



# Synthesis of WG3 meeting and topics for future activity

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**Fairmode Technical meeting**  
**Zagreb, 27-29 June 2016**

# First intercomparison for Receptor (RM) and Chemical Transport models (CTM).

The intercomparison is useful for:

- Evaluating the overall source apportionment model performance on the basis of pre-established criteria,
  - ✓ *for the purposes of air quality management (AQM)*
- Obtaining an indirect measure of the overall output uncertainty,
- Generating more robust SA results (from a single outcome to an ensemble)
- Cross-validating results (to overcome the lack in observed data)
- Providing insights to understand the models behavior:
  - ✓ *influence of specific factors (e.g. input data, type of site, type of pollutant, meteorological conditions, etc...)*
  - ✓ *sensitivity to modelling approaches (e.g. RMs vs CTMs) and assumptions*
- Learning about CTMs performance when used for purposes other than SA

# Evaluation in this IE

**RM**

**CTM**

**BOTH**

**SINGLE SITE**

**SINGLE SITE**

**MULTI SITE**

**Complementary tests:**

Mass apportionment  
Number of factor/sources

**Preliminary tests:**

Chemical profiles  
Contribution-to-species (all)  
Time-trends

**Performance tests**

Z-scores  
zeta-scores  
RMSD\*

**Complementary tests:**

Mass apportionment  
Number of factor/sources

**Preliminary tests:**

Chemical profiles  
Contribution-to-species (selected ones)  
Time-trends

**Performance tests:**

Z-scores  
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**Complementary tests:**

Mass apportionment  
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**Preliminary tests:**

Chemical profiles  
Contribution-to-species (selected ones)  
Time-trends

**Performance tests:**

Z-scores  
zeta-scores  
RMSD\*

# Participants



European  
Commission

## RM: 33 participants – 38 results

AGH-UST	ISAC LE	RIVM
APPATN	FMI	SAGE
ARPA ER	IDAEA_T	UCC
ARPA LO	IDAEA_A	UMH
ARPA PU	IMROH	UNIBO
ARSO	ISSeP	UNIHE
AUTH	IST	UNIMI
CARES	LGGE+	UNMIB
CNR IIA	NCSR	UNIFI
ENEA	PSI	UNIGE
ISAC BO	PUC	WUT

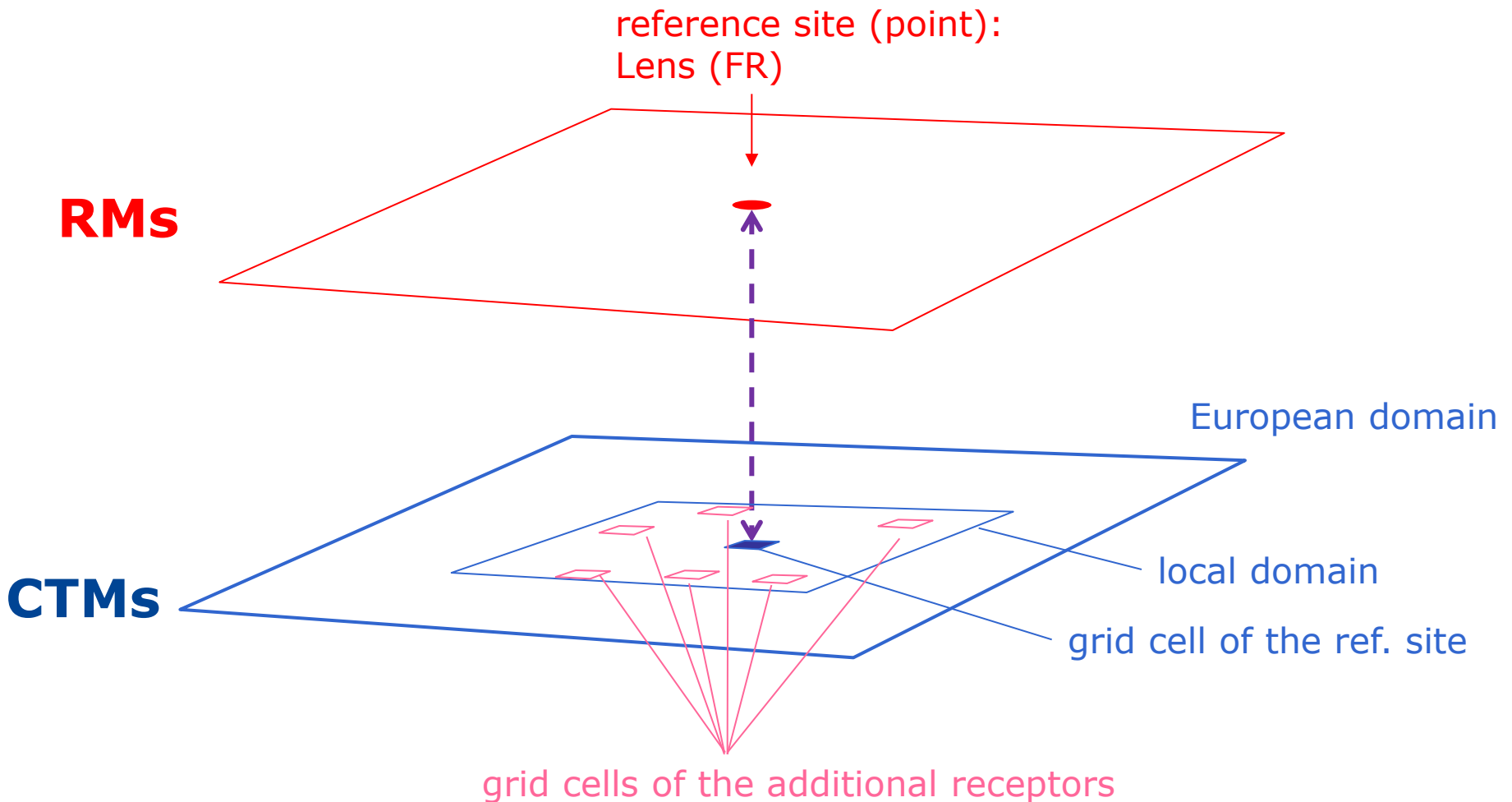
## CTM: 7 participants – 11 results

ENEA /ARIANET/ ARPA PIEMONTE	joint result
CIEMAT/LISA CNRS	joint result
RIER- UNI KOLN	independent result
TNO	independent result
ARPAV	coordinated result
RSE	coordinated results
UNIAVE	coordinated results

A,B,C,D,E,F,G,H,I,J,K,L,M,N,O,P,Q,R,S,  
T,U,V,W,X,Y,Z,\*A,\*B,\*C,\*D,\*E,\*F,\*G,\*  
H,\*I,\*J,\*K,\*L

cA,cAo,cAs,cAso,cAs2,cB,cBo,cD,cDo,  
cE,cEo,cF

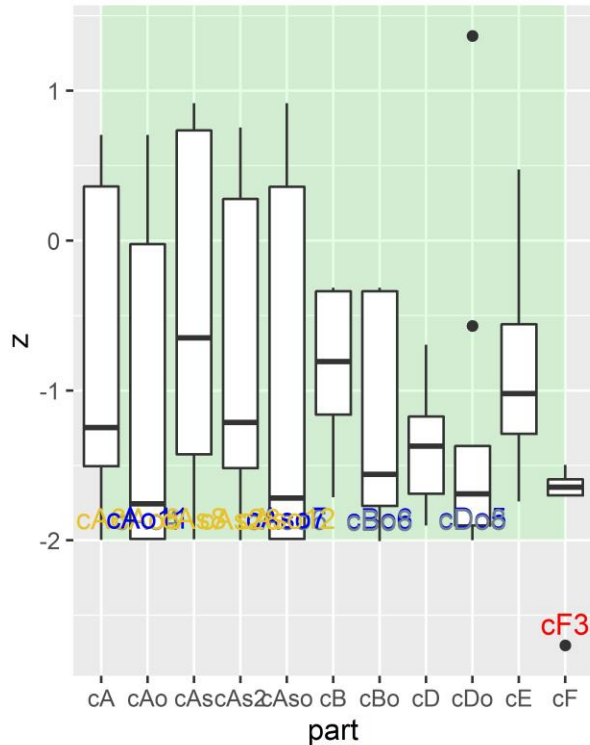
# Domains



# Performance of CTMs using RM as reference

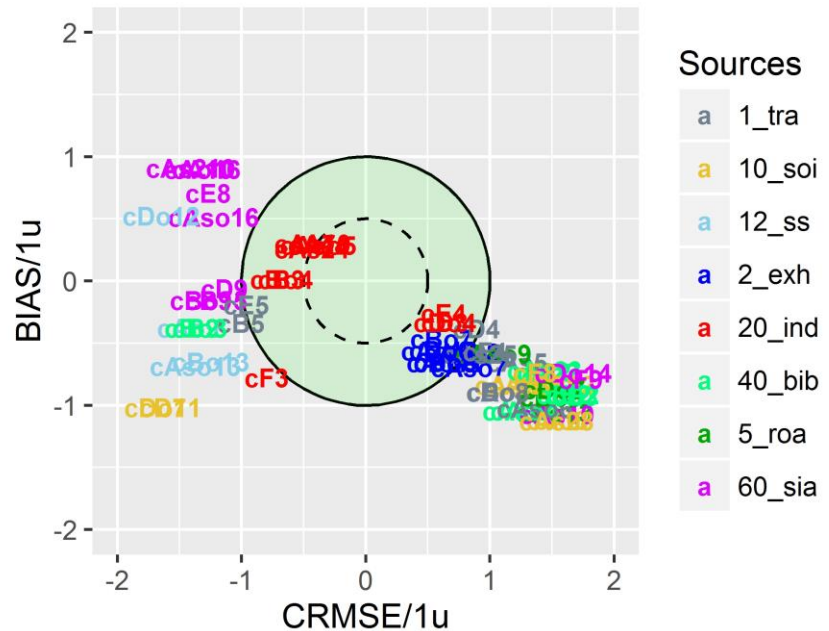
## Site: Lens

### z-score



SOURCE	Source ID	Description
a	1	traffic
a	10	soil
a	12	marine
a	2	exhaust
a	20	industry
a	40	biomass
a	5	road
a	60	SIA

### target



In both plots the best possible value is zero. The green background represents the acceptability area.

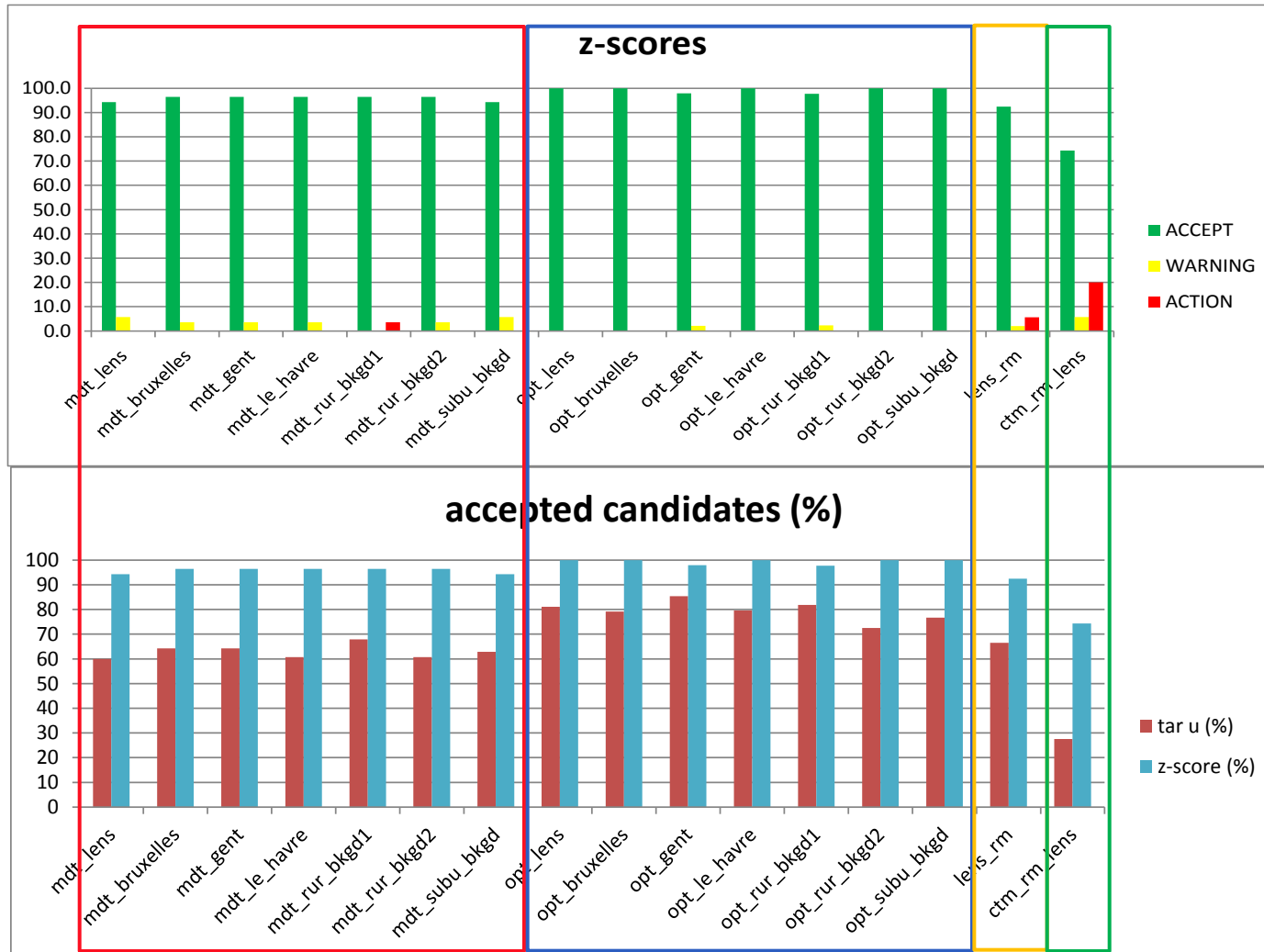
# Performance RM and CTMs ALL RECEPTORS



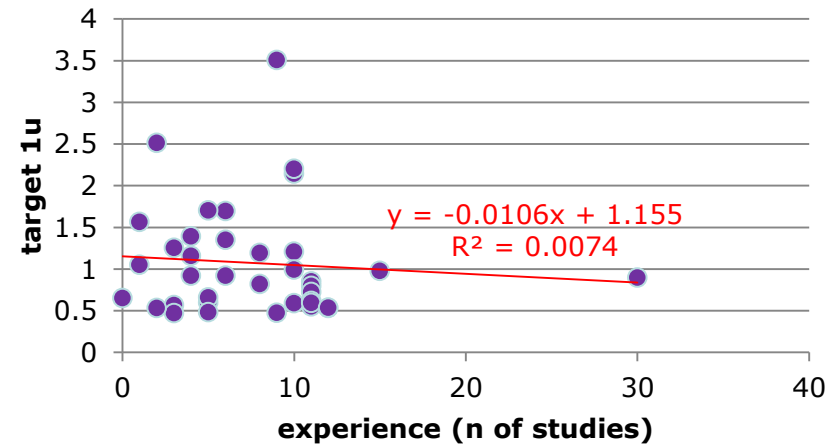
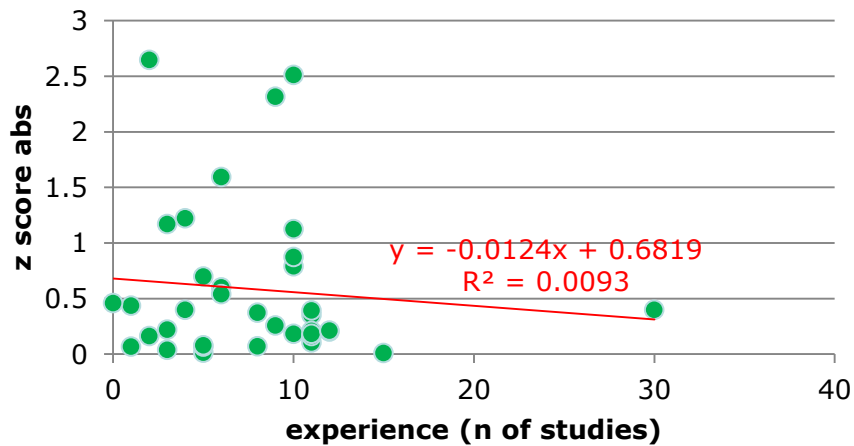
MDT:7 results 180 t. steps

OPT:4 results 180 t. steps

38 res. 7 res.  
116 ts 57 ts



## RM: analysis of practitioner experience



Users with more experience (at least 10 studies) obtain better performance.



# Preliminary conclusions of the IE

- In RMs convergence towards PMF5 (in part due to the good performances in previous IE) contributes to more homogeneous results.
- Industry source category needs better definition because too generic.
- CTMs show quite homogeneous behaviour when using exactly the same input data.
- the comparison of CTM with RM reference points out the underestimation of the some sources.
- Good performance for exhaust and biomass burning source categories which are comparable in the two families of models.
- Sensitivity analysis for CTM quantified the influence of vertical dispersion coefficient and of the grid scale in particular for urban areas.

# Intercomparison follow up

- E.V. more technical discussions of factors influencing RM results
- Dalia (organics, importance of uncertainty)
- Constrained analysis can be useful to improve the results? e.g. force sensible factor profiles
- PP importance of pre-treatment
- Constraints beyond EPA PMF5 to be explored
- G.P first glance to the performance of CTM now should explore the dataset more in detail to learn more about the CTM (detailed set of questions see slide by G.P.) WHO CAN DO WHAT
- G.C. spatial aspects of source apportionment with the LENS Data (timing to be decided)
- MM seasonal analysis of Lens data



European Commission

# On-line Delta SA tool

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**Chemical profile Similarity**

**Source Apportionment Model performance**

## Delta tool for Source Apportionment

### DeltaSA

It is an on-line tool to assess source apportionment model outputs. It works in two different modes. The first is the source chemical profiles similarity, the second mode consists in a complete test of the model result.



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## Delta tool for Source Apportionment

### DeltaSA

It is an on-line tool to assess source apportionment model outputs. It works in two different modes. The first is the source chemical profiles similarity, the second mode consists in a complete test of the model result.

### Chemical profile Similarity

Compares the chemical profile of a candidate source (e.g. a factor chemical profile) with the chemical profiles in SPECIATE (US-EPA) and SPECIEUROPE (EC-JRC) repositories. The similarity is computed using the Standardized Identity Distance (SID, Balle et al., 2013) and the Pearson Distance (PD, Pearson correlation coefficient).

**Upload the file(s) containing the chemical profile(s). There are two options (see examples in main page):**

- 1) zip file with three csv (comma separated values) files containing: a) the concentrations of the species in the profiles (mandatory), b) the time series of the contribution of the candidate sources, c) the uncertainties of the species concentrations in the profiles, respectively CCINC, TREND, and CUS.
- 2) The information in point 1 in one single xls or excel file.

All the data shall be expressed in  $\mu\text{g}/\text{m}^3$ .

Chemical Profile:

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**Chemical profile Similarity**

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## Delta tool for Source Apportionment

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It is an on-line tool to assess source apportionment model outputs. It works in two different modes. The first is the source chemical profiles similarity, the second mode consists in a complete test of the model result.

### Source Apportionment Model performance

The second of the tool uses a complete test of the results obtained with source apportionment models.

**The first step of the procedure is to download a testing dataset using the selection window on the right.**

Select a testing dataset (corresponding to an intercomparison) and download the package containing the information and data needed by the user to run the source apportionment model. For chemical receptor models (CRM) the input data are available from: [SHOULDERS@ipcc.at](#) or [ipcc.at](#)

Available datasets for receptor models: Iannuzzi, Lens, Synthesis. Datasets for CRM: Lens (mandatory set of sources (MSI) and optional set of sources (OPT)).

**The second step of the procedure is the run of the source apportionment by the user using the testing data set in order to produce a complete result.**

**The third step is to upload the source apportionment results. Upload the file(s) containing the results according to one of the following options (see examples in main page):**

- 1) zip file with three csv (comma separated values) files containing: a) the concentrations of the species in the profiles (mandatory,  $\mu\text{g}/\text{m}^3$ ), b) the time series of the contribution of the candidate sources (mandatory,  $\mu\text{g}/\text{m}^3$ ), c) the uncertainties of the species concentrations in the profiles (optional, in  $\mu\text{g}/\text{m}^3$ ), and d) the contribution to receptor (optional, in %), respectively CCINC, TREND, USC and CUS.
- 2) The information in point 1 in one single xls or excel file.

SA result:

DeltaSA is an on-line tool to assess source apportionment model outputs. It works in two different modes. The first is the source chemical profiles similarity test accomplished by comparing those obtained by the user with more than one thousand  $\text{PM}_{10}/\text{PM}_{2.5}$  source measured chemical profiles from the online SPECIATE (US-EPA) and SPECIEUROPE repositories. This configuration is intended to support practitioners in the identification of factors during the execution of factor analytical tools. The second mode consists in a complete test of the model result using a testing dataset and reference values generated in the framework of inter-comparison exercises organized by the European Commission- JRC.

The output of the source apportionment models are Source Contribution Estimates (sce), in other words, the estimation of the contribution from source categories ("candidate sources" or simply "candidates") to the total mass of the studied pollutant(s). In the present release of the tool, are only available particulate matter testing datasets. The minimum data required for the chemical profiles similarity test are the chemical profiles for each candidate source, reporting the mass concentration ( $\mu\text{g}/\text{m}^3$ ) of every species, plus the mass concentration ( $\mu\text{g}/\text{m}^3$ ) of the total pollutant (e.g.  $\text{PM}_{10}$  or  $\text{PM}_{2.5}$ ) apportioned by the user to each candidate source. For the model performance tests, the result of the source apportionment study on a testing dataset associated with a specific intercomparison exercise (provided in the tool), is required. A complete source apportionment result consists of: a) the chemical profiles ( $\mu\text{g}/\text{m}^3$ ), b) the time series of source contribution ( $\mu\text{g}/\text{m}^3$ ) for each candidate source, c) the uncertainty of the chemical profiles ( $\mu\text{g}/\text{m}^3$ ) and d) the contribution of candidate sources to every single chemical species in the profiles ("contribution-to-species", in %). The first two set of parameters are essential while the last two are optional.

The DeltaSA input files can be either .csv (comma delimited) or xls/xlsx (excel) format. For a better understanding on how to prepare the source apportionment model output to be uploaded in the DeltaSA tool, an example of input data is provided for the two tool modes by clicking the buttons on the right.

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## New on-line tool to test SA model performance using existing testing datasets developed by JRC.

## WG3 topics for future activity

**Guidelines:** development of CTM area and update the RM existing document (M. Mircea coordinator, G. Pirovano, G. Calori, O. Favez, I. El Haddad.)

**E-reporting:** creation of dedicated task force inter WGs to address the different aspects. In particular, propose sensible and robust SA approach

**Standardization:** continue collaboration for the Technical Specification, comments to the method are welcome, take advantage of the intercomparison, use the Delta SA tool

**Specific pollutants** put an emphasis on the apportionment of key pollutants like BC and PAHs

**Delta SA tool:** test and implementation for online model evaluation (D. Salameh, E. Venturini, Z. Kertesz test users)