

# Model Evaluation Toolkit

## What's New in Version 5.4?

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*June 2026*

This document describes the changes in version 5.4 of the Model Evaluation Toolkit, compared with the last 'What's new' document released with version 4.0 in 2016. A list of changes is given for each tool, followed by notes on updating existing files from version 4.0 to version 5.4.

### Data Input Tool

Full details of all the options described below are given in Section 3.1 of the User Guide.

1. More **modelled data file formats** are now supported, including MAQS, WRF-Chem, EMEP, CMAQ, CAMx and CHIMERE. Defra modelled background map data files are also supported.
2. There is now an option to use a **species mapping file** to map modelled species to the required pollutants, for example, to combine modelled NO and NO<sub>2</sub> to obtain modelled NO<sub>x</sub> for comparison with NO<sub>x</sub> observations.
3. The downloading of **observed data from online monitoring networks** has been extended and made more flexible:
  - a. Observed data can now be downloaded from more networks; the complete list is given in the User Guide.
  - b. Observed data can now be downloaded for different networks for different stations. A 'network' column has been added to the stations input file for the user to specify which network the station belongs to. An 'auto.download' column has also been added; "yes" means the data will automatically be downloaded from the appropriate network for that station and "no" means the observed data for that station will be imported from the local file.
  - c. Metadata for online network monitoring stations is now easily accessible, to assist with choosing monitoring stations for evaluation, using the options under the new 'Tools' menu.
4. **Meteorological data** can now be included to facilitate polar plots in the Model Diagnostics Tool. A range of ADMS input / output meteorological file formats are supported, as well as WRF model gridded netCDF files.
5. There is now an option to **use a template file path** for selecting multiple files for the modelled data.
6. There is now an option to enter the **time difference** between modelled and observed data.
7. There is now more flexibility around the averaging times and statistics of input modelled and observed data. Previously, observed data was required to either be 1-hour mean data, or to have the same averaging time and statistic as the modelled data. Now, the averaging time and

statistic is set through the avg.time and statistic columns in the pollutant definitions file and these will be applied to both the modelled and observed data.

## Model Evaluation Tool

Full details of all the options described below are given in Section 3.2 of the User Guide.

1. There is now an option to calculate the **ensemble median modelled dataset** and include this in the evaluation.
2. **Composite pollutants** can now be evaluated, for example NO<sub>2</sub>/NO<sub>x</sub> or PM<sub>10</sub>-PM<sub>2.5</sub>.
3. Two new graph options have been added:
  - a. **Statistical scatter plots** compare modelled and observed statistics (mean, maximum standard deviation, AOT40, SOMO35 or a specified percentile) for each station, with the option to plot custom reference lines and filter by station type using different colours, symbols or graphs.
  - b. **Time variation analysis plots** compare modelled and observed diurnal, monthly and weekday profiles.
4. There is now an option to **specify stations to exclude** from the analysis.
5. If ozone is included in the evaluation, **AOT40 and SOMO35** are now calculated and added to the statistical output. These can also be plotted on the statistical scatter plot.
6. There is now an option to specify the **station data coverage threshold**, in addition to the averaging period data coverage threshold. This means that only monitoring stations that meet the required valid data coverage over the selected analysis period (or full analysis period if not specified) will be included in the evaluation.
7. There is now an option for **NO<sub>2</sub> to be set as the lower limit for NO<sub>x</sub>** to avoid issues with measured NO<sub>2</sub> being greater than measured NO<sub>x</sub>.
8. The **target plot** has been updated to be consistent with version 7.2 of the FAIRMODE DELTA tool (release date April 2023).
9. There is now an option to specify the **modelled dataset colours** to be used on the time variation and box and whisker plots.
10. Statistical output files now contain **additional statistics**, including mean square error and its components (MSE, MSEs, MSEu, MSE.cor and mMSE).
11. The forecast index evaluation now calculates information about **pollution episodes**, where a pollution episode is defined as the observed concentration being above a user-specified alert threshold for a user-specified number of consecutive days.
12. The concentration evaluation time plot is now compatible with any **forecast index scale**, e.g. DAQI, EUAQI, EEA, etc.

## Model Diagnostics Tool

Full details of all the options described below are given in Section 3.3 of the User Guide.

1. Plots can now be produced for **all stations, pollutants and modelled datasets at once**, or for a selection of stations, pollutants and modelled datasets.
2. There is now an option to select a **date range** for analysis.
3. **Polar plots** have been added to the list of plot options. These plots require meteorological data to be provided to the Data Input Tool.
4. **Axes limits** can now be specified for time plots and scatter plots.
5. There is now an option to **Add markers** to time plots, which adds small solid circles to represent each data point.

## Universal changes

1. The format of averaging times has been changed to increase flexibility. Instead of specifying the averaging time in terms of the number of hours, the averaging time is now specified as a string, for example, '1 hour', '24 hour', 'day', 'week' or 'month'.
2. The CRAN mirror setting and 'Update R packages' option have been moved to the 'R Support' menu in all tools.

## Notes on updating from version 4.0 to version 5.4

Any workspaces saved using previous versions of the Data Input tool will need to be re-created by running version 5.4 of the Data Input tool, in order to be used in version 5.4 of the Model Evaluation and Model Diagnostic tools.

TKI, TKM and TKD files from previous versions of the toolkit can be opened in the interface and the user will be prompted to upgrade the file to the latest version. The user will then need to check the correct options are selected for their desired run.

It is recommended to run the Toolkit using R version 4.5.3 or later:

1. Install R from <https://cran.r-project.org/>
2. Start the Data Input Tool
3. From the Data Input Tool menu select 'R Support' then 'Detect current R installation folder'. For full Toolkit installation instructions see Section 2.2 in the Toolkit User Guide.

A number of Toolkit improvements have led to changes in the formats of some of the input parameter files required to run the Data Input Tool and Model Evaluation Tool. The specific changes required for each Tool and each file are listed below:

- Data Input Tool (User Guide Section 3.1):
  - Pollutant definitions file:
    - Add an extra column with the header 'ozone'. This should be 'yes' or 'no' for each pollutant. If 'yes' then ozone-specific statistics can be calculated for this pollutant.
    - Add two extra columns with the headers 'avg.time' and 'statistic'. The modelled and observed data will be averaged to the averaging time (avg.time) using the statistic given.

- Station definitions file:
  - Add an extra column with the header 'network'. For each station this should be set to one of the recognised online networks or a user-specified network. Each user-specified network should have separate pollutant definitions in the observed pollutant definitions file.
  - Add an extra column with the header 'auto.download'. This should be 'yes' or 'no' for each station. If 'yes' then observed data for this pollutant will be downloaded from the specified online network. If 'no' then observed data for this pollutant will be imported from the local observed data file.
- Modelled pollutant definitions file:
  - Change the 'mod.avg.time.hours' column header to 'mod.avg.time'
  - Change the averaging time from a numeric value to a string, for example, '1 hour', '24 hour', 'day', 'week' or 'month'.
- Observed pollutant definitions file:
  - This file is now only required if observed data for one or more stations is to be imported from the local observed data file.
  - Change the 'obs.avg.time.hours' column header to 'obs.avg.time'
  - Change the averaging time from a numeric value to a string, for example, '1 hour', '24 hour', 'day', 'week' or 'month'.
  - Add an extra column with the header 'network'. This is user-specified and should match the user-defined network names used in the station definitions file. Observed pollutant definitions should be provided for every user-defined network used in the station definitions file.
  - Add an extra column with the header 'hour.ending'. This should be 'yes' or 'no' for each pollutant for each user-defined network. Hourly observed data will be assumed to represent the hour leading up to the timestamp if 'yes' or starting from the timestamp if 'no'. The Toolkit assumes that hourly modelled data represents the hour leading up to the timestamp (i.e. hour.ending = yes).
- Model Evaluation Tool (User Guide Section 3.2):
  - Output averaging times file:
    - Change the 'output.avg.time.hours' column header to 'output.avg.time'
    - Change the averaging time from a numeric value to a string, for example, '1 hour', '24 hour', 'day', 'week' or 'month'.
  - Index scales file:
    - Change the 'index.avg.time.hours' column header to 'index.avg.time'
    - Change the averaging time from a numeric value to a string, for example, '1 hour', '24 hour', 'day', 'week' or 'month'.