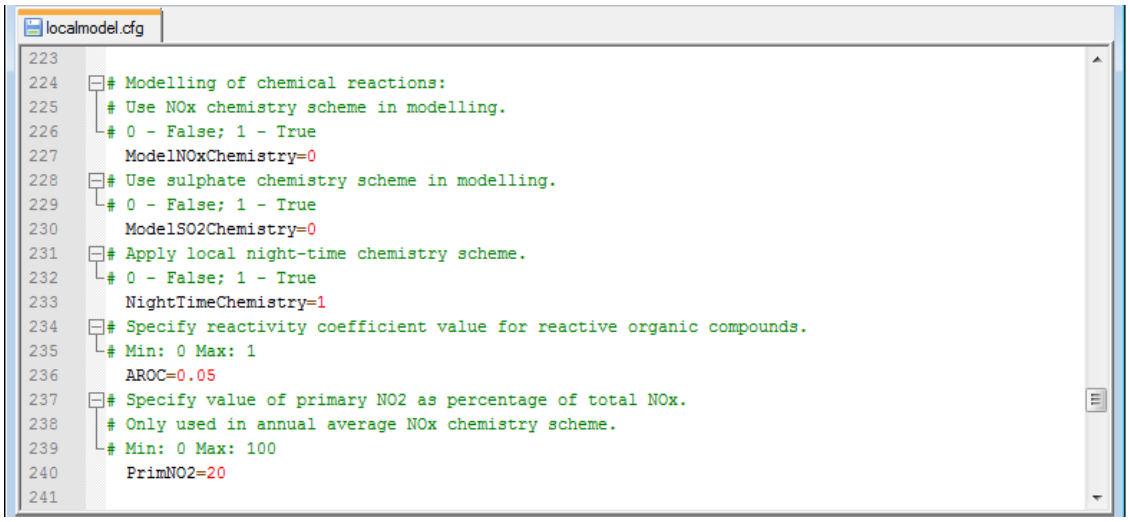


Figure 4.44 The chemistry variables in the *localmodel.cfg* file

- **Nitrate chemistry scheme**

  Set the variable `ModelNOxChemistry=1` in *localmodel.cfg* to use NO_x chemistry scheme.

- **Sulphate chemistry scheme**

  Set the variable `ModelSO2Chemistry=1` in *localmodel.cfg* to use sulphate chemistry scheme.

- **Night-time chemistry**

  Set the variable `NightTimeChemistry=1` in *localmodel.cfg* to use night-time chemistry scheme for NO_x chemistry.

- **AROC value**

  AROC represents the weighted reactivity coefficient for ROC or Reactive Organic Compounds (a fixed proportion of VOCs) used in the GRS scheme (refer to Section 8.3.7), taken to be 0.05 by default. This value can be modified by users by adjusting the variable `AROC` in the *localmodel.cfg* file.

- **Primary NO_2 fraction value**

  If modelling NO_x chemistry effects with annual average regional model concentrations, ADMS-Local assumes that a fixed percentage of NO_x is emitted as NO_2. Specify the percentage of 'NO_x as NO_2' using the variable `PrimNO2` in the *localmodel.cfg* file.

4.7.12 Conversion factors (ADMS-Local only)

ADMS-Local contains pre-defined µg/m^3 to ppb conversion factors for a palette of pollutants, shown in **Table 4.15**. This option allows user-defined conversion factors for new pollutants to be defined, or for the pre-defined pollutants to be altered. User-defined pollutants and conversion factors for ADMS-Urban are defined via the *.upl* file(s).

Pollutant name	Conversion factor µg/m^3 to ppb
NO_x	0.52
NO_2	0.52
NO	0.8
VOC	0.31
O_3	0.5
SO_2	0.37
SO_4	0.25

Table 4.15 Default conversion factors in ADMS-Local

Specify the conversion factors by entering the number of pollutants using the variable `NumConvFactors` in *localmodel.cfg* and setting the variable `ConvPolName<N>` to the

pollutant name and `ConvFactor<N>` to the corresponding conversion factor, adding new variables as necessary replacing `<N>` with the pollutant number, for example `ConvPolName1` and `ConvFactor1`.

The pollutant names must be consistent with the local model output pollutant names.

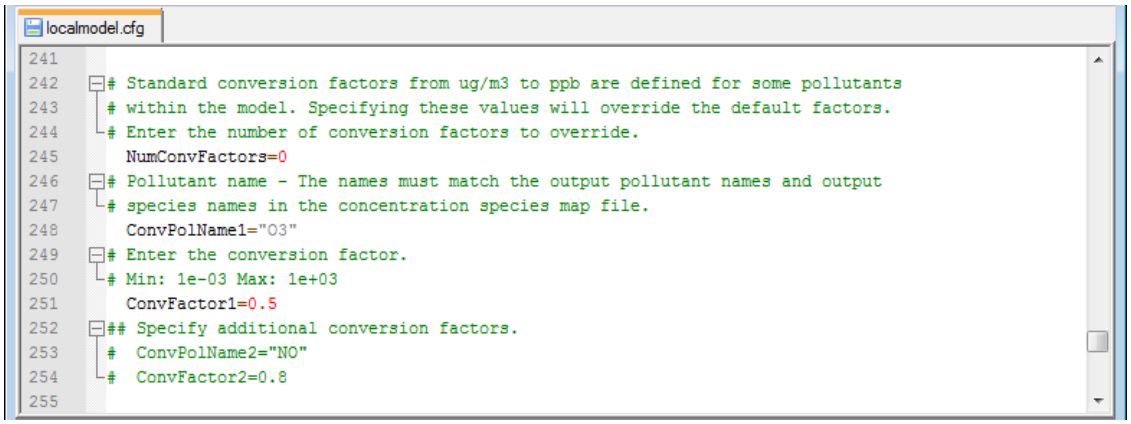


Figure 4.45 The conversion factors variables in the *localmodel.cfg* file

4.7.13 ADMS-Urban .upl files

If ADMS-Urban is the selected local model in *options.cfg* (refer to Section 4.1.3), the parameters for the local model runs are specified using an input *.upl* file(s) and all ADMS-Local input options above (Section 4.7.2 to 4.7.12 inclusive) are not used by the system. The ADMS-Urban *.upl* file path(s) are specified by setting the variables `ExplicitInputFilePath` and (optionally) `GriddedInputFilePath` in *localmodel.cfg*. Please refer to the ADMS-Urban User Guide for general information about how to create *.upl* files.

For each *.upl*, the MAQS coupled system control scripts will apply appropriate spatial and temporal truncation for each regional model grid cell covered by the nesting domain and substitute the *.met* and *.bgd* file paths corresponding to the relevant cell, please refer to Appendix APPENDIX I for more information. The coupled system will also alter the output locations when required.

The main differences between the *.upl* files used in the MAQS coupled system are the sources which they contain:

- the *.upl* with explicit emissions for the main nesting run uses emissions at the highest known resolution, which may include both explicitly defined road and point sources and gridded sources for minor road or domestic heating emissions; while
- the *.upl* with gridded emissions for the main nesting and background runs uses emissions matching those used in the regional model.

If the gridded emissions used in the regional model are also suitable for use in the run with explicit emissions, only one *.upl* needs to be specified by the user, with the system ensuring that it is run with only gridded emissions modelled when required.

Regional model emissions can be most closely matched in ADMS-Urban using a 3D grid source input file. If the option for automatic conversion of regional model emissions is in use (described in Section 4.4.1), only a single .upl *containing explicit source emissions needs to be specified, as the system will create 3D grid files and apply them to the* .upl *files automatically. This approach is recommended for runs of the MAQS coupled system using either the CMAQ or WRF-Chem regional models.*

For other regional models where the automatic conversion approach is not available, if the emissions data can be converted into Generic 3D grid source input file format by the user, this can be applied manually to one or both .upl *files.*

Elevated point sources may be included explicitly in .upl *files with 2D gridded emissions, if their emissions are represented at sufficient height in the regional model that they will not affect surface layer concentrations within the same grid cell. However, this approach should be used with caution in combination with the option to interpolate regional model concentrations (described in Section 4.1.7).*

Both *.upl* files should include the same **Meteorology** and **Background** settings. There are differences in the permitted and recommended settings for **Setup** for the two input *.upl* files, while the system makes changes to the **Grids** settings. Common aspects for both files are discussed below, while settings specific to a particular *.upl* are discussed in Sections 4.7.13.1 and 4.7.13.2.

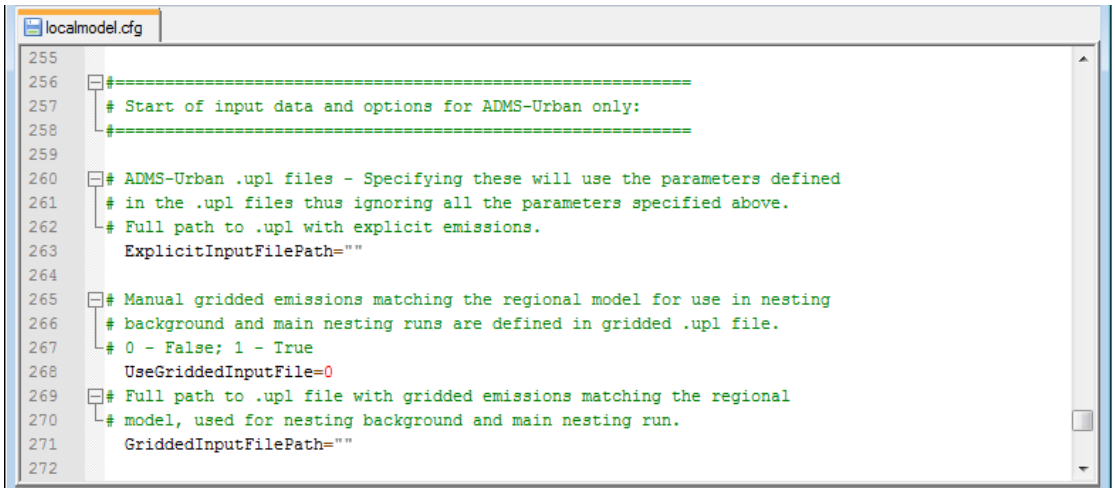


Figure 4.46 The ADMS-Urban *.upl* file paths in the *inputdata.cfg* file.

Setup

If you wish to include the effects of deposition in the locally-modelled concentrations, select the **Dry deposition** and/or **Wet deposition** option(s) and ensure that deposition parameters are set to match those used in the regional model. Note that the MAQS coupled system is currently only set up to calculate concentration values, not deposition, so no deposition rates will be included in the final outputs.

The **Odours** and **Buildings** options are not currently permitted in the MAQS coupled system.

If you wish to model NO_x chemistry, or the contribution of SO_2 to particulate

concentrations, select the **Chemistry** option, click on the **Enter parameters**... button and select the **Chemical reaction scheme** option. If the nesting domain contains areas with very low emission rates, the **Local night-time chemistry** *.uai* file option should be also be selected.

The Trajectory Model, which is used in standard ADMS-Urban modelling to take into account long-range chemical effects for emissions from distant grid source cells, should not be used in the MAQS coupled system .upl *files as these effects are captured by the regional model chemistry*.

The **Complex terrain** option should only be considered for use in the *.upl* file with explicit emissions if all three of the following conditions can be satisfied:

- the nesting domain is significantly smaller than the corresponding meteorological model domain;
- terrain elevation and/or roughness length data are available for the modelling region at significantly higher resolution than the regional meteorological model grid resolution; and
- the complex terrain modelling resolution selected in the ADMS-Urban interface corresponds to a substantially higher grid resolution across the terrain or roughness file extent than was used in the regional meteorological model.

Use of the ADMS-Urban **Complex terrain** module may lead to inconsistent nesting results, as local meteorological data from the current meteorological model grid cell is used as 'upstream' input to the whole area covered by the terrain or roughness file data, so should be treated with extreme caution.

The **Complex terrain** option should not be used in any *.upl* file with gridded emissions, as the meteorology extracted from the meso-scale meteorological model will include complex terrain effects at the resolution used by the regional air quality model.

Source groups

User-defined groups may be defined in the *.upl* file(s), but only the output from the first group in the output netCDF files, which will be the **All Sources** group, will be used for the final MAQS coupled system output.

Meteorology

The **Met. measurement site** parameters, such as surface roughness, should be set equal to the **Dispersion site** parameters, as local meteorological data from the corresponding cell of the meteorological model will be used. A central latitude for the nesting domain should be defined. The **Dispersion site Surface roughness** and any advanced options should be set based on the corresponding values used in the meso-scale meteorological model.

The MAQS coupled system control scripts will supply the file path of a *.met* file extracted from the regional model meteorological data for the relevant grid cell at run time, so any *.met* file specified in the *.upl* file will not be used. The met data extracted from the WRF output does not have wind directions in sectors and is always hourly sequential.

The **Use a subset of met. data** option should not be selected, as the MAQS coupled system control scripts will set this as required by the dates given for the nesting period.

Vertical profile data are not currently extracted from WRF for use in the MAQS coupled system, so this option should not be selected.

Background

A background concentration file containing either local upwind background from the regional model or nesting background concentrations is supplied by the MAQS coupled system control scripts so any *.bgd* file specified in the *.upl* file will not be used. If the **Chemistry** option is selected, either **From file** with a default background file or **Enter by hand** must be selected on the **Background** screen to allow the *.upl* file to be saved with output of non-emitted pollutants such as ozone (O_3) selected.

Output

An output should be defined for each ADMS pollutant listed in the species map file (described in Section 4.3.1). The outputs should be defined as:

- long-term (LT),
- units of $\mu g/m^3$ and
- averaging times of 1 hour.

The **All sources** group output and **Comprehensive output file** options should be selected.

4.7.13.1 .upl with explicit emissions

This *.upl* should be set up according to the best practice for local modelling with ADMS-Urban, with advanced modelling of road sources in street canyons if required. Select the desired explicit *.upl* by setting the variable `ExplicitInputFilePath` to an appropriate file path in the *inputdata.cfg* control file. This *.upl* is always required.

Setup

Please refer to the *Other inputs* section below for a discussion of additional input (*.uai*) file options for this run.

Sources and emissions

Sources should be set up in this *.upl* according to the best available explicit and gridded emissions data. Please refer to the ADMS-Urban User Guide for information about the source types available in ADMS-Urban. Time-variation of emissions can be defined on a source-by-source basis if this information is available.

If the option for automatic conversion of regional model emissions is in use, this *.upl* file will not contain any gridded emissions as the automatically converted 3D gridded emissions file will be applied by the system. If different gridded emissions are required for this run, the automatic regional model emissions option should not be used, but the regional model emissions could be converted outside the system using a stand-alone run of the conversion utility (described in Appendix B) and applied manually to the *.upl* file with gridded emission.

The grid source geometry for this run may use a higher spatial resolution than used for the regional model grid, if corresponding emissions data are available. The grid source emissions used in this run should include all the explicit emissions, so they may be different from those used in the run with gridded emissions if there are explicit sources in this run which are not included in the regional model emissions or if improved local emissions data are in use. The user may select a 2D or 3D grid source for this run depending on the available data and any required manipulations. Further considerations related to creating manual gridded emissions to match regional model emissions are given in Section 4.7.13.2.

Grids

If the **Receptor** output type has been specified in *inputdata.cfg*, as described in Section 4.5, specified point locations should be defined as required for final output. Only specified points defined in the ADMS-Urban interface or in an *.asp* file will be included in the final run; any gridded output settings will be overridden.

If the **Contour** option is selected, the gridded output locations specified in this run and the explicit source locations will be used for the **Create ASP** run to allow the creation of an *.asp* file including source-oriented grid point locations. Please refer to Section 8.4 and Appendix G for more details of the additional processes involved in the **Grid for contouring** option, including the **Create ASP** mode ADMS-Urban run.

When defining a regular output grid for this *.upl* in ADMS-Urban, ensure that it is offset from regional model grid cell boundaries and has spacing smaller than the regional model grid resolution, so that there are a consistent number of output points per regional model grid cell, ideally at least 5 points in each direction.

Further tips for model set-up and data processing to generate high-resolution contour plots of concentrations are given in Section 6.1.

Other inputs

Any of the additional model options available in ADMS-Urban may be used in this run, for example the Urban Canopy flow field and/or street canyon modules. If you wish to alter the number and/or locations of source-oriented grid points for road or line sources (intelligent grid points), to improve the resolution of concentration contours, the options in the *.uai* file sections for **Along-source locations** and **Across-source locations** of **Source-oriented grids** should be used for this run. Please refer to the ADMS-Urban User Guide for more details of the available *.uai* options.

Note that the .uai *file guidelines for numbers of points will be applied across the whole modelling domain, so if high resolution contour output is required for a large modelling domain, very large point number guidelines may need to be defined in the* .uai *file, as suggested in Section 6.1. Only those output points within a single regional model grid cell will be modelled in each ADMS-Urban run within the system.*

If the **Local night-time chemistry** *.uai* option is used in this *.upl* file it should also be selected for the *.upl* with gridded emissions, if used.

4.7.13.2 .upl with gridded emissions

Specify that a separate *.upl* file with gridded emissions has been defined by setting the option `UseGriddedInputFile=1` and the variable `GriddedInputFilePath` to an appropriate path in the *inputdata.cfg* control file.

This *.upl* should use gridded emissions matched as closely as possible to those used in the regional model, in both magnitude and time-variation. If the option for automatic conversion of regional model emissions is in use, described in Section 4.4.1, this *.upl* file will not contain any user-defined emissions and is not required. Details of the recommended input options which differ from those in the other *.upl* file are given below, arranged in the order of the main screens of the ADMS-Urban interface.

Setup

If including **Dry Deposition** or **Wet Deposition** in this run, ensure that pollutant deposition parameters are set to match those used in the regional model.

An additional input file (*.uai*) should only be supplied for this run in order to specify one or both of:

- manual use of the 3D grid source option, if the option for automatic conversion of regional model emissions is *not* in use; and
- use of the **Local night-time chemistry** option, which is recommended for nesting domains which contain areas with very low emission rates, such as rural or marine areas.

Sources and emissions

This *.upl* should include gridded emissions, in order to match the behaviour of the regional model as closely as possible. If the option for automatic conversion of regional model emissions is in use, or if gridded emissions equivalent to the regional model emissions have manually been specified in the *.upl* with explicit emissions, this *.upl* file is not required.

If the option for automatic conversion of regional model emissions is *not* in use, gridded emissions should be defined to cover the whole of the selected nesting domain. A larger extent of emissions may be defined in the *.upl* file, for example covering the whole of the regional model domain, as the emissions will be spatially truncated to the extents of each regional model grid cell within the nesting domain before running.

The emissions for this run should match those used in the regional model as closely as possible, so use of the 3D grid source option is recommended, where a netCDF file including hourly emissions for each pollutant species on a 3D grid is used in ADMS-Urban. Generic 3D gridded emissions files (with format as defined in Section 4.4.6) must be created outside the MAQS coupled system if a regional model other than CMAQ or WRF-Chem is in use.

If it is not possible to use a 3D grid source, a 2D grid source should be used, as described in the following paragraphs. The 2D grid source should be defined with horizontal geometry matching the regional model horizontal grid definition, and depth equal to twice the height of the regional model grid layer(s) containing the majority of the

ground-level emissions. For example, if the lowest regional model grid layer is 20 m deep and contains 95% of the emissions from non-point sources, an ADMS-Urban grid source depth of 40 m would be suitable. The doubling of the grid source depth takes into account the vertical plume spread which occurs across the initial cell.

The magnitude of the emission rate in each 2D grid cell should correspond to the annual average emission from the corresponding regional model grid cell. Note that unit and species conversions may be required to obtain emissions suitable for an ADMS-Urban grid source from those used in the regional model.

Any time-variation used in the regional model emissions should be applied to the 2D grid source in this *.upl* file using either a *.fac* file or hourly factors specified in the ADMS-Urban interface. The *.fac* file allows monthly profiles to be included in addition to daily variation on weekdays, Saturdays and Sundays or each day of the week. If different time-varying profiles are used for different source types in the regional model, a weighted average profile should be calculated for use in ADMS-Urban.

Poor matching between the emissions used in this run and the regional model emissions can lead to invalid nesting background calculations. If large numbers of negative nesting background hours are reported as warnings from the ***Processor*** *utility in nesting background mode, the emission factors and time-variation profiles used in this run should be assessed for consistency with those used in the regional model.*

If a 2D grid source is in use, elevated point sources, for example power stations, may be included as explicit sources in this *.upl* file if they are included in the regional model emissions in upper layers of the regional model grid, such that they will have no effect on local near-ground concentrations. This will prevent the emissions from being modelled at ground level by ADMS-Urban, which can lead to invalid nesting background calculations. However, this approach should not be used in combination with the option to interpolate regional model concentrations.

Grids

If the **Receptor** output type has been chosen in the *inputdata.cfg* file, identical specified point locations should be defined in both *.upl* files. If the **Contour** option is selected, the output locations specified in the *.upl* file with gridded emissions will not be used. Please refer to Section 8.4 and Appendix G for more details of the additional processes involved in the C**ontour** option.

4.7.13.3 Options not included in final system output

User-defined group output and deposition rates are not currently included in the final MAQS coupled system output files. These options may still be specified in the input *.upls*, for example to take account of the plume depletion caused by deposition, or for investigations of the contributions of different source types in the explicitly-modelled ADMS-Urban concentrations.

4.7.13.4 Options not permitted in system input .upls

The **Odours**, **Buildings** and **Aircraft Sources** options must not be included in the MAQS coupled system input *.upl(s)*.

4.8 Remote machine options

The *sshlogin.cfg* input file is required if the GNU parallel option is being used for parallelisation of the main utility and local model runs, as described in Sections 2.2.2 and 4.1.12. The *sshlogin.cfg* file contains a list of machines to use for the runs with ssh login details, with an optional setting of the number of runs which can be sent to each machine. The template file created using the `make_def_inputs.sh` script specifies use of the local machine on which the top level `run-maqs` script is run with the special indicator :, as shown in Figure 4.47.

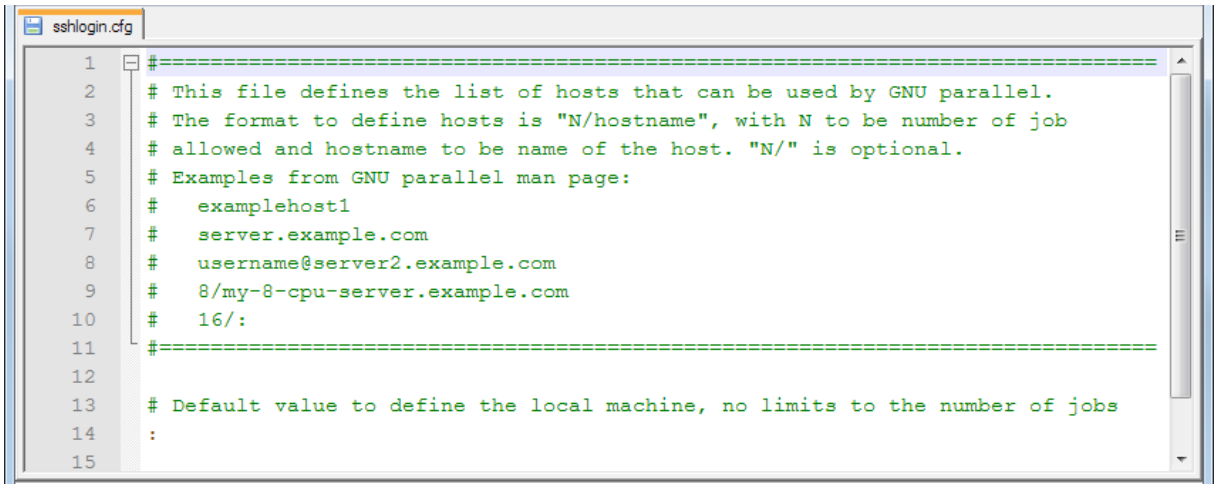


Figure 4.47 The default *sshlogin.cfg* file, defining an unlimited number of runs on the local machine.

For each remote machine, the ssh login details are specified in the format `user@hostname`. The number of permitted runs for each machine are defined by a prefix in the format `n/` where n is the number of permitted runs. For example, if 4 runs are permitted for the account `user1` on the machine with host name `node2`, this is defined as `4/user1@node2`. The hostname can alternatively be defined as an IP address or an internet server address. Further examples of valid ssh login definitions can be found through the GNU parallel `man` pages and the initial comments in the template *sshlogin.cfg* file.

Remote machines must be set up to allow ssh logins from the local machine without entering a password i.e. using ssh keys.

SECTION 5 System output

This section describes the outputs which are produced by the MAQS coupled system. The main output files, which will be produced by all successful system runs, are a log file and an ADMS format netCDF file containing concentration data, these are described in Sections 5.1 and 5.2 respectively. Other files which may be returned by the system are described briefly in Section 5.3. The MAQS Post Processor utility (CERC, 2023b) is a dedicated tool for spatial and temporal processing of the final output netCDF file produced by the MAQS coupled system. Some of the functions of the Post Processor were based on a precursor tool, the ADMS Comprehensive Output File Processor (CERC, 2020a), which has its own user guide.

5.1 System log file

The MAQS coupled system generates a log file which records activities from each component of the system, with details of the inputs and whether the component ran without errors.

The MAQS coupled system log file is created with a name according to the pattern <project name>_YYYY-MM-DD_HH_mm_<output type>.log, where <project name> is the value of `ProjectName` in *inputdata.cfg*, described in Section 4.5.2, the date and time is the starting date and time of the run, and <output type> is an abbreviation of the local model output type from Section 4.5.1. For example, if your `ProjectName` is "`Cambridge`", and the run was launched at 10:21 on 25/05/2023 with a `CONTOUR` output type, then the log file would be found at:

/disk/output/Cambridge_2023-05-25_10_21_con.log.

The local model and utility version information can be found in the log files of each individual model and utility run.

Each entry in the main section of the log file consists of date and time information, followed by a message about the current stage of the coupled system. For example, a call to the utility which extracts meteorological data would be recorded as follows:

```
[2023-05-25 10:21:17] Launched RMMetData utility for (22000.00,-
676500.00) with command line:

  "/disk/user/working/C100C22000.00C-676500.00/RMMetDataInput.txt"
```

The end of the *.log* file (and terminal output) gives the final status of the coupled system run, and the location of the output files, such as in the example shown below.

```
[2023-05-25 10:21:20] Process succeeded.

[2023-05-25 10:21:20] Final comprehensive output file can be found
here:

 /disk/output/Cambridge_2023-05-25_10_21_con.nc

[2023-05-25 10:21:20] Other files can be found here:

 /disk/output/Cambridge_2023-05-25_10_21_con_files/
```

When the GNU Parallel option is in use, as described in Section 4.1.12, additional partial log files will be created on each remote machine, recording the utility and model runs carried out on that remote machine. At the end of the parallelised tasks the remote log files are copied back to the host machine. The log files from remote machines have extended file names with a final component of `-remote-<machine name>`. To extend the example above, if the `ProjectName` is `"Cambridge"`, the run was launched at 10:21 on 25/05/2023 with a `CONTOUR` output type and it was run on remote machines node1 and node2, then the additional remote log files will have the names

/disk/output/Cambridge_2023-05-25_10_21_con-remote-node1.log

/disk/output/Cambridge_2023-05-25_10_21_con-remote-node2.log

When all processes for a particular cell have completed on a remote machine, the remote log will include the statement: `Stored scripts executed for cell X`. where X is the cell index number within the nesting domain.

5.2 Final output file

The concentrations output by the MAQS coupled system are stored in a netCDF (*.nc*) file which follows the ADMS Comprehensive Output File conventions. This differs from regional model output as in general, the data points do not form a regular grid and the point locations are only supplied in a projected coordinate system. This format is described in **Table 5.1** to **Table 5.3**. The dimensions, variables and attributes listed below the thicker black line in each table are not relevant to ADMS-Local but are included for consistency with the format of ADMS-Urban netCDF output files.

Name	Description
nPoints_XYZ	Number of output points
nMetLines	Number of met. lines (netCDF 'unlimited' dimension)
nDatasets	Number of hourly datatests
nAveDatasets	Number of period average datasets
MetLineStringLength	*Maximum length of the met line description (=11)*
DatasetNameStringLength	*Maximum length of the dataset names (=44)*
PointNameStringLength	*Maximum length of an output point name (=44)*
OutputTypesUsed	*Number of output types (=2; hourly and period average)*
OutputTypesStringLength	*Maximum length of the output type description (=14)*
nPoints_XY	Number of output points
nGroups	*1*
OutputOptionsUsed	*3*
NumberOfTypesOfOutputPoint	*5*
GroupStringLength	*30*
OutputOptionsStringLength	*14*
OutputPointTypesLength	*16*

Table 5.1 Dimensions in the netCDF output file. The dimensions in italics are required as part of the netCDF format and are the same for all coupled system output files.

Name	Dimensions	Description
PointX_XYZ	nPoints_XYZ	X-coordinate of each output point
PointY_XYZ	nPoints_XYZ	Y-coordinate of each output point
PointZ_XYZ	nPoints_XYZ	Z-coordinate of each output point
PointName_XYZ	nPoints_XYZ, *PointNameStringLength*	"Receptor, *name*", where *name* is the name given by the user for each output point
Met_Line	nMetLines, *MetLineStringLength*	Date and time of met line in the format YYYY_DDD_HH, where YYYY is the year, DDD is the Julian day and HH is the hour (local solar time, hour ending convention)
Met_Uat10m	nMetLines	10 m wind speed for each met line
Met_Phi	nMetLines	Wind direction for each met line
Met_H_over_LMO	nMetLines	Boundary layer height divided by Monin-Obukhov length for each met line
Number_Of_Output_ Points_Of_Each_Type	NumberOfTypesOfOutputPoint	(0, 0, number of output points, 0, 0)
Output_Types_Description	OutputTypesUsed, *OutputTypesStringLength*	("Hourly", "Period average")
Output_Types_Used	OutputTypesUsed	Indicates whether hourly and/or period average data are included in the file, e.g. (1,0)
DatasetNames	nDatasets, *DatasetNameStringLength*	Descriptive name for each dataset, including the pollutant name, e.g. "NOx_conc_1hour"
Dataset#	nMetLines, *nGroups*, nPoints_XYZ	Datasets containing hourly concentration data for each output pollutant
Ave_DatasetNames	nAveDatasets, *DatasetNameStringLength*	Descriptive name for each period average dataset, including the pollutant name, e.g. "NOx_conc_Ave"
Ave_Dataset#	*nGroups*, nPoints_XYZ	Datasets containing period average concentration data for each output pollutant
PointX_XY	nPoints_XY	X-coordinate of each output point
PointY_XY	nPoints_XY	Y-coordinate of each output point
PointName_XY	nPoints_XY, *PointNameStringLength*	"Receptor, *name*", where *name* is the name given by the user for each output point
Met_Freq	nMetLines	Set 1 for each met line
Output_Options_ Description	OutputOptionsUsed, *OutputOptionsStringLength*	("Concentration", "Dry deposition", "Wet deposition")

Name	Dimensions	Description
Output_Options_Used	OutputOptionsUsed	(1, 0, 0)
Output_Points_Type	NumberOfTypesOfOutputPoint, *OutputPointTypesLength*	(“Grid Horiz”, “Grid All”, “Specified Points”, “Grid Nested”, “Grid Intelligent”)
Group	*nGroups*, *GroupStringLength*	“<All sources>”

Table 5.2 Variables in the netCDF output file. Dimensions are listed with the fastest varying last and the string length dimension is indicated in italics for character variables.

Associated with	Name	Description
Global	File_Version	Version number of the netCDF output file
Global	File_Type	Indicator that this is an ADMS output file
Global	Site_Name	The name of the modelling site
Global	Project_Name	The name of the modelling project
Global	Model_Name	Name of the model that created the file
Global	Model_Version	Version number of the model that created the file
Global	Model_Build_Number	Build number of the model that created the file
Global	Model_Release_Date	Build date of the model that created the file
Global	Date_Created	The date the file was created
Global	Time_Created	The time the file was created
Variables	Units	Units of the variable
Dataset#	Dataset_Name	Name of an hourly dataset
Dataset#	Pollutant_Name	Name of the pollutant for an hourly dataset
Dataset#	Av_Time_s	Averaging time (= 3600 s for hourly datasets)
Dataset#	Units	Units of an hourly dataset
Dataset#	ugm3_to_ppb_conv_factor	$\mu g/m^3$ to ppb conversion factor for the pollutant associated with an hourly dataset
Ave_Dataset#	Dataset_Name	Name of a period average dataset
Ave_Dataset#	Pollutant_Name	Name of the pollutant for a period average dataset
Ave_Dataset#	Av_Time_s	Averaging time (= 3600 × nMetLines s for period average datasets)
Ave_Dataset#	Units	Units of a period average dataset ($\mu g/m^3$)
Ave_Dataset#	ugm3_to_ppb_conv_factor	$\mu g/m^3$ to ppb conversion factor for the pollutant associated with a period average dataset
Global	Is_Data_Hourly_Sequential	“YES”
Global	Grid_Description	“Sp. Pts. Only”
Dataset#	Output_Type	“Concentration”
Ave_Dataset#	Output_Type	“Concentration”

Table 5.3 Global and variable attributes in the netCDF output file.

There is a dedicated utility for processing the MAQS Coupled System output files, the Post Processor utility, which allows for spatial and temporal processing of the netCDF file output by the coupled system. These processed concentration data can be output in text-based *.csv* format for use in other processing or as Surfer Grid files (*.grd*) for gridded data. The Surfer Grid files can then be converted to image format. Please refer to the Post Processor Utility User Guide for more details of the available processing options.

Other netCDF processing tools can be used to extract the data from the coupled system output file on Linux, for example Python or R.

5.3 Intermediate files

The number and type of intermediate files retained by the MAQS coupled system depends on the user input for file save options, as described in Section 4.1.9.

Each local model run within the coupled system produces standard output files, for example **.nc*, **.log*. The input and output files associated with each of the utility programs are described in the Appendices.

5.3.1 Intermediate file names

Intermediate files are stored in a directory created with the file-name stem of the log and output files, appended with *'_files'* within the specified `ARCH_DIR` directory where output files are stored. For example, if your output file is */disk/output/Cambridge_2023-05-25_10_21_con.nc* then the intermediate files would be saved in */disk/output/Cambridge_2023-05-25_10_21_con_files/*.

Within this directory, additional directories will be created for each regional model grid cell included in the nesting domain if it includes any output points, named according to the x and y coordinates of the centre of the grid cell, as well as their run order. For example, if your nesting domain covers the region (0, 0) to (2000, 2000), with regional model resolution of 1000 m, all files associated with the lower-left cell of the domain would be filed in */disk/output/Cambridge_2023-05-25_10_21_con_files/C0C500.00C500.00/*.

Strict naming conventions are used by the coupled system to ensure that every file has a unique name without an excessively long file path. **Table 5.4** shows the file naming conventions used for each stage of the MAQS coupled system.

Stage	Inputs	Description	File name stem	Each cell?
Step 2	4.3	Extraction of regional model grid information	GridInfo	N
Step 3	4.4	Extraction of regional model emissions	RMEmissions	N
Step 4	4.7.8	Create *.asp* file with source-oriented grid locations	CreateAsp	N
Step 5	4.2	Extraction of met data	RMMetData	Y
Step 6		Extraction of local upwind background	LocalUpwind	Y
Step 7	4.7	Local model run for nesting background	BgdGrid	Y
Step 8		Calculation of nesting background	NestingBgdCalc	Y
Step 9	4.7	Main local model runs: explicit emissions	MainExpl	Y
Step 9	4.7	Main local model runs: gridded emissions	MainGrid	Y
Step 10		Calculate nesting output concentrations	NestingOutput	Y
Step 11		Combine output files	CombineCOF	N
		Add interpolated source-oriented grid points	CombineCOF.out	N

Table 5.4 Summary of file naming conventions used in the MAQS coupled system. Please refer to Section 8.2 for a detailed description of each Stage. Please refer to the sections in the User inputs column for information about corresponding control file inputs. The 'Each cell?' column indicates whether files are created for each regional model grid cell covered by the nesting domain.

5.3.2 Additional parallel process log files

When the GNU parallel option is in use, as described in Section 4.1.12, an additional log file is created which records the parallel commands that distribute cell processes between remote machines, along with the start times and durations for these commands. This log file contains one line for each grid cell within the nesting domain and is given the standard name *Parallel.log*.

When the option for transferring files from the host machine to remote machines is in use, as discussed in Section 4.1.12, a separate log file will be created to record the file transfers. This file contains one line for each remote machine to which files are being transferred and includes details of the time taken for each transfer and the command used for the transfer. It is given the standard name *ParallelRemoteTransfer.log*.

SECTION 6 Troubleshooting

This section gives guidance on how to investigate common errors from the MAQS coupled system. Section 6.1 gives tips for improving the appearance of high-resolution contour plots. Section 6.2 outlines a procedure for investigating cells which are reported as 'failed' in the coupled system log file. The remaining errors are arranged according to the component of the coupled system from which they would be issued or with which they are associated. This is not a comprehensive list of errors which can be issued by all components of the MAQS coupled system if run as stand-alone utilities, as the scripts ensure correct settings for many inputs.

6.1 Tips for creating high-resolution contour plots

Users are strongly advised to run MAQS in model verification mode and create a test plot of the output before starting a large contour run for a long modelling period. This will allow you to ensure that the output grid settings are suitable for high-resolution concentration contours. The following problems may be encountered:

Problem 1: The contour boundaries are uneven, particularly near the boundaries between regional model grid cells.

Solution 1: Consider using the option to interpolate regional model concentrations, as described in Section 4.1.7. When defining a regular output grid in *localmodel.cfg* in Section 4.7.84.1.7, ensure that it is offset from regional model grid cell boundaries and has spacing smaller than the regional model grid resolution, so that there are a consistent number of output points per regional model grid cell, ideally at least 5 points in each direction. For example, if the nesting domain is defined as extending from (1000, 1000) to (3000, 3000), with 1 km regional model grid resolution, a suitable output grid might extend from (1100, 1100) to (2900, 2900), with 19 points in each direction, to give a regular grid spacing of 200 m. If ADMS-Urban is the selected local model, the output grid is defined in the *.upl* file **Grids** settings.

The nearest or natural neighbour gridding methods are recommended for creating smooth contour plots from irregularly spaced modelling locations.

Problem 2: The contour resolution is poor near the explicitly-modelled road sources

Solution 2: View the locations of the output points used as input to the contour process. There should be output points along each of the explicitly-modelled road sources, with spacing similar to the desired output image resolution, eg. 10 m. If the output points near roads do not form a sufficiently high-density network, either set the **Along-source locations** of **Source-oriented grids** option in *localmodel.cfg* described in Section 4.7.9.2 with an increased guideline number of source-oriented grid points for road sources (when modelling with ADMS-Local). In ADMS-Urban, use the *.uai* file section for **Along-source locations** of **Source-oriented grids** and apply it to the *.upl* with explicit emissions. The following settings for the **Along-source locations** parameters have been found suitable for large nesting domains to create images at resolutions of 10 – 20 m:

- **NumIGPLimit** – increase to a large number, consider values up to 5000000;
- **IGPPercentageSpacing** – recommended setting 0.1;

- **IGPAbsoluteSpacing** – recommended setting 60 m, this will give a final output resolution along roads of 15 m after interpolated points are added.

Consider using the natural neighbour method for creating contours.

Problem 3: The concentration contours for night-time hours in areas with low emission rates are not smooth, showing unwanted artefacts.

Solution 3: Use the **Night-time chemistry** option in *localmodel.cfg* described in Section 4.7.11. In ADMS-Urban, use the **Local-night-time chemistry** option in the *.uai* file.

6.2 Investigating failed cells

If the MAQS coupled system log file summary of the run indicates that one or more cells have failed, the following steps will help to identify the cause of the failure:

The location of `WORK_DIR` *should be altered in the* folders.cfg *control file before investigating, so that the working files for the run with the failed cell(s) are not overwritten by any subsequent run attempts.*

- Open the coupled system *<run name>.log* file from the run in a text editor, such as Notepad.
- Search the file for the word 'failed' (without the inverted commas). Note which cell(s) have failed, e.g. (-4000.00,-665500.00) and at which stage of the system run, e.g. Local Upwind Background.

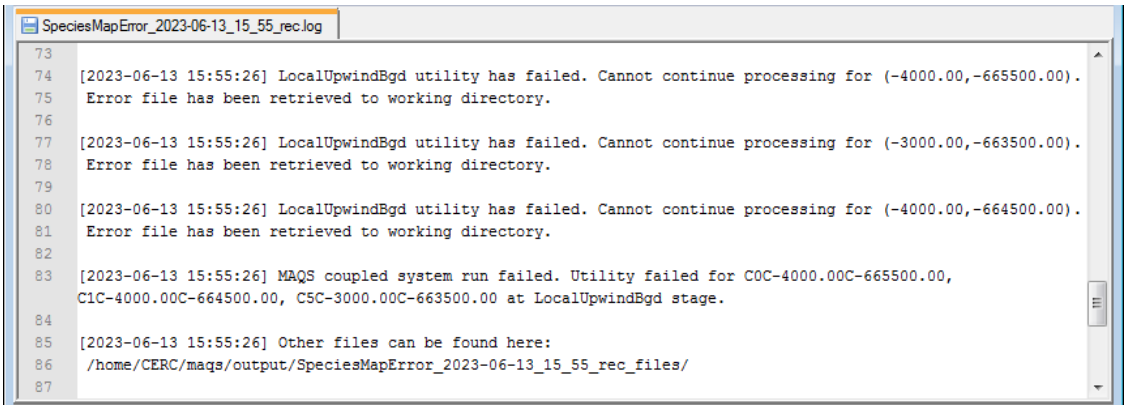


Figure 6.1 System log file error messages

- For each failed cell:
  - Open the *<run name>_files* directory and go to the subdirectory for the failed cell e.g. *C0C-4000.00C-665500.00.*
  - Use a text editor to open any Error file for the failed stage, which can be identified following the naming conventions described in **Table 5.4** . The contents of the file will give additional information about which stage of the MAQS coupled system failed for this cell.
  - Use a text editor to open any Warning file for the failed stage in a text editor, again identified by the naming conventions. In some cases the warning messages may

give more information about problems identified by the utilities before the final failure.

- If there is no error file or the error does not have an obvious cause, try re-running the failed stage manually to see whether the error is repeated. Instructions for running each of the utility programs can be found in the appendices. Make sure that you have selected the option to keep all files to be able to use the input files for the failed stage in the cell's subdirectory of the MAQS coupled system output directory. If the error is not repeated when the failed stage is re-run, it may have been caused by a temporary problem, for example an interruption in the network connections between HPCs or file storage locations used by the coupled system. If the error is repeated and you cannot identify its cause, contact the CERC helpdesk for support.

- Once you have corrected the error(s) and re-run the failed stage for each failed cell, consider re-running the remaining stages of the MAQS coupled system manually, following the instructions given in the Appendices, or re-running the complete coupled system run. If a cell has failed in the initial stages of the coupled system run, i.e. before the main local model runs have been performed, it is likely to be necessary to rerun the complete system run. However, if a cell has failed during the main local model runs or one of the post-processing stages, re-running the failed stages manually may be less time-consuming.

6.3 MAQS coupled system control scripts

Error messages from the coupled system are written to the current run's log file and to the terminal via `stdout`.

6.3.1 File path template does not match the regional model files

CaseSensitive_2023-09-08_09_59_rec.log

```
1  [2023-09-08 09:59:44] MAQS coupled system run started.
2
3  [2023-09-08 09:59:44] MAQS coupled system version 1.1.0
4  [2023-09-08 09:59:44] $ProjectRevision: SVN 9463 (2023-09-04) $
5
6  [2023-09-08 09:59:44] Writing utility input file:
7   /home/CERC/maqs/working/GridInfoInput.txt
8
9  [2023-09-08 09:59:44] Launched GridInfo utility for (-4000.000,-665500.000) with command line:
10   "/home/CERC/maqs/working/GridInfoInput.txt"
11
12 [2023-09-08 09:59:44] GridInfo utility has failed. Cannot continue processing.
13  Error file has been retrieved to working directory.
14
15 [2023-09-08 09:59:44] MAQS coupled system run failed. Utility failed for whole domain at GridInfo stage.
16
17 [2023-09-08 09:59:44] Other files can be found here:
18  /home/CERC/maqs/output/CaseSensitive_2023-09-08_09_59_rec_files/
19
```

Figure 6.2 Log file error message entries for missing regional model file

Problem: **Figure 6.2** shows the error message which will be issued if the regional model files cannot be found by the MAQS coupled system scripts as indicated by failure at the **RM Grid Info** utility stage.

GridInfo.wng

```
3  /home/CERC/maqs/utils/RMGridInfo.out
4  ============================
5  Problem:      The regional model file
   /home/CERC/maqs/Data/CAMx/CAMx.20100303_4x5.ncf does not exist.
6  Date/time:    08/09/2023 09:59:44
7  Input directory:  "/home/CERC/maqs/working"
8  Output file:  "/home/CERC/maqs/working/GridInfoOutput.txt"
9  Version:      1.1
10 Build number: 9446
11
```

Figure 6.3 Utility warning message for missing regional model file

Solution: Go to the top level directory of `WORK_DIR` and check the **RM Grid Info** utility error and warning files as in **Figure 6.3**. The specified file directory and/or file name template for the regional model files may be inaccurate in the MAQS user inputs, as described in Section 4.3.2. Ensure that the file quoted in the warning file is correct. Note that file paths and variable names are case sensitive on Linux systems.

6.3.2 Nesting domain not covered by regional grid cells

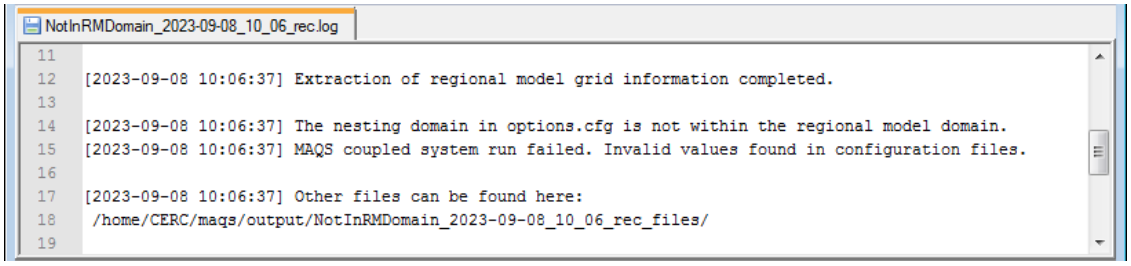


Figure 6.4 Log file error message entries for incorrect nesting domain settings

Problem: **Figure 6.4** shows the error message which will be issued if the nesting domain coordinates are not fully within the extents of the regional model grid, based on the regional model grid definition that is extracted by the **RM Grid Info** utility.

Solution 1: Check that the correct regional model concentration output files are being used by the system.

Solution 2: Check that the same projected coordinate system, with units of metres, has been used to define both the regional model grid and the nesting domain corner coordinates. The regional model grid must be regular and orthogonal in this coordinate system.

6.3.3 Nesting domain boundary not aligned with regional model cell boundary

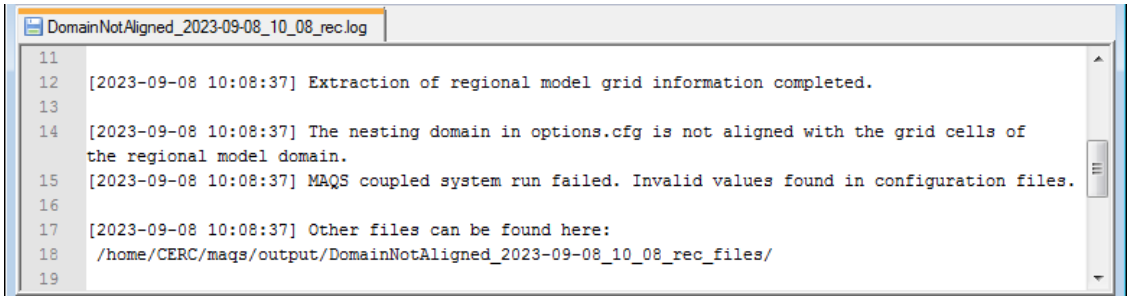


Figure 6.5 Error message issued if the nesting domain boundaries do not align with regional model grid cell boundaries

Problem: The coupled system requires the input nesting domain boundaries to be aligned with regional model grid cell boundaries to within 0.01 of the cell spacing. If this is not the case, the error message shown in **Figure 6.5** will be issued.

Solution: Check that the boundaries of the nesting domain you have defined align with regional model grid cell boundaries. The nesting domain and regional model grid must both be defined in the same projected coordinate system with units of metres, in which the regional model grid is regular and orthogonal.

6.4 ADMS-Local model

Errors from the ADMS-Local model are written to the ADMS-Local *.log* file, in addition to an *.err* or *.wng* file in the same directory as the ADMS-Local primary input text file. All ADMS-Local runs in the MAQS coupled system are carried out with spatial truncation to a single regional model grid cell. Hence the associated *.log* files from the model are stored in directories for each grid cell, as described in Section 5.3.

6.4.1 Error in reading the input road data files

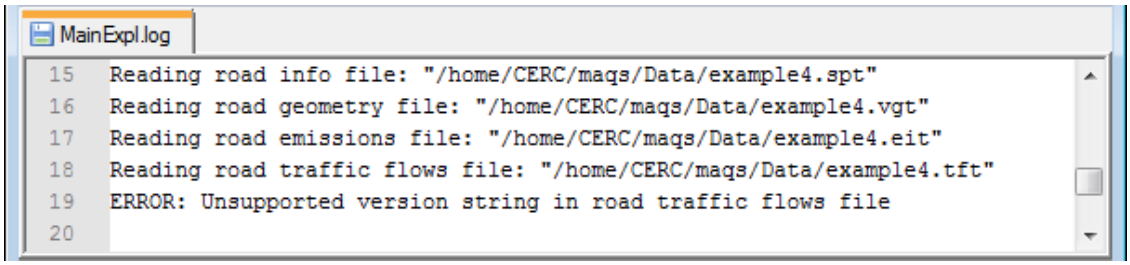


Figure 6.6 Error message if there is a problem reading the road data files.

Problem: **Figure 6.6** shows the message if an input road data file is invalid or in an unsupported format.

Solution: Check that the road data files are in the correct format for the specified regional model, defined in Sections 4.7.2 and 4.7.3. Note that the MAQS coupled system directly supports the equivalent files used by the ADMS-Urban import and export facility for the road source properties (*.spt*) file and the corresponding vertex information (*.vgt*) and pollutant emissions (*.eit*) file with the exception of the traffic flow data (*.tft*) file which should be converted to the ADMS-Local specific *.rdt* file. It is important for users to ensure the correct formatting of road data files as they are read in the main local model runs with explicit emissions, which are one of the later stages of a MAQS coupled system run.

6.5 ADMS-Urban model

Errors from ADMS-Urban model runs are written to the ADMS-Urban *.log* file, in the same directory as the relevant *.upl* file. All ADMS-Urban model runs in the MAQS coupled system are carried out with spatial truncation to a single regional model grid cell, except the run in **Create ASP** mode if the **Grid for contouring** output type option is selected. Hence the *.upl* files and associated *.log* files are stored in directories for each grid cell, as described in Section 5.3.

6.5.1 Spatial truncation removes all output points

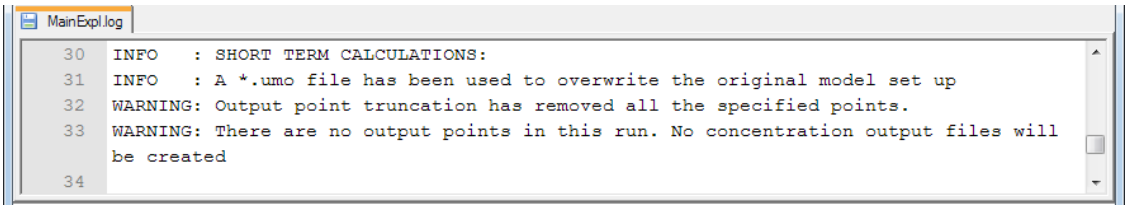


Figure 6.7 Example warning message if no output points are within the spatial truncation limits.

Problem: ADMS-Urban will give a warning if there are no output points to be modelled after spatial truncation has been applied. The warning message for no output points remaining within the truncation region is shown in **Figure 6.7**.

When the MAQS coupled system is run with the **ADMS-Urban Output type** set to **Receptor**, the initial check run (described in Step 4 of Section 8.2) runs ADMS-Urban over the whole domain and then analyses each grid cell. A regional model grid cell which contains no output points will be excluded from further processing by the MAQS coupled system control scripts. The coupled system run containing excluded cells is likely to complete successfully, provided at least one cell is included in the run.

When the MAQS coupled system is run with the **ADMS-Urban output type** set to **Contour**, the initial check run is not performed. The **Create ASP** run (described in Section 8.4.1) will fail if there is no overlap between the nesting domain and the output points defined in the *.upl* with explicit sources. If one or more grid cells within a larger nesting domain do not contain any output points, these cells will generate warnings at the main ADMS-Urban runs stage and fail in the calculation of output concentrations as the required *.nc* input files are not available.

Solution: Check that the nesting domain and all output point locations in the input *.upl* files are defined in the same coordinate system. If there are cells which do not include output points, use the **Receptor** run type instead of **Contour**.

6.6 RM Grid Info utility

Errors or warnings from the **RM Grid Info** utility are written to an *.err* or *.wng* file, in the same directory as the relevant input text file. **RM Grid Info** is run once at the start of the system run, so any error files from the utility are stored in the top level of the `WORK_DIR`.

6.6.1 Errors with regional model files

GridInfo.wng

```
3   /home/CERC/maqs/utils/RMGridInfo.out
4   ==========================
5   Problem:      The regional model file
    /home/CERC/maqs/Data/CAMx/CAMx.20100302_4X5.ncf does not exist.
6   Date/time:    01/09/2023 11:06:10
7   Input directory:  "/home/CERC/maqs/working"
8   Output file:  "/home/CERC/maqs/working/GridInfoOutput.txt"
9   Version:      1.1
10  Build number: 9446
11
```

GridInfo.err

```
3   /home/CERC/maqs/utils/RMGridInfo.out
4   ==========================
5   Problem:      The first regional model file must not be missing. Please check the
    regional model file path and naming pattern and alter the start date/time to match
    regional model file availability
6   Date/time:    01/09/2023 11:06:10
7   Input directory:  "/home/CERC/maqs/working"
8   Output file:  "/home/CERC/maqs/working/GridInfoOutput.txt"
9   Version:      1.1
10  Build number: 9446
11
```

Figure 6.8 Warning and error messages if the regional model concentration output files cannot be found.

The error message issued if the **RM Grid Info** utility could not locate a regional model concentration output file is shown in **Figure 6.8**. There are two possible causes for this error, which are described below with suggested solutions.

Problem 1: This error may indicate an inaccuracy in the file directory and/or file name template for the regional model concentration output files, if the file path quoted in the error message is incorrect.

Solution 1: Check the file directory and file name template specified for the regional concentration model output files in the MAQS user inputs, as described in Section 4.3.2. As in Section 6.3.1, note that file paths are case sensitive on Linux systems. Also, if using tags in the file name template, check the modelling period specified in the user inputs will result in the expected file name.

Problem 2: If the file path quoted in the error message is correct, the utility may not be able to access the relevant file.

Solution 2: Check the access permissions for the directories containing the regional model output data and any network connection between the MAQS coupled system host machine and the data storage directory.

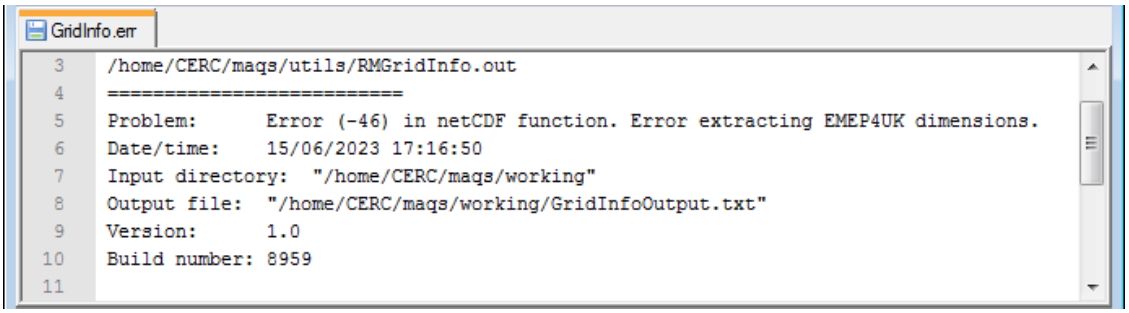


Figure 6.9 Error message if there is a problem reading the regional model concentration output files.

Problem 3: **Figure 6.9** shows the message if the input regional model concentration file is invalid or corrupt.

Solution 3: Check that the regional model concentration data files are in the correct format for the specified regional model, defined in Section 4.1.2.

6.6.2 Unknown vertical coordinate type (CMAQ only)

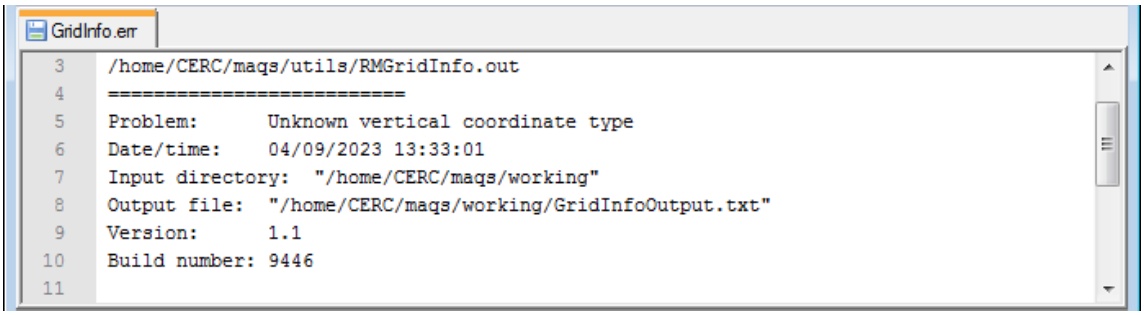


Figure 6.10 Error message if the regional model grid heights file cannot be found.

Problem: CMAQ output concentration files that use hybrid vertical coordinate system are not defined with a valid vertical coordinate type in the file attributes. **Figure 6.10** shows the message if the vertical coordinate type read from the file is invalid.

Solution: When using CMAQ output files with the hybrid vertical coordinate system, the MAQS coupled system requires an additional data file to extract the vertical layer heights. Please refer to Section 4.3.3 for details on the regional model grid heights data file for CMAQ.

6.7 RM Emissions utility

Any error or warning messages from the **RM Emissions** utility are written to an *.err* or *.wng* file in the same directory as the input text file. **RM Emissions** is run once at the start of the system run, so any error files from the utility are stored in the top level of the `WORK_DIR`.

6.7.1 Regional model emissions file does not exist

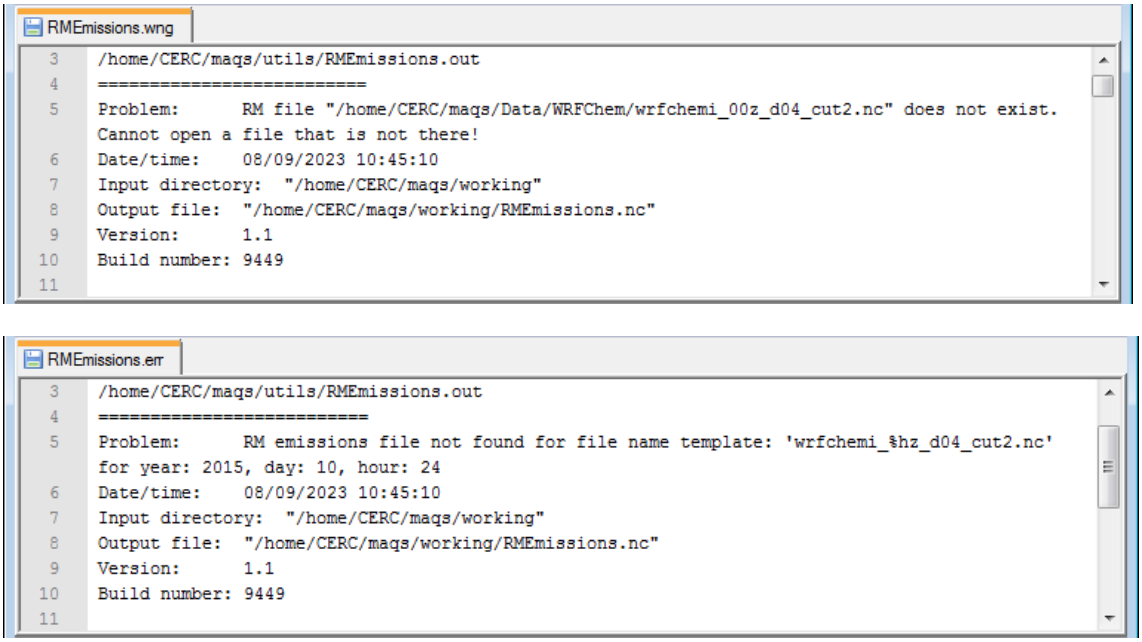


Figure 6.11 Warning and error messages if the regional model emissions files cannot be found.

The warning and error messages issued if the **RM Emissions** utility could not locate a regional model concentration output file are shown in **Figure 6.11**. There are two possible causes for this error, which are described below with suggested solutions.

Problem 1: This error may indicate an inaccuracy in the file directory and/or file name template for the regional model emissions files, if the file path quoted in the error message is incorrect.

Solution 1: Check the file directory and file name template specified for the regional model emissions files in the MAQS coupled system user inputs, as described in Section 4.4.2.

Problem 2: If the file path quoted in the error message is correct, the utility may not be able to access the relevant file.

Solution 2: Check the access permissions for the directories containing the regional model output data and any network connection between the MAQS coupled system host machine and the data storage directory.

6.7.2 Error reading emissions file attributes

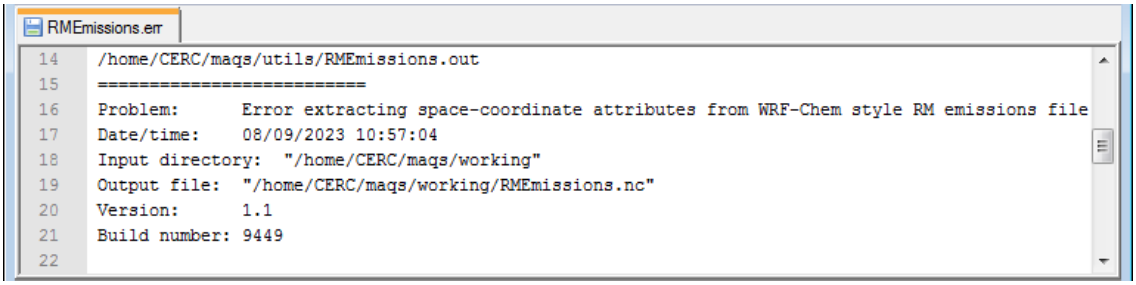


Figure 6.12 Error message if there is a problem reading attributes from the regional model emissions files.

Problem: **Figure 6.12** shows the message if the input regional model emission file is invalid or corrupt.

Solution: Check that the regional model emissions files are in the correct format for the specified regional model, defined in Section 4.1.2. The emissions files are expected to match the regional model defined for the concentration data files. Currently only emissions files from the CMAQ and WRF-Chem regional models are supported. If a different regional model is in use, the data must be re-gridded and re-formatted into the generic emissions data file format described in Section 4.4.6 before it can be used by the MAQS coupled system.

6.7.3 Error finding emissions species

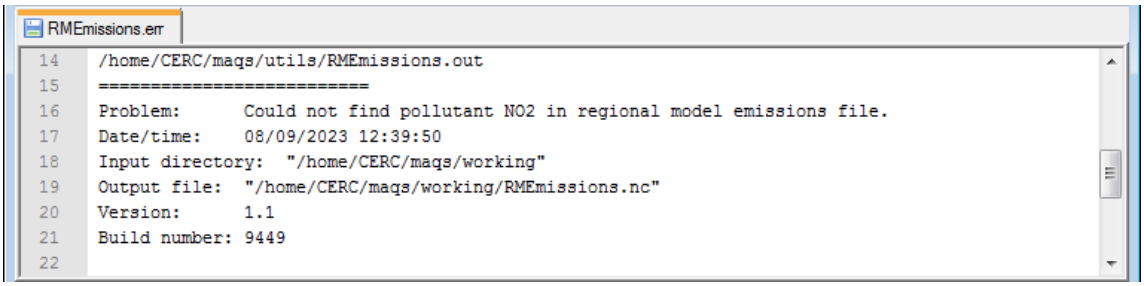


Figure 6.13 Error message if there is a problem finding a regional model emissions species in the emissions file.

Problem: **Figure 6.13** shows the message if a regional model pollutant species is not found in the regional model emission file.

Solution: Check that the regional model species names listed in the emissions species map file exactly match the variable names in the netCDF emissions files, including capitalisation. Note that in general emissions and concentration species have different names and different species mapping files are required.

6.7.4 Error in number of vertical levels

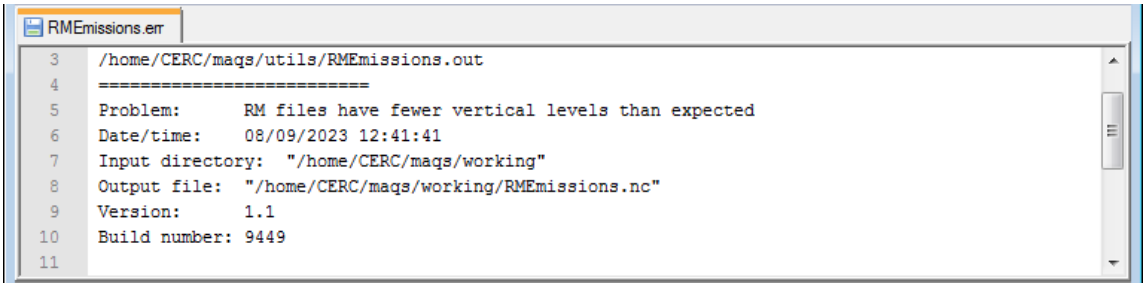


Figure 6.14 Error message if the regional emissions files contain fewer vertical levels than requested in the input file.

Problem: **Figure 6.14** shows the message if the regional model emissions files contain fewer vertical levels than the specified **Number of layers of emissions data to extract** (`EmNumLayers`).

Solution: Ensure that the specified number of layers to extract does not exceed the number of vertical levels of data available in the regional model emissions files. When processing different sectors, this will be the number of levels included in the emissions files for the sector with the most layers. Where multiple sectors have different numbers of layers, the **RM Emissions** utility will set emissions for the vertical levels above the available layers for sectors with smaller numbers of layers to zero.

6.7.5 Input WRF heights file does not exist (WRF-Chem only)

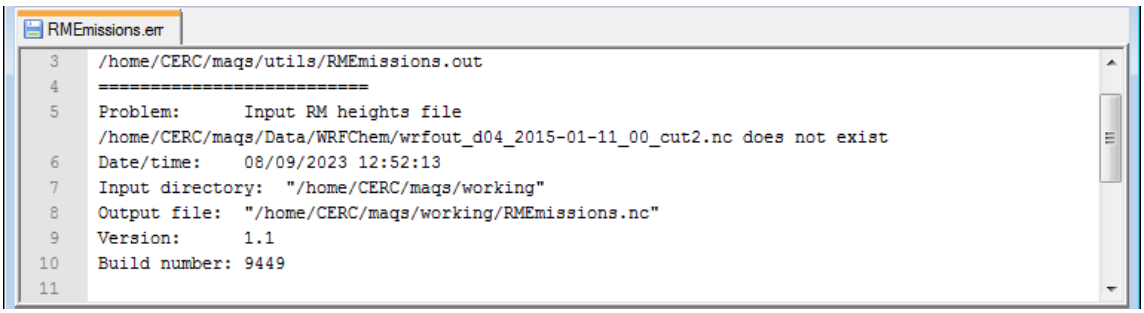


Figure 6.15 Error message if the WRF output file used to determine model layer heights for WRF-Chem emissions file cannot be found.

WRF-Chem regional model emissions files do not contain information about the vertical heights, so the utility which extracts emissions data uses a WRF output file to define these heights. **Figure 6.15** shows the message if the required WRF file cannot be found. Please refer to Section 6.8.1 for possible problems and solutions relating to the locations of WRF output files.

6.8 RM Met Data utility

Errors from the **RM Met Data** utility are written to an *.err* file in the same directory as the relevant input text file. The **RM Met Data** utility is run separately for each regional model grid cell within the nesting domain. Hence any error files from the utility are stored in directories for each grid cell, as described in Section 5.3.

6.8.1 Could not open meteorological model output file

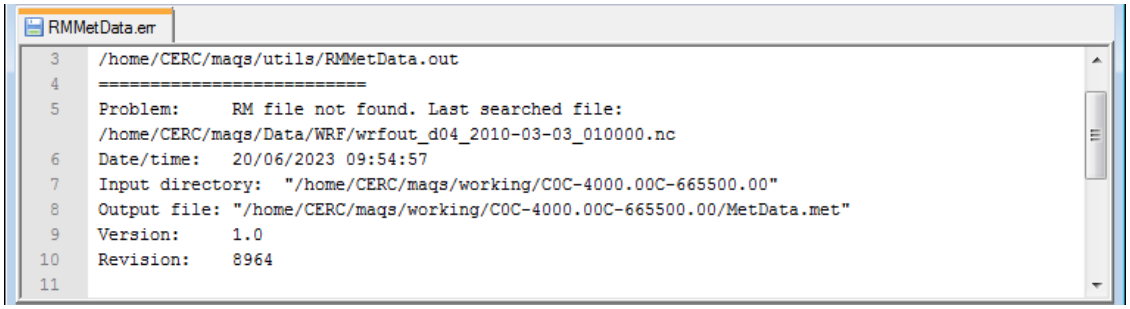


Figure 6.16 Warning message if RM Met Data cannot open a WRF output file

The error message issued if the **RM Met Data** utility could not open a meteorological model output file is shown in **Figure 6.16**. There are two possible causes for this error, which are described below with suggested solutions.

Problem 1: This error may indicate an inaccuracy in the file directory and/or file name template specification for the met output files, if the file path quoted in the error message is incorrect.

Solution 1: Check the meteorological model file directory and file name template inputs, as described in Section 4.2.1.

Problem 2: If the file path quoted in the error message is correct, there may be a problem with the utility accessing the file.

Solution 2: Check that:

- the access permissions for the directories containing the data files are set appropriately;
- any network connection between the MAQS coupled system host machine and the directory containing the data files is operating correctly; and
- the files are not simultaneously being used by any other user or process.

6.8.2 Error extracting variable from WRF

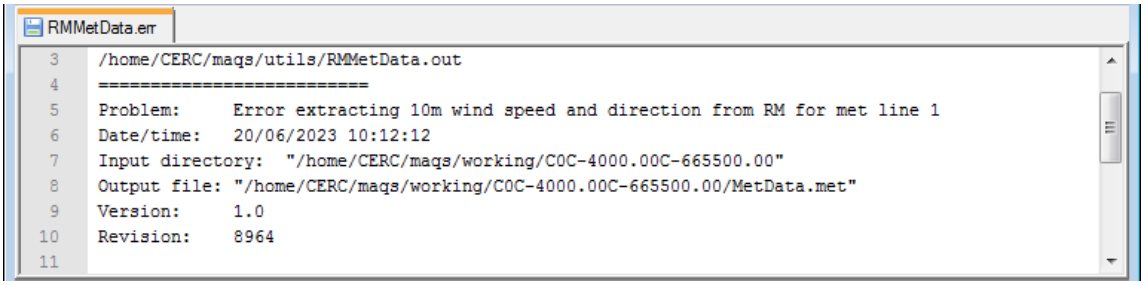


Figure 6.17 Error message if a specified variable name is not available in the WRF output files

Problem: **Figure 6.17** shows an example of the error message which will be issued if a variable cannot be found in the WRF output files. This may indicate an error in the custom WRF extraction configuration file, such that the variable name specified in the file does not correspond to a variable name in the WRF output file.

Solution: Check that the variable names being used in the custom WRF extraction configuration file correspond to netCDF variable names in the WRF output file(s).

6.9 Processor utility

Errors and warnings from the **Processor** utility are written to *.err* files in the same directory as the relevant input text file. The **Processor** utility is run separately for each regional model grid cell within the nesting domain, in three different modes. Hence any error files from the utility are stored in directories for each grid cell, as described in Section 5.3.

6.9.1 Regional model output file does not exist

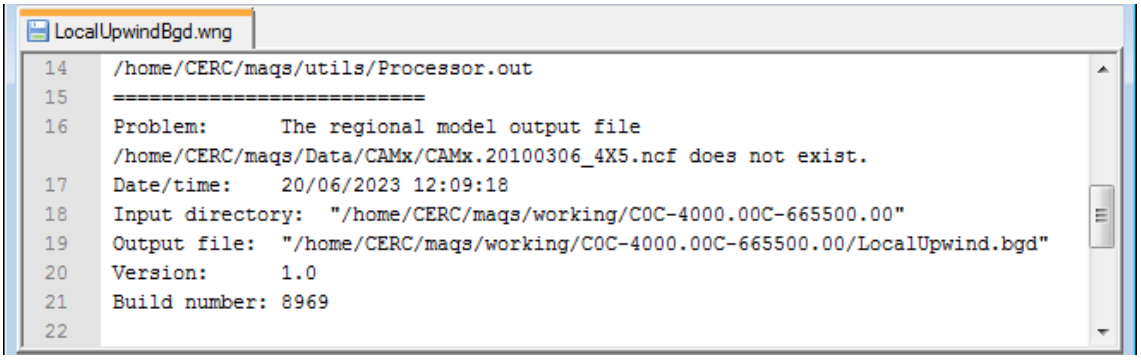


Figure 6.18 Warning message if a specified regional model concentration output file does not exist

The warning message issued if the **Processor** utility could not locate a regional model concentration output file is shown in **Figure 6.18**. As the **RM Grid Info** utility uses the same file location information as the **Processor** utility, this suggests that access to the files has been lost during the system run or the run duration exceeds the availability of regional model data.

Problem: If the file path quoted in the error message is correct, the utility may not be able to access the relevant file.

Solution: Check the access permissions for the directories containing the regional model output data and any network connection between the MAQS coupled system host machine and the data storage directory.

6.9.2 Specified regional model output file not opened correctly

Problem: An error message that a specified regional model output file has not been opened correctly indicates that the utility cannot access the relevant file.

Solution: Check any network connection between the MAQS coupled system host machine and the data storage directory and that the files are not simultaneously being used by any other user or process.

6.9.3 Regional model pollutant not found

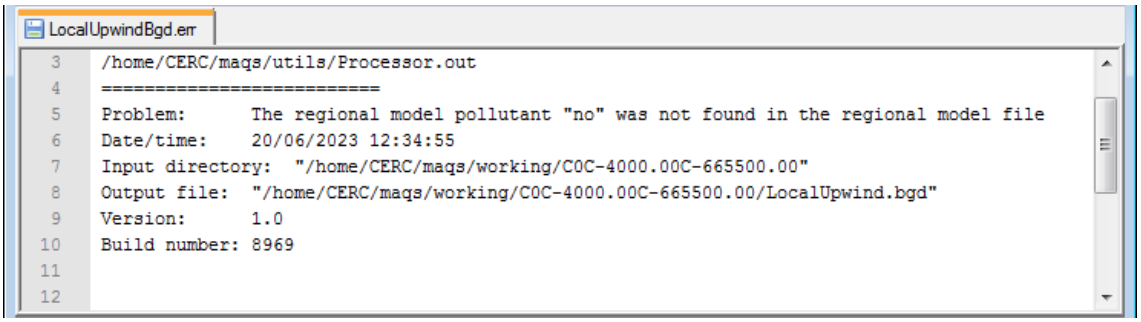


Figure 6.19 Error message for a problem with finding a regional model pollutant

Problem: The error message shown in **Figure 6.19** indicates that one or more of the regional model species names given in the species map file may not be a valid variable name for the concentration output files.

Solution: Check that the names used in the concentration species map file exactly match the species variable names in the regional model concentration output files, including capitalisation.

6.9.4 Error in reading input text file

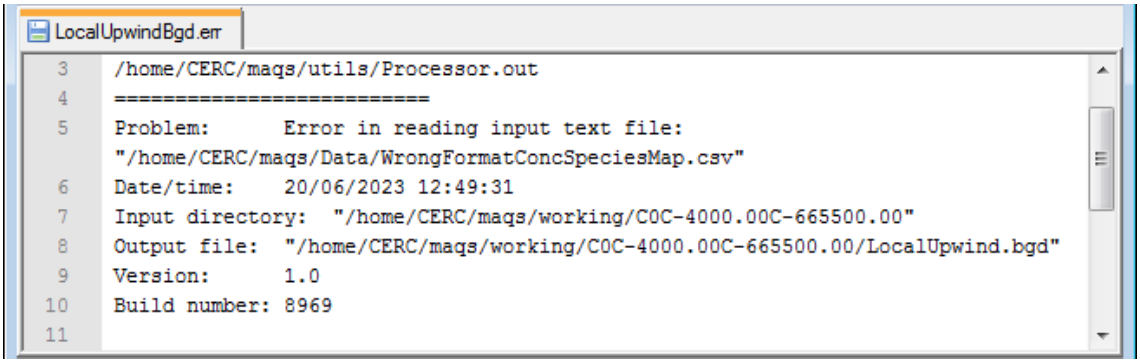


Figure 6.20 Error message for a problem with the species map file contents

Problem: An "Error in reading input text file" message, as shown in **Figure 6.20**, will be issued if the concentration species map file is not in the correct format.

Solution: Check that the concentration species map file format matches the definition given in Section 4.3.1.

6.9.5 Negative nesting background (nesting background mode only)

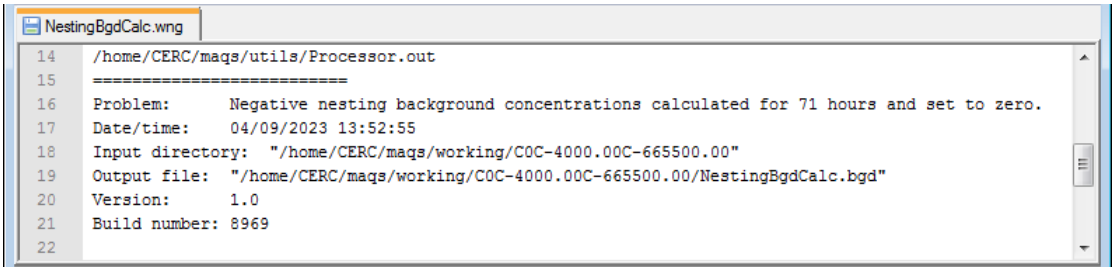


Figure 6.21 Warning message about the number of hours when negative nesting background concentrations were calculated

Problem: Nesting background concentrations are calculated as a difference between regional and local model concentrations excluding background from the local model run with gridded emissions matching those used in the regional model. If the local model concentration is larger than the regional model concentration, a negative nesting background concentration can be calculated. The **Processor** utility will set negative nesting background concentrations to zero in the output background file, but will output a warning with the total number of hours where a negative concentration was calculated for any pollutant, as shown in **Figure 6.21**. Negative values for a small proportion of modelled hours, which may be of very small magnitude, can be caused by minor differences in dispersion calculations between the local and regional dispersion models and may be ignored.

Negative nesting background concentrations calculated for a substantial proportion of the modelled hours, for example more than 5%, indicate inconsistencies between the local model set-up for the model run with gridded emissions for nesting background and the regional model. If the 3D grid source option with direct conversion of regional model emissions to ADMS 3D emissions is chosen, these inconsistencies should be minimal.

Solution: Check that:

- the factor values in the concentration species map convert the regional model concentrations into ADMS species in units of µg/m^3;
- the horizontal grid definition for the local model grid source cells and the regional model grid cells is consistent.

If running with ADMS-Urban using 2D grid sources, also check that:

- the 2D grid source depth is twice the height of the lowest regional model grid layer;
- the total magnitude of emissions from each 2D grid source cell is the same as that from the corresponding regional model cell;
- the time-variation of emissions from the 2D grid source corresponds as closely as possible to the time-variation of emissions from the regional model within the nesting domain; and
- elevated point sources, which will not affect local ground-level concentrations, are included explicitly in the run.

Analysis of the diurnal profiles of:

- regional model concentrations;
- local upwind background concentrations;
- local model concentrations output from the model run with gridded emissions for nesting background; and
- nesting background concentrations

may assist with identifying inconsistencies with the magnitude and/or time-variation of emissions used in the local and regional models. Selecting the 'key files' option for file storage (as described in Section 4.1.9) will retain the background concentration files and local model outputs for each grid cell in order to facilitate this analysis.

6.9.6 ADMS species not found (nesting background and output modes only)

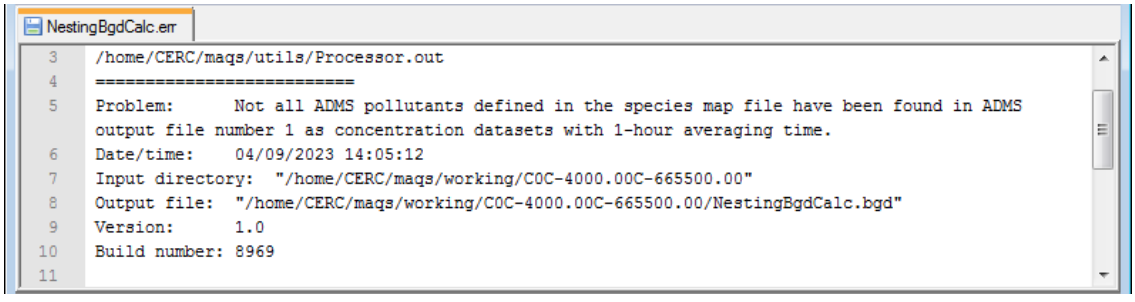


Figure 6.22 Error message if any ADMS species have not been found in the input *.nc* file

Problem: **Figure 6.22** shows the error message that will be issued by the **Processor** utility if any ADMS species were not found in the input *.nc* file. This may indicate that the species map list of ADMS species does not match the species names used in the local model, or that not all the ADMS species listed in the species map have been included as

output in the local modelling.

Solution: For ADMS-Local, Check that the ADMS species names in the species map file match those used in *localmodel.cfg*. For ADMS-Urban ensure that all ADMS species from the species map file are defined as outputs with one hour averaging time in the *.upl* files, as described in Section 4.7.13.

6.10 Combine COF utility

Errors or warnings from the **Combine COF** utility are written to an *.err* or *.wng* file in the same directory as the input text file. **Combine COF** is run at the end of the system run, so any error files from the utility are stored in the top level of the `WORK_DIR`.

6.10.1 Insufficient disk space

Problem: The **Combine COF** utility will stop abruptly if there is not enough storage on the disk where the utility is being run. The output *.nc* file will contain incomplete data and Linux will give the error message `"No Space left on device"`, this may not be written to an *.err* file.

The size of the final output *.nc* file created by the MAQS coupled system can be substantial as it contains the full set of output points including specified points and regular grid and/or source-oriented grid points.

Solution: Ensure that the runs machine has enough free space or use a shared data drive to run the **Combine COF** utility.

SECTION 7 Worked Examples

This section describes worked examples to guide you through setting up some basic MAQS coupled system runs and presenting their results. It is recommended that you work through these examples when starting to use the system. Note that a complete set of the resulting input and output files can be found in the *Data* sub-directory of the installation package. The examples can be run with either ADMS-Local or, if available, ADMS-Urban as the local model.

Section 7.1 gives a brief description of the example regional model data files which are supplied with the MAQS coupled system installation. The first two examples use the same regional model data files while the final example uses data files from a different model, location and period.

It is strongly recommended that you create a new directory for setting up and running these examples, as you would when starting a new project. The example output files are supplied with the system for reference.

7.1 Regional model data

The first set of example regional model data files which are supplied as part of the MAQS coupled system installation consist of 72 WRF meteorological output files, each containing one hour of data, and three CAMx concentration output files, each containing 24 hours of data and converted to CMAQ format. Although the models were originally run with larger modelling domains, the supplied data has been extracted to cover a rectangular area of 4 x 5 cells. The grid resolution is 1 km in each direction. The number of chemical species contained in the CAMx output files has also been reduced compared to the internal model speciation.

The time period covered by the regional model data files is midnight on 3rd March 2010 to 11 pm on 5th March 2010 in UTC. There is a time difference of eight hours between local solar time and UTC, so the time period in local time is 8 am on 3rd March 2010 to 7 am on 6th March 2010. Concentrations of NO_2 from the CAMx output file for 6 pm on 3rd March 2010 in UTC are shown in **Figure 7.1**, as displayed in the free VERDI visualisation software (Adams and Brandmeyer, 2014).

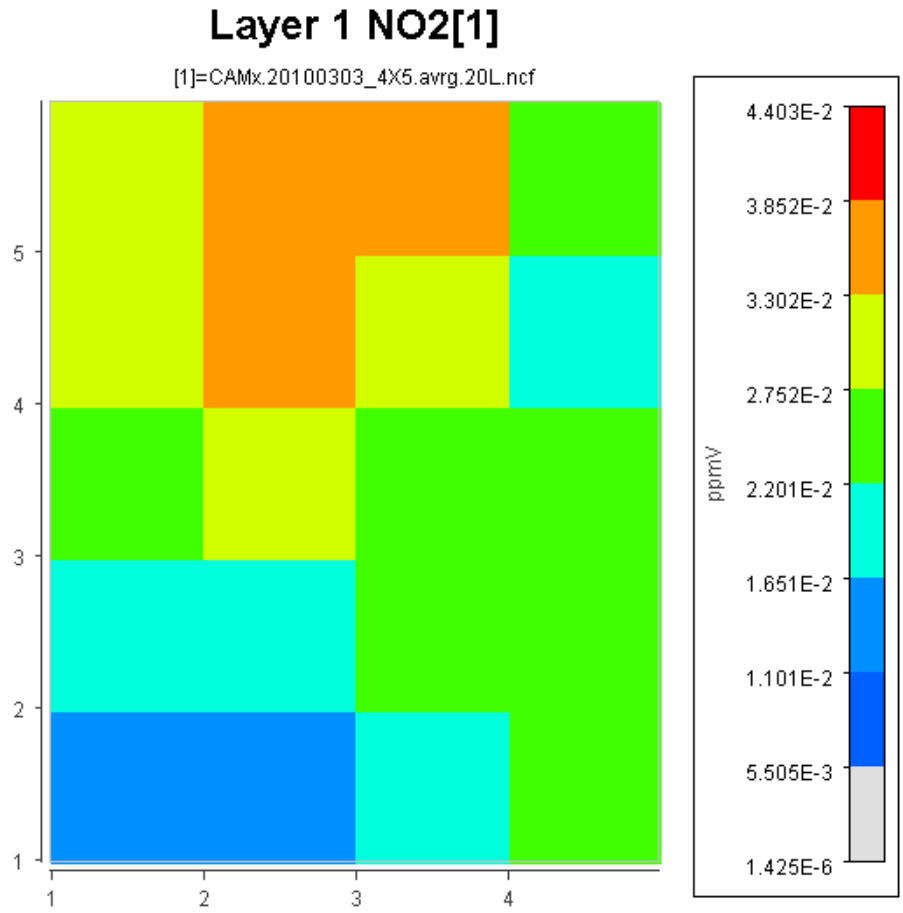


Figure 7.1 Plot of example CAMx ground-level NO_2 concentrations in ppmV for 3rd March 2010 at 18:00 UTC (4th March 2010 at 00:00 local time), visualised in VERDI.

The second set of example regional model data files which are supplied as part of the MAQS coupled system installation consist of 25 WRF-Chem output files, each containing one hour of meteorological and concentration data, and two WRF-Chem emissions files, each containing 12 hours of data. Although the model was originally run with a larger modelling domain, the supplied data has been extracted to cover a rectangular area of 5 x 4 cells. The grid resolution is 1.67 km in each direction. The number of chemical species and meteorological parameters included in the WRF-Chem output files has also been reduced compared to the internal model speciation.

The time period covered by the regional model data files is midnight on 11th January 2015 to midnight on 12th January 2015 in UTC. There is a time difference of 5 hours between local solar time and UTC, so the time period in local time is 5 am on 11th January 2015 to 5 am on 12th January 2015. Concentrations of NO_2 from the WRF-Chem output file for 9 am on 11th January 2015 in UTC are shown in **Figure 7.2**, as displayed in the free Panoply visualisation software (www.giss.nasa.gov/tools/panoply).

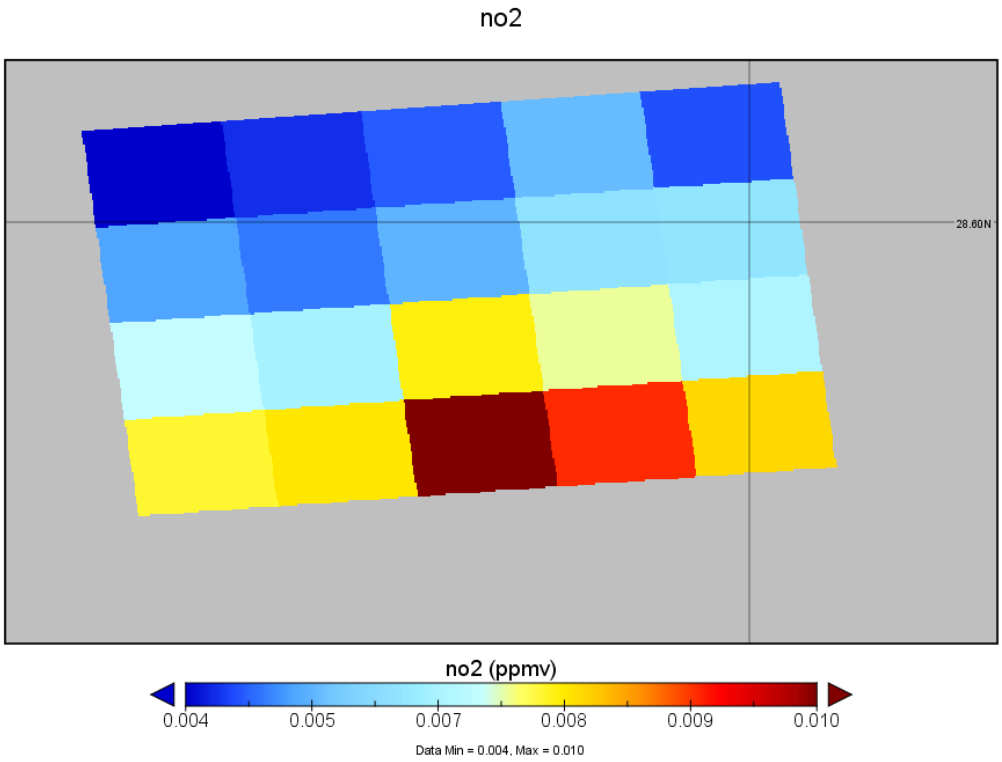


Figure 7.2 Plot of example WRF-Chem ground-level NO_2 concentrations in ppmV for 11th January 2015 at 09:00 UTC (11th January 2010 at 14:00 local time), visualised in Panoply.

7.2 Example 1: Modelling with output at receptor locations

In this example you will carry out a simple MAQS coupled system run, with output at receptor locations, as may be used for model validation.

7.2.1 Setting up the run

Step 1 If running the system using ADMS-Local as the local model, skip to Step 4. Otherwise if using ADMS-Urban, start by copying the ADMS-Urban input (*.upl*) file. Find the file called *Example1.upl* in the *<install_path>/Data* directory and copy it to a new working location, preferably outside the installation directory. This *.upl* file contains the explicit ADMS-Urban sources that are present within the ADMS-Urban modelling area, gridded emissions equivalent to those in the regional model and the receptor points at which final concentration output will be obtained.

Step 2 The *.upl* file contains several fields with paths to auxiliary input files that are in the *<install_path>/Data* directory. These all have an `<installdir>` placeholder that must be replaced across the file with the parent directory of *Data*. There are various ways to do this, such as using `sed`.

```
sed -i 's:<installdir>:/home/user/maqs:g' Example1.upl
```

Step 3 Once the ADMS-Urban run file has been set up, the MAQS coupled system input parameters can be defined.

Step 4 Define the system input parameters by running *<install_path>/default inputs/make_def_inputs.sh*. This will create a fresh set of control files (*options.cfg, inputdata.cfg, localmodel.cfg, run.cfg, sshlogin.cfg*) in the same directory. Copy these to a new location, preferably outside the installation directory. Note that *sshlogin.cfg* is only required if the system will be run in parallel using the GNU parallel option, as described in Section 4.1.12, and will not be used in this example.

Step 5 Open *options.cfg* in a text editor of your choice.

Step 6 The `Meteorological data` section is where some of the details of the regional model meteorological data files are defined. In this example, WRF files are being used, so set the regional model used to `'WRF'`. Set the time difference between local and model time to 8 hours.

Step 7 The `Concentration and emissions data` section is where some of the details of the regional model concentration and emissions data files are defined. In this example, CAMx files are being used. As files in CAMx format are not directly supported, the CAMx data have been converted into CMAQ format for the purposes of this example, so set the `Regional model used` to `'CMAQ'`. Set the time difference between local and model time to 8 hours.

Step 8 The `Local model configuration` section is where the local model to be used to calculate the high-resolution concentrations is selected. Select the local model that will be used in this example.

Step 9 The step size in the `Advanced nesting settings` section can be left as the default value.

Step 10 In the `Reference conditions` section, set the Sea-level temperature to 25°C. Choose to specify pressure for the top of the model and set the value to be 5000 Pa. You do not need to specify the height for the regional model concentration and emissions grids.

Step 11 Fill in the `Nesting domain definition` section in the file. This is where the extent of the nested area is defined, as explained in Section 4.1.6. Set the `Lower coordinates` to be (-4000, -665500) and the `Upper coordinates` to be (-2000, -662500).

Step 12 Select the option to interpolate regional model concentrations (`InterpRMConc=1`).

Step 13 In the `Meteorological variables` section, select the options to extract the wind speed at 10 m, temperature at 2 m, boundary layer height, incoming solar radiation and surface sensible heat flux. This example does not require shifting invalid surface sensible heat flux values to within valid range (`AmendHeatFlux=0`).

Step 14 In the logging option section, you can choose whether to preserve all intermediate files, intermediate output files, or just log files. Change this value to `$ALL_FILES` to save all files.

Step 15 Ensure that the coordinate transform datum is set to be consistent with CAMx by setting the `RMDatum` variable to `'EMEPSPHERE'`. As this is a relatively small-scale run, the `Job limit count` can be left as the default

value and it is not necessary to use the options for running scripts in parallel.

Step 16 Save the *options.cfg* file and open the *inputdata.cfg* file from the same directory.

Step 17 The `Meteorological data` section is where details of the regional meteorology files must be defined. Set the directory that contains the meteorology files, for example *<install_path>/Data/WRF*, and set the naming pattern (folder/file name template) for the files as *%Y%M/wrfout_d04_%Y-%M-%D_%h%m%s.nc*. The `Number of hours per file` should be set to 1. You do not need to specify a custom WRF extraction configuration file.

Step 18 The `Concentration data` section is where details of the concentration files must be defined. Enter the path of the provided species map file, for example *<install_path>/Data/ADMS_CAMx_SpeciesMap.csv*. Enter the directory that contains the concentration files, for example *<install_path>/Data/CAMx*, and set the naming pattern for the files as *CAMx.%Y%M%D_4X5.ncf*. There are 24 hours of data in each concentration file. It is not necessary to supply a `Regional model grid heights file` for this example.

Step 19 The `Annual average background concentration data` section is only used when modelling with Defra background map files as regional model concentration data and can be ignored for all worked examples.

Step 20 The path for the *.cco* file is only used with the CHIMERE regional model and can be ignored for all worked examples.

Step 21 The `Emissions data` section relates to the method used to incorporate regional model emissions into the local modelling as gridded emissions. The option to automatically import the regional model emissions into ADMS cannot be used for this example so make sure that it is not selected (`UseEmissionsData=0`). If ADMS-Urban is the chosen local model, the regional model emissions has been provided for you within the *.upl* file.

Step 22 If ADMS-Local is the chosen local model, an ADMS-format 3D gridded emissions file will be used. Set `UseCustomEmissionsFile` to 1 and enter the full path of the file containing the regional model emissions, for example *<install_path>/Data/Example1_3DEmissions.nc*. The disaggregation options can be left with their default values.

Step 23 In the `Output Type` section, enter `$RECEPTOR` as the output type.

Step 24 Finally enter a suitable name such as “Example1” for the project name. This allows you to easily distinguish the output files from each MAQS coupled system run.

Step 25 Save the *inputdata.cfg* file and open the *localmodel.cfg* file from the same directory.

Step 26 The options in the `Shared local model parameters` section are relevant to both ADMS-Local and ADMS-Urban, but will not be used in this example. If ADMS-Local is the chosen local model, continue to the next step. Otherwise if using ADMS-Urban, skip to Step 37.

Step 27 In the `Road sources data` section, select the option to use explicit road source emissions in the main model runs (`UseRoadEmissionsData=1`). Enter the full path of the road source data files for this example (*Example1.rdi*, *Example1.rdg* and *Example1.rde*) which are in the *<install_path>/Data* directory.

Step 28 The options in the `Traffic flow data` section are not used in this example and can be ignored.

Step 29 The `Time-varying emission factors` section is where details about how the local emissions vary with time can be specified. The emission factors are specified in this example via a 'time-varying profiles' *.fac* file (`UseTVEFFacFile=1`). Enter the full path of the file, for example *<install_path>/Data/TVEF_vkt.fac*. No 'time-varying hourly factors' *.hfc* file will be used (`UseTVEFHfcFile=0`).

Step 30 You do not need to suppress warnings from the time-varying emission factors processing, or to adjust the factors for daylight saving time / British summer time.

Step 31 The `Site properties` section is where details about the surface properties for meteorology using spatially varying site parameters for each grid cell must be defined. The data are input using text file format. Enter the full path to the site properties file, for example *<install_path>/Data/Example1_SiteProperties.csv*. This example does not use urban canopy buildings data.

Step 32 The `Output specifications` section is where details about the locations of the receptors and/or output grid must be specified. For this example, the option to produce output at receptor locations should be selected. Enter the full path to the receptor locations file *<install_path>/Data/Example1.asp*.

Step 33 You do not need to fill in the next sections relating to the output grid and source-oriented gridding options as gridded output is not required for this example.

Step 34 In the `Output pollutant names` section, enter the number of pollutants and the pollutant names for this example: `"SO2"`, `"PM10"`, `"PM2.5"`, `"CO"`, `"NOx"`, `"NO2"`, `"O3"`.

Step 35 The `Modelling of chemical reactions` section is where the chemistry schemes can be selected. Select the options to use NO_x and sulphate chemistry. Local night-time chemistry will not be applied for this example. The reactivity coefficient (AROC) can be left as the default value. You do not need to specify the percentage of NO_x emitted as primary NO_2 as this option is not used in this example.

Step 36 The option to override default conversion factors is not required for this example.

Step 37 If ADMS-Urban is the chosen local model, in the `ADMS-Urban .upl files` section, enter the full path to the working copy of your *.upl* file. In this example there is no separate *.upl* file with only gridded emissions.

Step 38 Save the *localmodel.cfg* file and open the *run.cfg* file from the same directory.

Step 39 Set the start and end dates to cover the full extent covered by the regional model files. Set the start date to be 03 March 2010 at 09:00 and the end date to be 06 March 2010 at 07:00.

Step 40 Save the file.

Step 41 To carry out the nesting run, open your terminal and run the *run-maqs* bash script with the inputs argument set to the folder containing the working copies of the control files. An example command line would be

```
bash ./maqs/run-maqs –i '/home/user/example1/'
```

Once the nesting run has completed, the end of the terminal output gives the final status of the MAQS coupled system run, and the location of the output files, as in the example shown in Section 5.1. Check the location of the output files. The first points to the main netCDF output file and second to the additional files. This latter contains all of the files created during the run. As you selected to keep all files, this folder will contain a large number of files, including input, intermediate and output files for each grid cell divided between subfolders, labelled by the cell's lower left coordinate. The cells that do not contain output points are excluded from the run and do not have corresponding folders.

7.2.2 Analysing output data

The final output from the MAQS coupled system is a netCDF Comprehensive Output file. This differs from regional model output as in general the data points do not form a regular grid and the point locations are only supplied in a projected coordinate system.

The Post Processor utility is a command line application developed for the MAQS coupled system which reads the ADMS Comprehensive Output File (COF) and allows spatial and temporal processing of the file. Please refer to the Post Processor User Guide (CERC, 2023) for details about the utility and the format of the input file.

A Post Processor utility input text file for this example has been provided in the *<install_path>/Data* directory to enable you to process the coupled system output netCDF file for visualisation.

Step 1 Find the Post Processor input file *PostProcessorInput_Example1.txt* in the *<install_path>/Data* directory and copy it to a new location, preferably outside the installation directory.

Step 2 The input file contains fields using placeholders in the paths that must be replaced with the appropriate directories. Replace the `<output file path>` placeholder with the path to the final output netCDF file generated by the coupled system for this example. Then, replace the `<outputdir>` placeholder with the directory for storing the files to be created by the Post Processor utility. Finally, replace the `<installdir>` placeholder with *<install_path>*.

The full file path entries should be given with quote delimiters, but the output directory path should not use quotes.

Step 3 Save the *PostProcessorInput_Example1.txt* file.

Step 4 The utility is run using the syntax

```
<executable file path> <input text file_path>
```

For example, if the executable is saved in the default installation directory, *<install_path>/utils*, the command line to run the utility would be

```
./maqs/utils/PostProcessor.out
/home/user/example1/PostProcessorInput_Example1.txt
```

This will produce ADMS-style concentration (*.pst* and *.plt*) files containing all output pollutants. These files have an underlying comma-separated variable format which can be used for creating time series plots of the concentrations e.g. in R or Excel.

Alternatively, the Comprehensive Output File may be transferred to a Windows system in order to use the ADMS-Urban Comprehensive Output File Processor (COFP).

The full Comprehensive Output file format definition can be found in Section 5.2 and could also be used to develop custom Linux-based post-processing code. Output data is contained in datasets for each output concentration variable, where the Pollutant_Name attribute can be used to identify the required dataset. A custom data processing tool can be used to identify the point index for a particular receptor (listed in PointName_XYZ), extract and plot the time-series of data for that point.

7.3 Example 2: Modelling with gridded output for contours

This example uses the same regional and local model inputs as Example 1 but changes the output settings to generate gridded output for concentration contour mapping.

7.3.1 Setting up the run

Step 1 If running the system using ADMS-Local as the local model, skip to Step 3. Otherwise if using ADMS-Urban, start by copying the ADMS-Urban input (*.upl*) file. Find the file called *Example2.upl* in the *<install_path>/Data* directory and copy it to a different location to the one used in Example 1 (Section 7.2).

Step 2 As before, the *.upl* file contains several fields with paths to auxiliary input files that are in the *<install_path>/Data* directory. These have an `<installdir>` placeholder that must be replaced across the file with the parent directory of *Data*. There are various ways to do this, such as using `sed`.

```
sed –i 's:<installdir>:/home/user/maqs:g' Example2.upl
```

Step 3 Instead of creating new control files from scratch, copy the ones used in Example 1 to a new location.

Remember that all .cfg *files required for a MAQS run must always be saved together in one folder.*

Step 4 We do not need to keep all of the run files this time, so in *options.cfg*, choose

the logging option to preserve only key files (`$KEY_FILES`).

Step 5 Save the *options.cfg* file and open the *inputdata.cfg* file from the same directory. In the `Output type` section, enter `$CONTOUR` for the output type.

Step 6 Change the project name to "Example2".

Step 7 Save the *inputdata.cfg* file and open the *localmodel.cfg* file from the same directory.

Step 8 If ADMS-Urban is being used as the local model in the coupled system, skip to Step 10. If running the system using ADMS-Local as the local model , move to the `Output specifications` section of the file where the parameters of the output grid are defined. In the `Regular gridded output extents` section, specify a grid extending from (-3900,-665400, 0) to (-2100, -662600, 0). In the `Regular grid output resolution` section, set the number of x-points to 40, the number of y-points to 60 and the number of z-points to 1.

Step 9 The system will automatically add extra output points or source-oriented grid points in locations where concentration gradients are high, for example close to road sources, as explained in Section 4.7.9. In this example, we will use the default settings.

Step 10 If ADMS-Urban is being used as the local model in the coupled system, in the `ADMS-Urban .upl files` section, change the path of the *.upl* file to the new location of *Example2.upl*.

Step 11 Save the *localmodel.cfg* file and open *folders.cfg*, which is saved in the top-level MAQS installation directory (<*install_path*>). Note that *folders.cfg* does not need to be recreated for each run, unlike the other input *.cfg* files. Change the value of `DEF_INPUT_DIR` to the full path of the folder containing the control files (*.cfg*) that have been edited for this example.

Step 12 Save the *folders.cfg* file, then run *run-maqs*. You do not need to use the `-i` argument as the location of the edited control files has been specified by `DEF_INPUT_DIR` in *folders.cfg*. This will take slightly longer than Example 1 as there are a greater number of output points and calculations will be performed for all six regional model grid cells.

7.3.2 Analysing output data

The Comprehensive Output file produced by the MAQS coupled system contains gridded output, such as could be used to create a concentration contour plot. Please refer to Section 5.2 for a full definition of the Comprehensive Output File format. The Post Processor utility is a command line application developed for the MAQS coupled system which reads the ADMS Comprehensive Output File and allows for spatial and temporal processing of the file. Please refer to the Post Processor User Guide (CERC, 2023b) for details about the utility and the format of the input file.

A Post Processor utility input text file for this example has been provided in the <*install_path*>*/Data* directory to enable you to process the coupled system output netCDF file for visualisation.

Step 1 Find the Post Processor input file *PostProcessorInput_Example2.txt* in the <*install_path*>*/Data* directory and copy it to a new location, preferably outside the installation directory.

Step 2 As before, the input file contains fields using placeholders in the paths that must be replaced with the appropriate directories. Replace the `<output file path>` placeholder with the path to the final netCDF (*.nc*) file generated by the coupled system for this example. Then, replace the `<outputdir>` placeholder with the directory for storing the files to be created by the Post Processor utility. Finally, replace the `<installdir>` placeholder with <*install_path*>.

Step 3 Save the *PostProcessorInput_Example2.txt* file.

Step 4 The utility is run using the syntax

```
<executable file path> <input text file_path>
```

For example, if the executable is saved in the default installation directory, <*install_path*>*/utils*, the command line to run the utility would be

```
./maqs/utils/PostProcessor.out
/home/user/example1/PostProcessorInput_Example2.txt
```

This will produce regular grid (*.grd*) files covering the modelling area at 10 metre resolution for all output pollutants, which can then be used for visualising the concentration values using plotting tools such as GDAL, Python or R libraries. Other visualisation tools such as the ADMS-Urban Mapper or ArcGIS can also be used for viewing the concentration contour plots on Windows. A natural neighbour gridding method is usually the most successful for contour plots including source-oriented output points.

Alternatively, a contour plot of the output data can be created by transferring the Comprehensive Output File to a Windows system in order to use the ADMS-Urban Comprehensive Output File Processor (COFP) and ADMS-Urban Mapper interpolation.

7.4 Example 3: Using regional model emissions

The regional and local model data files used for this example are different from those used in the first two examples. This example will demonstrate the option for automatic conversion of regional model emissions for use in the local model. The use of WRF-Chem output means that the same files are used for both meteorological and concentration data.

7.4.1 Setting up the run

Step 1 If running the system using ADMS-Local as the local model, skip to Step 4. Otherwise if using ADMS-Urban, start by copying the ADMS-Urban input file. Find the file called *Example3.upl* in the <*install_path*>*/Data* directory and copy it to another new working location.

Step 2 The *.upl* file contains several fields with paths to auxiliary input files that are in the <*install_path*>*/Data* directory. These all have an `<installdir>`

placeholder that must be replaced across the file with the parent directory of *Data*. There are various ways to do this, such as using `sed`.

```
sed -i 's:<installdir>:/home/user/maqs:g' Example3.upl
```

Step 3 Once the ADMS-Urban run file has been set up, the MAQS coupled system input parameters can be defined.

Step 4 Define the system input parameters by running *<install_path>/default inputs/make_def_inputs.sh*. This will create a fresh set of control files (*options.cfg, inputdata.cfg, localmodel.cfg, run.cfg, sshlogin.cfg*) in the same directory. Copy these to a new location, preferably outside the installation directory.

Step 5 Open *options.cfg* in a text editor of your choice.

Step 6 The `Meteorological data` section is where some of the details of the regional model meteorological data files are defined. In this example, WRF-Chem files are being used, so set the `Regional model used` to `'WRF'`. Set the time difference between local and model time to 5 hours.

Step 7 The `Concentration and emissions data` section is where some of the details of regional model used to model concentration and emissions are defined. Set the `Regional model used` to `'WRFChem'`. The time difference for this example is 5 hours, which is generally the same for the concentration and the meteorological data. In this case the same files include both concentration and meteorological variables.

Step 8 Set the `Local model used` to match the local model that will be used in this example.

Step 9 The step size in the `Advanced nesting settings` section can be left as default. The `Reference conditions` will not be used for WRF-Chem and can also be left as default values.

Step 10 Fill in the `Nesting domain definition` section. This is where the extent of the nested area is defined, as explained in Section 4.1.6. Set the `Lower coordinates` to be (-796667.41, 465000.30) and the `Upper coordinates` to be (-791667.86, 468333.30).

Step 11 Set the option to interpolate regional model concentrations (`InterpRMConc=1`).

Step 12 In the `Meteorological variables` section, select the options to extract the wind speed at 10 m, temperature at 2 m, incoming solar radiation and surface sensible heat flux. This example does not require shifting invalid surface sensible heat flux values to within valid range (`AmendHeatFlux=0`).

Step 13 The logging option can be left at its default value for this example. The coordinate transform datum can be left at its default setting of EMEP sphere. The `Job limit count` can be left as the default value and the parallel running option will not be used.

Step 14 Save the *options.cfg* file and open the *inputdata.cfg* file from the same directory.

Step 15 The `Meteorological data` section is where details of the regional meteorology files must be defined. Set the directory that contains the WRF-Chem output files, such as *<install_path>/Data/WRFChem/output*, and set the folder/file name template for the files as *wrfout_d04_%Y-%M-%D_%h_cut2.nc*. The `Number of hours per file` should be set to 1. Set the option to use a custom WRF extraction configuration file (`UseCustomWRFConfigFile=1`). Enter the path of the provided file, for example *<install_path>/Data/Modified_WRF_Input.txt*.

Step 16 The `Concentration data` section is where details of the regional concentration files must be defined. Enter the path of the provided species map file, for example *<install_path>/Data/WRFCHEM_conc_species.csv*. Enter the same directory, file name template and number of hours per file as for the Meteorological data files (Step 15). The `Regional model grid heights file` is only used with CMAQ regional model and can be ignored for this example.

Step 17 This example will use the `Emissions data` section. Set `UseEmissionsData=1`.

Step 18 In the second part of the `Emissions data` section, it is possible to use multiple types of emissions files by setting a higher value for `EmNumDataDirs`, and copying and renumbering the `directory file sets` section to match that value. There is only one type of emissions files supplied in this case, so we leave `EmNumDataDirs` at its default value and use the first directory sets section provided. Set the directory that contains the WRF-Chem emissions files, for example *<install_path>/Data/WRFChem/emissions.* Set the folder/file name template for the files as *wrfchemi_%hz_d04_cut2.nc* and the number of hours per file as 12. Enter the path of the provided emissions species map file, for example *<install_path>/Data/WRFCHEM_em_species.csv*. Note that both the listed regional model species and the conversion factors are different between the concentration and emissions species maps.

Step 19 In the third part of the `Emissions data` section, set the number of layers to extract as 7. The option to automatically import the regional model emissions into ADMS is selected for this example so you do not need to specify a custom 3D emissions data file. In the following section, set `EmDisaggSurfaceRoads=1`, but leave the other disaggregation options with their default values.

Step 20 In the `Output Type` section, enter `$CONTOUR` as the output type.

Step 21 Finally enter a suitable name such as “Example3” for the project name. This allows you to easily distinguish the output files of different model inputs.

Step 22 Save the *inputdata.cfg* file and open the *localmodel.cfg* file from the same directory.

Step 23 The options in the `Shared local model parameters` section are relevant to both ADMS-Local and ADMS-Urban, but will not be used in this example. If ADMS-Local is the chosen local model, continue to the next step. Otherwise if using ADMS-Urban, skip to Step 35.

Step 24 In the `Road sources data` section, select the option to use explicit road source emissions in the main model runs (`UseRoadEmissionsData=1`). Enter the full path of the road source data files for this example (*Example3.rdi*, *Example3.rdg* and *Example3.rde*) which are supplied in the *<install_path>/Data* directory.

Step 25 The `Traffic flow data` section is where the traffic flow information may be specified for the purpose of improving the estimate of traffic-induced turbulence. Set UseTrafficFlowDataFile and enter the full path of the file, for example *<install_path>/Data/Example3.rdt*. Leave the vehicle split percentage value with its default value.

Step 26 The `Time-varying emission factors` section is where details about how the local emissions vary with time can be specified. The emission factors are specified in this example via a 'time-varying profiles' *.fac* file (`UseTVEFFacFile=1`). Enter the full path of the file, for example *<install_path>/Data/tvef_road_rail.fac*. No 'time-varying hourly factors' *.hfc* file will be used (`UseTVEFHfcFile=0`).

Step 27 You do not need to suppress warnings from the time-varying emission factors processing, or to adjust the factors for daylight saving time / British summer time.

Step 28 The `Site properties` section is where details about the surface properties for meteorology using spatially varying site parameters for each grid cell must be defined. The data are input using text file format. Enter the full path to the site properties file, for example *<install_path>/Data/Example3_SiteProperties.csv*. This example does not use urban canopy buildings data.

Step 29 The `Output specifications` section is where details about the locations of the receptors and/or output grid must be specified. For this example, the option to produce gridded output will be selected. It is not necessary to supply a receptor locations file.

Step 30 Move to the `Regular gridded output extents` section of the file and specify the parameters to define an output grid extending from (-796617,465050, 0) to (-791717, 468283.3, 0). In the `Regular grid output resolution` section, set the number of x-points to 50, the number of y-points to 31 and the number of z-points to 1.

Step 31 The system will automatically add extra output points or source-oriented grid points in locations where concentration gradients are high, for example close to road sources, as explained in Section 4.7.9. In this example, we will use the default settings.

Step 32 In the `Output pollutant names` section, enter the number of pollutants and the pollutant names for this example: `"NOx"`, `"NO2"`, `"O3"`, `"SO2"`, `"PM10"`, `"PM2.5"`, `"CO"`.

Step 33 The `Modelling of chemical reactions` section is where the chemistry schemes can be selected. Select the options to use NO_x and sulphate chemistry. Local night-time chemistry will not be applied for this example. The reactivity coefficient (AROC) can be left as the default value. You do not need to specify the percentage of NO_x as primary NO_2 as this option is

not used in this example.

Step 34 The option to override default conversion factors is not required for this example.

Step 35 If ADMS-Urban is the chosen local model, in the `ADMS-Urban .upl files` section, enter the full path to the working copy of your *.upl* file.

Step 36 Save the *localmodel.cfg* file and open the *run.cfg* file from the same directory.

Step 37 Set the start and end dates to cover the full extent covered by the regional model files. Set the start date to be 11 January 2015 at 05:00 and the end date to be 12 January 2015 at 04:00.

Step 38 Save the *run.cfg* file.

Step 39 To carry out the nesting run, open your terminal and run the *run-maqs* bash script with the inputs argument set to the folder containing the working copies of the control files. An example command line would be

```
bash ./maqs/run-maqs –i '/home/user/example3/'
```

Once the nesting run has completed, the end of the terminal output gives the final status of the MAQS coupled system run, and the location of the output files, as in the example shown in Section 5.1. Check the location of the output files. The first points to the main netCDF output file and second to the additional files. This latter contains the key files created during the run.

7.4.2 Analysing output data

The Comprehensive Output file produced by the MAQS coupled system contains gridded output, which can be used to create a concentration contour plot. Please refer to Section 5.2 for a full definition of the Comprehensive Output File format. The Post Processor utility is a command line application developed for the MAQS coupled system which reads the ADMS Comprehensive Output File and allows for spatial and temporal processing of the file. Please refer to the Post Processor User Guide (CERC, 2023) for details about the utility and the format of the input file.

A Post Processor utility input text file for this example has been provided in the *<install_path>/Data* directory to enable you to process the coupled system output netCDF file for visualisation.

Step 1 Find the Post Processor input file *PostProcessorInput_Example3.txt* in the *<install_path>/Data* directory and copy it to a new location, preferably outside the installation directory.

Step 2 The input file contains fields using placeholders in the paths that must be replaced with the appropriate directories. Replace the `<output file path>` placeholder with the path to the final netCDF (*.nc*) file output by the coupled system for this example. Then, replace the `<outputdir>` placeholder with the directory for storing the files to be created by the Post Processor utility. Finally, replace the `<installdir>` placeholder with *<install_path>*.

Step 3 Save the *PostProcessorInput_Example3.txt* file.

Step 4 The utility is run using the syntax

```
<executable file path> <input text file_path>
```

For example, if the executable is saved in the default installation directory, *<install_path>/utils*, the command line to run the utility would be

```
./maqs/utils/PostProcessor.out
/home/user/example1/PostProcessorInput_Example3.txt
```

This will produce regular grid (*.grd*) files for all output pollutants covering the modelling area at 10 metre resolution, which can then be used for visualising the concentration values using plotting tools such as GDAL, Python or R libraries. Other visualisation tools such as ADMS-Urban Mapper or ArcGIS can also be used for viewing the concentration contour plots on Windows. A natural neighbour gridding method is usually the most successful for contour plots including source-oriented output points.

Alternatively, a contour plot of the output data can be created by transferring the Comprehensive Output File to a Windows system in order to use the ADMS-Urban Comprehensive Output File Processor (COFP) and ADMS-Urban Mapper interpolation.

SECTION 8 Technical Summary

8.1 Concept

The concept of the MAQS coupled system (Figure 8.1) is based on a mixing time, T_m, defined as the length of time required after release for a plume from an explicitly-modelled source to be well-mixed on the scale of the regional model grid cells. For times longer than T_m after release, the regional model will give a good representation of dispersion and chemistry, whereas for the initial period, within T_m after release, a local model should be used to represent the detailed dispersion and chemistry. In general, T_m depends on the size of the regional model grid cells, the size and elevation of the explicitly modelled source, and the meteorological conditions. Earlier work has demonstrated that a fixed value of T_m of 1 hour is sufficient for modelling urban areas, and it is likely that shorter times could be used for finer resolution regional model domains.

In the following, the local dispersion model is referred to as ADMS, which represents either ADMS-Local (more information in Section 8.3) or ADMS-Urban (CERC, 2020b).

The theoretical expression for concentrations at an instantaneous output time t is as follows:

$$\text{Coupled system receptor concentration} = \text{RM}(0{:}\,t) - \text{RM}(t - T_m{:}\,t) + \text{ADMS expl}\,(t - T_m{:}\,t) \quad (1)$$

where the first term on the right hand side is the standard regional model (RM) concentration including emissions from all times up to t, the second is an adjustment to remove the regional model concentrations from emissions from times less than T_m prior to t, and the third is the replacement with concentrations from explicit modelling of emissions at times less than T_m before t.

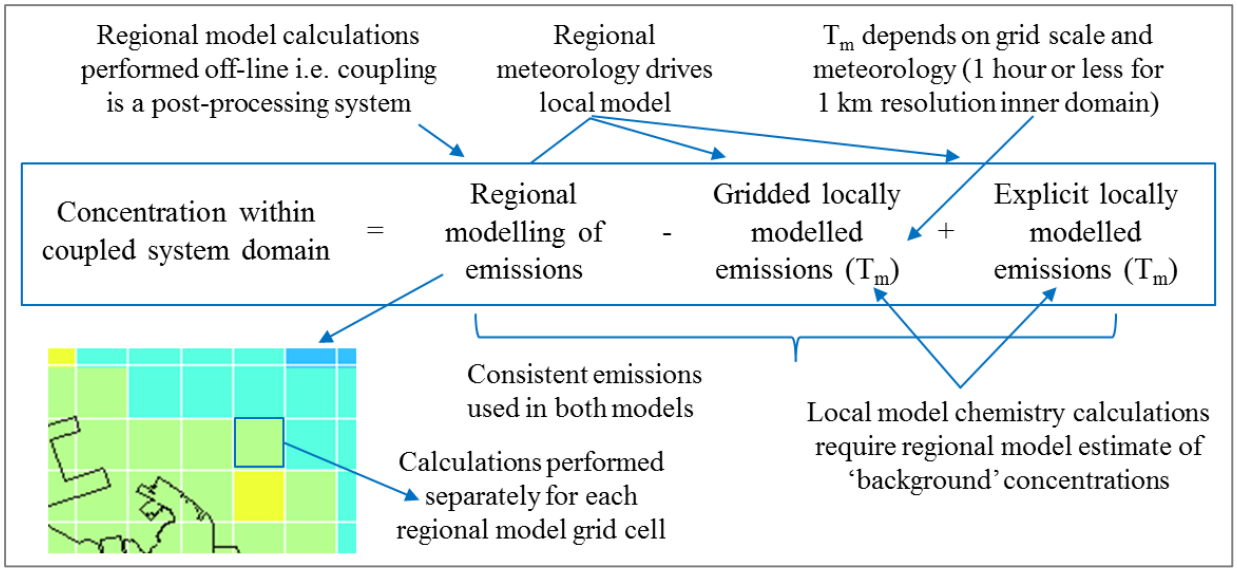


Figure 8.1 – MAQS coupled system concept

In practice, it is difficult and computationally inefficient to modify and re-run the regional model to obtain the second term in (1) above, so this part of the expression is substituted with gridded emissions modelled in ADMS-Local or ADMS-Urban, giving the following expression:

$$\text{Coupled system receptor concentration} = \text{RM}(0{:}\,t) - \text{ADMS grid}(t - T_m{:}\,t) + \text{ADMS expl}(t - T_m{:}\,t) \quad (2)$$

where

ADMS grid$(t - T_m{:}\,t)$ = the concentration field due to all emissions within the area of interest represented as gridded sources, dispersing from time $t - T_m$ to time t

ADMS expl$(t - T_m{:}\,t)$ = the concentration field due to all emissions within the area of interest represented at the highest known resolution, dispersing from time $t - T_m$ to time t

ADMS-Local or ADMS-Urban configured to model gridded emissions sources can adequately represent the dispersion and chemistry of the regional model over the small temporal and spatial scales implied by the mixing time (T_m) in one grid cell. Computer processing times for ADMS-Local or ADMS-Urban modelling of grid sources are orders of magnitude smaller than those of a multi-scale regional model with modified emissions.

The ADMS-Local or ADMS-Urban calculations use concentrations derived from the regional model as urban background boundary conditions, which are necessary for accurate calculations of local chemistry effects, and provide a further connection between the regional and local models in the MAQS coupled system. Only one set of regional model data is required for this type of system, which reduces the computational resources required for its implementation.

ADMS-Local and ADMS-Urban calculate 'steady-state' concentrations by assuming that the concentrations at each hour are independent; dispersion and chemistry calculations are truncated at the specified time, T_m. By only using regional model emissions from prior to T_m before the output time t (0: t - T_m), and local model emissions from after T_m before t (t - T_m: t) ensures that no double-counting of emissions can occur. Each model will satisfy conservation of mass, including dispersion and chemistry effects, for the subset of emissions that it includes, hence also ensuring overall mass conservation.

The calculations described above are executed separately for each regional model grid cell. The MAQS coupled system only considers explicit modelling of road sources when running with the ADMS-local local model; all other sources are modelled within a 3D grid of emissions. When running with ADMS-Urban, additional non-road source types can be modelled explicitly, including point, line, area and volume sources. If output concentrations are only required near ground level, then only the lowest grid level of regional model output will be used in the calculations.

For annual average regional concentrations (currently only available with ADMS-Local local modelling), calculations will be performed on an annual average basis as hourly data are unavailable:

$$\text{Coupled system receptor concentration} = \text{AAVE}(aa) - \text{ADMS-Local grid}(aa) + \text{ADMS-Local expl}(aa)$$

(3)

where aa indicates annual average concentrations and AAVE is the annual average 'regional model' concentration. The model uses hourly varying background concentrations to set the conditions for the calculation of local chemistry effects. For this coupling, hourly background concentrations are not available, so monthly average hourly diurnal profile values of NO_X, NO_2 and O_3 concentrations from a rural monitoring site are used as additional input. Then conservation of oxidant ($O_3 + NO_2$), along with an input estimate of typical primary NO_2 as a fraction of NO_X, is used to estimate the local hourly background concentrations from the annual average local NO_X and NO_2.

8.2 Implementation

The MAQS coupled system control scripts read the user input *.cfg* files and automates utility and local model runs. A nesting domain which covers multiple regional model grid cells is automatically divided into separate runs for each grid cell, with the results re-combined at the end of the system run. The user has the option of using the GNU parallel library to distribute procedures between nodes of an HPC or can modify the control scripts to customise the parallelisation of utility and local model runs in order to optimise the use of available computing resources.

The main procedures included in the MAQS coupled system are shown as a flow chart in **Figure 8.2**. A brief description of each stage follows the diagram, while more details about the individual utilities can be found in the Appendices.

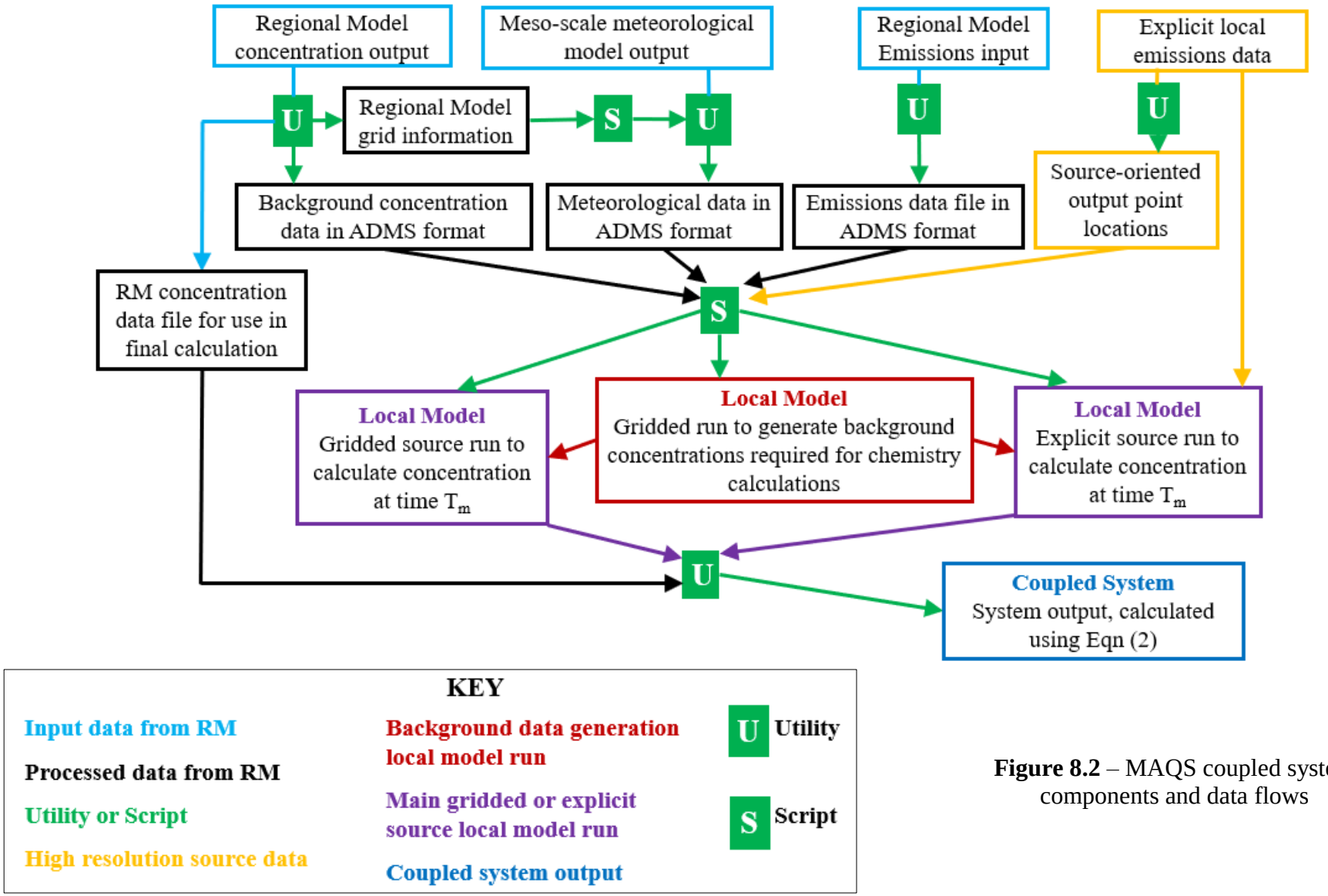


Figure 8.2 – MAQS coupled system components and data flows

Step 1 Initialisation of the MAQS coupled system

The control script reads the data from control files and command line options, then sets up the internal variables for the MAQS coupled system run.

Step 2 Utility 1 – Extract regional model grid information

The first utility used in the MAQS coupled system is the utility for extracting grid information from the regional model concentration files, described in Appendix A. This allows the control system to calculate the number and locations of the regional model grid cells which are included in the nesting domain, as most of the subsequent processes (Step 5 to Step 10) are replicated for each grid cell. In addition, an *.asp* file is created by this utility containing one output point in the centre of each surface layer regional model grid cell, for use in the local model (ADMS-Urban or ADMS-Local) 'background' run.

Step 3 Utility 2 – Extract regional model emissions (optional)

The second utility used in the MAQS coupled system is the optional utility for converting regional model emissions into ADMS 3D grid format, as described in Appendix B. Emissions for the whole nesting domain and nesting period are extracted into a single 3D gridded emissions file.

Step 4 Defining output point locations

(a) Utility 3 – Generate output receptors for the nesting domain

If using ADMS-Local as the local model for the MAQS coupled system run for producing regular gridded output for contours, the third utility is run to generate an Additional Specified Points (*.asp*) file containing the output points at which concentration values will be calculated for the whole nesting domain. The set of output points can be a combination of standard grid points and source-oriented grid points, including user-defined receptor locations, if specified. Details of this utility can be found in Appendix C. If the system output is for receptor locations only, the utility is not run and the user-specified *.asp* file (Section 4.7.7) is used for identifying grid cells which include output points.

(b) ADMS-Urban run for initial checking.

If using ADMS-Urban as the local model for the MAQS coupled system, an initial ADMS-Urban run is triggered using the *.upl* file with explicit emissions, with the **Create ASP** mode selected, in order to generate an Additional Specified Points (*.asp*) file containing the output points at which concentration values will be calculated. If running the system for producing gridded output for contours, the set of output points includes both standard regular grid points and source-oriented grid points for the whole nesting domain. If the system output is for receptor locations only, the *.asp* file includes the user-defined receptor locations in the *.upl* file (including any input *.asp* file locations). Please refer to the ADMS-Urban User Guide for details of the ADMS-Urban **Create ASP** mode.

(c) Identify cells containing output points (receptor mode only).

The MAQS scripts process the generated *.asp* file to check which grid cells include output points. Any cells which do not contain any output points are excluded from further processing.

Step 5 Utility 4 - Extract meteorological data from WRF

The fourth utility used in the MAQS coupled system is the utility for extracting meteorological data from WRF files. This utility is run for each grid cell to create an ADMS format met file (*.met*) for each cell, which is used for all subsequent local model (ADMS-Urban or ADMS-Local) runs in that cell. Details of this utility can be found in Appendix D.

Step 6 Utility 5 – Extract local upwind background concentrations

The fifth utility used in the MAQS coupled system extracts local upwind background concentrations from the regional air quality model output files. These are defined as the concentrations from the neighbouring regional model cell in the upwind direction. The utility is run for each regional model grid cell included in the nesting domain and creates ADMS format background concentration files (*.bgd*).

Further details of the **Processor** utility can be found in Appendix E. Note that the same utility is used for the extraction of upwind background concentrations, the calculation of nesting background concentrations and the calculation of final output concentrations, with the required mode selected via the input file.

Step 7 Local model run with gridded emissions

The first full ADMS-Local or ADMS-Urban model run in the MAQS coupled system uses gridded emissions matched as closely as possible to the regional model emissions. The control program supplies file paths for the corresponding meteorology and background data files and sets spatial and temporal truncation limits of the grid cell boundaries and half an hour, respectively. The control program also applies the *.asp* file created by the grid information utility (Step 2) to define a single output point in the centre of each surface layer regional model grid cell.

If the option to use regional model emissions is in use, the control program will also supply the file path for the 3D gridded emissions file created in Step 3. If only a single input *.upl* file is supplied by the user, the control program will ensure that no non-grid source emissions are modelled in this run. In general the local model grid source resolution will match the regional model grid resolution and one output point will be specified at the centre of each grid source cell, so the truncated runs will each contain only one grid source cell for each vertical layer and one output point, leading to short run times.

The concentrations calculated by this run are relatively insensitive to both truncation time and averaging time, due to being output at the centre of the grid source. The output from this run is an ADMS-Urban Comprehensive Output File *(.nc*).

Step 8 Utility 6 - Calculate nesting background concentrations

The sixth utility used in the MAQS coupled system calculates the nesting background concentrations, defined as

$$\text{Nesting background} = \text{RM}(0:t) - \left[\text{ADMS grid}\left(t - \frac{1}{2} : t\right) - \text{local upwind background}\right]$$

where: '$\text{RM}(0:t)$' is the regional model concentration in the relevant grid cell;

'ADMS grid $\left(t-\frac{1}{2}:t\right)$' is the output concentration from the local model (ADMS-Local or ADMS-Urban) run with gridded emissions matching the regional model emissions and dispersion truncated at half an hour (Step 7); and 'local upwind background' is the background concentration extracted in Step 6.

This nesting background concentration dataset represents the regional model (RM) concentration in the nesting domain throughout the output hour by using the instantaneous value estimated at the middle of the output hour. The direct contribution of the nesting background to the final concentrations of inert pollutants is zero, due to the subtraction of the gridded runs from the explicit runs, which both use the same nesting background. However, an appropriate value of nesting background is important for accurate representation of the local chemistry processes.

Further details of the **Processor** utility can be found in Appendix E. Note that the same utility is used for the extraction of upwind background concentrations, the calculation of nesting background concentrations and the calculation of final output concentrations, with the required mode selected via the input file. The output from this utility is an ADMS format background concentration file (*.bgd*).

Step 9 Main local model runs

The main ADMS-Local or ADMS-Urban runs, with gridded and explicit emissions, are run using the regional meteorology extracted in Step 5 and the nesting background concentrations calculated in Step 8. If the option to use regional model emissions is selected, the 3D gridded emissions file created in Step 3 will also be used in both the gridded and explicit runs. If only a single *.upl* file is supplied by the user, the control program will ensure that the gridded run only models gridded emission sources.

The runs with gridded and explicit emissions must include exactly the same output locations. The outputs from these runs are ADMS Comprehensive Output File (COF) format netCDF files (*.nc*).

Step 10 Utility 7 - Calculate nesting output concentrations

The seventh utility used in the MAQS coupled system calculates nested concentrations, defined as follows:

$$C_N(t, \boldsymbol{X}_{OP}) = [\boldsymbol{S}]C_{RM}(t, \boldsymbol{I}_{OP}) + C_{ADMS_{Ei}}(t, \boldsymbol{X}_{OP}) - C_{ADMS_{Gi}}(t, \boldsymbol{X}_{OP})$$

where $C_N(t, \boldsymbol{X}_{OP})$ is the nested output concentration at time t (hours) and output point location $\boldsymbol{X}_{OP}$; $[\boldsymbol{S}]C_{RM}(t, \boldsymbol{I}_{OP})$ is the regional model concentration at time t and grid cell indices of the output point $\boldsymbol{I}_{OP}$, converted from regional model to ADMS speciation via the species map matrix $[\boldsymbol{S}]$; $C_{ADMS_{Ei}}(t, \boldsymbol{X}_{OP})$ is the concentration from the local model (ADMS-Local or ADMS-Urban) run with explicit emissions, at output time t and output point location $\boldsymbol{X}_{OP}$; and $C_{ADMS_{Gi}}(t, \boldsymbol{X}_{OP})$ is the concentration from the local model (ADMS-Local or ADMS-Urban) run with gridded emissions, at output time t and output point location $\boldsymbol{X}_{OP}$.

If the option to interpolate regional model concentrations is in use, which also changes the local model run settings, the regional model concentration $C_{RM}(t, \boldsymbol{I}_{OP})$

is calculated by bilinear interpolation of the concentrations at the four regional model grid cell centres which surround the output point. Note that this may use concentrations from regional model grid cells which neighbour the nesting domain but are not included within the nesting domain.

The utility is run for each regional model grid cell covered by the nesting domain. The output from this utility is an ADMS COF format netCDF file (*.nc*). Further details of the **Processor** utility can be found in Appendix E. Note that the same utility is used for the extraction of upwind background concentrations, the calculation of nesting background concentrations and the calculation of final output concentrations, with the required mode selected via the input file.

Step 11 Utility 8 - Combine output files

The eighth utility used in the MAQS coupled system combines the output concentration files from each regional model grid cell covered by the nesting domain into a single output file for the whole domain. The output from this utility is an ADMS COF format netCDF file (*.nc*). Please refer to Appendix F for more information about the **Combine COF** utility.

Step 12 Return final output and any required intermediate files to the output location designated by `ARCH_DIR` in *folders.cfg*.

The MAQS coupled system control scripts copy the final concentration output file, the main system log file, other system component log files and any additional files requested by the user to the requested output file directory.

8.3 ADMS-Local

ADMS-Local was developed as a local model component for the MAQS coupled system. It is closely related to the well-established ADMS-Urban model, with some simplifications in the range of source types available and the street canyon modelling approach implemented. It is a Gaussian plume dispersion model with the atmospheric boundary layer structure defined by boundary layer depth and Monin-Obukhov length. A skewed Gaussian distribution is used in convective conditions.

ADMS-Local includes a meteorological processor to calculate the boundary layer properties from the input meteorological data (more details are given in Section 8.3.1). Road sources are modelled as line sources with additional mixing due to traffic induced turbulence (Section 8.3.3) and a parameterised representation of street canyon effects (Section 8.3.4). Aggregate gridded sources are modelled by a 3D grid of volume sources (Section 8.3.6). For each of these source types, concentrations can be calculated at any output point location to ensure the required spatial resolution. Fast local chemistry can also be applied during the concentration calculations (Section 8.3.7).

8.3.1 Meteorological data input

ADMS-Local takes as input meteorological data as used by the regional meteorological model, extracted into ADMS format. Within the model this data is processed into the variables required to describe the atmospheric boundary layer. ADMS-Local requires

input values of wind speed, wind direction, screen-height temperature and surface heat flux for extracted from the regional model data for each hour. Optionally the boundary layer height may also be entered.

In addition, ADMS-Local requires three time-independent parameters, specifically: the site latitude (decimal degrees), an average surface roughness (m), and the minimum Monin-Obukhov length (m). This last parameter is used as a simple mechanism to account for the urban heat island effect, in which the radiative properties of urban surfaces and the presence of traffic can lead to increased heat production and mixing within the urban surface layer compared with the adjacent rural surface layer, thus preventing the occurrence of very stable atmospheric conditions.

ADMS-Local also takes into account the effects of the presence of buildings in an urban area on local air flow, causing changes in the wind speed and turbulence profiles (urban canopy flow). The characteristics of the urban area can be specified per cell as optional parameters; these include:

- H – average building height within the cell (m)
- G – average street canyon width within the cell (m)
- λ_P – ratio of the sum of the plan area occupied by buildings to the total plan area within the cell
- λ_F – ratio of total frontal area of buildings perpendicular to a specific wind direction to the total plan area within the cell for a range of wind directions ϕ_1 to ϕ_2 (degrees)
- z_{0s} – roughness length within the urban canopy (m)

8.3.2 Meteorological calculations and boundary layer profiles

The ADMS-Local meteorological processor routines take the input meteorological data for a given hour along with the additional time-independent parameters specified in the previous section and uses similarity theory to derive further boundary layer parameters as required for running the dispersion model. Similarity theory assumes universal relationships between non-dimensionalised atmospheric variables.

The meteorological processor routines use components of the meteorological pre-processor which is also included in CERC's other ADMS models to process data from a regional meteorological model. A full technical description of the ADMS meteorological pre-processor can be found in Technical Specification document P05/01 (CERC, 2023a). Some key concepts are included here, though for brevity readers are asked to refer to the referenced document for definitions of all the presented terms as well as for the original references on which the equations are based.

Key parameters that are calculated by the met processor include:

- u_* – friction velocity (m/s)
- w_* – convective velocity scale (m/s) if the surface sensible heat flux is positive (zero otherwise)

- L_{MO} – Monin-Obukhov length (m)
- h – boundary layer depth (m) if not provided as an input parameter

An iterative procedure is used to calculate u_* and L_{MO}, assuming a modified logarithmic surface layer wind profile following:

$$\frac{\kappa U_s}{u_*} = \log\left(\frac{z + z_0}{z_0}\right) + \Psi\left(\frac{z + z_0}{L_{MO}}\right) - \Psi\left(\frac{z_0}{L_{MO}}\right) \quad (1)$$

where L_{MO} is defined as:

$$L_{MO} = -\frac{u_*^3 \rho_a c_p T_0^K}{\kappa F_{\theta_0} g} \quad (2)$$

$U_s(z)$ is the wind speed at height z above ground (which is known at 10 m from the input met data) and Ψ is a stability-dependent function.

If the boundary layer depth is not provided directly, it is calculated as follows. In stable conditions ($F_{\theta_0} \leq 0$) it is taken as:

$$h = \frac{0.6u_*}{|\omega|\left(1 + \sqrt{1 + \frac{2.28u_*}{|\omega|L_{MO}}}\right)} \quad (3)$$

where ω is the Coriolis parameter. In unstable conditions ($F_{\theta_0} > 0$), h is assumed to evolve according to:

$$\frac{dh}{dt} = \frac{S}{\Delta\theta} \quad (4)$$

where $\Delta\theta$ is the potential temperature jump across the boundary layer and S is a function of T_0^K, F_{θ_0}, u_* and the current value of h.

Finally, w_* is calculated using:

$$w_*^3 = \frac{u_*^3 h}{\kappa |L_{MO}|} \quad (5)$$

Using the derived boundary layer parameters output by the met processor, the local model is able to calculate vertical profiles of mean wind speed, turbulence, temperature and other quantities throughout the boundary layer. The boundary layer structure algorithms that are used are described in detail in Technical Specification document P09/01 (CERC, 2023a), some are summarised below.

The mean wind profile is the same as that used in the met pre-processor (Equation (1)), i.e. a stability-dependent modified logarithmic profile is assumed. Above h, the wind speed is held constant.

If urban canopy flow parameters are provided, the wind profile is implemented in three parts depending on the displacement height d above the ground:

$$\frac{d}{H} = 1 + (\lambda_P - 1)\alpha^{-\lambda_P} \tag{6}$$

Above the buildings ($z > 2d$), the mean wind profile is displaced vertically upward. The profile above buildings $U_a(z)$ is calculated similarly as in Equation (1), using $(z - d)$ as the height. Here, u_{*b} is the frictional velocity representative of the buildings and z_{0b} is the local surface roughness derived from the input parameters.

$$U_a(z) = \frac{u_{*b}}{\kappa}\left\{\ln\left(\frac{z-d}{z_{0b}}\right) - \Psi\left(\frac{z-d}{L_{MO}}\right)\right\} \tag{7}$$

Near the ground ($z < d$), the flow within the building canopy is related in magnitude to the upwind flow but is reduced logarithmically. Here, u_{*s} is the frictional velocity representative of the wind profile within the building canopy. The roughness length z_{0s} represents the value of extrusions from the roads and pavements in an urban area with a typical value of 10 cm.

$$U_c(z) = \frac{u_{*s}}{\kappa}\ln\left(\frac{z}{z_{0_s}}\right) \tag{8}$$

A transition layer exists between the urban canopy flow regimes ($d < z < 2d$) where the profile is calculated using linear interpolation to allow for a continuous vertical profile. The Technical Specification document P34/01 (CERC, 2023a) contains a full technical description of the urban canopy flow formulation.

Turbulence profiles are calculated using one of three sets of formulae, depending on the atmospheric stability, namely whether $h/L_{MO} < -0.3$ (convective), $0.3 \leq h/L_{MO} \leq 1$ (neutral) or $h/L_{MO} > 1$ (stable). In convective conditions, contributions from convectively driven and mechanically driven turbulence are included, while in neutral conditions only mechanically driven turbulence contributes. In stable conditions, the turbulence profiles depend on the friction velocity, roughness length and boundary layer depth alone. A minimum value is also applied to the turbulence components depending on the specified minimum Monin-Obukhov length.

If the urban canopy flow is considered, turbulence profiles above the building canopy ($z > d$) are calculated using the same atmosphere dependent formulae. Within the building canopy ($z < d$), the turbulence profile decays exponentially towards the ground.

The potential temperature profile assumes that T and θ are equal at screen height ($z_s = 1.22$ m), and the expressions used depend on whether h/L_{MO} is negative. The temperature profile relates to the potential temperature profile via:

$$T(z) = \theta(z) - \frac{g}{c_p}(z + z_0 - z_s) \tag{9}$$

and the pressure profile follows from the ideal gas equation:

$$p(z) = p_0 \left(\frac{T(z)}{\theta(z)} \right)^{\frac{c_p}{R}} \tag{10}$$

8.3.3 Road source dispersion

Road sources are modelled explicitly as line sources within ADMS-Local. Detailed information about each of the road sources is specified as input. Road and volume sources are modelled using Gaussian-plume formulations; a parameterised approach is used to account for the influence of street canyons on road source dispersion.

The Gaussian-plume dispersion equation used to model a two-dimensional crosswind-aligned ground-level line source of length L and source strength Q is:

$$C(x,y,z) = \frac{Q}{2\sqrt{2\pi}\sigma_z U}\left[\text{erf}\left(\frac{y+L/2}{\sqrt{2}\sigma_y}\right) + \text{erf}\left(\frac{y-L/2}{\sqrt{2}\sigma_y}\right)\right]\left\{\exp\left(-\frac{z^2}{2\sigma_z^2}\right) + \text{reflection terms}\right\} \tag{11}$$

where the crosswind and vertical plume spread, $\sigma_y(x,z)$ and $\sigma_z(x,z)$, and wind speed $U(z)$ are calculated at the mean plume height utilising the boundary layer profiles described in Section 8.3.1 above. In convective conditions a skewed Gaussian profile is used, in line with field experiments that show the probability density function of the vertical velocity to be non-Gaussian. The reflection terms are used to characterise the limits on plume spread formed by the ground surface and the temperature inversion at the top of the boundary layer in neutral and convective conditions.

To make use of this equation, the model divides up each road source segment into a number of two-dimensional crosswind 'elements', each with a source strength that varies in proportion to the fractional area of the segment that it represents and such that the sum over all elements equals the original source strength to conserve the mass released. The concentration C at a particular receptor location x, y, z due to emissions from that road segment is then the sum of the individual contributions from each element.

The division of each road segment into elements is done on a receptor-by-receptor basis, since the part of a segment that can contribute to the concentration at a particular receptor will vary, depending on their relative locations. Once the region of influence of a given segment for a particular receptor has been determined, this region is divided into a maximum of 10 crosswind elements. The along-wind spacing between elements is such that the elements closest to the receptor are closer together to reduce fractional error, while the spacing between any two adjacent elements is in general limited to change by no more than 10 %.

The initial vertical plume spread is taken as 1 m (and the height of release is also increased by 1 m) while the crosswind plume spread is calculated on a road-by-road

basis to account for the extra turbulence caused by the flow of traffic.

When the road source is located within a street canyon, adjustments are made to the dispersion calculations as outlined in the next section.

8.3.4 Street canyon influencing road source dispersion

Street canyons play an important role in altering the dispersion of pollutants from roads (Hood *et al.*, 2021). ADMS-Local incorporates the effects of street canyons on the dispersion from road sources in two ways. Firstly, within street canyons, concentrations resulting from road source dispersion are modified based on the properties of the street canyon. Then outside the street canyon, the dispersion from the road is modelled as a coverage-weighted combination of the standard (i.e. no-canyon) road source and a volume source representing the release of material from the top of the canyon. For a given road source segment, the concentration contribution at an output point within the canyon is calculated as a coverage-weighted combination of the standard (i.e. no-canyon) road source segment concentration and the full-canyon (i.e. unit coverage) segment concentration at that output point. Details of how this full-canyon concentration is calculated are given below.

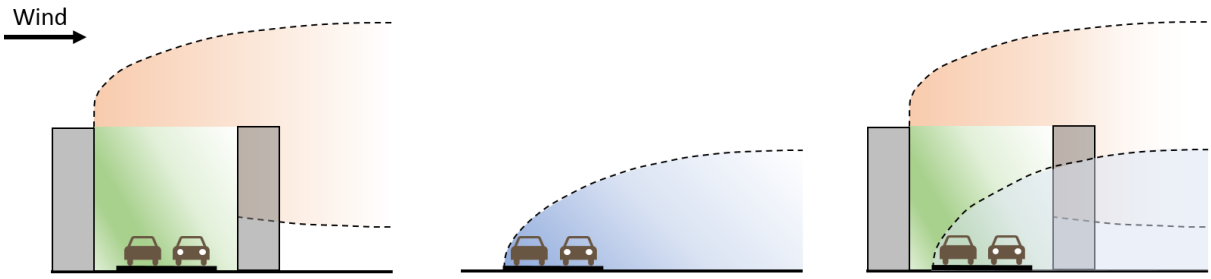


Figure 8.3 – Schematic showing ADMS-Local canyon parametrisation. Concentration pattern for a full-coverage canyon (left), a zero-coverage canyon equivalent to a standard road source (middle) and a partial-coverage canyon (right). In-canyon component (green) can only affect concentrations within the canyon; canyon top volume source component (orange) can only affect concentrations outside the canyon; non-canyon road source component (blue) can affect concentrations anywhere. Weightings given to each component depend on the canyon coverage.

The full-canyon concentration, C_{canyon}, at a given output point within the canyon is calculated using a series of factors applied to the standard (i.e. no-canyon) road source segment centre point concentration, $\hat{C}_{\text{non-canyon}}$, at the release height (1 m) in the following way:

$$C_{\text{canyon}} = \hat{C}_{\text{non-canyon}} f_{\text{lateral}} \left(f^{\parallel}_{\text{canyon}} f^{\parallel}_{H/W} f^{\parallel}_{\varphi} + f^{\perp}_{\text{canyon}} f^{\perp}_{H/W} f^{\perp}_{\varphi} \right)$$

where:

- f_{canyon} introduces a vertical profile that adjusts the non-canyon centre point concentration, $\hat{C}_{\text{non-canyon}}$, to a canyon centreline concentration at the output height, z;
- $f_{\text{H/W}}$ adjusts concentrations to account for the canyon aspect ratio, H/W;

- f_{φ} adjusts concentrations to account for the wind direction, φ;
- f_{lateral} is a lateral factor to convert from canyon centreline to canyon off-centreline locations;
- superscripts ∥ and ⊥ denote factors relating to along-road (parallel) and across-road (perpendicular) upstream flow respectively.

Here, H is the building height and W the canyon width.

summarises the canyon factor dependencies and provides variable definitions.

Dependent variable		**Factor**			
Variable	**Description**	f_{canyon}	$f_{\text{H/W}}$	f_{φ}	f_{lateral}
W	Canyon width (m)	✓	✓	✓	✓
r_w/W	Ratio of road carriageway width to canyon width (-)	✓	✓	✓	✓
z	Vertical height above ground (m)	✓	×	×	✓
ρ	Fractional distance from centreline towards upstream wall (-1 to +1)	×	×	×	✓
φ	Angle between road and wind direction	(✓)*	(✓)*	✓	✓
H/W	Canyon aspect ratio	×	✓	×	✓
U_{10}	Wind speed at 10 m	✓	✓	✓	✓
h/L_{MO}	Stability parameter	✓	✓	✓	✓

Table 8.1 Dependent variable list for the four ADMS-Local canyon parameterisation scaling factors; * f_{lateral} and f_{φ} vary with all values of φ, whereas f_{canyon} and $f_{\text{H/W}}$ only have values relating to $\varphi = 0$ (parallel flow) and $\varphi = 90°$ (perpendicular flow).

Values for the four factors have been derived from analyses of concentration outputs from multiple runs of ADMS-Urban, where the model has been configured to represent a single in-canyon road source using the advanced canyon module (Hood *et al.*, 2021). A wide range of representative source parameter ranges have been considered, for example: aspect ratios up to 2; $0.3 \leq r_w/W \leq 0.95$; and wind speeds and atmospheric stabilities representative of those experienced in urban areas.

The canyon-top volume source for a given road segment has the same horizontal footprint as the segment and is vertically centred on the canyon top (building height) with a depth of twice the initial road mixing height (2 m).

8.3.5 Volume source dispersion

Dispersion from a volume source is calculated in a similar way to a road source, but with each element representing a vertical slice of finite length and height. The concentration contribution from an individual crosswind element of length L_S, height L_V, vertical mid-point z_c and source strength Q is given by:

$$C(x,y,z) = \frac{Q}{4U}\left[\text{erf}\left(\frac{y+L_S/2}{\sqrt{2}\sigma_y}\right) + \text{erf}\left(\frac{y-L_S/2}{\sqrt{2}\sigma_y}\right)\right]\left[\text{erf}\left(\frac{z+\frac{L_V}{2}-z_c}{\sqrt{2}\sigma_z}\right) + \text{erf}\left(\frac{z-\frac{L_V}{2}-z_c}{\sqrt{2}\sigma_z}\right)\right] + \text{reflection terms} \quad (12)$$

A modified profile is adopted in convective conditions.

8.3.6 Gridded aggregate source dispersion

Aggregate, gridded, hourly emissions are modelled by ADMS-Local in order to represent the total emissions from each grid cell that correspond to the regional model's 3D hourly grid emissions. The gridded emission input files for ADMS-Local are created either by the emissions processing utility within the MAQS coupled system or externally by users. The emissions files are in netCDF format that complies with 'Climate and Forecast' (CF) metadata conventions (Eaton *et al.*, 2011) and contains hourly emissions data on a regularly-spaced horizontal (and potentially variably-spaced) vertical grid encompassing the local model domain. This format is described in Section 4.4.6.

For the run where road sources are explicitly represented in ADMS-Local, the model disaggregates road source emissions from the grid source to avoid double counting, scaling emissions using the time-variation factors as appropriate. Where roads cross more than one grid cell, the amount of emissions disaggregated from each cell is proportional to the length of road lying within that cell. The total emissions for each grid cell are used for the gridded run.

The remaining aggregated emissions from each individual grid cell are modelled as a volume source. In contrast to road sources, grid cell dispersion calculations are only performed for one cell per grid cell height, using a unit emission rate. Results for each individual grid cell are calculated by spatial translation and applying an emission rate scaling factor.

8.3.7 Chemistry

Chemical reactions have significant effects on ambient concentrations for many pollutants. Multiple complex atmospheric chemical processes are modelled within the regional model component of the MAQS coupled system; these reactions are modelled over large temporal and spatial extents, usually at hourly temporal resolution and at spatial grid scales of 1 km or larger. Chemical reactions on short time-scales govern concentrations of some pollutants in urban areas, for instance, NO_x chemistry strongly influences NO_2 concentration gradients in the vicinity of road sources. ADMS-Local incorporates local scale chemistry schemes; pollutants not included in these chemistry schemes are still modelled within ADMS-Local, but treated as locally inert.

Total concentrations are required in order to accurately model atmospheric chemical reactions. Consequently, for ADMS-Local, both local dispersion and long-range pollutant transport must be accounted for in chemical reactions. Within the coupled system an estimate of long-range pollutant transport is derived from the regional model

concentration files, taking account of the prevailing wind direction and other meteorology.

ADMS-Local includes two chemistry schemes, with the same basic principles shared by both schemes. They are essentially the same as those currently used in ADMS-Urban. The chemical reactions included in the schemes are simplified to represent the most important reactions over the short-to-medium-range time periods associated with local dispersion processes.

The chemistry calculations are uncoupled from the dispersion calculations; that is, dispersion processes are modelled first to generate an initial estimate of concentrations for each emitted pollutant. Individual 'travel times' are calculated as the time taken for each plume to reach each receptor. If only one plume was being modelled, this 'travel time' would be the appropriate time over which to apply the chemical reactions; with multiple sources in ADMS-Local, a concentration-weighted average travel time is used.

Each time the chemical reactions are applied, an adaptive stepping technique is adopted to reduce finite difference errors during periods of fast chemical conversions while allowing faster computation during periods when concentration changes are small.

The two chemistry schemes are discussed in more detail below.

NOx – GRS chemistry scheme

The ADMS-Local model uses a scheme based on the Generic Reaction Set (GRS) to model chemical processes that occur due to vehicular emissions of oxides of nitrogen (NO_x, consisting of NO and NO_2) and volatile organic compounds (VOCs), and their reactions with ozone (O_3). The GRS scheme (Venkatram *et al.*, 1994) is a semi-empirical photochemical model that reduces the complex series of chemical reactions involving the above pollutants to just seven reactions (1-7 below). An additional eighth reaction is added for the reaction between NO and O_2.

1. $ROC + hv \rightarrow RP + ROC$
2. $RP + NO \rightarrow NO_2$
3. $NO_2 + hv \rightarrow NO + O_3$
4. $NO + O_3 \rightarrow NO_2$
5. $RP + RP \rightarrow RP$
6. $RP + NO_2 \rightarrow SGN$
7. $RP + NO_2 \rightarrow SNGN$
8. $2NO + O_2 \rightarrow 2NO_2$

where

ROC = Reactive Organic Compounds (a fixed proportion of VOCs)

RP = Radical Pool

SGN = Stable Gaseous Nitrogen products

SNGN = Stable Non-Gaseous Nitrogen Products

Reactions 3. and 4. represent exact chemical reactions that occur very quickly, while reaction 8. occurs far more slowly. The remaining equations are approximations involving bulk species.

During the day, the reaction rate for reaction 3. is modified by assuming the background values are in chemical equilibrium. No such adjustment is made at night-time. The full list of reaction coefficients are given below, where e.g. R_1 corresponds to the reaction coefficient used for reaction 1 above:

$$R_1 = \mathrm{AROC} \times R_3 \times \exp\left(-4700\left(\frac{1}{T_0} - \frac{1}{316}\right)\right) \tag{13}$$

$$R_2 = \frac{358.1}{6T_0} \tag{14}$$

$$R_3 = \min(R_3(Q_{\max}), \overline{R_3}) \tag{15}$$

$$R_4 = 4.405 \times 10^{-2} \exp\left(\frac{-1370}{T_0}\right) \tag{16}$$

$$R_5 = \frac{1}{6} \tag{17}$$

$$R_6 = 2 \times 10^{-3} \tag{18}$$

$$R_7 = 2 \times 10^{-3} \tag{19}$$

$$R_8 = 4.61 \times 10^{-10} \exp\left(\frac{530}{T_0}\right) \tag{20}$$

where

$$R_3(Q) = 8 \times 10^{-4} \exp\left(\frac{-10}{Q}\right) + 7.4 \times 10^{-6} Q \tag{21}$$

$$\overline{R_3} = \frac{C_{\mathrm{BGD}}(O_3) \times C_{\mathrm{BGD}}(NO) \times R_4}{C_{\mathrm{BGD}}(NO_2)} \tag{22}$$

Q is solar radiation in W/m^2, $Q_{\max}$ is the maximum value of Q possible (assuming a solar elevation angle of 90 degrees and zero cloud cover), T_0 is temperature in Kelvin, and AROC represents the weighted reactivity coefficient for ROC, taken to be 0.05 by default as a result of validation work, though this value is modifiable via ADMS-Local's primary input file. $\overline{R_3}$ is calculated from the background concentrations of ozone, NO and NO_2 ($C_{\mathrm{BGD}}(O_3)$, $C_{\mathrm{BGD}}(NO)$ and $C_{\mathrm{BGD}}(NO_2)$ respectively). If any of these values are zero, R_3=$R_3(Q)$ is used. The above formulation assumes that a photochemical reaction rate derived from the background concentrations is more representative than a rate calculated from solar radiation values. In case of erroneous background data, a

minimum of $R_3(Q_{\max})$ and $\overline{R_3}$ is taken to ensure that the reactions occur at a realistic rate.

If processing annual average data, the hourly background concentrations of NO_X, NO_2 and ozone are derived using their monthly average hourly diurnal profile values from a rural monitoring site (Section 4.3.5), the primary NO_2 value as a fraction of NO_X (Section 4.7.11) and the annual average local background values of NO_X and NO_2 from the regional model. The hourly background concentrations are calculated assuming conservation of NO_X, conservation of OX (i.e. the sum of NO_2 and ozone) and, during the daytime, photo-stationary equilibrium.

$$C_{BGD}(NO_2) = \frac{R4}{R3} \times C_{BGD}(NO) \times C_{BGD}(O_3) \quad (23)$$

Sulphate chemistry scheme

The sulphate reaction scheme in ADMS-Local is the same as that currently used in ADMS-Urban and is taken from the EMEP model (Simpson *et al.*, 2012). Any SO_2 in the atmosphere is assumed to oxidise to SO_3:

1. $2SO_2 + O_2 \rightarrow 2SO_3$

with a rate constant, R_{S1}, defined as:

$$R_{S1} = 3 \times 10^{-6} + 2 \times 10^{-6} \sin\left(2\pi \frac{(\text{Day} - 80)}{365}\right) \quad (24)$$

where Day is the Julian day of the year. This SO_3 is then assumed to undergo the following immediate chain of reactions to form ammonium sulphate:

2. $SO_3 + H_20 \rightarrow H_2SO_4$
3. $H_2SO_4 + 2NH_3 \rightarrow (NH_3)_2SO_4$

Oxygen (O_2), water vapour (H_20) and ammonia (NH_3) are assumed to be available in abundance. Practically, the model can therefore perform the above three reactions in one step, namely, $2SO_2 \rightarrow (NH_3)_2SO_4$, using rate constant R_{S1}. This ammonium sulphate is added to the particulate matter concentrations, with 100% of it assumed to be PM_{10} and 73% assumed to be $PM_{2.5}$.

8.4 Additional system procedures for high-resolution contour output

When generating high-resolution contours of concentration using stand-alone local model runs, three types of output locations are included in the final output files:

- a regular grid of output points which provide the underlying grid resolution away from explicitly modelled sources;
- primary source-oriented grid points, which are added to increase the resolution where the highest concentration gradients are expected, such as along explicitly modelled

roads, and which are included in the main concentration calculations; and

- secondary or interpolated intelligent grid points, which are inserted in between pairs of primary source-oriented grid points at the end of the run and given concentrations interpolated between the adjacent modelled concentrations.

This combination of output point types helps to generate smooth concentration contours at high resolution without requiring excessive modelling calculations. In order to allow the same type of high resolution contour output from the MAQS coupled system, two procedures are required in addition to those described in Section 8.2, firstly to define a consistent set of output points for the main nesting runs with and without explicit emissions, and secondly to add interpolated intelligent grid points to the final output.

An additional user option is available to apply interpolation to the regional model concentrations, which makes the output concentration contours smoother across the boundaries of regional model cells. This option also changes the settings for grid modelling in the ADMS-Urban runs in order to apply similar interpolation, as described in Appendix I.3.

8.4.1 Defining output point locations: Create ASP

As described in Step 4 of the main MAQS coupled system procedures described in Section 8.2, when ADMS-Local is used as the local model, the **Create ASP** utility is run in order to generate an Additional Specified Points (*.asp)* file. This *.asp* file contains any specified points, the regular grid points and the primary source-oriented grid points for the whole nesting domain.

If ADMS-Urban is the selected local model, the *.upl* with explicit emissions is run with spatial truncation to the whole nesting domain using the ADMS-Urban **Create ASP** mode. Please refer to the ADMS-Urban User Guide for more details of the ADMS-Urban **Create ASP** mode.

Creating the *.asp* file for the whole nesting domain rather than for individual regional model grid cell regions allows high-resolution contours to be created across the boundaries between regional model grid cells, which are otherwise run independently in the MAQS coupled system.

8.4.2 Adding interpolated concentrations

The **AddInterpIGP** utility is run after the nested concentration files have been combined for the whole nesting domain in Step 11. This ensures that pairs of source-oriented grid points which lie on different sides of a boundary between adjacent regional model grid cells can be used to create interpolated source-oriented grid points. The output from this utility is an ADMS COF format netCDF file (*.nc*), with the points reclassified as regular or source-oriented grid points as appropriate. Please refer to Appendix G for more information about the **AddInterpIGP** utility.

8.5 System limits

8.5.1 Permitted characters

Users are advised to restrict the characters used in file paths to a-z, A-Z, and 0-9. The use of the character : is not permitted in file paths. Note that file paths and variable names are case sensitive in Linux systems, and that there is a distinction between the use of single and double quotes. Refer to Section 2.3.2 for more details of valid number and string formats for the Linux system input files.

The main MAQS working directory must not have a name beginning with C and containing two further C characters, in order to avoid conflicts with automatic cell folder names.

8.5.2 Numbers of sources in ADMS-Urban .upl files

The numbers of explicit and gridded sources defined in the *.upl* input to the MAQS coupled system may be very large, to include all sources within the urban area of interest. The maximum number of each source type which can be defined in the ADMS-Urban interface is 100000 road sources, 100000 industrial sources and 100000 grid source cells.

The number of explicit and gridded sources which can be included in each regional model grid cell within the nesting domain is controlled by the terms of your ADMS-Urban license.

SECTION 9 References

Adams, L. and Brandmeyer, J., 2014: Visualization Environment for Rich Data Interpretation (VERDI 1.5): User's Manual. Available online at https://www.cmascenter.org/verdi/documentation/1.5/VerdiUserManual1.5.pdf (accessed September 2023).

Brookes, D., Stedman, J., Kent, A., Whiting, S., Rose, R., Williams, C. and Pugsley, K., 2020: Technical report on UK supplementary assessment under The Air Quality Directive (2008/50/EC), The Air Quality Framework Directive (96/62/EC) and Fourth Daughter Directive (2004/107/EC) for 2018. Ricardo report reference ED12633 - Issue Number 1. Ricardo Energy & Environment/R/3470.

Byun, D. and Schere, K.L., 2006: Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modelling system. *Applied Mechanics Reviews* **59**, 51-77.

CERC, 2020a: Comprehensive Output File Processor User Guide, Version 4.0. Available online at www.cerc.co.uk/UserGuides (accessed September 2023).

CERC, 2020b: ADMS-Urban User Guide, Version 5.0. Available online at www.cerc.co.uk/UserGuides (accessed September 2023).

CERC, 2022: EMIT Atmospheric Emissions Inventory Toolkit User Guide, Version 3.9. Available online at www.cerc.co.uk/UserGuides (accessed September 2023).

CERC, 2023a: ADMS Technical Specification. Available online at www.cerc.co.uk/environmental-software/technical-specifications.html (accessed September 2023).

CERC, 2023b: MAQS Post Processor User Guide, Version 1.0. Available online at www.cerc.co.uk/UserGuides (accessed September 2023).

Coats, C.J., 2004: The BAMS/EDSS/Models-3 I/O API: User Manual. Available online at https://www.cmascenter.org/ioapi/documentation/all_versions/html/ (accessed September 2023).

Dudhia, J., Gill, D., Manning, K., Wang, W. and Bruyere, C., 2005: PSU/NCAR Mesoscale Modeling System Tutorial Class Notes and Users' Guide (MM5 Modeling System Version 3). Available online at http://www2.mmm.ucar.edu/mm5/documents/ (accessed September 2023).

Eaton, B., Gregory, J., Drach, B., Taylor, K., Hankin, S., Caron, J., Signell, R., Bentley, P., Rappa, G., Hock, H., Pamment, A and Juckes, M., 2011: NetCDF Climate and Forecast (CF) Metadata Conventions, Version 1.6. Available online at http://cfconventions.org/cf-conventions/v1.6.0/cf-conventions.pdf (accessed September 2023).

ENVIRON, 2016: User's Guide to the Comprehensive Air Quality Model with Extensions Version 7.2. Available online at https://camx-wp.azurewebsites.net/Files/CAMxUsersGuide_v7.20.pdf (accessed September 2023).

Grell, G.A., Peckham, S. E., Schmitz, R. and McKeen, S. A., 2005: Fully coupled 'online' chemistry in the WRF model. *Atmospheric Environment* **39**, 6957 – 6976.

Hood, C., Stocker, J., Seaton, M., Johnson, K., O'Neill, J., Thorne, L. and Carruthers, D., 2021: Comprehensive evaluation of an advanced street canyon air pollution model. *Journal of the Air & Waste Management Association*, **71**, 247-267.

McHugh, C.A., Carruthers, D.J., and Edmunds, H.A., 1997: ADMS-Urban: an air quality management system for traffic, domestic and industrial pollution. *International Journal of Environment and Pollution* **8**, 437–440.

Otte, T.L. and Pleim, J.E., 2010: The Meteorology-Chemistry Interface Processor (MCIP) for the CMAQ modeling system: updates through MCIPv3. 4.1. *Geoscientific Model Development*, **3**, 243-256.

Schmidt, H., Derognat, C., Vautard, R. and Beekmann, M., 2001: A comparison of simulated and observed ozone mixing ratios for the summer of 1998 in Western Europe. *Atmospheric Environment* **35**, 6277-6297.

Seaton, M., O'Neill, J., Bien, B., Hood, C., Jackson, M., Jackson, R., Johnson, K., Oades, M., Stidworthy, A., Stocker, J. and Carruthers, D., 2022: A multi-model air quality system for health research: road model development and evaluation. *Environmental Modelling & Software*, **155**, 105455.

Simpson, D., Benedictow, A., Berge, H., Bergström, R., Emberson, L. D., Fagerli, H., Flechard, C. R., Hayman, G. D., Gauss, M., Jonson, J. E., Jenkin, M. E., Nyíri, A., Richter, C., Semeena, V. S., Tsyro, S., Tuovinen, J.-P., Valdebenito, Á., and Wind, P., 2012: The EMEP MSC-W chemical transport model – technical description. *Atmospheric Chemistry and Physics*, **12**, 7825–7865.

Skamarock, W., Klemp, J., Dudhia, J., Gill, D., Barker, D., Duda, M., Huang, X., Wang, W., and Powers, J., 2008: A Description of the Advanced Research WRF Version 3. NCAR Technical Note NCAR/TN-475+STR. Available online at https://opensky.ucar.edu/islandora/object/technotes:500 (accessed September 2023).

Stidworthy, A., Carruthers, D., Stocker, J., Balis, D., Katragkou, E. and Kukkonen, J., 2013: MyAir Toolkit for Model Evaluation. 15th International Conference on Harmonisation, Madrid, Spain, May 2013. Available online at www.harmo.org/Conferences/Proceedings/_Madrid/publishedSections/H15-186.pdf (accessed September 2023).

Venkatram, A., Karamchandani, P., Pai, P. and Goldstein, R., 1994: The development and application of a simplified ozone modelling system (SOMS). *Atmospheric Environment*, **28**, 3665-3678.

Vieno, M., Dore, A.J., Stevenson, D.S., Doherty, R., Heal, M.R., Reis, S., Hallsworth, S., Tarrason, L., Wind, P., Fowler, D., Simpson, D., and Sutton, M.A., 2010: Modelling surface ozone during the 2003 heat-wave in the UK. *Atmospheric Chemistry and Physics* **10**, 7963-7978.

APPENDIX A RM Grid Info utility

The **RM Grid Info** utility is a command line application which extracts information about the spatial grid used in regional model concentration files. It can also write an *.asp* file defining an output point at the horizontal centre and layer boundary height of each regional model grid cell in the surface layer. This utility was developed for the MAQS coupled system.

The **RM Grid Info** utility is able to read spatial grid information directly from regional model concentration output files from the CMAQ, CAMx (converted into I/OAPI format), EMEP4UK, WRF-Chem and CHIMERE models. The utility can also read data from annual average regional model output such as Defra's 1 km resolution background map datasets. Output from any other model may also be used after re-gridding and re-formatting the data into the Generic file formats.

A.1 Calculation of Regional Model output heights

Some regional meteorological and air quality models run with vertical grid structure defined by pressure (sigma) coordinates, whereas ADMS-Local uses absolute heights above ground level in metres. The conversion from sigma values to heights in general requires knowledge of the terrain height, which can vary in space, and the surface temperature and pressure, which can vary in both space and time.

Within the **RM Grid Info** utility, heights are calculated from CMAQ or EMEP4UK sigma values using the simplified 'reference state' assumptions with constant surface temperature and pressure, and assuming a constant terrain height. This is based on the approach used in the MM5 meteorological model (Dudhia *et al.*, 2005), which was a precursor to the WRF model. It avoids the need to re-read all the WRF data purely to obtain the regional model grid heights, and enforces constant grid heights, both of which speed up the processing time for the utility. The spatial and temporal variations of absolute grid cell heights are generally small relative to cell depths and can be neglected for near-ground cells. The conversion of pressure coordinates to heights is more sensitive to the value of temperature than the value of terrain height, such that the use of a user-specified typical temperature and zero terrain height gives sufficient accuracy for the grid heights.

The expression used to calculate height from a sigma coordinate value σ is as follows:

$$z = -\frac{RA}{2g}\left(\left(\ln\left(\frac{(p_0 - p_T)\sigma + p_T}{p_0}\right)\right)^2 + \frac{2T_0}{\mathrm{A}}\ln\left(\frac{(p_0 - p_T)\sigma + p_T}{p_0}\right)\right)$$

where: z is height above ground in metres; R is the gas constant for air (287 J/kgK); A is an atmospheric lapse rate (50 K); g is gravitational acceleration (9.81 m/s^2); p_0 is the standard atmospheric pressure at sea-level (1.013x10^5 Pa); p_T is the pressure at the top of the model grid, which may be obtained from the concentration output files or specified by the user; and T_0 is the standard temperature at sea-level in Kelvin, which is specified by the user.

For the CHIMERE model, heights are given explicitly in the model output file. The **RM Grid Info** utility calculates an average height for each layer for the first hour of data. For the WRF-Chem model, the layer heights are calculated from base and perturbed geopotential values, gravity and terrain height. Again an average is taken over all cells in each layer for the first hour of data. The bottom of the lowest grid cell is assumed to be at ground level.

The use of hybrid vertical coordinates was introduced in CMAQ version 5.3, and from this version CMAQ output files using hybrid vertical coordinates do not contain sufficient information to define the vertical grid structure. If modelling with these files, the **RM Grid Info** utility extracts height values from a separate netCDF file produced by the CMAQ modelling system. The utility requires that the file contains 3D gridded data and the grid top height values (in metres) are stored in the variable called 'ZF', varying in space (dimensioned x, y, z) and time. It is recommended that the METCRO3D output file from the Meteorology-Chemistry Interface Processor (MCIP) component of CMAQ (Otte and Pleim, 2010) for the same domain as the CMAQ concentration output is used for defining the regional model grid heights. Similarly to the approach with WRF-Chem, an average grid top height is taken over all cells in each layer for the first hour of data while the bottom of the lowest grid cell is assumed to be at ground level.

A.2 Definition of coordinate system datum

It is important to define a suitable datum for the shape of the earth when converting from latitude-longitude grid coordinates, as used in WRF-Chem and CHIMERE output files, to projected coordinates for use in ADMS-Local and the MAQS coupled system. A datum is generally defined either as spherical or ellipsoid, with controlling parameters semi-major axis and inverse flattening. The semi-major axis length, a, is defined as half the longest axis of the ellipsoid, i.e. the radius of the equator, while the semi-minor axis length, b, is the distance along the ellipsoid axis from equator to pole. The inverse flattening is calculated as $\frac{a}{a-b}$.

The **RM Grid Info** utility offers two pre-set datum options and also the possibility of defining a custom spherical or ellipsoid datum. The 'EMEPSPHERE' datum setting indicates the assumption of a spherical datum with radius 6370000 m, as used in the EMEP, WRF and CMAQ models. The 'WGS84' datum indicates use of the WGS84 ellipsoid, commonly associated with GPS and other satellite data, with semi-major axis 6378137 m and inverse flattening 298.257223563. A 'CUSTOM' setting allows the user to define an alternative spherical or ellipsoid datum using values of semi-major axis and inverse flattening. The special inverse flattening value of 0.0 is used to indicate a spherical datum, otherwise for ellipsoid datum settings the inverse flattening value should be greater than 1.0.

A.3 Annual average processing

The MAQS coupled system allows linking with annual average datasets, for instance when using Defra's 1 km background maps. These datasets are available in a *.csv* format file for a particular pollutant and year. The **RM Grid Info** utility extracts the needed information as with other regional models. As the coordinate system used in the Defra background maps is OSGB (with Airy 1830 datum), the datum options in the previous section are ignored. The height of the regional model surface layer is set to a default of 10 m or specified by the user. The utility

also creates an additional intermediary file in ADMS generic average format containing the annual average concentrations; this is mainly used in the subsequent **Processor** utility for reading the regional model concentrations but can also be input to the **RM Grid Info** utility to allow faster re-runs of the system. The format of the Generic 2D average concentration data file is described in Section 4.3.7.

A.4 Input file format

The input file for the **RM Grid Info** utility is a text file which contains a version string and three or more sections of input data. Three sections are compulsory and the rest, which includes advanced parameters, are optional. The three compulsory sections are described in **Table A.1** while the optional sections are defined in **Table A.2**. The 'REGIONALMODEL' section is identical to that used in the **Processor** utility. The sections may be listed in any order but the order of the variables within each section must be as defined in the tables. Each element should be given on a new line, blank lines may be included before each section keyword but not within a section. If the 'ADVANCEDNESTING' section is included, all the Y/N elements must be included, with values for any 'Y' elements. An example input file is shown in **Figure A.1**. The 'RMHEIGHTINFOFILE' section is identical to that used in the **RM Emissions** utility.

GridInfoInput.txt

```
1   RMGRIDINFOINPUTVERSION1
2
3   REGIONALMODEL
4   'CMAQ'
5   2010,03,03, 9
6   2010,03,06, 7
7   PATH="/home/CERC/maqs/Data/ADMS_CAMx_SpeciesMap.csv"
8   "/home/CERC/maqs/Data/CAMx/"
9   'CAMx.%Y%M%D_4X5.ncf'
10  24
11  8
12
13  RMGRIDINFOOUTPUT
14  PATH="/home/CERC/maqs/working/GridInfoOutput.txt"
15  Y
16  PATH="/home/CERC/maqs/working/GridInfoCellCentres.asp"
17
18  ADVANCEDNESTING
19  Y
20  100000
21  Y
22  298.15
23  Y
24  5000
25  N
26
27  RMCOORDINFO
28  'EMEPSPHERE'
29
```

Figure A.1 Example input text file for the **RM Grid Info** utility

Element type	Description	Sample element	Comment
Version string	File version description	RMGRIDINFOINPUTVERSION1	Must be the first line of the file
Section keyword	Start of section containing general variables	REGIONALMODEL	Also used in the **Processor** utility, must be included, although the species map file is not used in this utility. Please refer to **Table E.1** for details
Variable	Regional model name	'CMAQ'	
Variable	Start date-time	2018,01,01,01	
Variable	End date-time	2018,12,31,24	
Variable	File path to species map file	PATH="/disk/cmaq/smap.csv"	
Variable	File path to date-independent directory containing regional model output file	"/disk/cmaq/Output"	
Variable	File name template for regional model output files	'%Y%M/cctm.%Y%M%D.nc'	
Variable	Number of hours in each regional model output file	24	
Variable	Time difference between local solar and regional model times	1	
Section keyword	Start of section containing coordinate datum definition	RMCOORDINFO	Also used in **RM Met Data** and **RM Emissions** utilities, must be included.
Variable	Datum type	EMEPSPHERE	EMEPSPHERE, WGS84 or CUSTOM
Variable	Semi-major axis (m)	6378137.0	Only included if datum type above is 'CUSTOM'. Special inverse flattening value of 0 used to indicate sphere.
Variable	Inverse flattening	298.257223563	
Section keyword	Start of section with variables specific to RM Grid Info	RMGRIDINFOOUTPUT	Must be included
Variable	File path of output grid information file	PATH="/disk/maqs/run/out.txt"	
Variable	Whether to output cell centre points *.asp* file	Y	Y or N
Variable	File path of output cell centre *.asp* file	PATH="/disk/maqs/run/Centres.asp"	Only included if Y above

Table A.1 Specification of compulsory elements of the input file format for the **RM Grid Info** utility

Element type	Description	Sample element	Comment
Section keyword	Start of optional section containing advanced settings	ADVANCEDNESTING	May be omitted, must be included in full if required.
Variable	Whether to specify frequency of checking output point locations match – not used in this utility	N	
Variable	Whether to specify sea-level temperature	Y	Y or N
Variable	Average sea-level temperature in Kelvin	298	Only included if Y above, default value 288.15
Variable	Whether to override the model top pressure	Y	Y or N
Variable	Model top pressure in Pascals	5000	Only included if Y above, default to use the value from the regional model concentration output files
Variable	Whether to specify a file path to a *.cco* file, which is required for CHIMERE regional model files.	Y	Y or N
Variable	The file path to a *.cco* file	PATH= "/disk/chimere/coords.cco"	Only included if Y above
Section keyword	Start of optional annual average background map files section	AABACKFILE	
Variable	File path of output generic average data file	PATH="/disk/maqs/run/generic.nc"	
Variable	Number of input annual average background map file	4	
Variable	Annual average background map species	NOx	Must list each pollutant and corresponding file path
Variable	File path to the annual average background map file	PATH="/disk/pcm/mapnox2018.csv"	
Section keyword	Start of annual average background map domain section	AABACKDOMAIN	
Variable	Lower left x coordinate (m)	407000	
Variable	Lower left y coordinate (m)	284000	
Variable	Upper right x coordinate (m)	410000	
Variable	Upper right y coordinate (m)	287000	

Element type	Description	Sample element	Comment
Section keyword	Start of regional model surface layer height section	RMSURFACEHEIGHT	
Variable	Whether to specify the top of the regional model surface layer as height or sigma value	HEIGHT	HEIGHT or SIGMA
Variable	Height or sigma value of the regional model surface layer	25.0	
Section keyword	Start of optional section for specifying a file with vertical height information, which is required for CMAQ regional model files that use hybrid vertical coordinate system.	RMHEIGHTINFOFILE	Also used in the **RM Emissions** utility
Variable	Whether specifying a single file path to the vertical height information file or otherwise specifying the directory and file name template for the file	Y	Y or N
Variable	File path to the file with vertical height information	PATH=”/disk/cmaq/METCRO 3D.nc”	For alternate option of specifying directory and file name template, please refer to **Table B.2**.

Table A.2 Specification of optional elements of the input file format for the **RM Grid Info** utility

A.5 Command line structure

To run the **RM Grid Info** utility from the command line or a script, the following syntax should be used:

```
<executable file path> <input text file path>
```

where `<executable file path>` is the full path to the utility executable (*.out*), enclosed in inverted commas, and `<input text file path>` is the full path to the input text file that contains the information required to run the executable, enclosed in inverted commas.

For example, if the executable is saved in the default installation directory, */disk/maqs/utils/*, and the input text file is saved as */home/user/maqs_work/input.txt*, the command line to run the utility would be

```
‘/disk/maqs/utils/RMGridInfo.out’ ‘/home/user/maqs_work/input.txt’
```

A.6 Utility outputs

The **RM Grid Info** utility creates an output text file containing information about the regional model spatial grid. It will stop with an error if an existing file is found with the same file path as specified for the output file, i.e. it will not overwrite or append to an existing file.

The initial line contains a version string, RMGRIDINFOOUTPUTVERSION1, which is checked by other programs reading the file. A header section specifies when the file was created, the name and version number of the utility and the input control and regional model file paths. The information about the regional model grid is then presented as a list, described in **Table A.3**. An example output *.txt* file is shown in **Figure A.2**. The last three elements are only included in the grid information file for input files in I/O API (CMAQ or CAMx) format. The elements below the thicker black line in **Table A.3** are relevant only if calculating the CMAQ heights from sigma values, as described in A.1.

GridInfoOutput.txt

```
RMGRIDINFOOUTPUTVERSION1
!*********************************************************!
! File created at date/time:   18/05/2023 13:04:10
! Grid info file produced by the RM Grid Info program
! Version 1.0
! Build number 8959
! Input control file: /home/CERC/maqs/working/GridInfoInput.txt
! Input regional model file: /home/CERC/maqs/Data/CAMx/CAMx.20100303_4X5.ncf
!*********************************************************!

&RM_GridInfo
RM_MinX = -5000.00
RM_MinY = -666500.00
RM_MaxX = -1000.00
RM_MaxY = -661500.00
RM_SpacingX = 1000.00
RM_SpacingY = 1000.00
RM_NumCellsX = 4
RM_NumCellsY = 5
RM_NumVerticalLevels = 20
RM_GroundLevelIndex = 1
RM_GroundLevelDepth = 17.43
RM_VerticalList = .00 17.43 36.55 57.37 79.91 104.17 130.16 161.28 198.39 242.43 295.18
358.49 433.42 522.83 629.74 756.47 908.27 1089.00 1304.89 1561.98 1869.34
RM_GridName = "???????????????"
RM_TopPressure = 5000.00
RM_SigmaList = 1.0000 .9979 .9956 .9931 .9904 .9875 .9844 .9807 .9763 .9711 .9649 .9575
.9488 .9385 .9263 .9120 .8951 .8753 .8521 .8251 .7937
/
```

Figure A.2 Example output text file from the **RM Grid Info** utility

Name	Description
RM_MinX	The minimum x-coordinate, relating to the left edge of the regional model grid.
RM_MinY	The minimum y-coordinate, relating to the bottom edge of the regional model grid.
RM_MaxX	The maximum x-coordinate, relating to the right edge of the regional model grid.
RM_MaxY	The maximum y-coordinate, relating to the top edge of the regional model grid.
RM_SpacingX	The spacing between regional model grid points in the x-direction.
RM_SpacingY	The spacing between regional model grid points in the y-direction.
RM_NumCellsX	The number of regional model grid cells in the x-direction.
RM_NumCellsY	The number of regional model grid cells in the y-direction.
RM_NumVerticalLevels	The number of regional model grid cells in the vertical direction.
RM_GroundLevelIndex	The index of the regional model grid layer that is closest to the ground.
RM_GroundLevelDepth	The average depth of the regional model ground level layer.
RM_VerticalList	A list of the average heights of the vertical layer boundaries in the regional model, including the upper and lower edges.
RM_GridName	The name associated with the grid (CMAQ or CAMx only)
RM_TopPressure	The model top pressure associated with the sigma levels (CMAQ without hybrid vertical coordinates or CAMx only)
RM_SigmaList	A list of the sigma values of the vertical layer boundaries in the regional model, including the upper and lower edges. (CMAQ without hybrid vertical coordinates or CAMx only)

Table A.3 Specification of output file format from the **RM Grid Info** utility

The **RM Grid Info** utility can optionally create an *.asp* file for input to ADMS-Urban or ADMS-Local, defining an output point at the horizontal centre and layer boundary height of each regional model grid cell in the surface layer. It will stop with an error if an existing file is found with the same file path as specified for the output *.asp* file, i.e. it will not overwrite or append to an existing file. The *.asp* file is a list of output points, each defined by a comma-separated list of name, x, y and z coordinate values. The point names are generated using truncated integer x and y coordinate values, separated by an underscore ('_'). An example *.asp* file output by the **RM Grid Info** utility is shown in Figure A.3.

GridInfoCellCentres.asp

```
-4500_-666000, -4500.00, -666000.00, 17.43
-4500_-665000, -4500.00, -665000.00, 17.43
-4500_-664000, -4500.00, -664000.00, 17.43
-4500_-663000, -4500.00, -663000.00, 17.43
-4500_-662000, -4500.00, -662000.00, 17.43
-3500_-666000, -3500.00, -666000.00, 17.43
-3500_-665000, -3500.00, -665000.00, 17.43
-3500_-664000, -3500.00, -664000.00, 17.43
-3500_-663000, -3500.00, -663000.00, 17.43
-3500_-662000, -3500.00, -662000.00, 17.43
-2500_-666000, -2500.00, -666000.00, 17.43
-2500_-665000, -2500.00, -665000.00, 17.43
-2500_-664000, -2500.00, -664000.00, 17.43
-2500_-663000, -2500.00, -663000.00, 17.43
-2500_-662000, -2500.00, -662000.00, 17.43
-1500_-666000, -1500.00, -666000.00, 17.43
-1500_-665000, -1500.00, -665000.00, 17.43
-1500_-664000, -1500.00, -664000.00, 17.43
-1500_-663000, -1500.00, -663000.00, 17.43
-1500_-662000, -1500.00, -662000.00, 17.43
```

Figure A.3 Example output grid cell centre *.asp* file from the **RM Grid Info** utility

The **RM Grid Info** utility can also generate concentration data netCDF (*.nc*) files in Generic 2D average format from annual average datasets such as Defra's 1 km background maps. The height of the regional model spatial grid is 10 m by default, unless specified by the user. As the annual average background concentration maps are not necessarily rectangular, the utility fills in any missing cells to create a rectangular grid. The format of this file is described in Section 4.3.7.

Any error or warning messages are written to *Error.txt* or *Warning.txt* text files in the same directory as the input text file. Error messages relate to problems which cause the program to fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.

APPENDIX B RM Emissions utility

The **RM Emissions** utility is a command line application which creates ADMS format hourly 3D gridded emissions files from regional air quality model emissions files. This utility was developed for the MAQS coupled system but may also be useful for stand-alone ADMS-Urban or ADMS-Local modelling where regional model emissions files are available. An alternative method for creating ADMS 3D gridded emissions files from 2D gridded emissions and associated time-variation and vertical profiles is included in CERC's EMIT (Emissions Inventory Toolkit) software (CERC, 2022).

The **RM Emissions** utility currently supports regional model emissions files from the CMAQ and WRF-Chem models. Emissions from any other model which can be manipulated to comply with the Models-3 I/O API netCDF gridded file conventions (Coats, 2004) may also be used by selecting the CMAQ option.

Multiple regional model emissions files, for example including data for different emissions sectors, can be combined by the utility into a single generic 3D gridded emissions file.

B.1 3D emissions processing

The output 3D gridded emissions rate $E_{ADMS}(p,i,j,k,t)$ of ADMS pollutant p from a given cell with indices i,j,k at time t, is calculated from the input regional model emissions rate(s) $E_{RM}(f,q,i,j,k,t)$ of regional model pollutant(s) q from regional model emissions file(s) f, according to:

$$E_{ADMS}(p,i,j,k,t) = \sum_{f=1}^{F} \sum_{q=1}^{Q} S_{Em,f}(p,q) * E_{RM}(f,q,i,j,k,t)$$

Where $S_{Em,f}(p,q)$ is the conversion factor from the emissions species map for converting regional model pollutant q to ADMS pollutant p for the current file type; Q is the number of regional model pollutants defined in the emissions species map; and F is the number of types of regional model emissions files defined in the utility input file. The emissions species map factor values should include any unit conversions required to obtain ADMS species emission rates in units of g/m^2/s from the regional model emission rates.

Note that although the emissions species map file has the same format as the concentration species map file, in general the species and factor values included will not be the same for emissions as for concentrations, due to different unit conversion requirements and regional model speciations.

Different regional emission variables may be included in different file types, for example representing anthropogenic and biogenic sources. All emissions species maps should include the same ADMS emissions variables.

For the WRF-Chem model, the heights are not available in the regional model emissions files. The heights are calculated from WRF meteorological model output files for the same domain as the WRF-Chem emissions using terrain heights, base-state and perturbation geopotentials.

The heights in the CMAQ model can be defined by pressure (sigma) coordinates. However, from CMAQ version 5.3 when hybrid vertical coordinates are used, the sigma values in the regional model emission files are not sufficient for calculating heights. If modelling with these files, the utility extracts the layer boundary height values from an additional file from the Meteorology-Chemistry Interface Processor (MCIP) component of CMAQ (Otte and Pleim, 2010), similar to the **RM Grid Info** utility (see Appendix A.1).

B.2 Input file format

The input file for the **RM Emissions** utility is a text file which contains a version string and three or more sections of data. Three (in some cases, four) sections are compulsory and the rest are optional. The first two compulsory sections are described in **Table B.1**, the rest of the compulsory sections in

Variable	File path to date-independent directory containing file with vertical height information	"/home/WRF/Output"	For alternate option of specifying a single file path, please refer to **Table A.2.**
Variable	File name template for the heights file	'%Y%M/cctm.%Y%M%D.nc'	

Table B.2 and the optional sections in **Table B.3**. The version string must be the first line in the file, following which the sections may be listed in any order but the order of the variables within each section must be as defined in **Tables B.1** to **B.3**. Each element should be given on a new line, blank lines may be included before each section keyword but not within a section. An example input file is shown in **Figure B.1**. If the optional section 'ADVANCEDNESTING' is included, all the Y/N elements must be included, with additional values for any 'Y' elements.

If the input regional model emissions files contain 24 hours or fewer, the utility allows matching of time but not date values when selecting data to include in the output file, for example if a single day input file is used to represent each day of a month for output. However, if date tags are included in the file name templates, these will be set based on the output dates, so these may need to be defined with care.

The 'RMHEIGHTINFOFILE' section is identical to that used in the **RM Grid Info** utility. If converting from emissions files in WRF-Chem format or if processing CMAQ emission files that use a hybrid vertical coordinate system, the 'RMHEIGHTINFOFILE' section must be included in the input file.

RMEmissionsInput.txt

```
1  RMEMISSIONSVERSION1
2
3  RMEMISSIONSINPUTS
4  PATH="/home/CERC/maqs/working/RMEmissions.nc"
5  'WRFChem'
6  1
7  "/home/CERC/maqs/Data/WRFChem/emissions"
8  'wrfchemi_%hz_d04_cut2.nc'
9  12
10 PATH="/home/CERC/maqs/Data/WRFCHEM_em_species.csv"
11
12 RMEMISSIONSEXTENTS
13 2015,01,11, 5
14 2015,01,11, 6
15 5
16 -798334.011
17 463333.780
18 5
19 4
20 7
21
22 ADVANCEDNESTING
23 Y
24 288.15
25 N
26
27 RMCOORDINFO
28 'EMEPSPHERE'
29
30 RMHEIGHTINFOFILE
31 N
32 "/home/CERC/maqs/Data/WRFChem/output"
33 'wrfout_d04_%Y-%M-%D_%h_cut2.nc'
34
```

Figure B.1 Example input file for the **RM Emissions** utility

Element type	Description	Sample element	Comment
Version string	File version description	RMEMISSIONSVERSION1	Must be the first line of the file
Section keyword	Start of section containing regional model emissions file information	RMEMISSIONSINPUTS	
Variable	Output 3D emissions file path	PATH="/home/maqs/3DEmis.nc"	
Variable	Regional model name	'CMAQ'	CMAQ or WRFchem
Variable	Number of types of input emission file to combine. 4 lines below are repeated for each type.	1	
Variable	File path to date-independent directory containing regional model emissions files	"/home/CMAQ/Emissions"	
Variable	File name template for regional model emissions files	'%Y%M/cctm.%Y%M%D.nc'	
Variable	Number of hours in each regional model emissions file	24	
Variable	File path to emissions species map file[1]	PATH="/home/maqs/emSmp.csv"	Factors converting to $g/m^2/s$
Section keyword	Start of section containing the spatial and temporal domain to extract	RMEMISSIONSEXTENTS	
Variable	Start date-time	2018,01,01,01	
Variable	End date-time	2018,12,31,24	
Variable	Time difference between local solar and regional model times	1	
Variable	X coordinate of lower-left corner of emissions domain	11000	Coordinates in the projected coordinate system in units of m
Variable	Y coordinate of lower-left corner of emissions domain	-5000	
Variable	Number of cells to extract in x direction	10	
Variable	Number of cells to extract in y direction	10	
Variable	Number of layers to extract in z direction	5	

Table B.1 Specification of first two sections of elements which must be included in the input file for the **RM Emissions** utility. [1]The species map file format is defined in Section 4.3.1.

Element type	Description	Sample element	Comment
Section keyword	Start of section containing coordinate datum definition	RMCOORDINFO	Also used in **RM Met Data** and **RM Grid Info** utilities, must be included.
Variable	Datum type	'EMEPSPHERE'	Refer to **Table A.1** for details
Variable	Semi-major axis (m)	6378137.0	Only included if Datum type is 'CUSTOM'
Variable	Inverse flattening	298.257223563	
Section keyword	Start of section for specifying the file with vertical height information, which is required when the WRF-Chem regional model has been selected or processing CMAQ regional model files that use hybrid vertical coordinate system.	RMHEIGHTINFOFILE	Also used in the **RM Grid Info** utility
Variable	Whether specifying a single file path to the heights file or otherwise specifying the directory and file name template for the file	N	Y or N
Variable	File path to date-independent directory containing file with vertical height information	"/home/WRF/Output"	For alternate option of specifying a single file path, please refer to **Table A.2**.
Variable	File name template for the heights file	'%Y%M/cctm.%Y%M%D.nc'	

Table B.2 Specification of the remaining sections of elements which must be included in the input file for the **RM Emissions** utility.

Element type	Description	Sample element	Comment
Section keyword	Start of optional section containing advanced settings	ADVANCEDNESTING	May be omitted, must be included in full if required. Not relevant to WRF-Chem.
Variable	Whether to specify sea-level temperature	Y	Y or N
Variable	Average sea-level temperature in Kelvin	298	Only included if Y above, default value 288.15
Variable	Whether to override the model top pressure	Y	Y or N
Variable	Model top pressure in Pascals	5000	Only included if Y above, default to use the value from the regional model emissions files
Section keyword	Start of regional model surface layer height section	RMEMISSIONSSURFACEHEIGHT	
Variable	Whether to specify the top of the regional model surface layer as height or sigma value	HEIGHT	HEIGHT or SIGMA
Variable	Height or sigma value of the regional model surface layer	20.0	

Table B.3 Specification of optional elements which may be included in the input file for the **RM Emissions** utility

B.3 Command line structure

To run the **RM Emissions** utility from the command line or a script, the following syntax should be used:

```
<executable file path> <input text file path>
```

where `<executable file path>` is the full path to the utility executable (*.out*), enclosed in inverted commas, and `<input text file path>` is the full path to the input text file which contains the information required to run the executable, enclosed in inverted commas.

For example, if the executable is saved in the default installation directory, */disk/maqs/utils/*, and the input text file is saved as */home/user/maqs_work/Input.txt*, the command line to run the utility would be

```
'/disk/maqs/utils/RMEmissions.out' '/home/user/maqs_work/Input.txt'
```

B.4 Utility outputs

The **RM Emissions** utility writes output emissions to a netCDF (*.nc*) file which follows the generic 3D grid emissions file conventions, as described in full in Section 4.4.6. This utility will always create a new *.nc* file - it will stop with an error if an existing file is found with the same file path as specified for the output file, so it will not overwrite or append to an existing file.

The Global 'History' attribute value contains details of the **RM Emissions** utility run. The emissions species datasets are defined according to the local model species listed in the species map file. The netCDF data contents can be viewed and processed using standard viewers which support CF-compliant netCDF files, such as Panoply (https://www.giss.nasa.gov/tools/panoply/).

Any error or warning messages are written to *Error.txt* or *Warning.txt* text files in the same directory as the input text file. Error messages relate to problems which cause the program to fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.

APPENDIX C Create ASP utility

The **Create ASP** utility is a command line application which defines the locations of the points at which concentration values will be calculated and generates an *.asp* file containing the output points, when running the system to produce regular gridded output for contours. The points can include any combination of a 2- or 3-D regular grid of receptors covering the whole nesting domain, source-oriented grid points and/or receptor locations, as specified by the user. This utility was developed for the MAQS coupled system but may also be used as standalone utility for generating *.asp* files for local model runs that require the same set of output points. It has similar functionality to running ADMS-Urban in **Create ASP** mode, as described in Section 8.4.1.

C.1 Generation of output points

The coupled system output can be set to be at specific receptor locations or a regular grid for contouring. There are three different types of output points:

- Receptor locations specified by the user via text file input coordinates (x, y, z in projected coordinates);
- A 3D regular grid of receptors covering the nesting domain, typically at a vertical height above ground less than the height of the lowest layer of the regional model grid; and
- Extra receptor points in and around roads that are required in order to resolve the high concentration gradients close to roads. The location of these extra receptor points is dependent on the road width and (if applicable) canyon width. The user can alter some parameters controlling the locations of these points relative to the road geometry, as described in Section 4.7.9.

The user must specify parameters relating to the output grid extent, in addition to the road source data, including geographical locations. The **Create ASP** utility writes an *.asp* file which includes all the output locations above.

The resolution of the output grid must be higher than the regional model grid, taking into account that the maximum number of points in each horizontal direction is 2001 points, with up to 501 vertical levels. Care should be taken with high-resolution output grids since the local model run time and memory requirements partly depend on the number of receptor points.

If the automatic method is used to generate the source-oriented grid points, the MAQS coupled system, via the **AddInterpIGP** utility, will also add further along-road receptor locations at which concentrations are interpolated from the locations with model calculations, to increase spatial resolution in the final output without excessively increasing run times.

The naming conventions used by the utility are as follows:

- Any user-defined specified output points retain their original names.
- The regular grid points are given names which indicate their type and their position in the regular grid point sequence, for example |G|0000001 for the bottom left hand corner of the grid.

- The primary source-oriented grid points for road sources ('intelligent' grid points) are given names which indicate their type and their 'pairing' to another point for the purposes of interpolating secondary source-oriented grid points, for example |I|000001_P000005 for the first primary source-oriented grid point, which forms a pair with the fifth primary source-oriented grid point. If the user has specified to omit interpolation points, the 'pairing' information will not be included in the names given to the primary source-oriented grid points.

C.2 Input file format

The input file for the **Create ASP** utility is a text file which can contain one section of data or more. There are five additional sections that are optional, including advanced parameters for setting up source-oriented grid points. The version string must be the first line in the file, following which the sections may be listed in any order but the order of the variables within each section must be as defined in the tables below. Each element should be given on a new line, blank lines may be included before each section keyword but not within a section. An example input file is shown in **Figure C.1**.

CreateAsp.txt

```
CREATEASPINPUTVERSION1

REGULARGRID
-796617
-791717
50
465050
468283.3
31
0
0
1

SPECIFIEDPOINTS
PATH="/home/CERC/maqs/Data/receptors.asp"

ROADDATA
PATH="/home/CERC/maqs/Data/roads.rdi"
PATH="/home/CERC/maqs/Data/roads.rdg"

IGPACROSSLOCATIONS
1
0.45
1
N
1.0

IGPALONGLOCATIONS
1000
0.5
0.0
Y

```

Figure C.1 Example input file for the **Create ASP** utility

Element type	Description	Sample element	Comment
Version string	File version description	CREATEASPINPUTVERSION 1	Must be the first line of the file
Section keyword	Start of section containing the extents of the output regular grid	REGULARGRID	
Variable	X coordinate of lower-left corner of output grid	11100.00	Coordinates in the projected coordinate system in units of m; similar for Y
Variable	X coordinate of upper-right corner of output grid	20900.00	
Variable	Number of grid points in X direction	99	
Variable	Y coordinate of lower-left corner of output grid	-4900.00	
Variable	Y coordinate of upper-right corner of output grid	900.00	
Variable	Number of grid points in Y direction	59	
Variable	Z coordinate of surface level of output grid	0.0	Height above ground in units of m
Variable	Z coordinate of top of output grid	0.0	Use same value as above for a 2D grid
Variable	Number of grid points in Z direction	1	

Table C.1 Specification of compulsory elements of the input file format for the **Create ASP** utility

Element type	Description	Sample element	Comment
Section keyword	Start of optional section containing the path to receptor locations file	SPECIFIEDPOINTS	Additional user-specified points to include in output
Variable	File path to receptor locations file	PATH=”/disk/maqs/receptors.asp”	
Section keyword	Start of optional section containing the paths to road data files	ROADDATA	Must be included to generate source-oriented grid points
Variable	File path to road info file	PATH=”/disk/maqs/roads.rdi”	
Variable	File path to road geometry file	PATH=”/disk/maqs/roads.rdg”	
Section keyword	Start of optional section containing parameters for source-oriented grid points across-source locations	IGPACROSSLOCATIONS	
Variable	Whether specifying parameters for across-source locations for standard (non-canyon) roads	Y	Y or N
Variable	Number of points on each side of roads. 3 lines below are repeated for each row of points.	2	Only included if Y above
Variable	Perpendicular distance for this row of points	0.45	
Variable	Unit of distance	1	
Variable	Whether to remove this row of points if within 1 m of the previous row	Y	Y or N
Variable	Whether specifying parameters for across-source locations for canyon sources	Y	Y or N
Variable	Number of points on each side of canyons. 3 lines below are repeated for each row of points.	2	Only included if Y above
Variable	Perpendicular distance for this row of points	0.45	
Variable	Unit of distance	1	
Variable	Whether to remove this row of points if within 1 m of the previous row	Y	Y or N
Variable	Minimum separation between points	1	Default value 1 m

Element type	Description	Sample element	Comment
Section keyword	Start of optional section containing parameters for source-oriented grid points along-source locations	IGPALONGLOCATIONS	
Variable	Guideline total number of points to add along road sources	5000000	
Variable	Minimum spacing expressed as a percentage of the grid length	0.1	
Variable	Absolute spacing between each pair of points	60	
Variable	Whether to add interpolation points between each pair of points	Y	Y or N
Section keyword	Start of optional section for specifying which sources will have source-oriented grid points	IGPINCLUDESOURCES	
Variable	Whether to add points to 'all but' or 'only' the road sources listed	2	1 to add points to all road sources except those listed, or 2 to add points to only the road sources in the list
Variable	Number of road sources in the list	2	
Variable	Names of each road source given on a new line	Road1	

Table C.2 Specification of optional elements of the input file format for the **Create ASP** utility

C.3 Command line structure

To run the **Create ASP** utility from the command line or a script, the following syntax should be used:

```
<executable file path> <input text file path>
```

where `<executable file path>` is the full path to the utility executable (*.out*), enclosed in inverted commas, and `<input text file path>` is the full path to the input text file which contains the information required to run the executable, enclosed in inverted commas.

For example, if the executable is saved in the default installation directory, */disk/maqs/utils/*, and the input text file is saved as */home/user/maqs_work/CreateAsp.txt*, the command line to run the utility would be

```
'/disk/maqs/utils/CreateASP.out' '/home/user/maqs_work/CreateAsp.txt'
```

C.4 Utility outputs

The **Create ASP** utility creates an *.asp* file containing the list of output points at which the MAQS coupled system modelled output will be calculated by the local model. By default a new file will be created with the same file stem and location as the input text file, i.e. existing files will be overwritten. The beginning of an example *.asp* file generated by the utility is shown in **Figure C.2**.

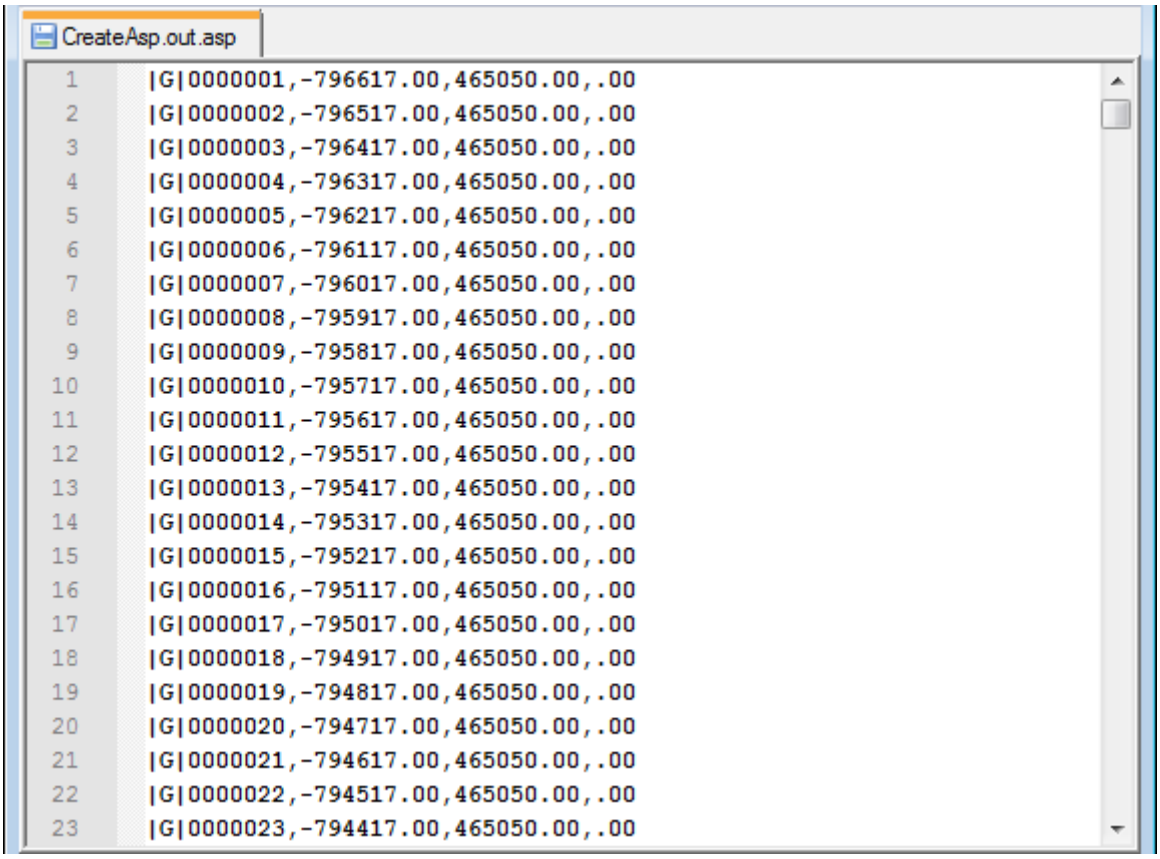


Figure C.2 Example output text file from the **Create ASP** utility

Any error or warning messages are written to text files with the same file stem and directory as the input text file but with the *.err* and *.wng* extensions, respectively. Error messages relate to problems which cause the program to fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.

APPENDIX D RM Met Data utility

The **RM Met Data** utility is a command line application which extracts meteorological data from WRF model output or generic 2D netCDF files and creates ADMS format *.met* files. It was developed for the MAQS coupled system but may also be useful for generating *.met* files for stand-alone local model runs. Please refer to the WRF model documentation (Skamarock et al., 2008) for details of the WRF variables and output file format. The generic 2D meteorological data file format is defined in Section 4.2.3.

D.1 Data requirements

The meteorological model output files must have file names and/or directory structures which indicate the date and time of the first hour of data they contain. This enables the utility to generate the file path for the file containing a specific hour of data from the supplied templates. The period over which meteorological data is required may span many files, but they should all have the same file-name pattern, differing only in date and time values.

The met output files must contain at least the following attributes or variables:

- Latitude and Longitude;
- Map projection type;
- Simulation start time;
- Wind speeds at 10 m (U10, V10);
- Temperature at 2 m; and
- Surface sensible heat flux.

If using WRF output files, additional options are available to use the following variables:

- Wind speeds at 10 m (U10, V10) or at grid heights; and if the latter, also terrain heights, base-state and perturbation geopotentials; and
- At least one of incoming solar radiation and surface sensible heat flux.

Some other requirements depend on the type of coordinates used to specify the location at which meteorological data should be extracted from met output: if grid indices are used, no additional information is required and no additional restrictions are applied to the choice of coordinate system. If lat-long or projected coordinates are used, the following additional requirements apply:

- The map projection type must be Lambert Conformal Conic, Polar Stereographic or Universal Transverse Mercator;
- The appropriate parameters for a full definition of the projected coordinate system must be present as attributes.
- The underlying coordinate datum for the projected coordinate system must be defined in the utility input file.

If OSGB-36 coordinates are used with WRF output files, the additional requirements above apply. Input projected coordinates (easting and northing values in m) are first converted to latitude and longitude values in decimal degrees, using the Airy 1830 ellipsoid. The calculations were based on the 2020 edition of the Ordnance Survey document A Guide to Coordinate Systems in Great Britain (Annexes A.1 and C). If used with generic 2D format files, the utility assumes that the coordinates are in the same projected coordinate system.

D.2 Processing assumptions

The meteorological data saved to WRF output files is instantaneous, giving a snapshot of the meteorological conditions at that particular time. For the purposes of using WRF data in the local model, it is assumed to represent the overall met conditions for the previous hour, hence matching the hour-ending ADMS convention.

The **RM Met Data** utility will extract data from the lowest grid layer if the U10, V10 option for wind speeds is not selected, otherwise the wind speed and direction will be extracted from the values at 10 m. The height at which the wind speed was extracted is written to the header of the *.met* output file. At present the utility does not create a profile file containing meteorological data at multiple heights.

The **RM Met Data** utility extracts most WRF variables with the assumption that their units in WRF are the same as those required by the local model, so does not perform any unit conversions, except for temperature where a conversion from Kelvin to Celsius is required. The units assumed in WRF and required in ADMS for the variables extracted by the **RM Met Data** utility are listed in **Table D.1**. The variables listed below the thicker black line in the table are relevant only if extracting from WRF output files for use in ADMS-Urban.

WRF met variable	WRF unit assumed	ADMS met file unit
Wind speeds	ms^{-1}	ms^{-1}
Temperature (2m)	K	°C
Surface sensible heat flux	Wm^{-2}	Wm^{-2}
Boundary layer depth	m	m
Solar radiation	Wm^{-2}	Wm^{-2}
Precipitation	mm (cumulative)	mm (per hour)
Heights	m	m
Geopotentials	m^2s^{-2}	m^2s^{-2}

Table D.1 The units used in the local model and assumed for WRF output files for selected meteorological variables

*Precipitation rates are only used by ADMS-Urban if wet deposition calculations are required. The precipitation variables in WRF store cumulative values of precipitation, whereas ADMS uses hourly rates of precipitation. The **RM Met Data** utility converts WRF precipitation to hourly rates by subtracting the previous hour's cumulative precipitation from the current hour. This requires all WRF files to be derived from the same WRF run, and for one hour of data to be available immediately before the first extracted hour.*

*Generic 2D met files may also contain cloud cover data. The values are expressed as a dimensionless fraction. The **RM Met Data** utility converts the values to oktas as required by ADMS-Local.*

D.3 Input file format

The input file for the **RM Met Data** utility is a text file which contains a version string, four sections of data that are compulsory and four optional sections. The compulsory sections are described in **Table D.2** and the optional sections in **Table D.3**. The version string must be the first line in the file, following which the sections may be listed in any order but the order of the variables within each section must be as defined in the tables below. Each element should be given on a new line, blank lines may be included before each section keyword but not within a section. An example file is shown in **Figure D.1**.

If using WRF output files, an additional input configuration file may be supplied to customise the names of WRF dimensions, attributes and variables to be extracted by the utility. This allows the user to specify the names if the files do not use default WRF names (shown in the example configuration file in **Figure D.2**). The file contains two sections. The start of a section is denoted by an ampersand ('&') and the section name, while the end of a section is denoted by a forward slash ('/'). Each variable within a section must be on a separate line, and text entries should be delimited by inverted commas (''). The sections must be listed in the order given below, but the variables within each section may be specified in any order.

The WRF_TableNames section contains information about the names of the WRF variables from which you wish to extract data. You do not have to include variable names for meteorological data you do not wish to extract. If a variable name for a variable you wish to extract does not exist in the WRF file then the utility will stop with an error. However, if a variable name for a variable which exists in the file but is not the intended variable is specified, the data values are within the valid ranges allowed by the local model and the variable dimensions are the same as those expected, the utility will extract the values from the named variable. Therefore it is important to ensure that the specified variable names correspond to the appropriate variables.

The WRF_DimAttNames section contains the names of the required WRF variables and attributes. All the entries in this section must be completed.

Tables D.4 to **D.5** list all the available options for each section in the WRF configuration file with descriptions and comments. An example file is shown in **Figure D.2**, and a default template is included in the MAQS Coupled System installation directory, by default *<install_path>/Data*.

If ADMS-Urban is the chosen local model and you wish to extract precipitation data from WRF, the WRF file including data for the hour before the specified extraction start time must be available and all of the WRF files must be output from the same WRF simulation. If the initial WRF file is missing, the utility run will stop with an error and no *.met* file will be created. If the WRF files are not all from the same WRF run a warning will be issued and a *.met* file will be created without precipitation data.

RMMetDataInput.txt

```
1   RMMETDATAINPUTVERSION1
2
3   RMMETINPUTS
4   'WRF'
5   2010,03,03, 9
6   71
7   "/home/CERC/maqs/Data/WRF"
8   '%Y%M/wrfout_d04_%Y-%M-%D_%h%m%s.nc'
9   1
10  8
11  2
12  -3500.000
13  -665000.000
14
15  RMMETOUTPUT
16  PATH="/home/CERC/maqs/working/C0C-4000.00C-665500.00/MetData.met"
17
18  RMMETVARIABLES
19  WIND10
20  Y
21  Y
22  Y
23  Y
24  N
25  N
26
27  RMCOORDINFO
28  'EMEPSPHERE'
29
```

Figure D.1 Example input file for the **RM Met Data** utility

Element type	Description	Sample element	Comment
Version string	File version description	RMMETDATAINPUTVERSION1	Must be the first line of the file
Section keyword	Start of section containing regional model file information	RMMETINPUTS	
Variable	Regional model name	'WRF'	WRF or Generic
Variable	Start date-time	2018,01,01,01	
Variable	Number of hours to be extracted	24	
Variable	File path to date-independent directory containing regional model output file	"/disk/WRF/Output"	
Variable	File name template for regional model output files	'%Y%M/cctm.%Y%M%D.nc'	
Variable	Number of hours in each regional model output file	1	
Variable	Time difference between local solar and regional model times	5	
Variable	Flag which identifies the form of the input coordinates	2	One of the following should be specified: • 0 to use grid indices • 1 to use lat-long in decimal degrees • 2 to use projected coordinates in m • 3 to use OSGB-36 coordinates in m
Variable	X coordinate of the point or index of the grid for which met data will be extracted	-795834.155	Coordinates in the system and units selected above
Variable	Y coordinate of the point or index of the grid for which met data will be extracted	465833.560	
Section keyword	Start of section containing output meteorological data file information	RMMETOUTPUT	
Variable	File path to the output meteorological data file	PATH= "/disk/maqs/WRFmet.met"	

Element type	Description	Sample element	Comment
Section keyword	Start of section containing information about which meteorological variables will be extracted	RMMETVARIABLES	
Variable	Whether to extract wind speed and direction from the values at 10 m or from the lowest grid layer data	WIND10	WIND10 or WINDHGTS
Variable	Whether to extract values of temperature at 2 m	Y	Y or N
Variable	Whether to extract values of boundary layer height	Y	Y or N
Variable	Whether to extract values of incoming solar radiation	Y	Y or N
Variable	Whether to extract values of surface sensible heat flux	Y	Y or N
Variable	Whether to extract values of precipitation	Y	Y or N
Variable	Whether to extract values of cloud cover	Y	Y or N
Section keyword	Start of section containing coordinate datum definition	RMCOORDINFO	Also used in **RM Grid Info** and **RM Emissions** utilities, must be included
Variable	Datum type	EMEPSPHERE	EMEPSPHERE, WGS84 or CUSTOM
Variable	Semi-major axis (m)	6378137.0	Only included if datum type above is 'CUSTOM'. Special inverse flattening value of 0 used to indicate sphere.
Variable	Inverse flattening	298.257223563	

Table D.2 Specification of compulsory elements of the input file format for the **RM Met Data** utility

Element type	Description	Sample element	Comment
Section keyword	Start of section containing the file path to the WRF configuration file	WRFDEFFILE	
Variable	File path to the WRF configuration file	PATH='disk/maqs/Data/WRF_Config.txt'	Refer to **Tables D.4** and **D.5** for details
Section keyword	Start of section containing the minimum wind speed setting	U10MINUSERDEF	
Variable	Minimum wind speed (m/s)	0.3	Ensures that the local model will treat low wind speeds as valid
Section keyword	Start of section containing the flag for amending the sensible surface heat flux	AMENDHEATFLUX	
Variable	Whether to shift invalid values to within valid range (-200 to 1000 W/m^2) to avoid errors in the local model	Y	Y or N
Section keyword	Start of section containing the flag for stopping the run with invalid values	STOPIFINVALID	
Variable	Whether to stop the run if any of the extracted values are invalid; otherwise, write -999 to the met file	Y	Y or N

Table D.3 Specification of optional elements of the input file format for the **RM Met Data** utility

WRF_Config.txt

```
&WRF_TableNames
  WRF_Name_WindU10 = 'U10',
  WRF_Name_WindV10 = 'V10',
  WRF_Name_WindU = 'U',
  WRF_Name_WindV = 'V',
  WRF_Name_TerrHgt = 'HGT'
  WRF_Name_GeopotBase = 'PHB'
  WRF_Name_GeopotPert = 'PH'
  WRF_Name_TempT2 = 'T2',
  WRF_Name_BLayerHgt = 'PBLH',
  WRF_Name_SolarRad = 'SWDOWN',
  WRF_Name_HeatFlux = 'HFX',
  WRF_Name_CumRain = 'RAINC',
  WRF_Name_GridRain = 'RAINNC'
/

&WRF_DimAttNames
  WRF_DimAttName_EastWest = 'west_east',
  WRF_DimAttName_NorthSouth = 'south_north',
  WRF_DimAttName_BottomTop = 'bottom_top',
  WRF_DimAttName_TimeDim = 'Time',
  WRF_DimAttName_Longitude = 'XLONG',
  WRF_DimAttName_Latitude = 'XLAT',
  WRF_DimAttName_Times = 'Times',
  WRF_DimAttName_MapProj = 'MAP_PROJ',
  WRF_DimAttName_RefLong = 'STAND_LON',
  WRF_DimAttName_RefLat = 'MOAD_CEN_LAT',
  WRF_DimAttName_StdPar1 = 'TRUELAT1',
  WRF_DimAttName_StdPar2 = 'TRUELAT2',
  WRF_DimAttName_SimStartTime = 'SIMULATION_START_DATE'
/

```

Figure D.2 Example WRF configuration file

Variable name	Required	Description	Comment
WRF_Name_WindU10	Y	WRF variable name for West-East wind speeds at 10 m above ground	
WRF_Name_WindV10	Y	WRF variable name for South-North wind speeds at 10 m above ground	
WRF_Name_WindU	Y	WRF variable name for West-East wind speeds at all heights	
WRF_Name_WindV	Y	WRF variable name for South-North wind speeds at all heights	
WRF_Name_TerrHgt	Y	WRF variable name for terrain heights	
WRF_Name_GeopotBase	Y	WRF variable name for base-state geopotentials	
WRF_Name_GeopotPert	Y	WRF variable name for perturbation geopotentials	
WRF_Name_TempT2	Y	WRF variable name for temperature at 2 m	
WRF_Name_BLayerHgt	Y	WRF variable name for boundary layer height	
WRF_Name_SolarRad	Y	WRF variable name for incoming solar radiation	
WRF_Name_HeatFlux	Y	WRF variable name for surface sensible heat flux	
WRF_Name_CumRain	Y	WRF variable name for cumulative cumulus (sub-grid scale) precipitation	
WRF_Name_GridRain	Y	WRF variable name for cumulative grid-scale precipitation	

Table D.4 Variables in the WRF_TableNames section of the WRF configuration file

Variable name	Required	Description	Comment
WRF_DimAttName_EastWest	Y	WRF East-West dimension name	
WRF_DimAttName_NorthSouth	Y	WRF North-South dimension name	
WRF_DimAttName_BottomTop	Y	WRF vertical dimension name	
WRF_DimAttName_TimeDim	Y	WRF time dimension name	Time dimension: number of time-steps included in the file
WRF_DimAttName_Longitude	Y	WRF Longitude variable name	
WRF_DimAttName_Latitude	Y	WRF Latitude variable name	
WRF_DimAttName_Times	Y	WRF Time variable name	Time variable: value of date/time at each time-step
WRF_DimAttName_MapProj	*Y*	WRF map projection attribute name	
WRF_DimAttName_RefLong	*Y*	WRF reference longitude attribute name	Parameters used to describe the map projection for coordinate transformations
WRF_DimAttName_RefLat	*Y (LCC)*	WRF reference latitude attribute name	
WRF_DimAttName_StdPar1	*Y*	WRF first standard parallel attribute name	
WRF_DimAttName_StdPar2	*Y (LCC)*	WRF first standard parallel attribute name	
WRF_DimAttName_SimStartTime	Y	WRF simulation start time attribute name	

Table D.5 Variables in the WRF_DimAttNames section of the WRFconfiguration file. The map projection attributes are only required if latitude-longitude or projected coordinates are used for specifying the input location. (LCC) in the 'Required' column indicates that this parameter is only required for the Lambert Conformal Conic projection.

D.4 Command line structure

To run the **RM Met Data** utility from the command line or a script, the following syntax should be used:

```
<executable file path> <input text file path>
```

where `<executable file path>` is the full path to the utility executable (*.out*), enclosed in inverted commas, and `<input text file path>` is the full path to the input text file which contains the information required to run the executable, also enclosed in inverted commas.

For example, if the executable is saved in the default installation directory, */disk/maqs/utils/*, and the input text file is saved as */home/user/maqs_work/RMMetInput.txt*, the command line to

run the utility would be

```
'/disk/maqs/utils/RMMetData.out' '/home/user/maqs_work/RMMetInput.txt'
```

D.5 Utility outputs

The **RM Met Data** utility creates a single ADMS format *.met* meteorological data file containing the variables selected in the input file over the period specified in the command line, from all the relevant meteorological model output files. The utility will create a new file or overwrite any existing file which is located in the same directory and has the same name. It does not append data to an existing *.met* file.

A header section indicates when the file was created, the location where the meteorological data was extracted in the input location specification (projected or longitude/latitude coordinates) and grid index values, and the height corresponding to the wind speed and direction values. An example output file created by the **RM Met Data** utility is shown in **Figure D.3**.

Any error or warning messages are written to *Error.txt* or *Warning.txt* text files in the same directory as the utility executable and input file. Error messages relate to problems which cause the program to fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.

MetData.met

```
1  ====================================================
2  File created by MAQS RMMetData
3  Date/time created:   18/05/2023 13:04:11
4  Model Version:     1.0
5  Model Revision:    8964
6  Location input for met data extraction (x, y): (-3500.00,-665000.00)
7  Met. data created for location with grid index (2,2)
8  Data created from RM directory: /home/CERC/maqs/Data/WRF
9  The height of the recorded wind is 10.0 m.
10 The met. data are hourly sequential.
11 ====================================================
12
13 VARIABLES:
14 10
15 YEAR
16 DAY
17 HOUR
18 U
19 PHI
20 T0C
21 H
22 SOLAR RAD
23 FTHETA0
24 U10MIN
25
26 DATA:
27 2010, 62,  9,   5.01, 153.2,  23.49,   454.6,   490.1,   159.6,  0.30
28 2010, 62, 10,   4.42, 137.3,  23.97,   650.0,   462.0,   190.2,  0.30
29 2010, 62, 11,   4.99, 144.7,  24.40,   792.3,   837.0,   356.4,  0.30
30 2010, 62, 12,   5.61, 140.9,  24.58,   876.7,   799.3,   404.4,  0.30
31 2010, 62, 13,   5.99, 143.8,  24.73,   802.0,   908.2,   472.8,  0.30
32 2010, 62, 14,   5.96, 145.8,  24.62,   783.6,   731.7,   418.0,  0.30
```

Figure D.3 Example *.met* file produced by the **RM Met Data** utility, viewed in Notepad++

APPENDIX E Core MAQS coupled system Processor utility

The **Processor** utility is a command line application which carries out the core processing in the MAQS coupled system. It has three modes:

- to calculate local upwind background concentrations, defined as an angular average of concentrations from cells immediately upwind of the area of interest, written to an ADMS format background data (*.bgd*) file;
- to calculate in-cell background concentrations, which represent the concentration in the area of interest during the modelling time, written to an ADMS format background data (*.bgd*) file; and
- to calculate in-cell output concentrations from ADMS and regional model outputs, written to an ADMS format netCDF (*.nc*) file.

The utility was developed for use in the MAQS coupled system, but the local upwind background mode may also be useful for stand-alone local model runs if rural monitoring data are not available outside the modelling area. Within the MAQS coupled system, the **Processor** utility is run separately for each regional model cell included in a larger nesting domain, but for a stand-alone utility run it could be used with a domain covering multiple regional model cells.

The **Processor** utility is able to read concentrations from regional model output files from the CMAQ, CAMx (converted into I/O API format), EMEP4UK, WRF-Chem and CHIMERE models. Defra's 1 km resolution background map files must be converted to generic 2D average netCDF file format, for example using the **RM Grid Info** utility, before they can be used as input to the **Processor** utility. Output from any other model can be used by re-gridding and re-formatting the data into the generic 3D hourly or 2D average concentration data file formats. Alternatively, if the regional model concentration data can be manipulated to comply with the Models-3 I/O API netCDF Gridded file conventions (Coats, 2004), these data can also be used by selecting the CMAQ option.

E.1 Calculation of local upwind background

The local upwind background mode of the **Processor** utility is illustrated in **Figure E.1**. The utility interpolates between concentrations found at the centres of two regional model cells immediately outside the current grid cell (indicated as 'nesting domain') and lying on each side of a line running upwind from the centre of the nesting domain, with weighting dependent on the wind direction.

The regional model concentrations will always be extracted from the lowest vertical layer of the regional model grid. The processing domain must be entirely within the regional model horizontal grid extent, with a border of at least one cell in each direction, to allow the adjacent upwind cells to be used.

The utility uses a species map to convert from regional model chemical species to the local model chemical species, please refer to Section 4.3.1 for more details of the species map concept and format. The output *.bgd* file concentration units are always written as `ug/m3` so the species map factors must include a conversion from regional model units to µg/m^3, if required.

The utility reads an ADMS-format *.met* file to identify the wind direction for each hour in order to find the upwind cells. The *.met* file must include year, day, hour and wind direction variables, with any of the permitted ADMS variable names, and should be in local time.

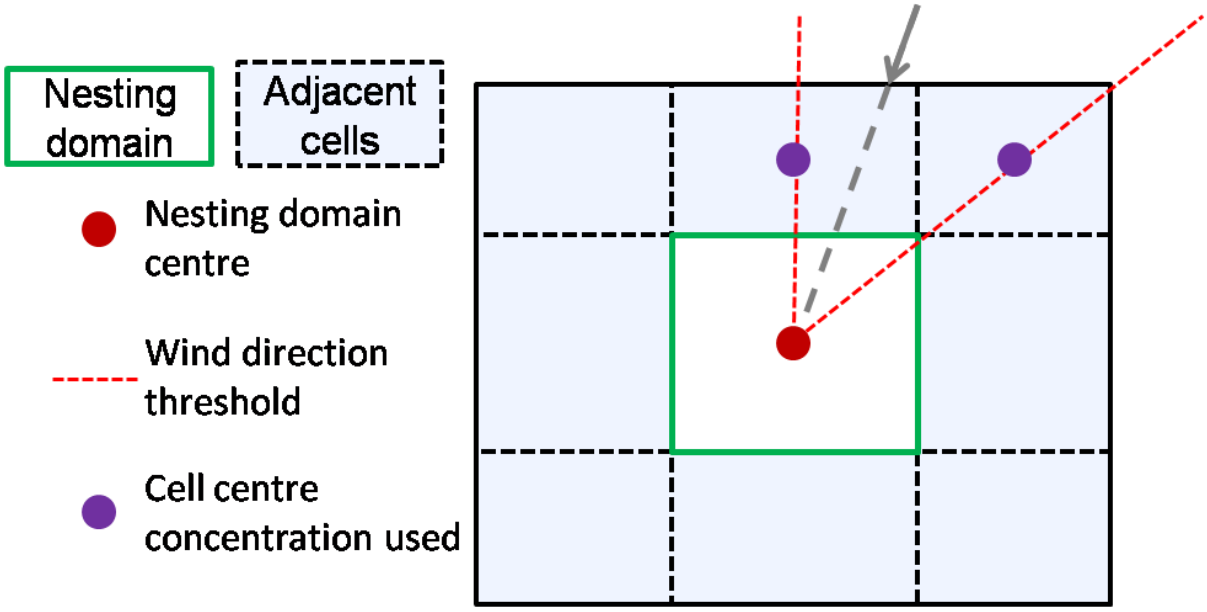


Figure E.1 Diagram of the local upwind background mode of the **Processor** utility. The output background concentration is interpolated between the upwind cell concentrations according to the wind direction.

E.2 In-cell background concentrations

The in-cell background concentrations mode of the **Processor** utility calculates background concentrations for the current grid cell, defined as:

$$\begin{aligned}\text{In-cell background} &= \text{RM}(0:t) \\ &- \left[\text{local modelled grid}\left(t-\frac{1}{2}:t\right) - \text{local upwind background}\right]\end{aligned}$$

where:

- 'RM' is the average regional model concentration in the lowest layer from the current grid cell;
- 'local modelled grid $\left(t-\frac{1}{2}:t\right)$' is the output concentration from the local model run with gridded emissions matching the regional model emissions and dispersion truncated at half an hour (Step 7 in the description of the MAQS coupled system procedures in Section 8.2); and

- 'local upwind background' is the background concentration calculated in the previous section.

This in-cell background represents the regional model (RM) concentration in the nesting domain throughout the mixing time by using the instantaneous value estimated at the middle of the mixing time.

For runs using annual average regional model concentration data, annual average in-cell background concentrations are calculated as follows:

$$\text{In-cell background}(aave) = \text{RM}(aave) - \text{ local modelled grid}\left(aave, t - \frac{1}{2} : t\right)$$

where:

- 'RM($aave$)' is the annual average regional model concentration in the lowest layer from the current grid cell; and
- 'local modelled grid $\left(aave, t - \frac{1}{2} : t\right)$' is the annual average output concentration from the local model run with the explicit local emissions aggregated to grid source(s) and dispersion truncated at half an hour.

The utility reads the local upwind *.bgd* file and the *.nc* (Comprehensive Output File version 2.0) file output from the initial local model run with gridded emissions. Both are required to contain concentrations in µg/m^3 units for the ADMS species listed in the species map file. The output *.bgd* file concentration units are always written as `ug/m3` so the species map factors must include a conversion from regional model units to µg/m^3, if required.

The local model output *.nc* file can include one or more receptors within the nesting domain. If more than one receptor is located in the nesting domain and listed in the input file, the *.nc* concentrations from all the listed receptors are averaged when calculating the in-cell background concentrations. When used in the MAQS coupled system, the *.nc* file is expected to include one receptor in the centre of each regional model grid cell, set by the *.asp* file created by the **RM Grid Info** utility, but the MAQS coupled system control scripts will include any receptors found within the cell.

If the nesting domain includes multiple regional model cells, the concentrations from each cell included in the nesting domain are averaged when calculating the in-cell background concentrations.

If a negative in-cell background concentration is calculated for any local model species at any hour, the output background concentration of that species is set to zero for that hour. The total number of hours with negative in-cell background concentrations for any pollutant is written to a warning file at the end of the utility run. If the number of hours with negative in-cell background is greater than 1% of the total number of hours included in the run, this may indicate a discrepancy in magnitude and/or time-variation between the regional and local model emissions, which should be investigated.

E.3 In-cell output concentrations

The **Processor** utility calculates the final hourly in-cell output concentrations, defined as follows:

$$C_N(t, \boldsymbol{X}_{OP}) = [\boldsymbol{S}]C_{RM}(t, \boldsymbol{I}_{OP}) + C_{ADMS_{Ei}}(t, \boldsymbol{X}_{OP}) - C_{ADMS_{Gi}}(t, \boldsymbol{X}_{OP})$$

where:

- $C_N(t, \boldsymbol{X}_{OP})$ is the coupled system output concentration at time t (hours) and output location $\boldsymbol{X}_{OP}$;
- $C_{RM}(t, \boldsymbol{I}_{OP})$ is the regional model concentration at time t and cell $\boldsymbol{I}_{OP}$ containing the output location $\boldsymbol{X}_{OP}$;
- $[\boldsymbol{S}]$ is the species map matrix used to convert from regional model to local model speciation and units;
- $C_{ADMS_{Ei}}(t, \boldsymbol{X}_{OP})$ is the local model output concentration including both gridded and explicit emissions at time t and output point location $\boldsymbol{X}_{OP}$; and
- $C_{ADMS_{Gi}}(t, \boldsymbol{X}_{OP})$ is the local model output concentration including gridded total emissions at time t and output point location $\boldsymbol{X}_{OP}$.

The final annual average in-cell output concentrations are calculated by the **Processor** utility as follows:

$$\begin{aligned} C_N(aave, \boldsymbol{X}_{OP}) \\ &= [\boldsymbol{S}]C_{RM}(aave, \boldsymbol{I}_{OP}) + C_{ADMS_{Ei}}(aave, \boldsymbol{X}_{OP}) - C_{bgd,eq}(aave, \boldsymbol{I}_{OP}) \\ &\quad - C_{ADMS_{Gi}}(aave, \boldsymbol{X}_{OP}) \end{aligned}$$

where:

- $C_N(aave, \boldsymbol{X}_{OP})$ is the coupled system annual average output concentration at output location $\boldsymbol{X}_{OP}$;
- $C_{RM}(aave, \boldsymbol{I}_{OP})$ is the regional model annual average output concentration at the cell $\boldsymbol{I}_{OP}$ containing the output location $\boldsymbol{X}_{OP}$;
- $[\boldsymbol{S}]$ is the species map matrix used to convert from regional model to local model speciation and units;
- $C_{ADMS_{Ei}}(aave, \boldsymbol{X}_{OP})$ is the local model annual average output concentration from the run with explicit emissions and local background at output point location $\boldsymbol{X}_{OP}$;
- $C_{bgd,eq}(aave, \boldsymbol{I}_{OP})$ is the annual average local background concentration, including adjustments for NO_X, NO_2 and O_3 equilibrium as applied in the local model, in the cell $\boldsymbol{I}_{OP}$ containing the output location $\boldsymbol{X}_{OP}$; and
- $C_{ADMS_{Gi}}(aave, \boldsymbol{X}_{OP})$ is the local model output concentration including gridded total emissions at time t and output point location $\boldsymbol{X}_{OP}$.

There is a user option to interpolate the regional model concentrations, such that $C_{RM}(t, \boldsymbol{I}_{OP})$ or $C_{RM}(aave, \boldsymbol{I}_{OP})$ will be replaced by a bilinear interpolation of concentrations from the four regional model cell centres surrounding the output point location. This requires regional model data to be available for cells neighbouring the overall output domain, as for the local upwind

background mode.

The local model concentrations are read from ADMS Comprehensive Output Files (version 2.0, netCDF format) and the calculated nested concentrations are written to a new netCDF file in the same format. The local model concentration datasets are required to have units of $\mu g/m^3$.

All the local model output files are required to contain the same output locations in the same order. This is usually achieved by using the same *.asp* file to specify output point locations for all runs. The horizontal extents of the nesting domain are calculated based on the output locations contained in the local model files. The vertical layer of the regional model grid matching each output location is determined relative to the list of regional model layer boundary heights in the **RM Grid Info** output file. All output locations must be within the horizontal and vertical extents of the regional model grid, and are not required to form a rectangular area.

If ADMS-Urban is selected as the local model, the utility will use concentrations only from the first group found in the Comprehensive Output File, which will be the 'All sources' group. Any non-concentration datasets in the input ADMS-Urban files, for example deposition rates, will be ignored by the utility.

E.4 Input file format

The input file for the **Processor** utility is a text file which contains a version string and at least three sections of data. The first two sections, whose elements are defined in **Table E.1** are common to all modes of the program. The third section, whose elements are defined in **Table E.2**, is required for both the local upwind background and in-cell background modes. The fourth section, with elements defined in **Table E.3**, contains elements only applicable to the in-cell output mode. The keyword and contents of the last section, defined in **Table E.4**, control which mode of the program will be run. The order of the sections and the variables within each section must be as defined in **Tables E.1** to **E.4**. Each element should be given on a new line; blank lines may be included before each section keyword but not within a section. An example input file is shown in **Figure E.2**.

When the **Processor** utility is running in local upwind or in-cell background modes, the required nesting domain must be defined in the input text file. The nesting domain should cover a whole number of regional model grid cells to within a tolerance of 10% of the regional model grid spacing. The nesting domain may cover any rectangular area of grid cells, it is not required to be square. When the utility is running in in-cell output mode the output domain is determined from locations in the local model output files.

Element type	Description	Example entry	Comment
Version string	File version description	PROCESSORINPUTVERSION1	Must be the first line of the file
Section keyword	Start of section containing variables common to all modes	REGIONALMODEL	Also used in the **RM Grid Info** utility, must be included
Variable	Regional model name	CMAQ	CMAQ, EMEP4UK, CHIMERE, WRFChem, GenericHourly or GenericAverage
Variable	Start date-time	2010,01,01,01	format YYYY, MM, DD, HH (year, month, day of month, hour)
Variable	End date-time	2010,12,31,24	
Variable	File path to species map file	PATH="/home/maqsinputs/SpecMap.csv"	Refer to Section 4.3.1 for details of the species map file format
Variable	File path to date-independent directory containing regional model output file	"/home/CMAQ/Output"	
Variable	File name template for regional model output files	'%Y%M/cctm.%Y%M%D.nc'	Refer to Section 4.2.1 for details of the file name template tags
Variable	Number of hours in each regional model output file	24	
Variable	Time difference between local solar time and regional model time	1	Time difference in whole hours, can be positive or negative
Section keyword	Start of section for regional model grid information file	GRIDINFO	Must be included
Variable	File path to grid information file	PATH="/home/maqsworking/GridInfo.txt"	Output file from **RM Grid Info** utility, containing regional model horizontal and vertical grid definition. Refer to Section A.6 for details of the grid information file format.

Table E.1 Specification of compulsory elements of the input text file for the **Processor** utility that are shared by other utilities

Element type	Description	Example entry	Comment
Section keyword	Start of section defining nesting domain	NESTINGDOMAIN	Must be included
Variable	Type of nesting domain definition	INDICES	COORDS or INDICES
Variable	Lower left x coordinate (m)	18000.00	Included if the nesting domain type is COORDS
Variable	Lower left y coordinate (m)	-676500.00	
Variable	Upper right x coordinate (m)	19000.00	
Variable	Upper right y coordinate (m)	-675500.00	
Variable	Lower left cell x index (column)	10	Included if the nesting domain type is INDICES
Variable	Upper right cell x index (column)	11	
Variable	Lower left cell y index (row)	15	
Variable	Upper right cell y index (row)	15	
Variable	Index of the grid layer nearest to the ground	1	

Table E.2 Specification of elements of the input text file format for the **Processor** utility that are compulsory for the local upwind background and in-cell background modes.

Element type	Description	Sample element	Comment
Section keyword	Start of optional section containing advanced settings	ADVANCEDNESTING	May be omitted, only applicable to in-cell output mode
Variable	Whether to specify frequency of checking output point locations match	Y	Y or N
Variable	frequency of checking output locations match	5	only included if Y above, default value 1
Section keyword	Start of optional section containing path to file containing annual average local background NO_x and NO_2 values	AABACKGROUND	May be omitted, only applicable to in-cell output mode
Variable	File path to annual average local background NO_x and NO_2 concentrations after values have been put into equilibrium by the local model	PATH=”/home/maqsworking/ AANOxNO2.bgd”	Output file from the local model

Table E.3 Specification of elements which may be included in the input file for the **Processor** utility when running in in-cell output mode.

Element type	Description	Example entry	Comment
Section keyword	Start of section defining local upwind mode inputs	LOCALUPWINDBACKGROUND	Included for the local upwind mode only
Variable	File path of the output *.bgd* file	PATH = "/home/maqs/upwind.bgd"	
Variable	File path of the input ADMS-format .met file	PATH = "/home/maqs/WRFmet.met"	
Section keyword	Start of section defining nesting background mode inputs	NESTINGBACKGROUND	Included for the nesting background mode only
Variable	File path of the output *.bgd* file	PATH = "/home/maqs/nesting.bgd"	
Variable	File path of the upwind *.bgd* file	PATH = "/home/maqs/upwind.bgd"	
Variable	File path of the input local model *.nc* file	PATH = "/home/maqs/NestBgd.nc"	
Variable	Number of *.nc* receptors to include in the calculations	1	
Variables	Names of *.nc* receptors to include in the calculations	Centre_1	List receptor names as used in the local model, one per line, must be within the nesting domain
Section keyword	Start of section defining nesting output mode inputs	NESTINGOUTPUT	Included for the in-cell output mode only
Variable	File path of output netCDF file	PATH="/home/maqs/Output.nc"	
Variable	Mixing time in whole hours	1	
Variable	List of file paths for gridded local model run output files	PATH="/home/maqs/MainGrd.nc"	
Variable	Mixing time in whole hours	1	Must be the same as above
Variable	List of file paths for explicit local model run output files	PATH="/home/maqs/Explicit.nc"	
Variable	Whether to interpolate regional model concentrations	Y	Y or N

Table E.4 Specification of optional elements for the input text file of the **Processor** utility. Note that one of the local upwind background, in-cell background mode and in-cell output sections must be included in the file.

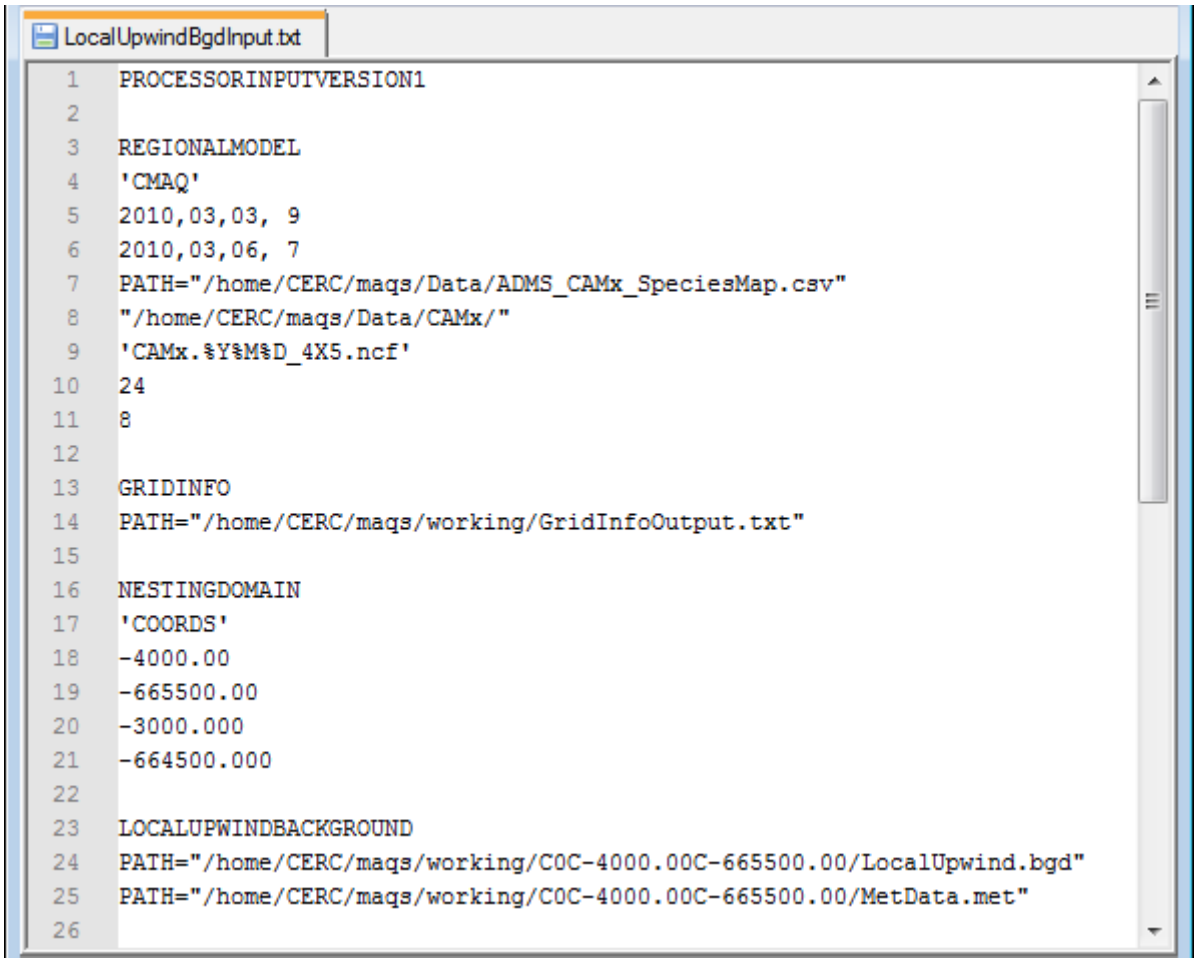


Figure E.2 Example input file for the **Processor** utility running in local upwind background mode, viewed in Notepad++

E.5 Command line structure

To run the **Processor** utility from the command line or a script, the following syntax should be used:

```
<executable file path> <input text file path>
```

where `<executable file path>` is the full path to the utility executable (*.out*), enclosed in inverted commas, and `<input text file path>` is the full path to the input text file which contains the information required to run the executable, enclosed in inverted commas.

For example, if the executable is saved in the default MAQS coupled system installation directory, */disk/maqs/utils/*, and the input text file is saved as */home/work/LocalUpwindBgdInput.txt*, the command line to run the utility would be

```
'/disk/maqs/utils/Processor.out' '/home/work/LocalUpwindBgdInput.txt'
```

E.6 Utility outputs

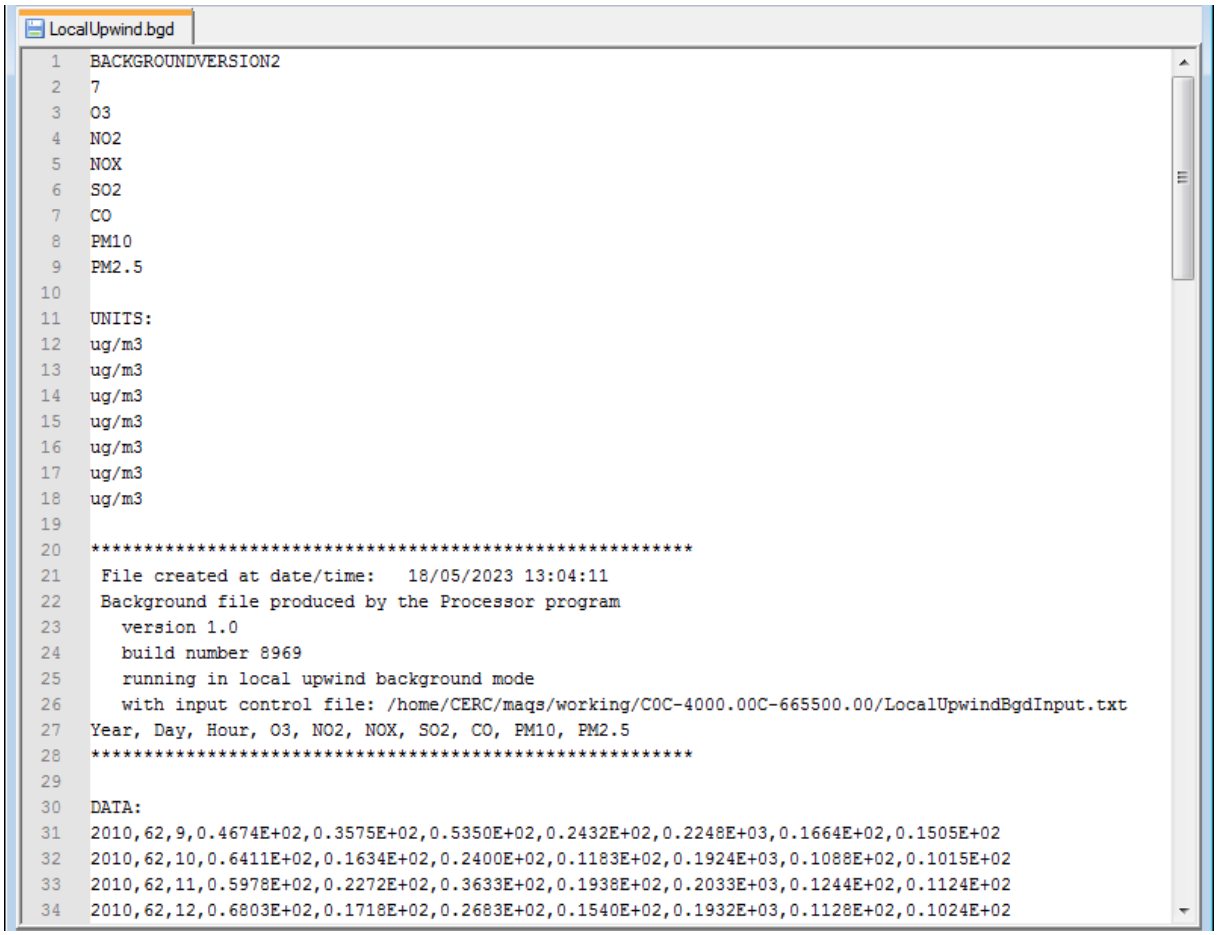
The **Processor** utility running in local upwind background or in-cell background mode creates an ADMS format *.bgd* file containing background concentrations for the output species defined in the species map file, for the period specified in the input file if sufficient data are available, in units of $\mu g/m^3$. This utility will create a new *.bgd* file. It will stop with an error if an existing file is found with the same file path as specified for the output file, i.e. it will not overwrite or append to an existing file.

A header section specifies when the file was created, in which mode the utility was run and the file path of the input text file used. An example output *.bgd* file is shown in **Figure E.3**. For runs using annual average regional model concentration data, the utility creates a slightly different format *.bgd* file containing only NO_x and NO_2 as required by the local model (**Figure E.4**).

The **Processor** utility running in in-cell output mode writes output concentrations to a netCDF (*.nc*) file which follows the ADMS Comprehensive Output File (Version 2.0) conventions. This format is described in full in Section 5.2. This utility will always create a new *.nc* file - it will stop with an error if an existing file is found with the same file path as specified for the output file, so it will not overwrite or append to an existing file.

Descriptive attribute values are copied from the first local model file, while the concentration datasets are defined according to the local model species specified in the species map file. The netCDF data contents can be processed using the Post Processor utility.

Any error or warning messages are written to *Error.txt* or *Warning.txt* text files in the same directory as the input text file. Error messages relate to problems which cause the program to fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.


LocalUpwind.bgd

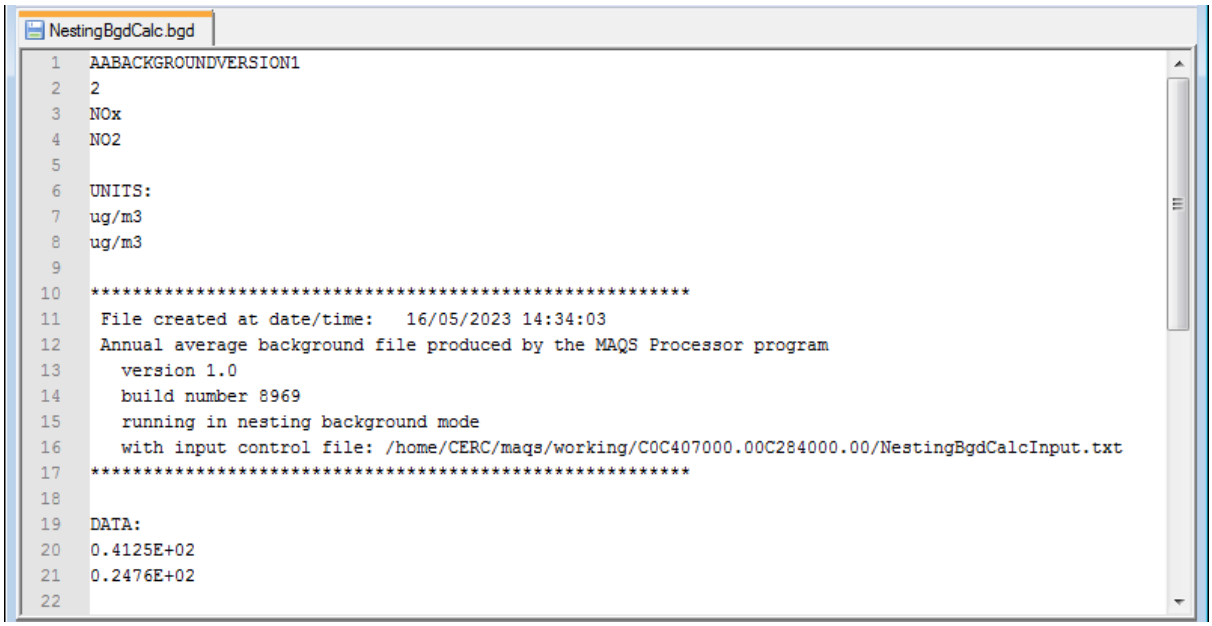
```
BACKGROUNDVERSION2
7
O3
NO2
NOX
SO2
CO
PM10
PM2.5

UNITS:
ug/m3
ug/m3
ug/m3
ug/m3
ug/m3
ug/m3
ug/m3

************************************************************
 File created at date/time:   18/05/2023 13:04:11
 Background file produced by the Processor program
   version 1.0
   build number 8969
   running in local upwind background mode
   with input control file: /home/CERC/maqs/working/C0C-4000.00C-665500.00/LocalUpwindBgdInput.txt
Year, Day, Hour, O3, NO2, NOX, SO2, CO, PM10, PM2.5
************************************************************

DATA:
2010,62,9,0.4674E+02,0.3575E+02,0.5350E+02,0.2432E+02,0.2248E+03,0.1664E+02,0.1505E+02
2010,62,10,0.6411E+02,0.1634E+02,0.2400E+02,0.1183E+02,0.1924E+03,0.1088E+02,0.1015E+02
2010,62,11,0.5978E+02,0.2272E+02,0.3633E+02,0.1938E+02,0.2033E+03,0.1244E+02,0.1124E+02
2010,62,12,0.6803E+02,0.1718E+02,0.2683E+02,0.1540E+02,0.1932E+03,0.1128E+02,0.1024E+02
```

Figure E.3 Output *.bgd* file produced by the **Processor** utility running in local upwind background mode, viewed in Notepad++


NestingBgdCalc.bgd

```
AABACKGROUNDVERSION1
2
NOx
NO2

UNITS:
ug/m3
ug/m3

************************************************************
 File created at date/time:   16/05/2023 14:34:03
 Annual average background file produced by the MAQS Processor program
   version 1.0
   build number 8969
   running in nesting background mode
   with input control file: /home/CERC/maqs/working/C0C407000.00C284000.00/NestingBgdCalcInput.txt
************************************************************

DATA:
0.4125E+02
0.2476E+02

```

Figure E.4 Output *.bgd* file produced by the **Processor** utility containing annual average background concentration data, viewed in Notepad++

APPENDIX F Combine COF utility

The **Combine COF** utility is a command line application which combines ADMS Comprehensive Output Files (netCDF) for different spatial and/or temporal modelling subsets into a single file in the same format. This utility was developed for the MAQS coupled system and for the parallel development of a system to distribute runs in a cloud computing environment. It may be useful for recombining output files if a large stand-alone local model run has been divided into multiple time periods or multiple spatial regions to allow efficient use of computing resources.

F.1 Data requirements

The input netCDF files may contain data for different spatial regions, different time periods or both, with the following restrictions:

- If combining files with period average data, the utility does not allow processing of multiple time-periods;
- If there are different time-periods, they must form an uninterrupted hourly sequence;
- If there are different spatial regions and different time-periods, the same spatial split between files must be maintained for all time-periods, i.e. the file for region 1 must contain the same output points during all time periods; and

The full set of output locations are included in the output netCDF file, this may include any combination of specified points, regular grids and/or source-oriented grids. The utility will re-order the gridded output points to fit the ADMS Comprehensive Output File (Version 2.0) conventions.

If gridded output points are included in the input files, the utility can check whether they form a regular rectangle with consistent x and y coordinates in order to output a valid grid. If the gridded output points do not form a complete rectangular grid, there is an option for them to be converted into specified point outputs.

The **Combine COF** utility stores data for a number of files before writing to the output file to allow efficient use of resources. The number of files for which data is stored depends on the number of spatial regions or the available memory of the HPC system where the MAQS coupled system is run, whichever is more restrictive. Care must be taken when running large domains as the utility can take up to 90% of the available system memory (RAM) and may conflict with other processes.

F.2 Input file format

The components of the input text file for the **Combine COF** utility are defined in **Table F.1**. There is only one section in the input file for this utility. An example input file is shown in **Figure**

F.1.

The **Combine COF** utility can treat output points in two different ways, either as their original types (specified point, gridded or source-oriented), including checks for the consistency of gridded output locations and retaining the user-specified point names; or all as specified points, with numerical names. The 'Receptor option' element in the input file should be set to Y for the first method or N for the second method.

Element type	Description	Example element	Comment
Version string	File version description	COMBINECOFVERSION1	Must be the first line of the file
Section keyword	Start of section with input data	COMBINECOF	Must be included
Variable	Output file path	PATH="/disk/maqs/Combined.nc"	
Variable	Whether multiple time-periods are included	Y	Y or N
Variable	Number of time-periods	2	Only included if Y above, must be greater than 1
Variable	Whether multiple spatial regions are included	Y	Y or N
Variable	Number of spatial regions	2	Only included if Y above, must be greater than 1
Variable	Receptor option	Y	Y to check grid, N to convert all points to receptors
Variable	Whether setting the number of input netCDF files from which data should be stored before writing out	Y	Y or N
Variable	Number of input netCDF files to store data from before writing	2	Only included if Y above; otherwise defaults to the number of spatial regions
Variable	Total number of input netCDF files	4	Number of time-periods*number of spatial regions
Variable	List of netCDF file paths	PATH="/disk/maqs/Region1T1.nc" PATH="/disk/maqs/Region2T1.nc" PATH="/disk/maqs/Region1T2.nc" PATH="/disk/maqs/Region2T2.nc"	Must list all spatial files for the same time period together, and spatial regions in the same order for all time periods, with time periods in chronological order

Table F.1 Specification of input file format for the **Combine COF** utility

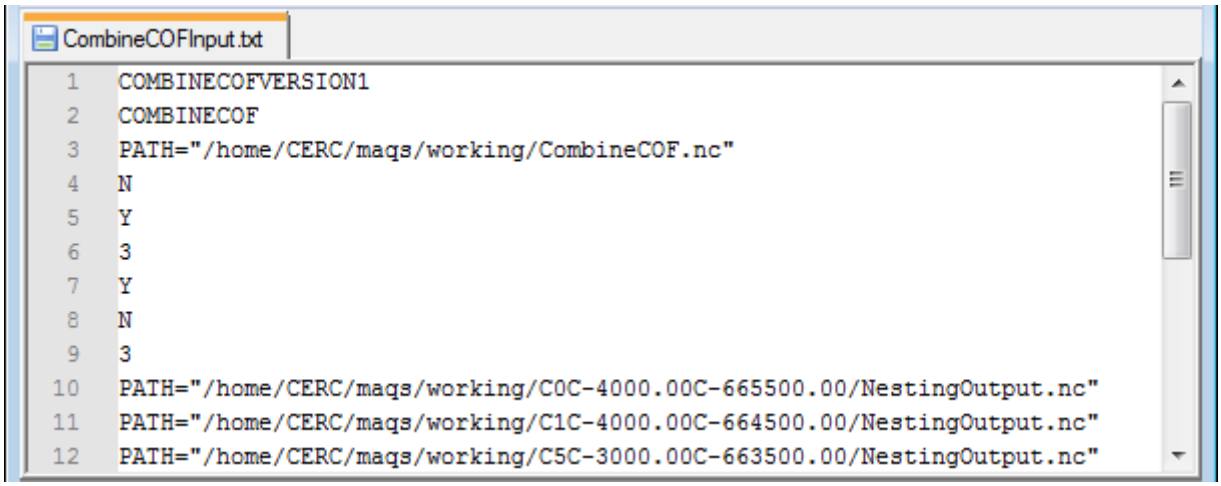


Figure F.1 Example input text file for the **Combine COF** utility

F.3 Command line structure

To run the **Combine COF** utility from the command line or a script, the following syntax should be used:

```
<executable file path> <input text file path>
```

where `<executable file path>` is the full path to the utility executable (*.out*), enclosed in inverted commas, and `<input text file path>` is the full path to the input text file which contains the information required to run the executable, enclosed in inverted commas.

For example, if the executable is saved in the default installation directory, */disk/maqs/utils*, and the input text file is saved as */home/working/CombineCOFInput.txt*, the command line to run the utility would be

```
'/disk/maqs/utils/CombineCOF.out' '/home/working/CombineCOFInput.txt'
```

F.4 Utility outputs

The **Combine COF** utility writes output concentrations to a netCDF (*.nc*) file which follows the ADMS Comprehensive Output File (Version 2.0) conventions. This format is described in full in Section 5.2. The utility will overwrite any existing file with the specified output file name and location.

Descriptive attribute values, such as the **Site Name**, are copied from the first input netCDF file. The netCDF data contents can be processed using the MAQS Post-Processor utility to get output which is useful for calculating health impact metrics, for example aggregating to spatial areas or calculating average concentrations over different periods of a day.

Any error or warning messages are written to *Error.txt* or *Warning.txt* text files in the same directory as the input text file. Error messages relate to problems which cause the program to fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.

APPENDIX G AddInterpIGP utility

The **AddInterpIGP** utility is a command-line application which adds interpolated intelligent grid points to an input ADMS-format netCDF file. This utility was developed for use in the MAQS coupled system but may also be useful when stand-alone modelling of high-resolution concentration contours is required over a large area. It allows the runs to be divided into smaller spatial regions for more efficient use of available computing resources and later re-combined without loss of contour resolution at the boundaries of the smaller regions. Please refer to Sections 4.7.9 and 8.4.2 for more details about source-oriented grid points and interpolated source-oriented grid points.

G.1 Data requirements

The **AddInterpIGP** utility reads an ADMS-format netCDF file, which must contain output from a local model run where the output locations were defined by an *.asp* file created using the **Create ASP** utility. Further specified points may have been defined for the local model run using the *.asp* file, but no gridded output should have been included. This ensures that the output locations in the netCDF file have the names required to allow the **AddInterpIGP** utility to determine where to locate interpolated source-oriented grid points, and to re-convert gridded output locations from specified points to gridded points.

If the runs using the *.asp* file have been split into multiple spatial regions and the output netCDF files re-combined using the **Combine COF** utility, the order of the *.asp* points in the final output file may not match that in the original *.asp* file. The **AddInterpIGP** utility will re-order the points before the calculations of interpolated point locations and concentrations.

G.2 Interpolation of concentrations

The **AddInterpIGP** utility uses the same method for determining the locations and output concentrations for interpolated source-oriented grid points as used by the ADMS-Urban model during a stand-alone run with source-oriented gridding for road and (if applicable) canyon sources. Interpolation points are three sets of points between sets or 'pairs' of points added along the same road segment by the **AddInterpIGP** utility, at which concentrations are calculated by linearly interpolating between the more sparsely located full calculation model output points. Please refer to Sections 4.7.9 and 8.4.2 for more details.

G.3 Input file format

The **AddInterpIGP** utility does not use an input text file.

G.4 Command line structure

To run the **AddInterpIGP** utility from the command line or a script, the following syntax should be used:

```
<executable file path> <input COF file path> <output COF file path>
```

where: `<executable file path>` is the full path to the utility executable (*.out*), enclosed in inverted commas; `<input COF file path>` is the full path to the input Comprehensive Output File (*.nc*, COF Version 2.0) to which interpolated source-oriented grid points should be added, enclosed in inverted commas; and `<output COF file path>` is the full path to the output Comprehensive Output File (*.nc*) including interpolated source-oriented grid points, enclosed in inverted commas. The output file path may be omitted, in this case the utility will create a file with the same file stem and location as the input file but with the *.out.nc* extension.

For example, if the executable is saved in the default installation directory, */disk/maqs/utils*, and the input netCDF file is saved as */home/maqsworking/Contour.nc*, the minimum command line to run the utility would be

```
'/disk/maqs/utils/AddInterpIGP.out' '/home/maqsworking/Contour.nc'
```

and in this case the output file would be saved as */home/maqsworking/Contour.out.nc*.

G.5 Utility outputs

The **AddInterpIGP** utility writes output concentrations for all input grid locations and added interpolated source-oriented grid point locations to a netCDF (*.nc*) file which follows the ADMS Comprehensive Output File (Version 2.0) conventions. This format is described in full in Section 5.2. The utility will overwrite an existing file with the specified output file name and location, but the output file path cannot be the same as the input file path.

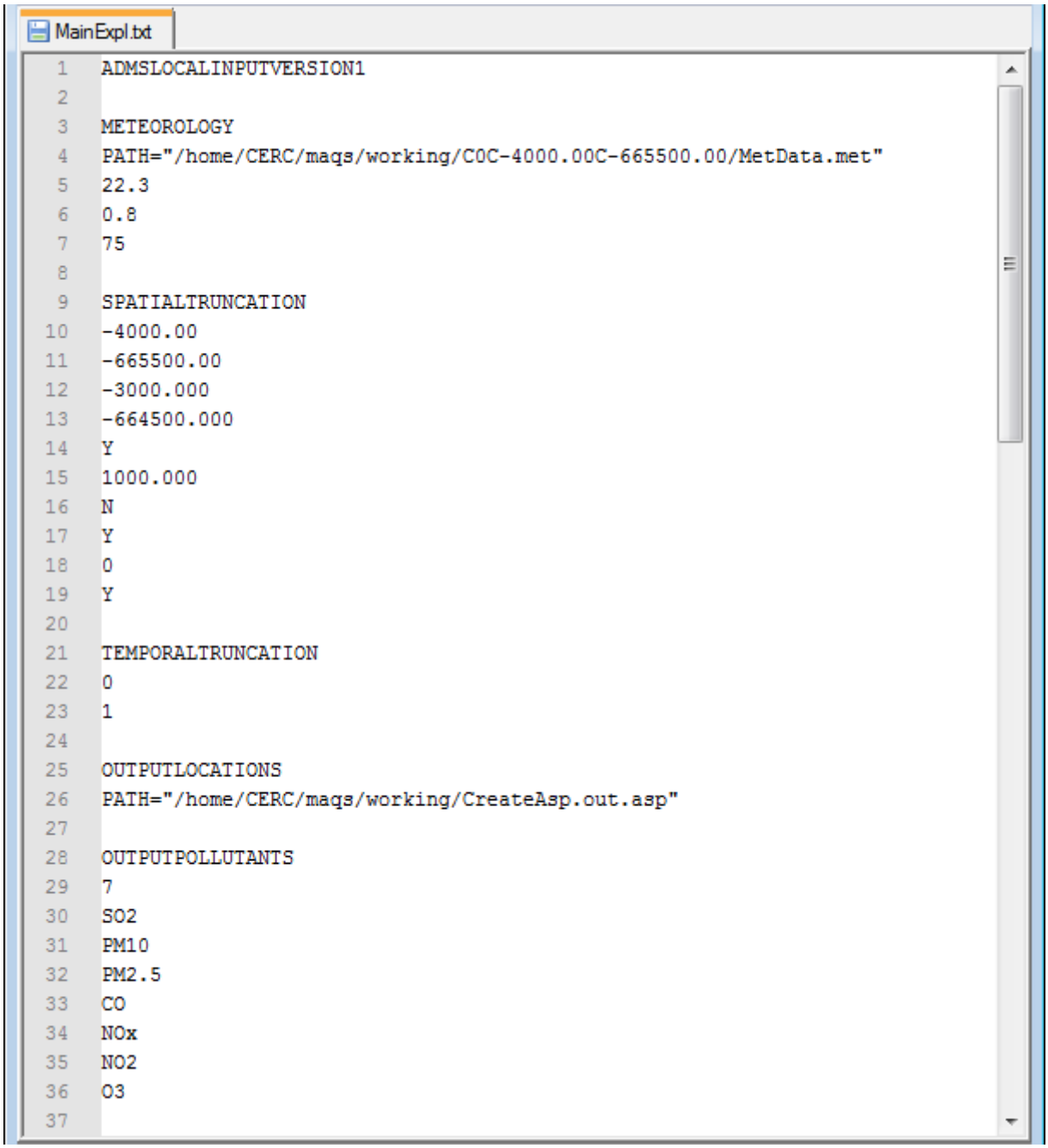
Descriptive attribute values, such as the **Site Name**, are copied from the input netCDF file. The netCDF data contents can be processed using the MAQS Post Processor utility.

Any error or warning messages are written to *Error.txt* or *Warning.txt* text files in the same directory as the input netCDF file. Error messages relate to problems which cause the program to fail, whereas warning messages give information or alerts about problems which may lead to unusual outputs but do not cause the program to fail.

APPENDIX H ADMS-Local primary input file format

The ADMS-Local primary input file is a text-based file which is generated by the coupled system, based on user inputs. The file contains a version string and at least six sections of data. The compulsory sections are described in **Table H.1** while the optional sections are described in **Table H.2**. There are a number of additional text-based files that can be output by ADMS-Local but are not created by default. These files can be requested by specifying the options described in **Table H.3**. The version string must be the first line in the file, following which the sections may be listed in any order but the order of the variables within each section must be as defined in the tables. Each element should be given on a new line, blank lines may be included before each section keyword but not within a section. An example file is shown in **Figures H.1** and **H.2**.

ADMS-Local was developed for the MAQS coupled system. The user-specified local model options described in Sections 4.7.2 to 4.7.12 are processed by the MAQS control scripts to write the appropriate sections to the primary input file in coordinating the ADMS-Local runs within the system. For technical information about the ADMS-Local modelling approach, please refer to Section 8.3.


MainExpl.txt

```
1  ADMSLOCALINPUTVERSION1
2
3  METEOROLOGY
4  PATH="/home/CERC/maqs/working/C0C-4000.00C-665500.00/MetData.met"
5  22.3
6  0.8
7  75
8
9  SPATIALTRUNCATION
10 -4000.00
11 -665500.00
12 -3000.000
13 -664500.000
14 Y
15 1000.000
16 N
17 Y
18 0
19 Y
20
21 TEMPORALTRUNCATION
22 0
23 1
24
25 OUTPUTLOCATIONS
26 PATH="/home/CERC/maqs/working/CreateAsp.out.asp"
27
28 OUTPUTPOLLUTANTS
29 7
30 SO2
31 PM10
32 PM2.5
33 CO
34 NOx
35 NO2
36 O3
37
```

Figure H.1 Example ADMS-Local primary input text file (first half)

MainExpl.txt

```
37
38  OUTPUTTYPES
39  Y
40  N
41
42  BACKGROUND
43  PATH="/home/CERC/maqs/working/C0C-4000.00C-665500.00/NestingBgdCalc.bgd"
44
45  3DGRIDSOURCE
46  PATH="/home/CERC/maqs/Data/example1_3DEmissions.nc"
47  N
48  N
49
50  GRIDDISPERSION
51  N
52  N
53
54  CHEMISTRY
55  Y
56  Y
57
58  ROADDATA
59  PATH="/home/CERC/maqs/Data/example1.rdi"
60  PATH="/home/CERC/maqs/Data/example1.rdg"
61  PATH="/home/CERC/maqs/Data/example1.rde"
62  N
63
64  TIMEVARYINGEMISSIONS
65  Y
66  PATH="/home/CERC/maqs/Data/TVEF_vkt.fac"
67  N
68
```

Figure H.2 Example ADMS-Local primary input text file (second half)

Element type	Description	Example element	Comment
Version string	File version description	ADMSLOCALINPUTVERSION1	Must be the first line of the file
Section keyword	Start of section containing meteorological information	METEOROLOGY	
Variable	File path to the input met file	PATH=”/disk/maqs/MetData.met”	
Variable	Latitude (decimal degrees)	52.5	
Variable	Roughness length (m)	0.5	
Variable	Minimum Monin-Obukhov length (m)	30	
Section keyword	Start of section containing information about the truncation area	SPATIALTRUNCATION	
Variable	X coordinate of lower-left corner of truncation region	11000.00	Coordinates in the projected coordinate system in units of m
Variable	Y coordinate of lower-left corner of truncation region	-5000.00	
Variable	X coordinate of upper-right corner of truncation region	21000.00	
Variable	Y coordinate of upper-right corner of truncation region	1000.00	
Variable	Whether to truncate road sources	Y	Y or N
Variable	Road buffer size (m)	1000.00	Only included if Y above
Variable	Whether to include road sources that touch the edge of the truncation region including the buffer	N	
Variable	Whether to truncate grid sources	Y	Y or N
Variable	Grid buffer size (m)	0.00	Only included if Y above
Variable	Whether to include grid sources that touch the edge of the truncation region including the buffer	Y	
Section keyword	Start of section containing information about the truncation time	TEMPORALTRUNCATION	
Variable	Minimum truncation time	0	Time in units of hours
Variable	Maximum truncation time	1	
Section keyword	Start of section containing the output locations file	OUTPUTLOCATIONS	
Variable	File path to the output locations file	PATH=”/disk/maqs/monitors.asp”	

Element type	Description	Example element	Comment
Section keyword	Start of section containing the output pollutants	OUTPUTPOLLUTANTS	
Variable	Number of output pollutants	4	
Variable	Name of output pollutant	NOx	Specify according to number of pollutants above; should match local species included in the concentration species map file (Section 4.3.1)
Section keyword	Start of section containing output type options	OUTPUTTYPES	
Variable	Whether to output hourly data	Y	Y or N
Variable	Whether to output period average data	N	Y or N

Table H.1 Specification of compulsory elements of the ADMS-Local primary input file

Element type	Description	Example element	Comment
Section keyword	Start of section containing road source data files	ROADDATA	Refer to Sections 4.7.2 and 4.7.3 for the file formats
Variable	File path to the road information file	PATH="/disk/maqs/roads.rdi"	
Variable	File path to the road geometry file	PATH="/disk/maqs/roads.rdg"	
Variable	File path to the road emissions file	PATH="/disk/maqs/roads.rde"	
Variable	Whether specifying a road traffic flow data file	Y	Y or N
Variable	File path to the road traffic flow data file	PATH="/disk/maqs/roads.rdt"	Only included if Y above
Section keyword	Start of section containing conversion factors	CONVERSIONFACTORS	
Variable	Number of pollutants	2	
Variable	Name of pollutant	O3	Specify according to number of pollutants above
Variable	Conversion factor (µg/m^3 to ppb)	0.5	

Element type	Description	Example element	Comment
Section keyword	Start of section containing the background concentration data file	BACKGROUND	
Variable	File path to the background data file	PATH="/disk/maqs/nesting.bgd"	
Section keyword	Start of section containing the time varying emission factors files	TIMEVARYINGEMISSIONS	
Variable	Whether specifying a time varying profiles file	Y	Y or N
Variable	File path to the time varying profiles file	PATH="/disk/maqs/tvef.fac"	Only included if Y above
Variable	Whether specifying an hourly factors file	Y	Y or N
Variable	File path to the hourly factors file	PATH="/disk/maqs/tvef.hfc"	Only included if Y above
Section keyword	Start of section for suppressing time varying emission factors warnings	SUPPRESSTVEFWARNINGS	
Variable	Whether to prevent warning messages relating to time varying emission factors from being written to the log file	Y	Y or N
Section keyword	Start of section containing information about daylight saving time (DST)	ADJUSTFACTORS_DST	Must not be included if also applying BST
Variable	Whether to take account of DST when applying time varying emission factors	Y	Y or N; the following elements are required if Y
Variable	Number of DST periods	2	
Variable	Start or end date-time of DST period in format YYYY, MM, DD, HH	2015,03,27,01	Must list the date-time for each DST period
Variable	Whether the above date and time is the start or end of DST period	START	START or END; period dates must alternate and be in sequential order
Variable	Number of hours to adjust for DST	1	
Section keyword	Start of section for taking account of British Summer Time (BST)	ADJUSTFACTORS_BST	Must not be included if also applying DST
Variable	Whether to take account of BST when applying time varying emission factors	Y	Y or N

Element type	Description	Example element	Comment
Section keyword	Start of section containing information about 3D grid sources	3DGRIDSOURCE	
Variable	File path to the 3D grid sources file	PATH="/disk/maqs/3DEmis.nc"	
Variable	Whether to suppress warning messages relating to 3D grid aggregation from being written to the log file	Y	Y or N
Variable	Whether to disaggregate all road emissions from the surface layer	Y	Y or N
Section keyword	Start of section containing the urban canopy flow parameters	URBANCANOPYFLOW	Refer to Section 4.7.6 for details
Variable	Average building height (m)	6.695109957	
Variable	Average street canyon width (m)	40.11609355	
Variable	Lambda P	0.111277362	
Variable	Lambda F value for a range of wind directions in degrees	0.093292657,337,022	Must specify values describing a complete range of wind directions
Variable	Surface roughness length within the canopy (m)	0.1	
Section keyword	Start of section containing the vehicle split for traffic flow calculation	VEHICLESPLIT	
Variable	Percentage of light vehicles	95	
Section keyword	Start of section containing the chemistry schemes to model	CHEMISTRY	
Variable	Whether to model NO_x chemistry	Y	Y or N
Variable	Whether to model sulphate chemistry	Y	Y or N
Section keyword	Start of section for using local night-time chemistry	NIGHTCHEM	
Variable	Whether to use the night-time NO_x chemistry option	Y	Y or N
Section keyword	Start of section containing the reactivity coefficient	AROCUSERDEF	
Variable	Weighted reactivity coefficient value for ROC	0.05	

Element type	Description	Example element	Comment
Section keyword	Start of section containing the minimum wind speed setting	U10MINUSERDEF	
Variable	Minimum wind speed (m/s)	0.3	Ensures that low wind speeds will be treated as valid
Section keyword	Start of section containing grid source dispersion parameters	GRIDDISPERSION	
Variable	Whether to choose the grid source centre point closest to the output points in calculating contributions from grid sources to output concentrations	N	Y or N
Variable	Whether to force a calculation height for output concentrations	N	Y or N
Variable	Grid calculation height (m)	17.43	
Section keyword	Start of section containing parameters for aggregating emissions from included road sources onto grids	GRIDAGGREGATION	
Variable	X coordinate of lower-left corner of the grid	-3500.00	Coordinates in the projected coordinate system in units of m
Variable	Y coordinate of lower-left corner of the grid	-4500.00	
Variable	Number of grid cells to aggregate in x direction	664	
Variable	Number of grid cells to aggregate in y direction	1218	
Variable	Spacing between grid cells in x direction (m)	1000.00	
Variable	Spacing between grid cells in y direction (m)	1000.00	
Variable	Height of the grid (m)	20.75	
Section keyword	Start of section containing files used in annual average NO_x chemistry	AABACKGROUND	
Variable	File path to annual average background concentration data file	PATH=”/disk/maqs/AANOxNO2.bgd”	Output file from the **Processor** utility in nesting background mode
Variable	File path to monthly diurnal background profile data file	PATH=”/disk/maqs/BgdProfiles.bgd”	Refer to Section 4.3.5 for the file format

Element type	Description	Example element	Comment
Variable	Primary NO_2 fraction value	20.0	

Table H.2 Specification of optional elements of the ADMS-Local primary input file

Element type	Description	Example element	Comment
Section keyword	Start of section for creating output .pst file	PSTFILE	Contains hourly output concentrations in a text-based file
Variable	Whether to create .pst file	Y	Y or N
Section keyword	Start of section for creating output .plt file	PLTFILE	Contains period average output concentrations in a text-based file
Variable	Whether to create .plt file	Y	Y or N
Section keyword	Start of section for creating output .mio file	MIOFILE	Contains input and processed met data for each met line
Variable	Whether to create .mio file	Y	Y or N
Section keyword	Start of section for creating output .blp file	BLPFILE	Contains boundary layer profiles of certain variables for each met line
Variable	Whether to create .blp file	Y	Y or N
Section keyword	Start of section for creating output .rds file	RDSFILE	Contains trapezoidal road segment geometry
Variable	Whether to create .rds file	Y	Y or N
Section keyword	Start of section for creating output .els file	ELSFILE	Contains the positions of the road source elements used for dispersion
Variable	Whether to create .els file	Y	Y or N

Table H.3 Specification of optional elements of the ADMS-Local primary input file for creating additional output files

APPENDIX I ADMS-Urban features

The MAQS control scripts coordinate a series of ADMS-Urban model runs, if ADMS-Urban is the selected local model, alongside utility programs. Some of the ADMS-Urban features used in the MAQS coupled system are specific to this system, so are not described in the standard ADMS-Urban User Guide. Sections I.1 to I.4 cover the key ADMS-Urban features used in the MAQS coupled system.

I.1 .umo model override files

A *.umo* file contains a subset of the information found in an ADMS-Urban model parameter (*.upl)* file, and is used to replace definitions found in the original *.upl*. For example, the MAQS control scripts use *.umo* files to specify appropriate *.met*, *.bgd* and *.uai* files for each regional model grid cell, without needing to edit the template *.upl*. Any input section of the *.upl* file structure which is not repeated can be overridden using a *.umo* file. For example, this means that meteorological or output settings can be changed but source and pollutant data cannot be redefined.

If a *.umo* file has been used, the ADMS-Urban *.log* file will include the statement:

```
INFO   : A *.umo file has been used to overwrite the original model set
up
```

All contents of the *.log* file will reflect the settings and file paths specified in the *.umo* file, where relevant. The *.umo* file must have the same file-name stem as the *.upl* and be saved in the same directory, with the *.umo* extension. For example, if the template *.upl* is saved as */home/maqsworking/Test.upl* then a *.umo* file would have to be saved as */home/maqsworking/Test.umo* in order to be used.

Note that a .uai *file path specified in a* .umo *file will replace any* .uai *file specified in the original* .upl.

I.2 Temporal truncation of dispersion

A key part of the MAQS coupled system concept is that the regional model outputs are used to represent dispersion over long time-scales, while ADMS-Urban modelling is used for short time-scales. When ADMS-Urban is run as a stand-alone model, it calculates dispersion of emissions separately for each hour and allows the emissions from that hour to disperse for all time. When used in MAQS, however, the ADMS-Urban model calculations must be restricted to short time-scales using an additional input option for temporal truncation.

The ADMS-Urban temporal truncation option is controlled by an additional input file (*.uai*) section. Both lower and upper time thresholds can be specified, although for a mixing time of one hour the lower threshold will always be set to 0.

When the temporal truncation option is in use, the log file from an ADMS-Urban run will include the following statement:

```
Dispersion time truncation in use, limits  0.00 to  1.00 hours
```

I.3 Grid dispersion modifications

In standalone ADMS-Urban runs, the output concentration within a grid source cell is interpolated towards those from neighbouring grid source cells in order to give a smooth variation throughout the modelling area. In the default MAQS coupled system approach each ADMS-Urban run is truncated to include only one grid source cell and so the interpolation of grid source concentrations is switched off via a *.uai* file section.

When the option to interpolate regional model concentrations is in use, in the main ADMS-Urban gridded and explicit runs the grid cell concentration interpolation option is retained and the run truncation is modified to include neighbouring grid cells. This allows the ADMS-Urban concentrations from the main gridded run to be consistent with the interpolated regional model concentrations.

For the gridded runs the calculation height of output points is forced to be equal to the depth of the lowest layer of the regional model grid (as calculated by the **RM Grid Info** utility), in order to match the regional model calculations as closely as possible.

I.4 Running only gridded sources

ADMS-Urban includes a *.uai* file option to only model gridded sources, which will ignore sources of any other type(s) defined in the *.upl*. When only a single *.upl* file is supplied to the MAQS coupled system by the user, this option is applied by the control program in order to model only gridded emissions in the run for background calculations and the main gridded run.

The *.uai* file section for using the **Only Grid Source** mode has the following format:

```
ONLYGRIDSOURCE
Y
```

CERC

Cambridge Environmental Research Consultants Ltd
3 King's Parade, Cambridge, CB2 1SJ, UK
Tel: +44 (0)1223 357 773
Email: help@cerc.co.uk
Website: www.cerc.co.uk