DELTA.TOOL.LIGHT (DTL)

USER MANUAL

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Version 1.0 - 07/11/2024
Version 1.1 – 22/11/2024 Beta_sliders
Version 1.2 – 16/12/2024 Re-organization of openings window; Added USERHRS.
Version 1.3 – 05/01/2025 Correction plot commands; added some examples.
Version 1.4 – 24/01/2025 Summary of Startup files: Station, NUTS, Species (ACTIONS/INFO tab)

Introduction

In a project focused on validating the CAMS re-Analysis and Forecast products, there was a need for efficient calculation of a large number of indicators, as defined in Fairmode publications ([1], [2], [3]). Although the well-known DeltaTool [1] provides extensive features for analyzing Air Quality model results, its batch mode is not well developed.

Delta.Tool.Light emphasizes the calculation and visualization of indicators in multi-model, multi-species, multi-domain, and multi-period studies, considering different approaches to parameters related to observational uncertainties (referred to in DeltaTool as Goals & Criteria). In addition to the graphical representation of these indicators, several supporting graphical options are implemented.

Delta.Tool.Light has a general setup, and specific applications are defined in an external file called 'GENERALinput.dat'. The input formats for Air Quality Model results, Observational data, and

Startup files (i.e., data regarding the monitoring stations) are identical to those used in DeltaTool [1].

The following Model Performance Indicators (in short, indicators) are implemented in DTL:

- MQI_HD, MQI_YR, MQI_FC (only in Forecast mode): Model Quality Indices
- TN(Bias), TN(1-R), TN(Stdev): Temporal (observational-uncertainty) normalized Bias (Model – Obs), 1-R (i.e. 1 minus Correlation), Stdev (i.e. Standard Deviation),
- T(W-S), T(Wk-We), T(D-N), For (T) Traffic stations temporal-related normalized differences between Winter (W) bias and Summer (S) bias, same for WeekDays (Wk) and WeekEndDays (We), and DayTimeHours (D) and NightTimeHours (N),
- B(W-S), B(Wk-We), B(D-N): same as before for (B) Background stations,
- I(W-S), I(Wk-We). I(D-N): same as before for (I) Industrial stations,
- SN(1-R), SN(Stdev): Spatial observational-uncertainty normalized 1-R, and Stdev,
- UT-UB: Spatial gradients of UrbanTraffic and UrbanBackground stations,
- UB-RB: Spatial gradients of UrbanBackground and RuralBackground stations.

The graphics have the following default ordering of the indicators:

MQI_HD, MQI_YR, (MQI_FC), TN(Bias), TN(1-R), TN(Stdev), T(W-S), T(Wk-We), T(D-N), B(W-S), B(Wk-We), B(D-N), I(W-S), I(Wk-We), I(D-N), SN(1-R), SN(Stdev), UT-UB, UB-RB

For definitions of the Indicators we refer to the Annex 1 of this manual.

Download, Installation, Launch

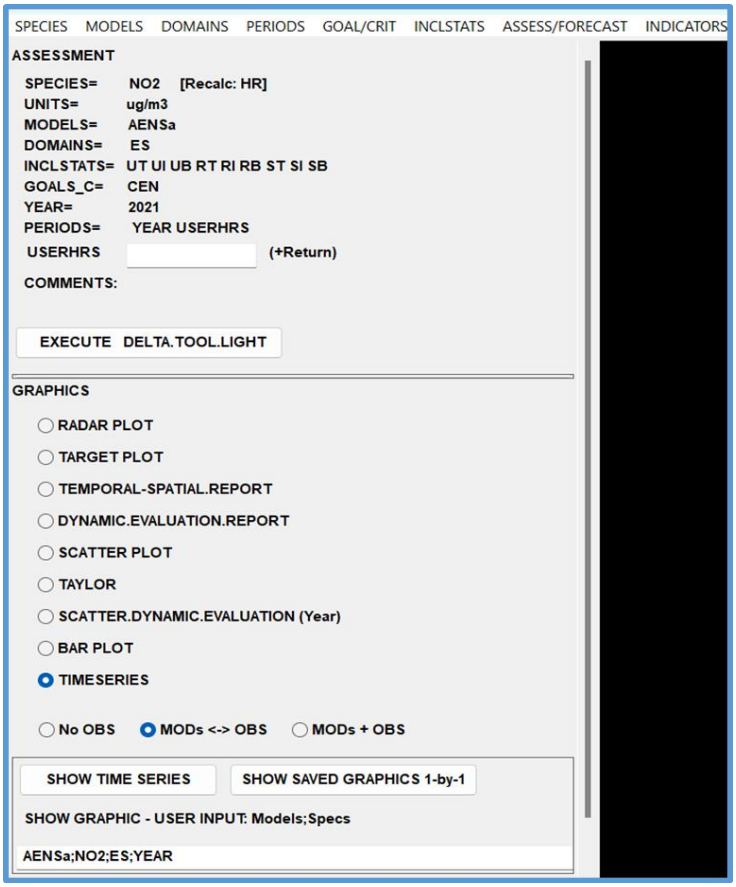
0) Windows environment needed on your pc.
1) Log in on the JRC box:
   https://jrcbox.jrc.ec.europa.eu/index.php/s/qAt8FqwJvxC1vSD
   with password: Fairmode_CT9!
2) Go to folder 'DeltaToolLight (DTL).
3) Go to folder DLT_Package.

4a) Download the contents of the DTL_Package into a local folder which will serve as the DTL home directory.

4b) The package contains all 9 CAMS re-analysis model results (total 4.5 Gb) in folder .\DTLinput\modeling\CAMS2021.
If you want to reduce the download size, 2 or 3 models are sufficient to explore all the features of the Tool.
Ensure the DTL home directory contains the following subdirectories: DTLinput, DTLoutput, and IDL88, as well as the following files: deltatoollight.sav, DTLTool.exe, DTLTool.ini, and splash_DTLTool.bmp.
For convenience, you may create a shortcut to the executable DTLTool.exe on the desktop.

5) Double click on the executable (or its shortcut) to launch the Tool and click 'continue' to start the IDL virtual machine.

The following DTL openings window will appear.



Left part of the DTL openings window.

Input

- Input to Delta.Tool.Light (DTL) consists of three folders, which are identical to those used in DeltaTool, and a text file with application-specific information.

- Startup
  This folder contains the startup.ini file or files, similar to those used in the DeltaTool.
  Remark 1: The first lines up to '[MONITORING]'+1 are not used.
  Remark 2: For each station line, only the following information is utilized:
  StationCode, Altitude, Longitude, Latitude, GMT, Station Type, Area Type, NUTS code, and the list of observational species.
  Accepted Station Types: Traffic, Industrial, Background (first 3 letters are used)
  Accepted Area Types: Urban, Rural, SubUrban (first 3 letters are used)
  Example:
  Milano;M1;M2;122;9.14;45.478;GMT+1;LOM;background;urban;ITC4C;NO2*O3*PM25;

- Modelling
  This folder contains (subfolders with) model files of type '*Year_Model*_TIME.cdf', similar to the model cdf files in the DeltaTool.

- Monitoring
  This folder contains (subfolders with) the monitoring file of type '*OBS_TIME*.cdf', similar to the monitoring cdf file in the DeltaTool.

- GENERALinput.dat
  This file contains all the application-specific information:

```
SPECS=     NO2,ug/m3; O3,ug/m3; PM25,ug/m3; PM10,ug/m3
; Next line: 0=HR; 1= DailyMax(NO2), HR8Max(O3), Mean(PM)
RECALC=    0,1,1,1
; 75% rule for hourly data availability
RULE75=    75
dIROBS=    DTLinput\monitoring\CAMS2021FC\
dIRMOD=    DTLinput\modeling\CAMS2021\
dIRSTART=  DTLinput\startup\
; Next lines: if 1 line then omit 'Start1=', 1 2 3 4 for species-dependent startup files
start1=    startup_CAMS2021NO2O3Nuts3AllvalSet13.ini
start2=    startup_CAMS2021NO2O3Nuts3AllvalSet13.ini
start3=    startup_CAMS2021PMNuts3AllvalSet13.ini
start4=    startup_CAMS2021PMNuts3AllvalSet13.ini
dIROUTP=   DTLoutput\
; Next lines: CNTRS in droplists, NUTS format; ALL= all available stations in startup
CNTRS=     ES,FR,IDF,PARIS,DE,POV,PL,DK,NL
CNTRSNUTS= ES,FR,FR1,FR101,DE,ITC+ITH,PL,DK,NL
; next line gives default indicators order. Can be changed - always contains all numbers from 1 to 19
INDORDER= DEFAULT
;INDORDER= 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19
YEAR=      2021
INITMODEL= AENSa
INITSPEC=  NO2
INITCNTR=  ES
INITPERD=  YEAR
INITGC=    CEN
ACROBAT= C:\Program Files\Adobe\Acrobat DC\Acrobat\acrobat.exe
; Next line defines user periods. If none then put NONE or delete line
USER_PERIODS= JAN+DEC, JUN+JUL+AUG
; Next line to change the color table: 0=DeltaToolLight, 1=DeltaTool
COLORTAB=  0
```

  with:

  - SPECS: List of species with units and Limit Values.
  - RECALC: Model and Monitoring data have hourly frequency. This line indicates whether or not a recalculation into DailyMax, hr8DailyMax, or DailyMean is required.
    0= Hourly, 1= DailyMax (NO2), HR8Max (O3), Mean (PM).
  - dirOBS, dirMOD, dirSTART: location of folders for Observations, Models, and Startup. These lines contain the location relative to the DTL home directory.
    Example: 'DTLinput\modeling\CAMS\').
  - Start*: location of startup files which may be species-specific (NO2, O3, PM2.5, PM10).
    If only 1 line (common to all species) is used then omit 'Start1='. 1, 2, 3, 4 for species-dependent startup files.

- dirOUTPUT: location of Output file (relative to the DTL home directory) for data and graphics. This folder contains subfolders for graphical output (Radars, Targets, TSsumms, DynEvals, Scatters, Taylors, ScatDynEvals, Bars, TimeSeries).
- CNTRS: List of Countries/Regions (user) names.
- CNTRSNUTS: List of NUTS codes corresponding to CNTRS. NUTS codes up to level 3 depending on what is available in the startup file. An R utility progam vor the conversion of Longitute, Latitude values to NUTS code is reproduced in Annex 3.
- INDORDER: Ordering of the 19 Indicators. For default order see Introduction. User specific ordering can be defined here.
- YEAR: The annual year
- INIT*: Initial settings for model, species, domain, period, GC in the DTL opening window. INITGC refers to the following uncertainty parameters: Fairmode (FM), CEN, and AAQD.
- ACROBAT: Link to the Acrobat reader for consultation of the (pdf) user's manual in the DTLinput directory.
- USER_PERIODS: The standard time periods available in the tool are: Year, Summer (JJA), Winter (DJF), and the 12 individual months. Specific user-defined periods can be added as the sum of individual months.
  Examples: 'JAN+FEB+DEC', 'JUL+AUG'.
- COLORTAB: 0 for the default colour table, 1 for the DeltaTool colour table

Drop lists and left panel of window

The drop lists at the top of the DTL window allow you to select which cases to run:

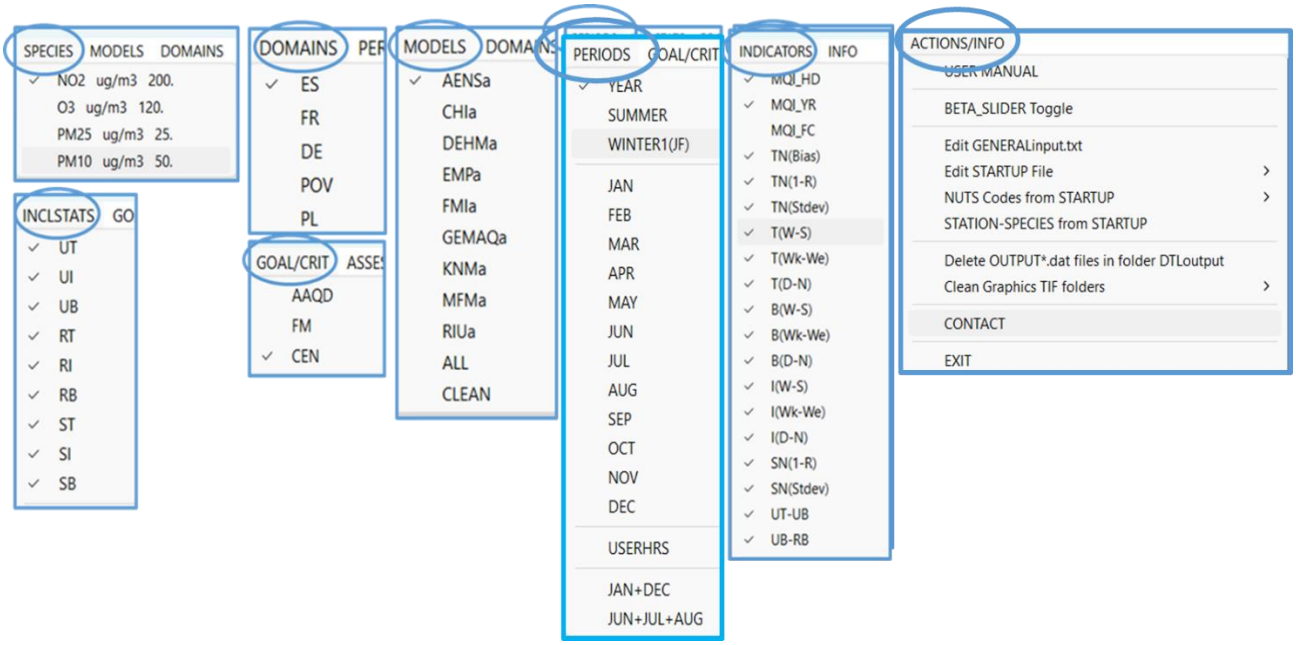
- SPECIES: List of species is taken from the GENERALinput.dat file.
- MODELS: A list is generated based on what is available in the modeling folder (dirMOD).
- DOMAINS: Countries/Regions are taken from the GENERALinput.dat file.
- PERIODS: This includes the default periods (Year, Summer, Winter, 12 months) as well as user-defined periods from the GENERALinput.dat file.
  The button 'USERHRS' can be used to define a specific time interval in the editable field USERHRS. The format is; Initial hour, followed by '-', followed by end hour.
  For example: 2000 – 3000.
- GOAL/CRIT: 3 types of parameters for the observational uncertainty are available: Fairmode (FM), CEN, and AAQD. For details, see Annex 2.

- INCLSTATS: This list provides options to include/exclude specific types of stations.

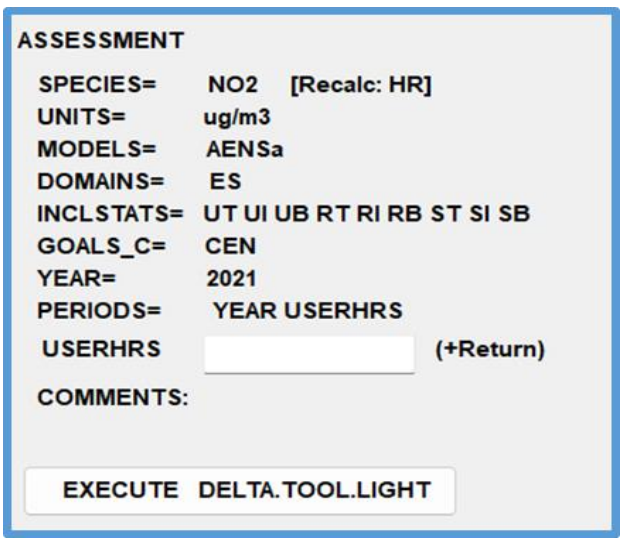
- ASSESS/FORECAST: The default mode is Assessment. In Forecast mode, the Persistence model can be selected here, and the indicator MQI_FC is calculated and appears in the Radar plot. There are three types of Persistence models:
  P1 is the mean value of Day -1 ,-2, -3 ,-4.
  P2 is the most recent hourly value at Day -1, -2, -3, -4.
  P3 is the value at the same hour on Day -1, -2, -3, -4.
  In the Target plot, normalization is with respect to the Persistence model (see [4]).

- INDICATORS: A list of Indicators that can be included or excluded from the visualization.

- ACTION/INFO: Provides useful editing and deletion options.



The selections made in the drop lists are summarized in the left panel. For example:



Execute DTL

The 'EXECUTE DELTA.TOOL.LIGHT' button runs de code and produces the following data output files in the 'DTLoutput' folder:

- OUTPUT_INDICATORS90p:
  All indicators (90p)

  Example:

```
Thu Aug 01 15:45:11 2024
ASSESSMENT
MODELS=  AENSa CHIa
SPECS=  NO2 O3
PERIODS=  YEAR SUMMER
DOMAINS=  ES FR
PERIODS= YEAR SUMMER
GOALS/CRIT=  FM CEN
StatAREA=  Urban|Rural
StatTYPE= Traffic|Industrial|Background
INCLUDES STATS=   UT  UI  UB  RT  RI  RB  ST  SI  SB
--------------------------------------------------------------------------------

SPEC=NO2  PERIOD=YEAR  GC=FM
              MQI_HD    MQI_YR    TN(Bias)  TN(1-R)   TN(Stdev) T(Wk-We)  T(D-N)    B(Wk-We)  B(D-N)    I(Wk-We)  I(D-N)    SN(1-R)   SN(Stdev) UT-UB     UB-RB
ES
AENSa         0.7793    1.3163    0.5381    0.1766    0.4589    0.6592    0.8413    0.3815    0.4346    0.4013    0.5447    0.3464    0.2320    1.2620    1.0841
CHIa          0.6782    0.9613    0.4044    0.2232    0.3600    0.5135    0.7405    0.3076    0.3838    0.2996    0.5208    0.2596    0.3323    1.3275    1.2158
FR
AENSa         0.9782    1.8558    0.7504    0.1955    0.4640    0.6122    1.5167    0.2743    0.4516    0.2557    0.3035    0.4392    0.5744    1.6908    1.4326
CHIa          0.8363    1.4795    0.6040    0.2090    0.3810    0.5106    1.3873    0.1959    0.4215    0.1660    0.2694    0.2942    0.7118    1.7639    1.2839
--------------------------------------------------------------------------------
SPEC=O3  PERIOD=YEAR  GC=FM
              MQI_HD    MQI_YR    TN(Bias)  TN(1-R)   TN(Stdev) T(Wk-We)  B(Wk-We)  I(Wk-We)  SN(1-R)   SN(Stdev) UT-UB     UB-RB
ES
AENSa         0.4015    0.5580    0.2915    0.0747    0.1791    0.1910    0.0991    0.0948    0.0749    0.1837    0.4516    0.4436
CHIa          0.3801    0.4913    0.2606    0.0830    0.1364    0.1717    0.1179    0.1091    0.0679    0.1649    0.4591    0.4835
FR
AENSa         0.2416    0.2770    0.1473    0.0351    0.1043    0.0380    0.0560    0.0391    0.0306    0.0581    ---       0.5077
CHIa          0.2569    0.2631    0.1386    0.0428    0.0819    0.0534    0.0673    0.0636    0.0323    0.0748    ---       0.4795
--------------------------------------------------------------------------------
SPEC=NO2  PERIOD=SUMMER  GC=FM
              MQI_HD    MQI_YR    TN(Bias)  TN(1-R)   TN(Stdev) T(Wk-We)  T(D-N)    B(Wk-We)  B(D-N)    I(Wk-We)  I(D-N)    SN(1-R)   SN(Stdev) UT-UB     UB-RB
ES
AENSa         0.7269    1.2010    0.4957    0.1224    0.4155    0.6724    0.8863    0.2746    0.5426    0.3633    0.6487    0.2794    0.1970    1.2940    0.6793
CHIa          0.6207    0.8185    0.3389    0.1730    0.3441    0.5313    0.9008    0.2490    0.6160    0.3244    0.6719    0.1862    0.3297    1.3111    0.8232
FR
AENSa         0.9915    1.9887    0.8140    0.1387    0.4709    0.6564    1.5948    0.2167    0.3971    0.2006    0.3882    0.3828    0.7782    2.0033    1.0711
CHIa          0.8804    1.6443    0.6803    0.1596    0.4332    0.5881    1.4801    0.1761    0.4020    0.1352    0.5011    0.2488    0.8772    2.0337    1.0163
--------------------------------------------------------------------------------
etc …
…
```

- OUTPUT_INDICATORSxSTATION:

  All indicators per station:
  (StatName, Area/Type, Model mean norm., Obs mean norm., TN(BIAS), TN(1-R), TN(STDEV), Mod-Obs Summer norm., Mod-Obs Winter norm., Mod-Obs WeekD norm., Mod-Obs WeekD norm., Mod-Obs WeekEnd norm., Mod-Obs WeekEnd norm., Mod-Obs DayHours norm., Mod-Obs NightHours norm., DynEval(W-S), DynEval(Wk-We), DynEval(D-N), statUB, UT-UB norm., StatRB, UB-RB norm.)

  Example:

```
Thu Aug 29 21:58:55 2024
ASSESSMENT
MODELS=  AENSa
SPECS=  NO2
DOMAINS=  ES
PERIODS= YEAR
GOALS/CRIT=  CEN
StatAREA=  Urban|Rural
StatTYPE= Traffic|Industrial|Background
INCLUDED STATS=   UT  UI  UB  RT  RI  RB  ST  SI  SB
-----------------------------------------------------------------------------------------------------------

DOMAIN=ES  MODEL=AENSa  SPEC=NO2  PERIOD=YEAR  GC=CEN
StatName  Area/Type MM        MO        TN(BIAS)  TN(1-R)   TN(STDEV) MS-OS     MW-OW     MWK-OWK   MWE-OWE   MD-OD     MN-ON     DE(W-S)   DE(Wk-We) DE(D-N)   StatUB    UT-UB     StatRB    UB-RB |
ES0016R   RB        0.3142    0.2285    0.0300    0.0022    0.0393    -0.004    0.2145    0.0897    0.0755    0.0394    0.1312    0.2194    0.0141    -0.091
ES0041A   UT        1.4153    3.0443    -0.472    0.0678    -0.276    -1.393    -1.692    -1.778    -1.257    -2.082    -1.179    -0.298    -0.520    -0.903    ES2127A   -1.149
ES0094A   RI        0.4077    0.1848    0.0780    0.0077    0.0200    0.1111    0.3456    0.2408    0.1786    0.2063    0.2390    0.2344    0.0622    -0.032
ES0110A   UT        1.5530    2.3005    -0.229    0.0486    -0.234    -0.560    -0.632    -0.900    -0.360    -0.788    -0.707    -0.072    -0.539    -0.081    ES2127A   -0.268
ES0118A   UT        2.5576    3.6185    -0.286    0.1072    -0.070    -1.303    -0.502    -1.175    -0.771    -1.444    -0.686    0.8009    -0.403    -0.757    ES1939A   -1.331
ES0120A   UT        2.3888    3.3923    -0.265    0.0946    -0.240    -1.047    -1.000    -1.139    -0.665    -1.522    -0.487    0.0470    -0.473    -1.035    ES1939A   -1.274
ES0125A   UB        2.5086    3.6432    -0.289    0.0550    -0.258    -0.949    -1.335    -1.207    -0.954    -0.968    -1.300    -0.386    -0.252    0.3316                        ES1806A   -1.272
ES0201A   SI        0.3913    0.4654    -0.025    0.0096    -0.045    -0.073    -0.089    -0.080    -0.058    -0.115    -0.033    -0.016    -0.021    -0.082
ES0339A   SI        0.3175    0.4802    -0.056    0.0145    -0.114    -0.051    -0.208    -0.187    -0.101    -0.210    -0.115    -0.157    -0.085    -0.094
ES0556A   SI        2.0026    1.0037    0.3364    0.1778    0.0578    1.0619    1.1961    1.0294    0.9244    0.8593    1.1373    0.1342    0.1050    -0.278
ES0557A   RI        1.9601    0.7760    0.4030    0.1951    0.0905    1.1497    1.1771    1.2234    1.0860    0.9249    1.4399    0.0274    0.1374    -0.514
ES0584A   ST        2.2195    3.0569    -0.243    0.0939    -0.115    -0.959    -0.664    -1.003    -0.421    -1.064    -0.613    0.2950    -0.581    -0.450
ES0587A   SI        1.2900    0.8880    0.1374    0.0626    -0.015    0.2676    0.6323    0.4217    0.3500    0.1304    0.6700    0.3646    0.0717    -0.539
ES0588A   SI        1.3816    1.6474    -0.084    0.0663    -0.261    -0.291    -0.254    -0.345    -0.061    -0.341    -0.191    0.0368    -0.284    -0.150
ES0624A   SI        0.5859    0.7968    -0.072    0.0311    -0.015    -0.271    -0.042    -0.191    -0.260    -0.245    -0.177    0.2287    0.0694    -0.068
ES0629A   UI        1.5099    1.4067    0.0336    0.0984    -0.109    0.0511    0.1725    0.0803    0.1597    -0.099    0.3019    0.1214    -0.079    -0.401
ES0633A   UI        1.8532    2.3396    -0.144    0.1826    -0.282    -0.386    0.0267    -0.533    -0.370    -0.616    -0.358    0.4131    -0.162    -0.258
ES0634A   SI        1.5649    1.2291    0.1113    0.1081    -0.066    0.3353    0.4468    0.3367    0.3336    0.1816    0.4874    0.1115    0.0031    -0.305
ES0651A   SI        0.8516    1.4641    -0.200    0.0619    -0.213    -0.547    -0.689    -0.669    -0.467    -0.730    -0.493    -0.141    -0.202    -0.236
ES0692A   UB        2.5478    2.4562    0.0275    0.0709    -0.146    0.2581    0.0724    0.0644    0.1592    -0.018    0.2007    -0.185    -0.094    -0.219                        ES2034A   0.3138
ES0712A   SI        1.6434    1.2526    0.1283    0.1179    -0.081    0.2767    0.4397    0.3920    0.3873    0.1855    0.5927    0.1629    0.0047    -0.407
ES0777A   RI        0.4986    1.0515    -0.188    0.0221    -0.098    -0.627    -0.353    -0.561    -0.531    -0.457    -0.646    0.2740    -0.029    0.1892
ES0787A   SI        0.6292    0.9601    -0.112    0.0314    -0.116    -0.361    -0.234    -0.357    -0.261    -0.404    -0.257    0.1274    -0.096    -0.146
ES0805A   UI        1.3746    2.2207    -0.262    0.0416    -0.243    -0.583    -0.969    -0.958    -0.560    -0.791    -0.901    -0.386    -0.397    0.1101
ES0817A   UT        1.4254    2.5048    -0.321    0.0545    -0.264    -0.896    -1.178    -1.220    -0.731    -1.316    -0.847    -0.281    -0.489    -0.468    ES1644A   -1.232
```

- OUTPUT_STATISTICSxSTATION:

  Statistics per station
  (StatName, Altitude, Lon, Lat, GMT, Area/Type, MQI_H, MQI_Y, mean Model, mean Obs, stdev M, stdev O, Bias M-O, CRMSE, RMSE, 1-R, Normalized Bias, Symmetrical Normalized RMSE)

  Example:

```
Thu Aug 01 15:43:24 2024
ASSESSMENT
MODELS=  AENSa CHIa
SPECS=  NO2 O3
DOMAINS=  ES FR
PERIODS= YEAR SUMMER
GOALS/CRIT=  FM CEN
StatAREA=  Urban|Rural
StatTYPE= Traffic|Industrial|Background
INCLUDED STATS=   UT  UI  UB  RT  RI  RB  ST  SI  SB
-----------------------------------------------------------------------------------------------------------

DOMAIN=ES  MODEL=AENSa  SPEC=NO2  PERIOD=YEAR  GC=FM
StatName  Alt     Lon         Lat         GMT   TA   MQI_H     MQI_Y     MEANM     MEANO     STDEVM    STDEVO    BIAS      CRMSE     RMSE      1-R       NBIAS     SNRMSE
ES0016R   506     -7.70472    42.6347     0     RB   0.0902    0.0930    2.7987    2.0360    2.0270    1.0278    -0.762    1.5583    1.7350    0.3432    0.5986    0.6526
ES0041A   32      -2.94565    43.2588     0     UT   0.8016    1.5243    13.400    28.822    6.9771    15.998    15.422    12.392    19.784    0.3233    0.5537    0.9207
ES0094A   478     -7.98860    43.4054     0     RI   0.1578    0.2422    3.6312    1.6464    2.0966    1.5859    -1.984    2.2967    3.0355    0.7540    1.3965    1.1643
ES0110A   4.0     -2.97724    43.3027     0     UT   0.5221    0.7420    14.309    21.195    7.7506    14.784    6.8865    9.6631    11.865    0.1916    0.3935    0.5963
ES0118A   672     -3.68222    40.4217     0     UT   0.5825    0.9434    24.894    35.220    18.770    21.302    10.326    12.068    15.883    0.1741    0.3558    0.4572
ES0120A   708     -3.67722    40.4517     0     UT   0.6241    0.9108    22.982    32.636    17.388    26.110    9.6538    14.176    17.150    0.1375    0.3653    0.5076
ES0125A   593     -3.70500    40.3469     0     UB   0.5989    1.0066    24.450    35.507    19.411    29.285    11.057    13.343    17.329    0.0708    0.3316    0.4637
ES0201A   362     -7.84780    43.4539     0     SI   0.1471    0.0803    3.4891    4.1505    2.1346    3.2998    0.6614    2.7719    2.8497    0.4491    0.4163    0.6650
ES0339A   60      -7.50778    43.6863     0     SI   0.2318    0.1761    2.8319    4.2821    2.1458    5.0806    1.4501    4.2705    4.5100    0.4414    0.5695    1.0567
ES0556A   9.0     -5.37697    36.1794     0     SI   0.7172    1.0663    17.945    8.9941    10.720    9.1815    -8.951    11.326    14.436    0.6397    1.2383    1.0289
ES0557A   15      -5.38081    36.1862     0     RI   0.7994    1.2735    17.520    6.9362    10.689    8.3121    -10.58    11.839    15.880    0.7570    1.8200    1.3274
ES0584A   34      2.18830     41.4820     0     ST   0.5396    0.7828    21.025    28.958    11.466    15.211    7.9328    10.646    13.276    0.2847    0.3389    0.4901
ES0587A   30      -3.11272    43.3207     0     SI   0.3780    0.4308    11.544    7.9471    6.0665    6.4831    -3.597    6.5635    7.4846    0.5455    0.7438    0.7148
ES0588A   136     -3.07414    43.3205     0     SI   0.4982    0.2753    12.516    14.924    6.5947    14.028    2.4080    10.428    10.703    0.2892    0.4785    0.6735
ES0624A   50      -2.03819    36.8475     0     SI   0.2533    0.2267    5.2380    7.1242    3.5421    3.9362    1.8861    4.5863    4.9591    0.7488    0.5114    0.7762
ES0629A   30      -5.48893    36.1856     0     UI   0.4416    0.1082    13.614    12.683    9.1915    12.227    -0.930    9.1889    9.2359    0.3346    0.4784    0.5871
ES0633A   1.0     -5.43277    36.1747     0     UI   0.7036    0.4815    17.095    21.582    10.460    19.253    4.4870    15.937    16.556    0.4387    0.4795    0.7541
ES0634A   32      -5.43027    36.2120     0     SI   0.4671    0.3553    14.068    11.049    8.9084    10.704    -3.019    9.0976    9.5856    0.4171    0.5837    0.6598
ES0651A   60      -0.913300   37.6033     0     SI   0.5084    0.6406    7.6870    13.215    4.9605    10.836    5.5279    9.0236    10.582    0.4364    0.4931    0.9215
ES0692A   29      2.11497     41.3705     0     UB   0.4035    0.0899    23.591    22.742    11.850    16.361    -0.848    9.3591    9.3975    0.1734    0.3016    0.3560
ES0712A   45      -5.48083    36.1754     0     SI   0.4965    0.4129    14.779    11.265    9.8166    12.054    -3.514    9.6637    10.282    0.3734    0.6432    0.6628
ES0777A   270     -8.49640    43.0935     0     RI   0.3433    0.5890    4.4716    9.4285    2.9131    5.5070    4.9568    4.6912    6.8248    0.4762    0.5518    0.9598
ES0787A   13      -6.90453    37.1903     0     SI   0.3177    0.3537    5.6356    8.5991    3.2947    6.3554    2.9634    5.5663    6.3060    0.5162    0.4517    0.8238
ES0805A   125     -2.88370    43.2411     0     UI   0.5449    0.8447    12.634    20.411    6.5312    13.759    7.7761    9.4228    12.217    0.2033    0.4244    0.6730
ES0817A   29      -5.95962    37.3843     0     UT   0.6313    1.0553    13.219    23.230    9.0521    17.290    10.011    10.984    14.862    0.1686    0.4604    0.7107
ES0822A   66      -6.93807    37.2796     0     UI   0.6789    0.8247    4.9230    11.975    3.0554    13.842    7.0526    12.423    14.285    0.4491    0.6689    1.5751
ES0823A   1.0     -6.96414    37.1857     0     UI   0.3571    0.5468    4.7857    9.3859    2.9081    6.4720    4.6002    5.4330    7.1189    0.4468    0.5420    0.9570
ES0824A   218     -5.70570    43.3069     0     SI   0.3335    0.2343    9.1511    11.144    5.3361    8.6706    1.9929    6.4760    6.7757    0.3331    0.3912    0.5878
etc …
…
```

- OUTPUT_STATISTICSmeans:

  Statistics mean values over stations
  (mean values over Stations: MQI_H, MQI_Y, Model, Obs, STDEV Model, STDEV Obs, BIAS (M-O), CRMSE, RMSE, 1-R, NBIAS, SNRMSE)

Example:

```
Thu Aug 01 15:43:24 2024
ASSESSMENT
MODELS=  AENSa CHIa
SPECS=  NO2 O3
DOMAINS=  ES FR
PERIODS= YEAR SUMMER
GOALS/CRIT=  FM CEN
StatAREA=  Urban|Rural
StatTYPE= Traffic|Industrial|Background
INCLUDED STATS=   UT  UI  UB  RT  RI  RB  ST  SI  SB
-------------------------------------------------------------------------------------------------------------------

DOMAIN=ES  SPEC=NO2  PERIOD=YEAR  GOALSC=FM
              MQI_H     MQI_Y     MEANM     MEANO     STDEVM    STDEVO    BIAS      CRMSE     RMSE      1-R       NBIAS     SNRMSE
AENSa         0.4910    0.6277    9.1906    13.996    5.9574    11.301    4.8063    8.7913    10.777    0.4078    0.5722    0.9316
CHIa          0.4736    0.4805    13.910    13.996    7.8954    11.301    0.0863    8.8942    10.261    0.4207    0.7757    0.7520
-------------------------------------------------------------------------------------------------------------------
DOMAIN=FR  SPEC=NO2  PERIOD=YEAR  GOALSC=FM
              MQI_H     MQI_Y     MEANM     MEANO     STDEVM    STDEVO    BIAS      CRMSE     RMSE      1-R       NBIAS     SNRMSE
AENSa         0.5450    0.8285    10.706    18.427    6.9716    12.570    7.7206    9.3725    12.835    0.3265    0.5008    0.8338
CHIa          0.4873    0.6545    14.286    18.427    8.3260    12.570    4.1406    8.8768    11.447    0.2837    0.5290    0.6359
-------------------------------------------------------------------------------------------------------------------
DOMAIN=ES  SPEC=O3  PERIOD=YEAR  GOALSC=FM
              MQI_H     MQI_Y     MEANM     MEANO     STDEVM    STDEVO    BIAS      CRMSE     RMSE      1-R       NBIAS     SNRMSE
AENSa         0.2762    0.2595    77.246    75.949    15.675    19.078    -1.297    8.5058    10.544    0.1142    0.1150    0.1372
CHIa          0.2716    0.2411    75.871    75.949    16.673    19.078    0.0773    8.5812    10.381    0.1223    0.1114    0.1358
-------------------------------------------------------------------------------------------------------------------
DOMAIN=FR  SPEC=O3  PERIOD=YEAR  GOALSC=FM
              MQI_H     MQI_Y     MEANM     MEANO     STDEVM    STDEVO    BIAS      CRMSE     RMSE      1-R       NBIAS     SNRMSE
AENSa         0.1824    0.1413    71.230    70.063    20.239    21.982    -1.167    5.9824    6.8926    0.0400    0.0761    0.0940
CHIa          0.1943    0.1379    70.198    70.063    21.158    21.982    -0.134    6.4924    7.3428    0.0465    0.0793    0.1005
-------------------------------------------------------------------------------------------------------------------
DOMAIN=ES  SPEC=NO2  PERIOD=SUMMER  GOALSC=FM
              MQI_H     MQI_Y     MEANM     MEANO     STDEVM    STDEVO    BIAS      CRMSE     RMSE      1-R       NBIAS     SNRMSE
AENSa         0.4136    0.5421    6.8399    10.913    3.8263    8.2300    4.0732    6.9478    8.7246    0.4962    0.5762    1.0055
CHIa          0.3994    0.4114    10.786    10.913    5.0085    8.2300    0.1270    7.1411    8.3650    0.5221    0.7556    0.7746
-------------------------------------------------------------------------------------------------------------------
DOMAIN=FR  SPEC=NO2  PERIOD=SUMMER  GOALSC=FM
              MQI_H     MQI_Y     MEANM     MEANO     STDEVM    STDEVO    BIAS      CRMSE     RMSE      1-R       NBIAS     SNRMSE
AENSa         0.4838    0.7882    6.8814    14.054    3.4381    8.5939    7.1728    7.5146    11.074    0.5216    0.5655    1.0297
CHIa          0.4506    0.6739    9.9715    14.054    4.1935    8.5939    4.0827    7.3783    10.277    0.4670    0.6471    0.7957
-------------------------------------------------------------------------------------------------------------------
etc …
…
```

Graphics

For the selections made in the drop lists, the following graphics can be generated:

- Radar plots
- Target plots
- Temporal.Spatial Reports
- Dynamic.Evaluation Reports
- Scatter plots
- Taylor plots
- Scatter.Dynamic.Evaluation plots
- Bar plots
- Time Series.

There are two ways to produce the graphics:

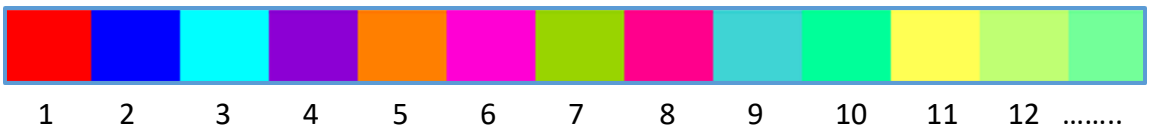
- SHOW SINGLE GRAPHICS: Graphics can be generated for a single species, a single model, a single domain, a single period, and a single G&C at a time based on the selections made in the droplists. These graphics will be saved in the DTLoutput subfolders.
  The produced and saved graphics can be visualized one by one using the 'SHOW SAVED GRAPHICS 1-by-1' button.
- SHOW MULTIPLE GRAPHICS: Graphics with multiple input parameters (species, models, domains, periods, G&C) can be generated using a line command in the editable field located at the bottom of the left-hand panel:
-

MODs; SPECs; CNTRs; PERDs [;GCs]

Generating Graphics with Uncertainty Parameters: For graphics dependent on uncertainty parameters (Radar, Target, Temporal_Spatial Report, Dynamic_Evaluation Report, and Scatter), indicators must first be calculated using the 'EXECUTE' button.
The line command may include multiple Models, Species, Domains, Periods, or Uncertainty Parameters, however, combining multiple values for different parameters simultaneously is not allowed.
Examples of valid commands:
Mod1,Mod2; NO2; ES; Year; CEN
Mod1; NO2,O3,PM10; FR; May; FM
Mod1; NO2,O3; ES,FR; Summer; CEN not allowed due to multiple combinations.

Generating Graphics without Indicator calculations: Without prior calculation ('EXECUTE') of the indicators, the graphics (Taylor, Scatter_Dynamic_Evaluation, Bar, and TimeSeries) can be generated for all Models, Species, Periods, and for all Station codes and Nuts codes available in the startup file. The G&C parameter in the command line can be omitted.
Examples of valid commands:
Mod1,Mod2; NO2; ES; Year
Mod1,Mod2; NO2; ES0041A; Year
Mod1; NO2,O3,PM10; FR; May
For Time Series double multiples are allowed:
Mod1,Mod2; NO2,O3; ES0094A; Summer
Mod1; NO2,O3,PM10; FR,FR1,FR101; July

The default (i.e. DTL) colour table is as follows:



For single-variable plots, the colour is determined by the rank number of the model in the model drop list sequence.
For multi-variable plots, the sequence of the variables determines the colours.

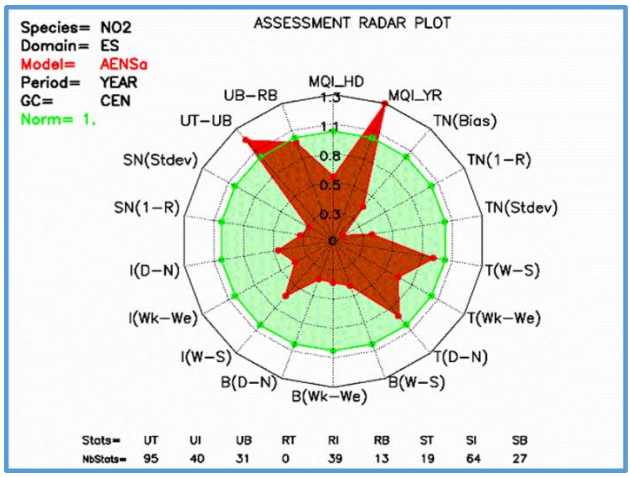
We now will show a number of graphics with one or more models, species, domains, and three different sets of observational uncertainty parameters. For each of the graphics, the corresponding line-commands is given between brackets in the legend,

RADAR PLOT

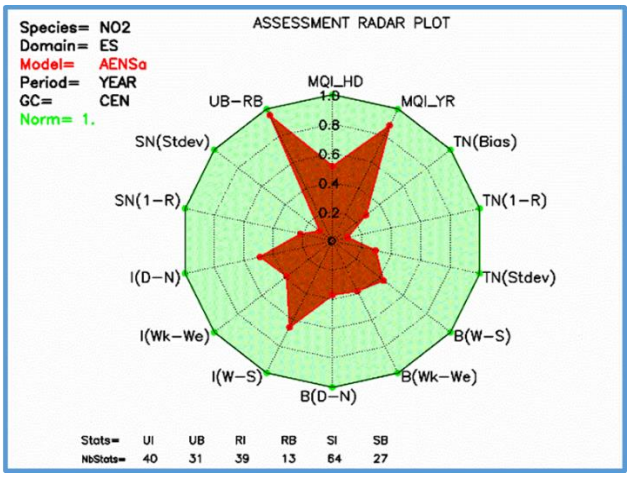
All active indicators are displayed in a radar setting. A specific MQO is met if the corresponding indicator (its 90th percentile) is less than 1, i.e., within the green zone.
The line below the plots indicates the types of stations included. For single plots (e.g., model, species, domain, period, GC), the "number of valid stations / the number of selected stations"

shows which stations meet the 75% rule of model and observational data coverage over the period.

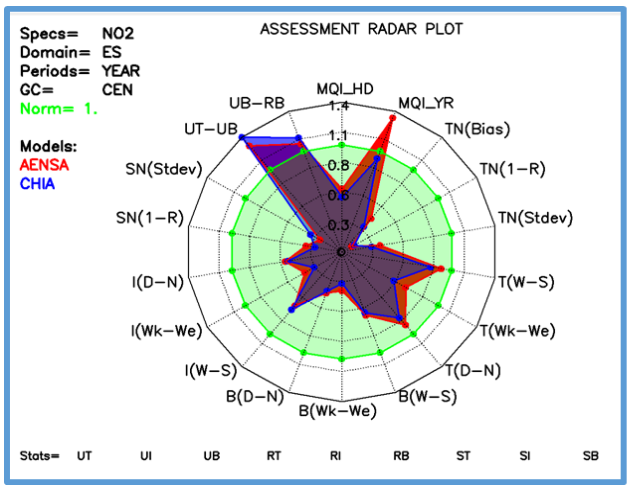
Examples of radar plots include:



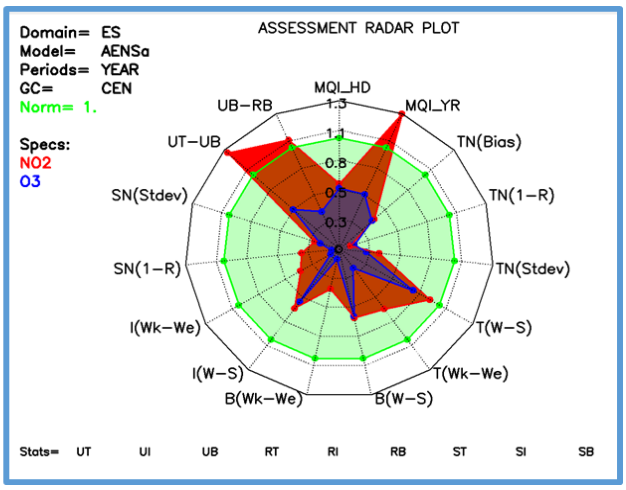
Radar plot with all ES stations. [AENSa;NO2;ES;YEAR;CEN].



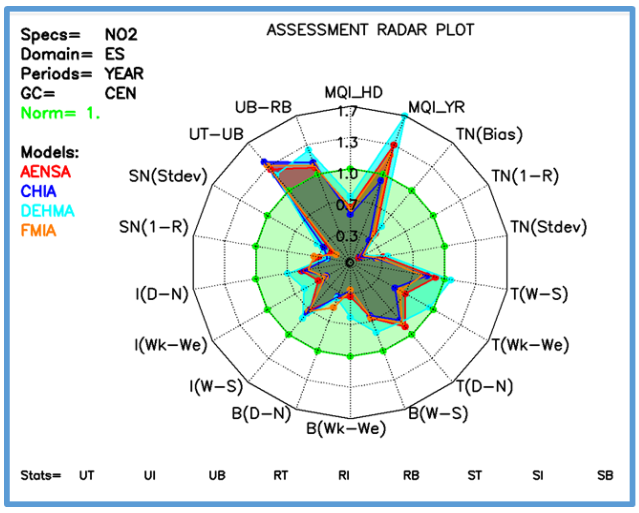
Same plot with Traffic stations excluded. [AENSa;NO2;ES;YEAR;CEN].



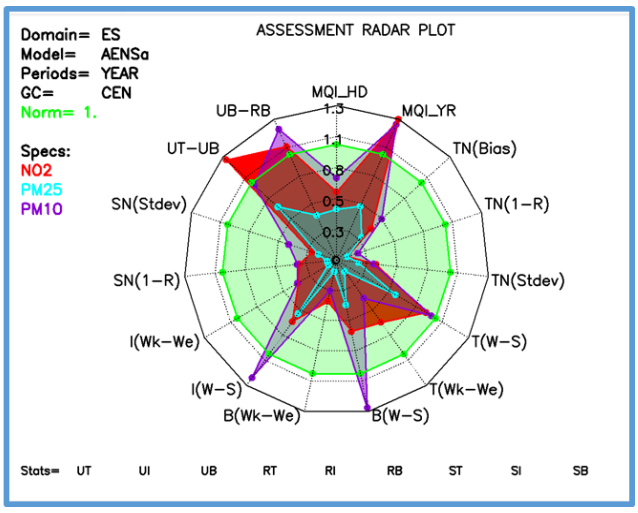
Radar plot with two models superimposed. [AENSa,CHIa;NO2;ES;YEAR;CEN].



Radar plot with two species superimposed. [AENSa;NO2,O3;ES;YEAR;CEN].



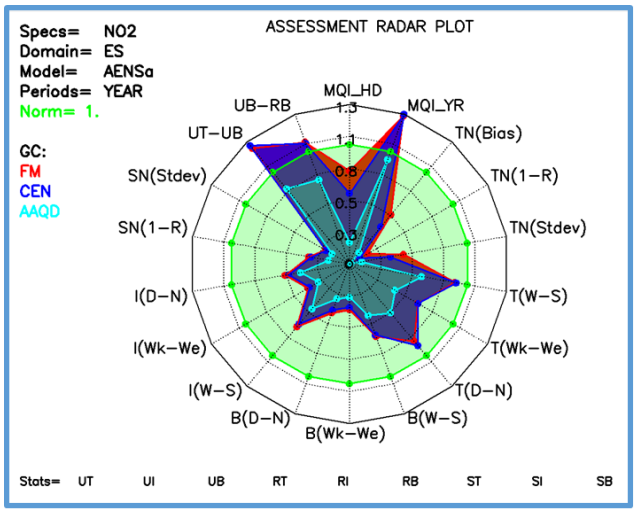
Radar plot with four models superimposed.

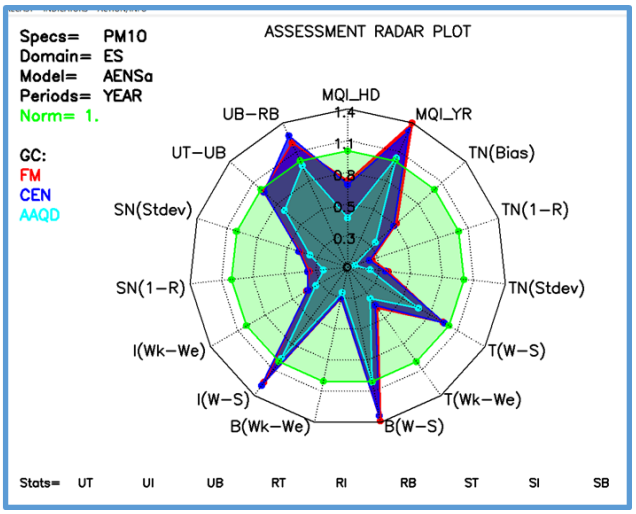


Radar plot with three species superimposed.

[AENSa,CHIa,DEHMa,FMIa;NO2;ES;YEAR;CEN].

[AENSa;NO2,PM25,PM10;ES;YEAR;CEN].



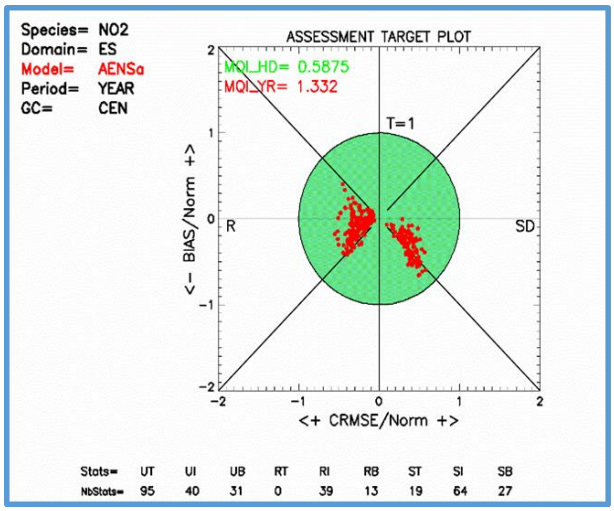


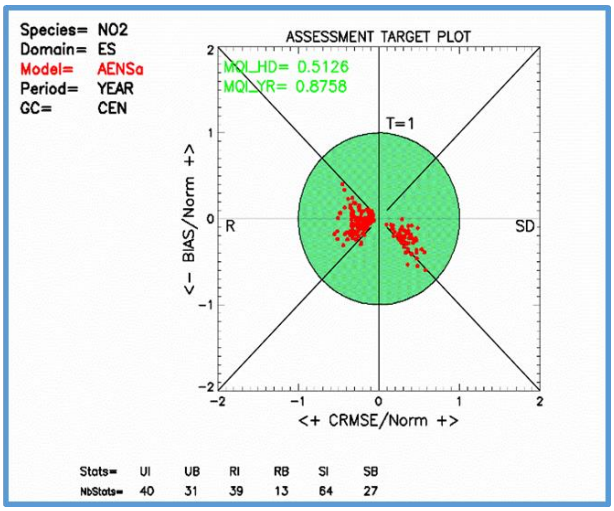
Radar plots (NO2 left, PM10 right) with three different sets of uncertainty parameters (FM, CEN, AAQD).
[AENSa;NO2;ES;YEAR;FM,CEN,AAQD].

[AENSa;PM10;ES;YEAR;FM,CEN,AAQD].

TARGET PLOT

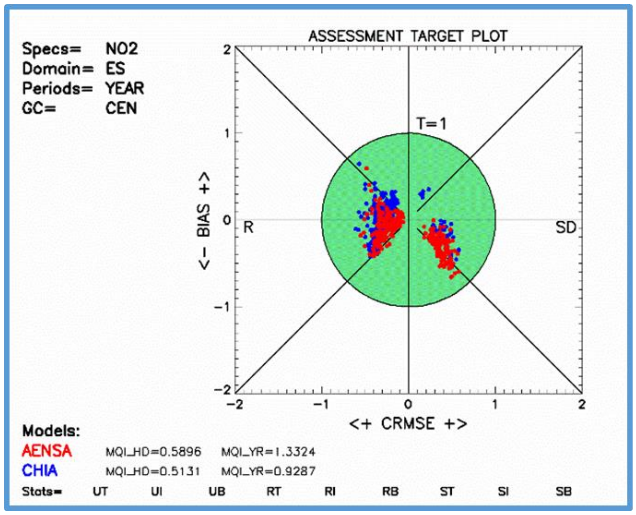
In the Target plot, observational-uncertainty normalized Bias is displayed on the vertical axis and similarly normalized CRMSE on the horizontal axis. The CRMSE is positive in both directions. A station dot appears on the right side of the diagram if the standard deviation (SD) dominates over the correlation coefficient (R) in the expression for CRMSE. Otherwise, it appears on the left side. Within the green area, the Target value (i.e., normalized RMSE) is less than or equal to 1 (T=1).
In Forecast mode, the Bias, CRMSE, and normalization are calculated with respect to the Persistence model (for details, see [4]).
Examples of Target plots include:



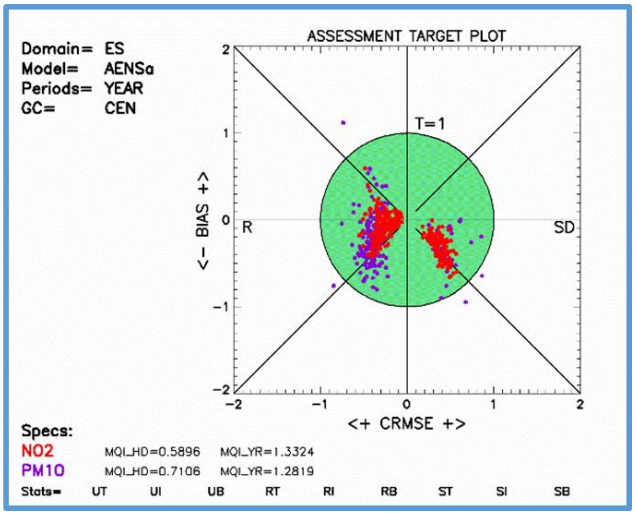


Target plot with all ES stations with MQI values in the diagram. [AENSa;NO2;ES;YEAR;CEN].

Target plot with Traffic stations excluded [AENSa;NO2;ES;YEAR;CEN].



Target plot with two models superimposed. [AENSa,CHIa;NO2;ES;YEAR;FM,CEN,AAQD].



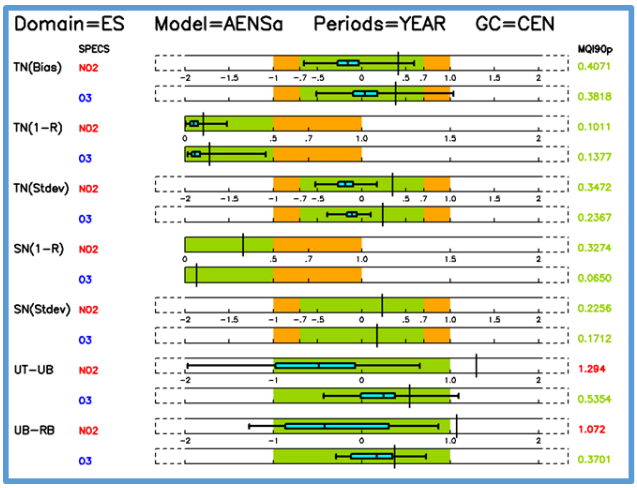
Target plot with two species superimposed. [AENSa;NO2,PM10;ES;YEAR;FM,CEN,AAQD].

TEMPORAL.SPATIAL (TS) REPORT

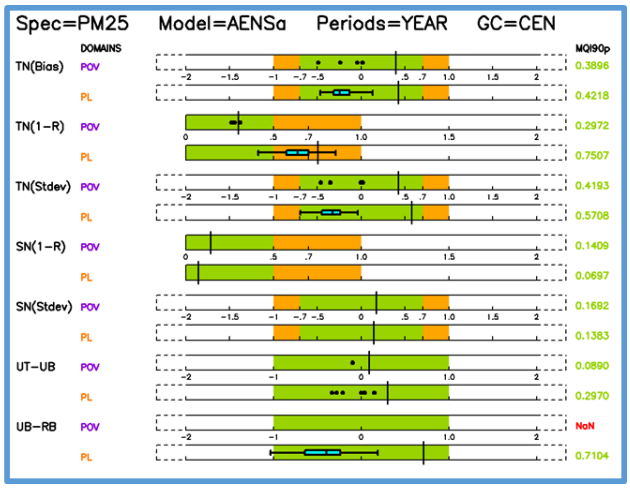
The TS Report shows bar plots with Temporal and Spatial indicators. Each horizontal bar represents station values using black dots. If the number of stations/dots on a bar exceeds 15, the stations are grouped into a blue box, extended by lines to the right and left. The values of the box indicate the 25th percentile, median, and 75th percentile. The extension to the left gives the minimum value, and the extension to the right gives the maximum value.

A vertical line on each bar shows the position of the 90th percentile MQI (Model Quality Indicator), with the value listed in the column on the right-hand side of the diagram. If this 90th percentile MQI is within the coloured part of the bar, the MQO (Model Quality Objective) is fulfilled (green if in the coloured zone, red otherwise). For the difference between orange and green we refer to [1].

Examples of TS Reports include:



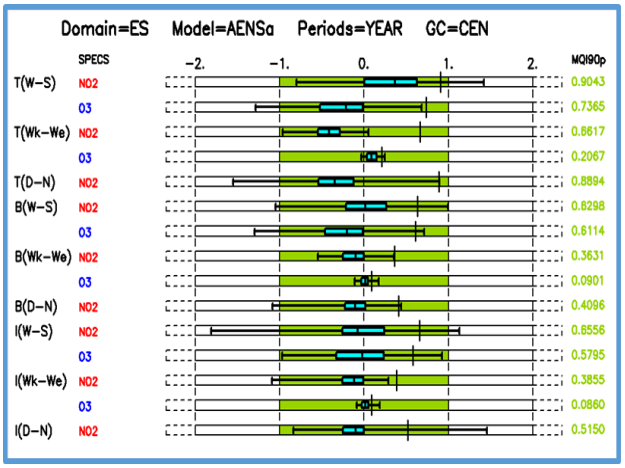
TS Report for two species with station dots and blue Boxes. [AENSa;NO2,O3;ES;YEAR;FM,CEN,AAQD]



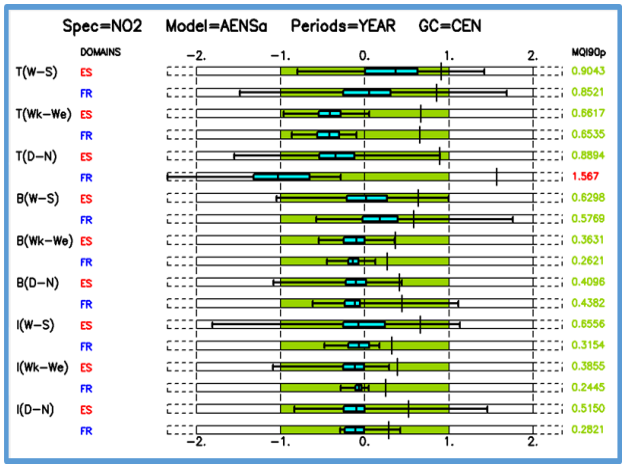
TS Report for two domains. [AENSa;NO2,O3;POV,POL;YEAR;FM,CEN,AAQD].

DYNAMIC.EVALUATION (DE) REPORT

The Dynamic Evaluation Report shows bar plots for Dynamic Evaluation indicators, with station dots and blue boxes presented similarly to the TS Report.
The vertical line on each bar indicates the position of the 90th percentile MQI, with the value shown in the right-hand column (green if in the green zone, red if outside).
The MQO is fulfilled if the 90th percentile MQI is within the green part of the bar.
Examples of DE Reports include:



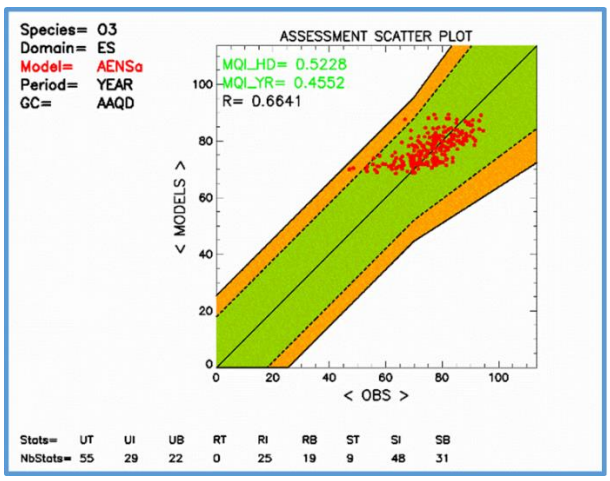
DE Report for two species. [AENSa;NO2,O3;ES;YEAR;CEN].



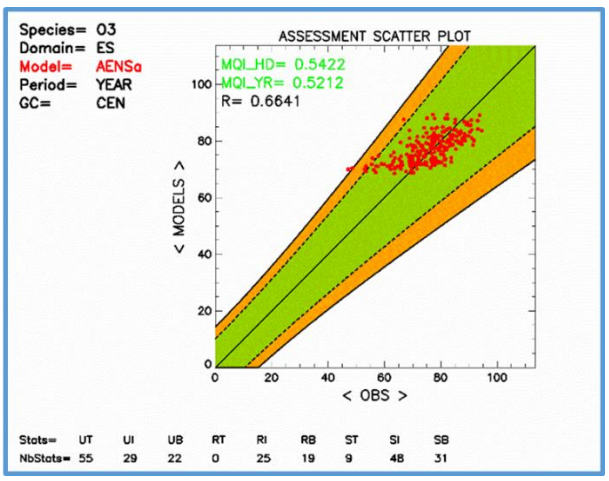
DE Report for two domains. [AENSa;NO2;ES,FR;YEAR;CEN].

SCATTER PLOT

The Scatter Plot is a classic comparison of Observations (on the horizontal axis) versus Model results (on the vertical axis). The plot includes a coloured area representing the uncertainty zone. For more details on the differences between green and yellow zones, refer to [1].

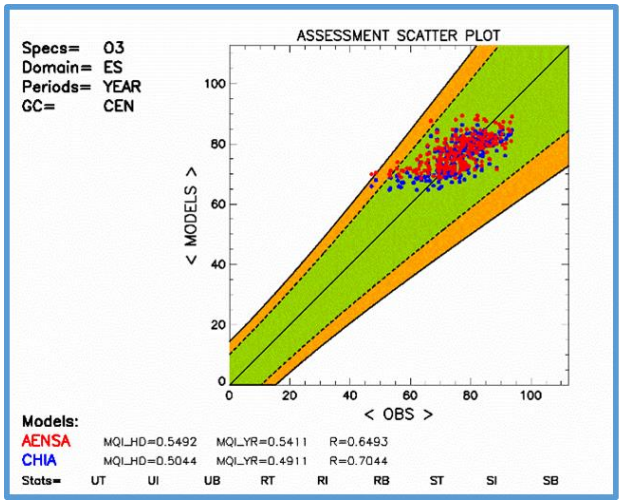


Scatter plot with CEN uncertainty zone. [AENSa;O3;ES;YEAR;AAQD].

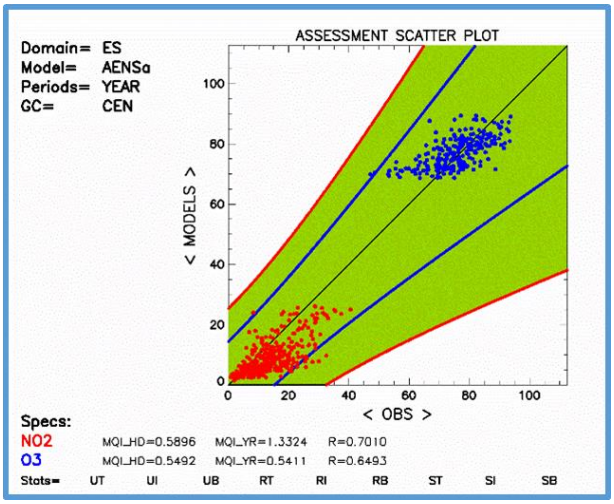


Scatter plot with AAQD uncertainty zone. [AENSa;O3;ES;YEAR;CEN].

Since the parameters for the uncertainty zone depend on the species, we indicate, in a multiple species scatter plot, the uncertainty zones by coloured borders (panel below right).



Scatter plot with two models [AENSa,CHIa;O3;ES;YEAR;CEN].

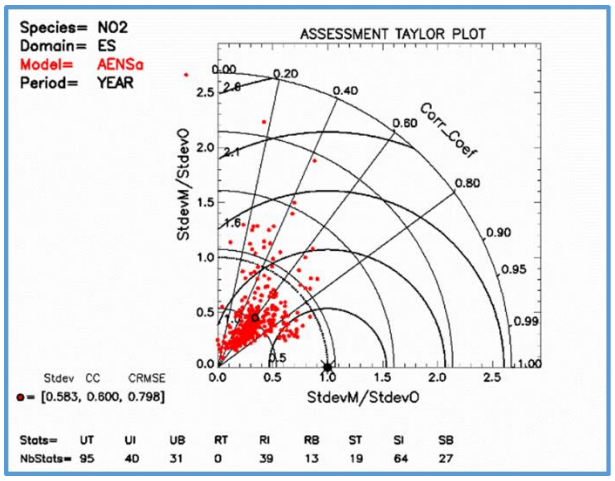


Scatter plot for 2 species with different uncertainty zones bounded by the species-fixed colours (red and blue in this case). [AENSa,CHIa;NO2,O3;ES;YEAR;CEN].

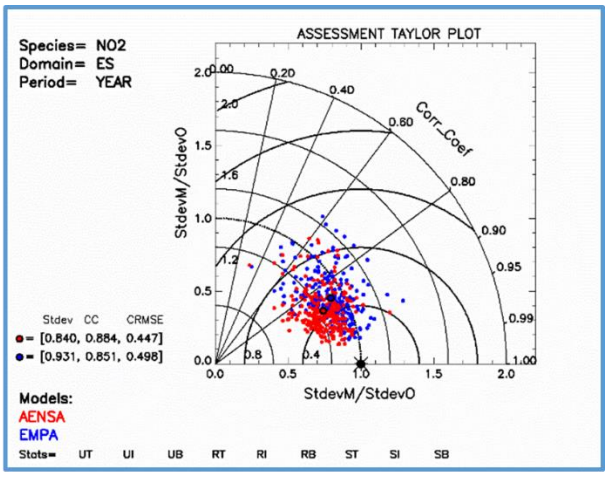
TAYLOR PLOT

The Taylor plot visualizes a combination of three statistics for each station: the Correlation Coefficient between model results and observations (represented by the azimuthal angle), the normalized Standard Deviation (StdevM) of the model results (represented by the radial distance from the station point to the origin of the diagram), and the normalized CRMSE (represented by the distance from the station point to the coordinates (1,0)). The normalization is based on the observational standard deviation (StdevO).

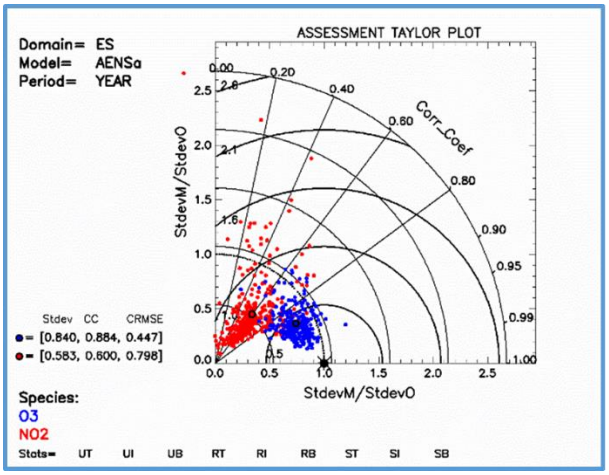
The values of MQI_HD and MQI_YR are displayed either in the upper right part or below the diagram.



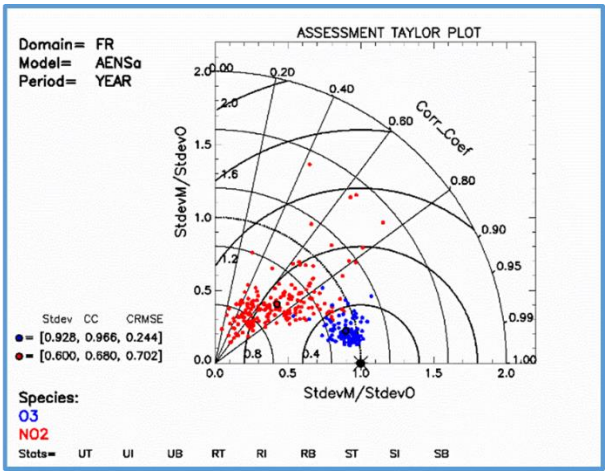
Taylor plot for NO2 and all ES stations for model AENSa [AENSa;NO2;ES;YEAR].



Taylor plot for O3 and two different models (AENSa, EMPa). [AENSa,EMPa;NO2;ES;YEAR].



Taylor plot for two species (NO2, O3) for ES stations [AENSa;O3,NO2;ES;YEAR].



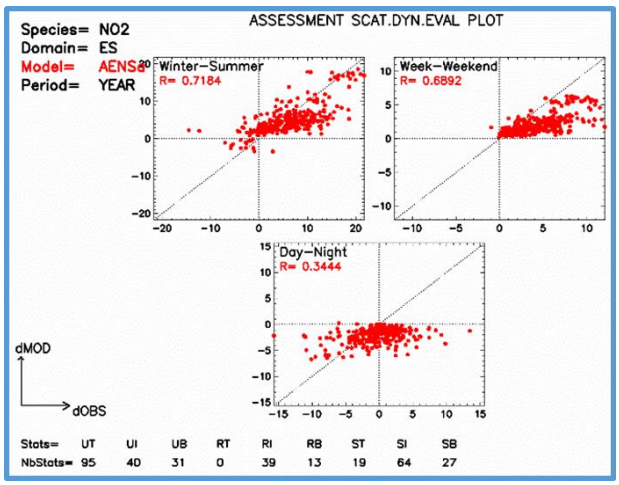
Taylor plot for two species (NO2, O3) for FR stations [AENSa;O3;FR;YEAR].

SCATTER.DYNAMIC.EVALUATION (SDE) PLOT

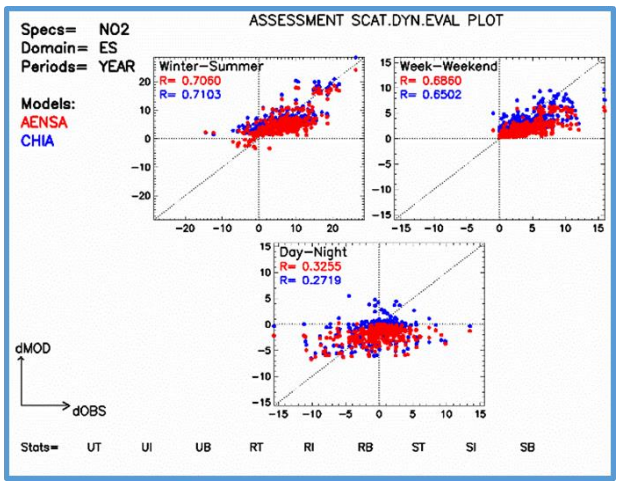
The following graphics show Scatter plots of differences Winter-Summer, WeekDays-WeekEndDays, and DayTimeHours-NightTimeHours. Observations on the x-axis, Models on the y-axis. In formulae:

Winter - Summer:	$(W - S)_{MOD}$ vs $(W - S)_{OBS}$
WeekDays - WeekEnd:	$(Wk - We)_{MOD}$ vs $(Wk - We)_{OBS}$
DayTimeHours - NightTimeHours:	$(D - N)_{MOD}$ vs $(D - N)_{OBS}$

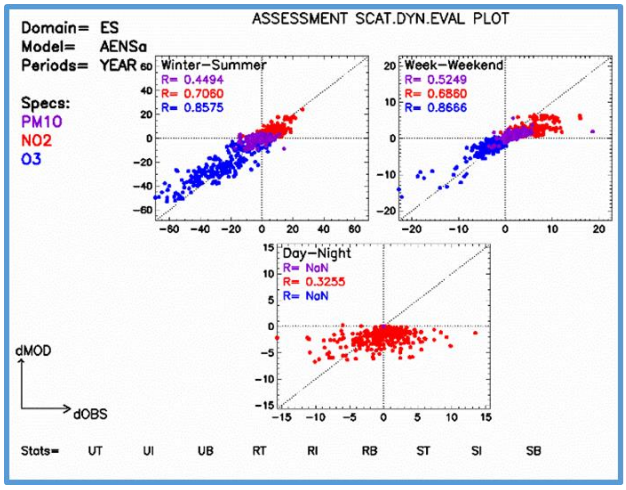
where W, S, Wk, We, D, and N refer to its mean values.



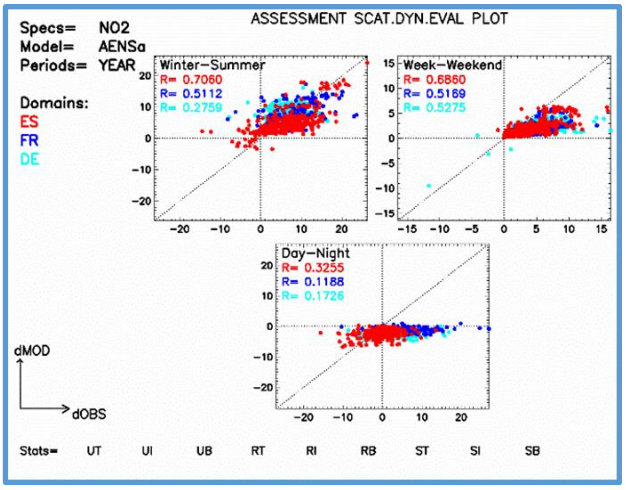
SDE plot for NO2 and ES stations. [AENSa;NO2;ES;YEAR].



SDE plot for NO2, and two models in red and blue. [AENSa,CHIa;NO2;ES;YEAR].



SDE plot for three species. No D-N dots for O3 and PM10, because of their daily values. [AENSa;PM10,NO2,O3;ES;YEAR].



SDE plot for NO2, and three domains. [AENSa;NO2;ES,FR,DE;YEAR].

BAR PLOT

The Bar Plot compares observations and model results for each group of station type and area. Observations are shown on the vertical axis as bars, with model results displayed as dots. Mean values (weighted over the number of TA stations) are indicated on the right-hand side of the panels: for Observations ▢, and coloured dots ● for models.

Bar plots can be generated to display the concentration of species for one or more individual stations (up to four) or for the mean values over a group of stations identified by a NUTS code (any level, e.g., ES112, ES11, ES1, or ES). The default time interval corresponds to the active Period, but this can be adjusted in the 'Time-Interval (Hrs)' editable field (e.g., 4000 4500).

The 'SHOW BAR PLOTS' button will produce all the Bar Plots for each of the selections made in the drop down lists (single graphics, i.e. one model, one species, one domain, and one period at the time). The GOAL/CRIT selection button is not active.

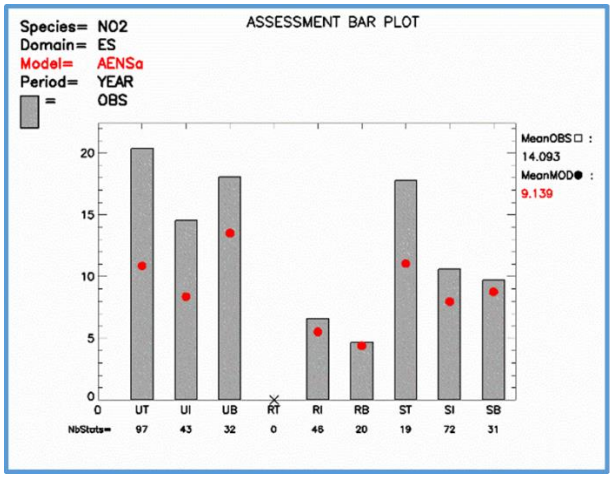
Multiple Bar Plots (i.e. for more than one species (less or equal to 4), or more than one domain, and more than one model) can be visualized directly (i.e. without executing DTL) using the editable field below the 'SHOW GRAPHIC' button.

Exemples of editable input are:

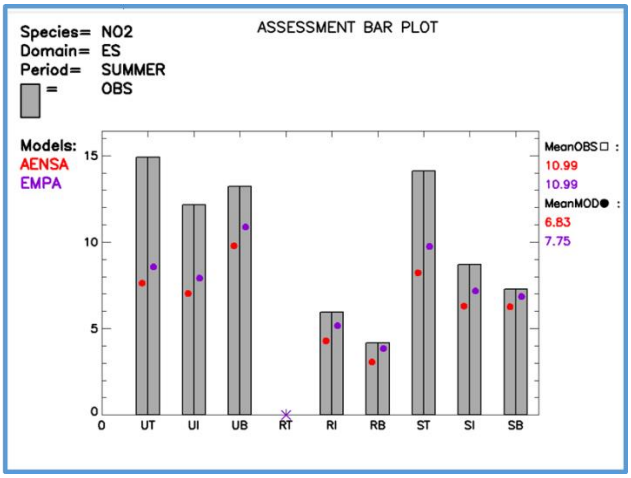
MOD1; NO2,O3; FR1 (Bar plot on NUTS FR1)
MOD1,MOD2; O3 ;FR,FR1 (Bar plot on NUTS FR and FR1 for 2 models)
MOD1,MOD2; O3,PM10 ;FR1 (Bar plot on NUTS FR1 for O3 and PM10)

There is an option to visualize i) Only Models (i.e. no Observations), ii) Models and Observations, which in the case of a NUTS code selection implies mean values on a common set of MOD and OBS stations, and iii) Both Models and Observations on all available Mod stations and OBS stations.

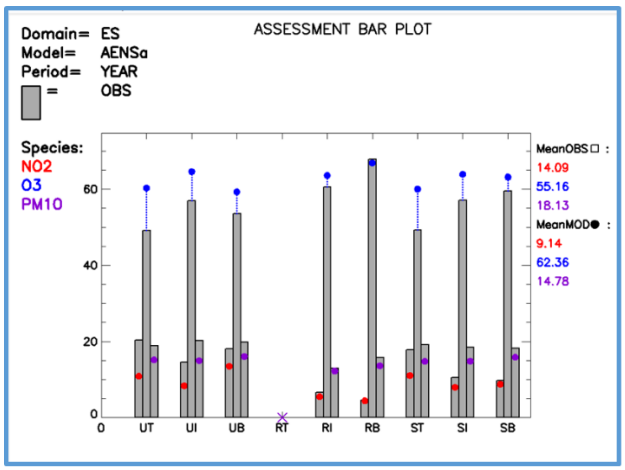
Examples of Bar Plots include:



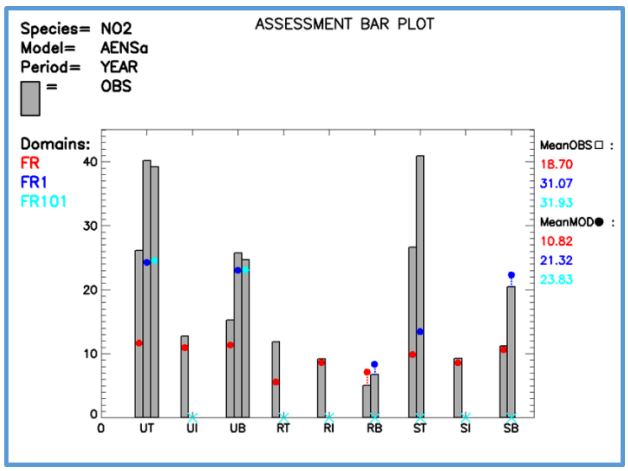
Bar plot with observation bars (grey) and red model dots. [AENSa;NO2;ES;YEAR].



Bar plot with observation bars (grey) and coloured dots for two models. Period is Summer. [AENSa,EMPa;NO2;ES;SUMMER].



Bar plot with observation bars (grey) and (coloured) model dots for three species. [AENSa;NO2,O3,PM10;ES;YEAR].



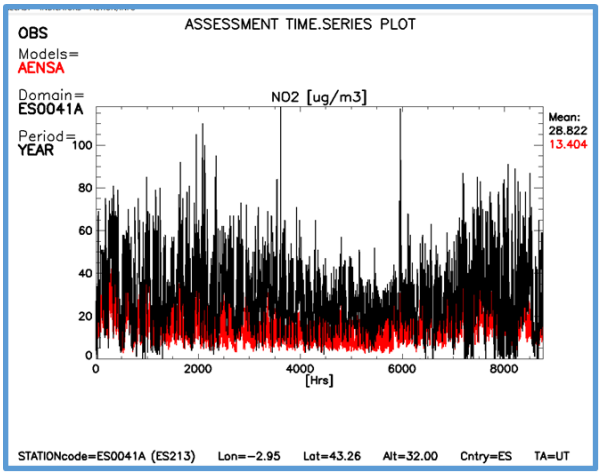
Bar plot with observation bars (grey) and coloured model dots for 3 domains (FR France, FR1 Ile-de-France, FR101 Paris-City). [AENSa;NO2;FR,FR1,FR101;YEAR].

TIME SERIES

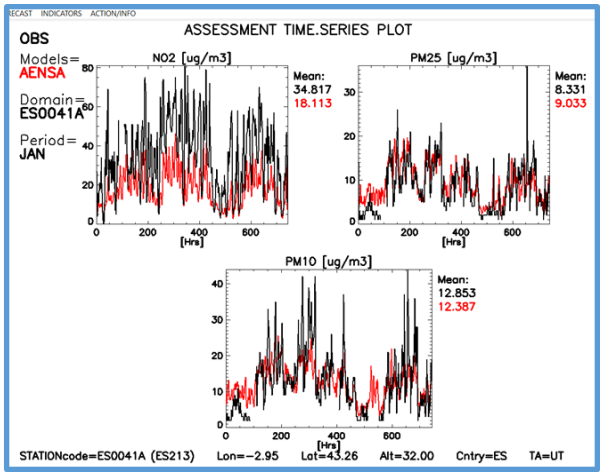
Time series plots can be generated to display the concentration of species for one or more individual stations (up to four) or for the mean values over a group of stations identified by a NUTS code (any level, e.g., ES112, ES11, ES1, or ES). The default time interval corresponds to the active Period, but this can be adjusted in the 'Time-Interval (Hrs)' editable field (e.g., 4000 4500).
The 'SHOW TIME SERIES' button will produce all the Time Series for each of the selections made in the drop down lists (single graphics, i.e. one model, one species, one domain, and one period at the time). The GOAL/CRIT sepection is not active.
Multiple Time Series (i.e. for more than one species (<= 4), or more than one domain (<= 4), and more than one model) can be visualized directly (i.e. without executing DTL) using the editable field below the 'SHOW GRAPHIC' button.

There is an option to visualize i) Only Models (i.e. no Observations), ii) Models and Observations, which in the case of a NUTS code selection implies mean values on a common set of MOD and OBS stations, and iii) Both Models and Observations on all available Mod stations and OBS stations.

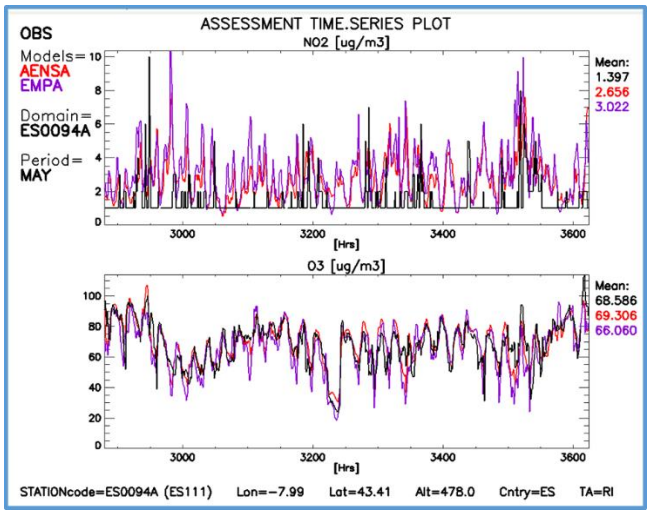
Mean values of observations and model concentrations are displayed on the right-hand side of the graphic.



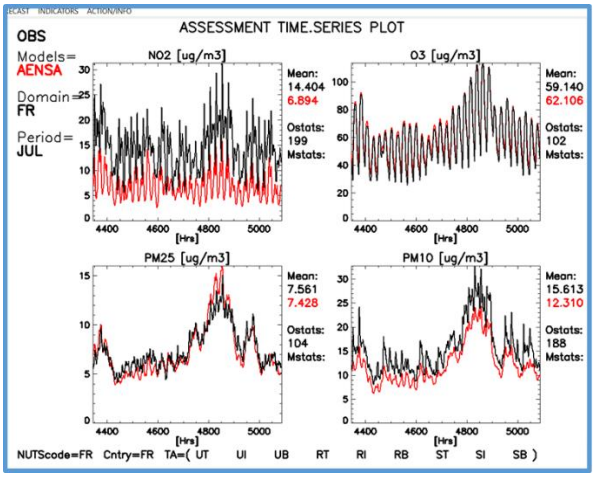
Time series NO2, model AENSa, full year at station ES0041A, including observations.
[AENSa;NO2;ES0041A;YEAR].



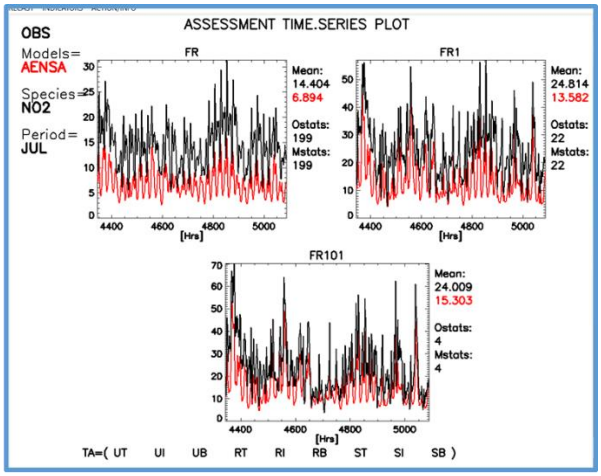
Time series NO2, PM2.5, PM10, Station ES0041A, time Interval January (0 - 744 hrs), model AENSa, [AENSa;NO2,PM25,PM10;ES0041A;JAN].



Time series for NO2 and O3, models AENSa and EMPa,
Station is ES0094A, covering the time interval May (2882 – 3624 hrs).
[AENSa,EMPa;NO2,O3;ES0094A;MAY].



Time series for NO2, O3, PM2.5 and PM10, model AENSa, mean values over a common set of Stations in NUTS FR (France), time interval July (4344 – 5088 hrs). [AENSa;NO2,O3,PM25,PM10;FR;JUL].



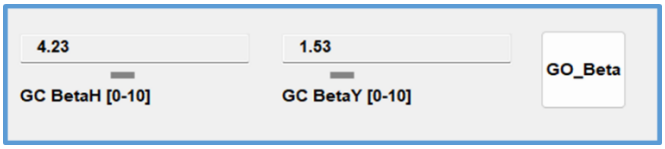
Time series for NO2, model AENSa, mean values over Stations NUTS FR (France), FR1 (Ile-de-France), and FR101 (Paris-City), time interval July (4344 – 5088 hrs). [AENSa;NO2;FR,FR1,FR101;JUL].

Beta Sliders

The factors betaH and betaY, which appear in the definitions of all the indicators, are proportionality coefficients specific to pollutants and measurements. These betas determine the maximum allowable modeling uncertainty and, consequently, the stringency of the validation process (i.e. the MQO).

Proposed values for three different sets of uncertainty parameters are provided in the tables in Annex 2. For the CEN values, we refer to [5], noting that the beta's in this DTL manual are equal to $\sqrt{(1 + betaC^2)}$, where betaC corresponds to the values in the CEN report.

To facilitate studying the impact of the beta values, beta sliders have been added to the Tool. The sliders can be activated via the second line in the ACTIONS/INFO tag.



The initial slider values are determined by the selected set of uncertainty parameters (Goals & Criteria: FM, CEN, or AAQD).

For the selected beta values, the 90th-percentile values of all indicators are saved in the 'MQI90p_Beta.dat' file located in the Output folder.

While multiple selections are allowed for Models and Domains, Species and Periods must be selected individually.

Note that the indicators MQI_HD, TN(Bias), TN(1-R), and TN(Stdev) depend on betaH, whereas all other indicators depend on betaY.

The following formula applies to the value of any indicator IND corresponding to beta (example: CEN, similarly for FM and AAQD):

$$IND = Beta_{CEN} * IND_{CEN} / Beta,$$

where IND_{CEN} is the indicator value for $Beta_{CEN}$.

To Do

Some features are still in development:

- A vertical scroll is needed in TS.Report and Dyn.Eval.Report.
- Development of R version.

References

[1] P. Thunis, C. Cuvelier, et al. Delta Tool version 7.0. Concepts, User's Guide, Diagrams. 2022.
[2] P. Thunis, L. Tarrasón. Proposal for a QA/QC protocol to support modelled assessments of air quality. Fairmode publication. 2020
[3] S. Janssen, P. Thunis. et al. FAIRMODE Guidance Document on Modelling Quality Objectives and Benchmarking. JRC Technical Report EUR 31068 EN. 2022.
[4] L. Vitali, C. Cuvelier, et al. A standardized methodology for the validation of air quality forecast applications (F-MQO). Lessons leant from its applications across Europe. Geosci. Model Dev. 16, 6029-6047, 2023.
[5] CEN-TC 264-WG 43_N297_V17 / WG 43 N 295/297 CEN working document, 2021.

Annex 1: Definition of Indicators

MQI_HD, MQI_YR, (MQI_FC), TN(Bias), TN(1-R), TN(Stdev), T(W-S), T(Wk-We), T(D-N), B(W-S), B(Wk-We), B(D-N), I(W-S), I(Wk-We), I(D-N), SN(1-R), SN(Stdev), UT-UB, UB-RB

MQI indicators:

1. MQI_HD = sqrt[crmse(Mod,Obs)^2 + bias(Mod,Obs)^2] / resH = rmse(Mod,Obs) / resH
   with resH= betaH*critH
2. MQI_YR = abs[mean(Mod)-mean(Obs)] /resY
   with resY= betaY*critY
3. MQI_FC = sqrt[rmse(Mod,Obs) / rmse(Pers,Obs)]

Temporal indicators:

4. TN(Bias) = abs[mean(Mod)-mean(Obs)] / (betaH*critH)
5. TN(1-R) = 2*stdev(Mod)*stdev(Obs)*(1-correlate(Mod,Obs)) / (betaH*critH)^2
6. TN(Stdev) = abs[stdev(Mod)-stdev(Obs)] / (betaH*critH)
7. T(W-S) = abs[[mean(Mod[Whrs])-mean(Obs[Whrs])] / (betaY*critY(Whrs)) -
   [mean(Mod[Shrs])-mean(Obs[Shrs])] / (betaY*critY(Shrs))]
   for Traffic (T) stations.
8. T(Wk-We) = similar WeekDayHrs – WeekEndHrs for T stations
9. T(D-N) = similar DayTimeHrs – NightTimeHrs for T stations
10. B(W-S) = similar for Background (B) stations
11. B(Wk-We) = similar for Background (B) stations
12. B(D-N) = similar for Background (B) stations
13. I(W-S) = similar for Industrial (I) stations
14. I(Wk-We) = similar for Industrial (I) stations
15. I(D-N) = similar for Industrial (I) stations

Spatial indicators:

16. SN(1-R) = 2*stdev(meanMS)*stdev(meanOS)*(1-correlate(meanMS,meanOS)) / (betaY*sumsq)^2
    with meanMS = mean Mod over stations
    with meanOS = mean Obs over stations
    with sumsq = sqrt[mean(critY^2)] over stations
17. SN(Stdev) = abs[stdev(meanMS)-stdev(meanOS)] / (betaY*sumsq)
18. UT-UB = abs[(mean(Mod(UT station)) – mean(Obs(UT station))) / (betaY*critY(UT station)) -
    (mean(Mod(nUB station)) – mean(Obs(nUB station))) / (betaY*critY(nUB station))]
    with nUB the nearest UB station to the UT station
19. UB-RB = similar for UB and RB stations

where:

for GC= FM, CEN: critH= (UrLVH/100)*sqrt[(1-alfaH^2)*(stdev(Obs)^2 + mean(Obs)^2) + (alfaH*LVH)^2)]
critY= (UrLVY/100)*sqrt[(1-alfaY^2)*(mean)Obs)^2)/NeffY + ((alfaY*LVY)^2)/NnpY]

for GC= AAQD: critH= relTH*mean(max(Obs,LVH))
critY= relTY*mean(max(Obs,LVY))

The Obs uncertainty (GC) parameters are given in the Tables of Annex 2.

Spatial-Temporal indicators: 4, 5, 6, 16, 17, 18, 19
Dynamic Evaluation indicators: 7, 8, 9, 10, 11, 12, 13, 14, 15
Winter - Summer indicators= 7, 10, 13
Week - WeekEnd= 8, 11, 14
Day - Night indicators= 9, 12, 15

Annex 2: Uncertainty parameters

FM	NO2	O3	PM2.5	PM10
alfaH	0.2	0.79	0.5	0.25
LVH	200	120	25	50
UrLVH	24	18	36	28
NeffH	5.2	11	20	20
NnpH	5.5	3	1.5	1.5
BetaH	2	2	2	2
alfaY	0.2	0.79	0.5	0.25
LVY	200	120	25	50
NeffH	5.2	11	20	20
NnpH	5.5	3	1.5	1.5
UrLVY	24	18	36	28
BetaY	2	2	2	2

GC parameters: FM

CEN	NO2	O3	PM2.5	PM10
alfaH	0.2	0.4	0.6	0.35
LVH	200	100	25	45
UrLVH	15	15	25	25
NeffH	1	1	1	1
NnpH	1	1	1	1
BetaH	3.35	2.42	2.69	2.42
alfaY	0.97	0.4	0.8	0.6
LVY	20	70	10	20
UrLVY	30	15	30	20
NeffH	1	1	1	1
NnpH	1	1	1	1
BetaY	1.72	1.93	1.97	1.64

GC parameters: CEN

AAQD	NO2	O3	PM2.5	PM10
LVH	200 / 50	70	25	45
RelTH	0.15	0.15	0.25	0.25
BetaH	3.35	2.42	2.69	2.42
LVY	20	70	10	20
RelTY	0.3	0.15	0.3	0.2
BetaY	1.72	1.93	1.97	1.64

GC parameters: AAQD

Annex 3: Conversion from Longitude, Latitude to NUTS code

R program for the conversion of Longitude/Latitude coordinates to NUTS code level 3:

```
# October 06, 2024
C. (Kees) Cuvelier

#Input file: 2 colums (Lons, Lats), 1= Longitudes, 2= Latitudes
LLinput <- "LonLatInput.dat"
setwd("C:/Rworkspace")
sep=" "   # separator in input file
digits=8  # number of digits in output

# Library:
library(giscoR)
library(sf)
library(stringr)
library(dplyr)
library(tibble)

# Read the input data file

conn <- file(LLinput,open="r")
linn <-readLines(conn)
nlines <- length(linn)
close(conn)

# Initialize vectors for longitudes and latitudes
Lons <- numeric(nlines - 1)
Lats <- numeric(nlines - 1)

# Extract longitudes and latitudes
for (i in 2:nlines) {
  hlp <- str_split_fixed(linn[i], sep, n = Inf)
  Lons[i - 1] <- as.numeric(hlp[1])
  Lats[i - 1] <- as.numeric(hlp[2])
}

# Create a data frame with longitudes and latitudes
df_latlon <- tibble( "longs" = Lons,"lats" = Lats)
Lons <- df_latlon$longs
Lats <- df_latlon$lats

# Convert to spatial data and join with NUTS regions
  df_latlon_sf <- df_latlon %>%
  st_as_sf(coords = c("longs","lats"), crs = 4326) %>%
  st_join(gisco_nuts) %>%
  filter(LEVL_CODE == 3 | is.na(LEVL_CODE))

# Extract NUTS region IDs
NUTS <- df_latlon_sf$NUTS_ID

# Combine longitudes, latitudes, and NUTS into a single data frame
df_combined <- data.frame(Lons = Lons, Lats = Lats, NUTS = NUTS)

# Save the combined data as a .dat file
write.table(format(df_combined,digits=digits),
"C:/Rworkspace/LonLatNUTS.dat", sep =  sep,
            row.names = FALSE, col.names = TRUE, quote = FALSE, na="")

# Display the data frame
print(df_combined)

print.noquote(" ")
print("END LonsLats2NUTS.R program ---- OUTPUT > LonLatNUTS.dat")
```

Example:

Input file LonLatInput.dat:

Lons	Lats
10.9292	44.6431
11.3336	44.4714
1.71699	42.5349
11.9611	44.8417
13.3934	45.9752
13.6711	48.3917
13.7945	45.6206
8.80384	45.8389
9.02640	45.6294
9.38466	46.1400
1.56525	42.5169

Output file LonLatNUTS.dat

Lons	Lats	NUTS
10.92920	44.6431	ITH54
11.33360	44.4714	ITH55
1.71699	42.5349	NA
11.96110	44.8417	ITH56
13.39340	45.9752	ITH42
13.67110	48.3917	AT311
13.79450	45.6206	ITH44
8.80384	45.8389	ITC41
9.02640	45.6294	ITC41
9.38466	46.1400	ITC42
1.56525	42.5169	NA

(NA = NUTS not identified)