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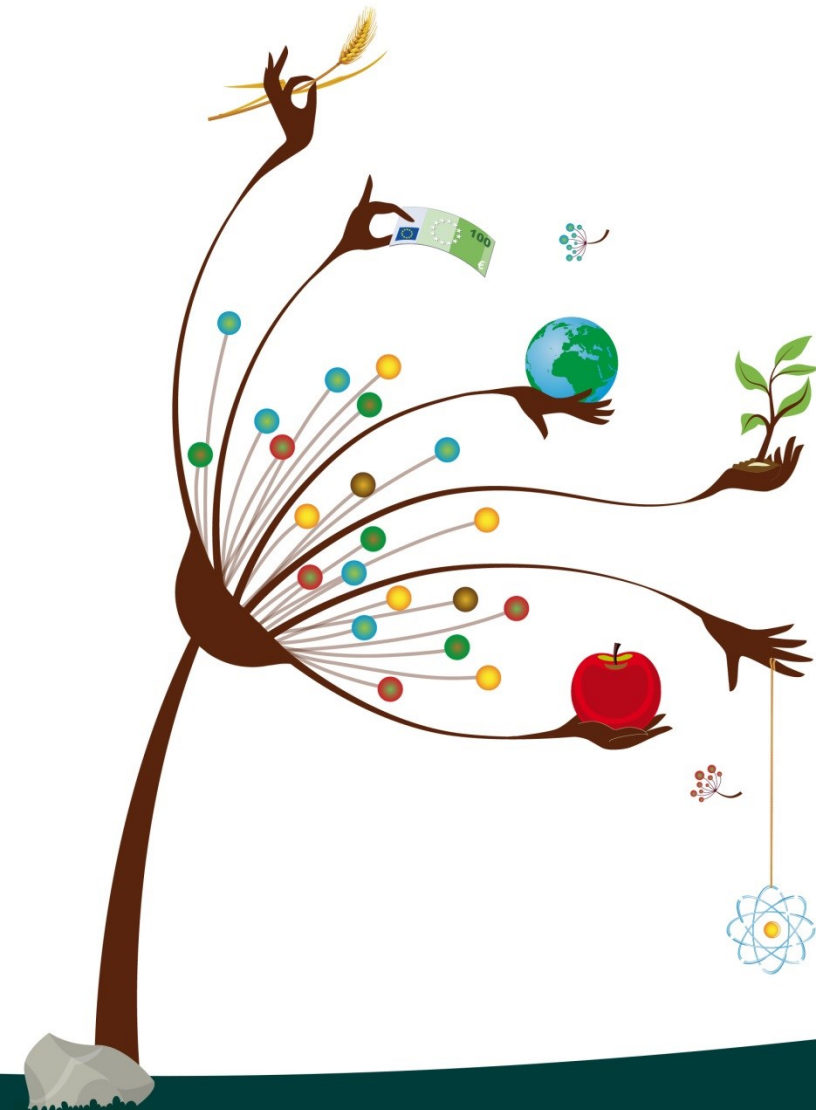
Joint Research Centre

WG 3 Source Apportionment tools

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FAIRMODE Warsaw, 12/2/2019



Outline of the presentation

- **What is source apportionment (SA)?**
- **SA techniques**
- **SPECIEUROPE online repository of source profiles**
- **DELTASA tool**
- **Technical documents to support SA**
- **How can these tools be useful for you?**



Source apportionment

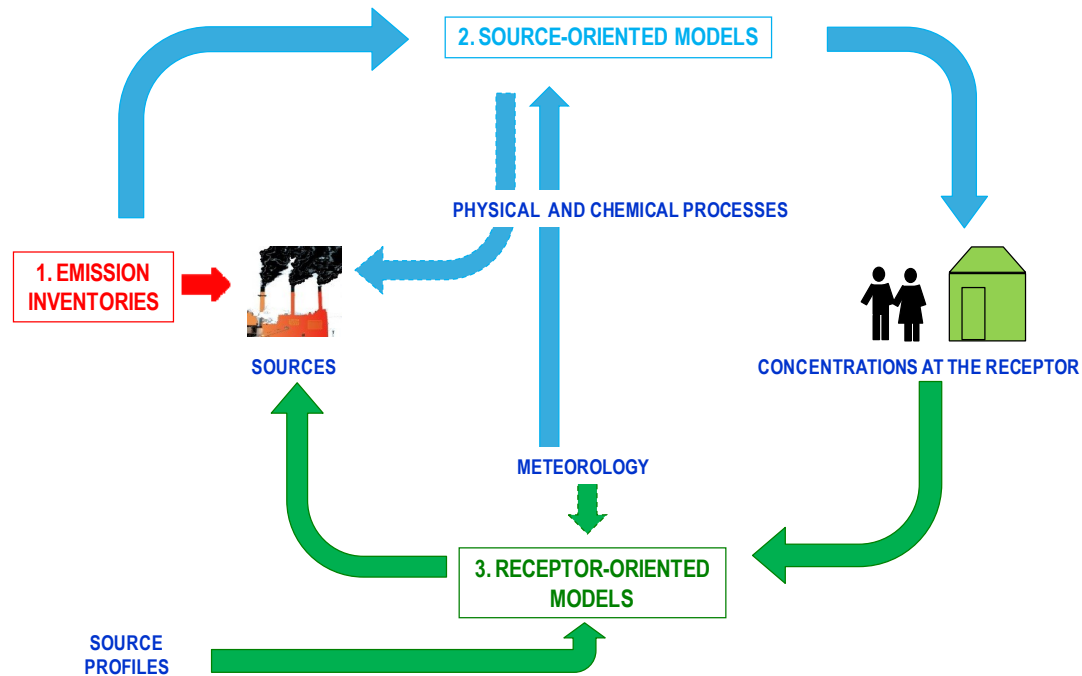
Source apportionment is the practice of quantifying the contribution of pollution sources to the concentration of pollutants in the atmosphere

Commonly used

SA techniques are:

- Receptor oriented models (RM)
- Source oriented models (SM)

- a) Lagrangian models
- b) Gaussian models
- c) Eulerian models



Typical source apportionment output

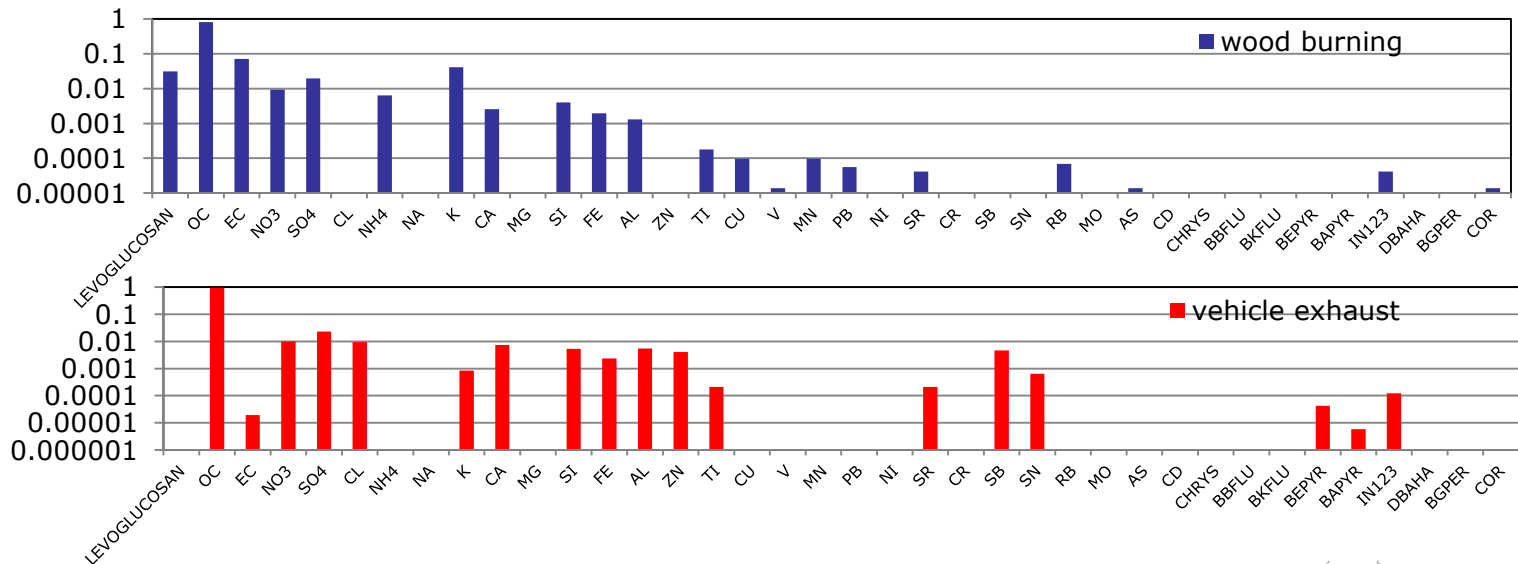


What is a source profile?

It describes the chemical composition of a source by depicting the relative concentration of the chemical species that compose that source

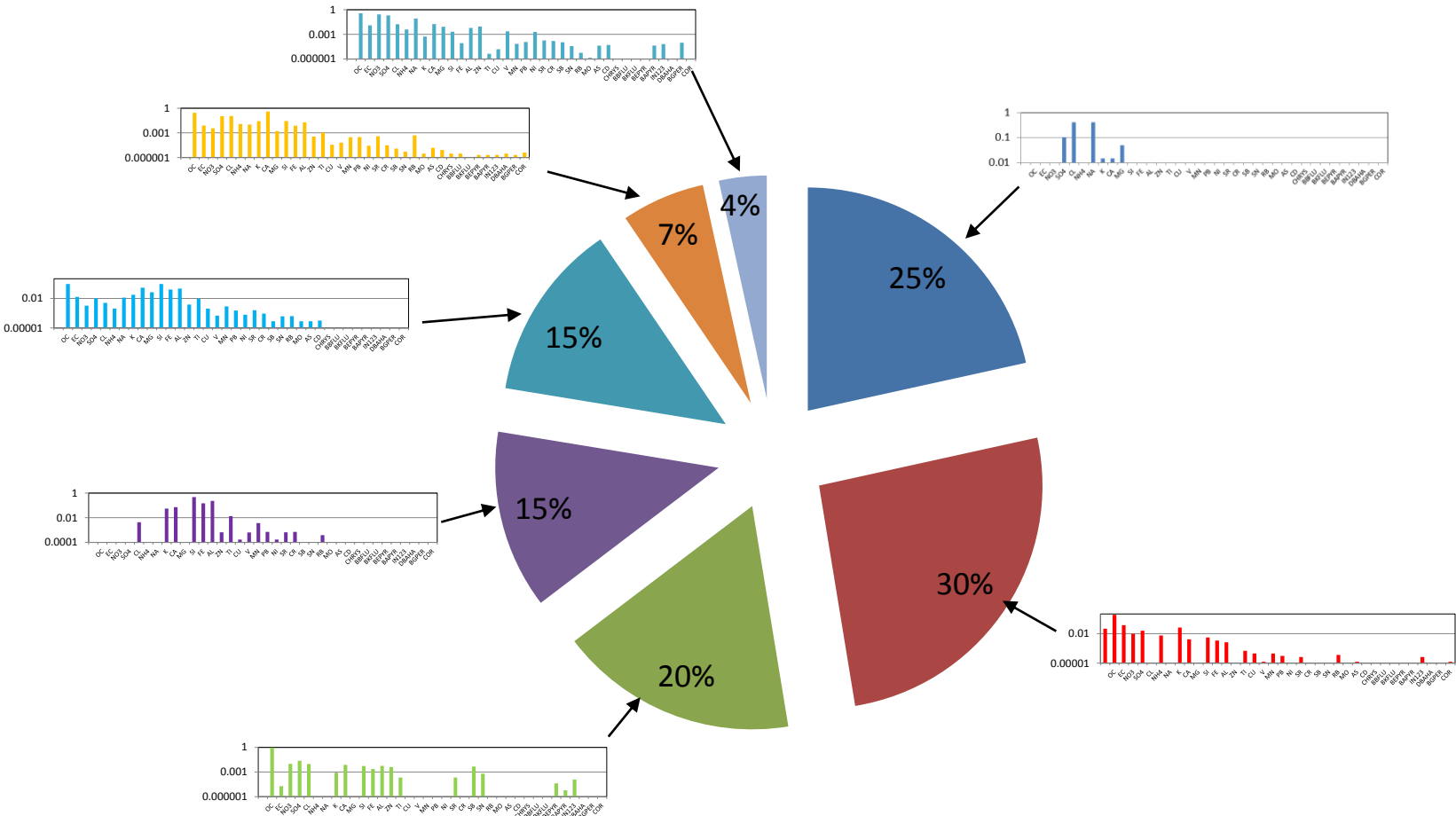
The source profile is the fingerprint of an air pollution source and makes it possible to identify it.

Examples of particulate matter source profiles



Example of SA output

In RM the souce profiles identify the source categories





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SPECIEUROPE

Source profiles for Europe database

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Welcome to SPECIEUROPE 2.0

SPECIEUROPE 2.0 is released on July 1st 2017. Near **eighty new profiles** have been added. The main changes concern the source categories industry, traffic, road dust, biomass burning, wood burning and secondary inorganic aerosol. A new source category "other combustion" has been created which includes a variety of combustion sources already present in other source categories excluding traffic and biomass burning.


SPECIEUROPE 2.0 has enhanced **search and download functionalities**. In the new version the profiles can be retrieved and downloaded by source category, species, year, PM size fraction, country or site. The architecture of the database is more clearly displayed to allow a better exploration of the source categories and subcategories.

Pernigotti, D., Belis, C.A., Spanó, L., 2016. SPECIEUROPE: The European data base for PM source profiles. Atmospheric Pollution Research, 7 (2), pp. 307-314. DOI: 10.1016/j.apr.2015.10.007

srcID	Source category name	#prof	srcID	Source category name	#prof
1	Traffic	28	24	Metal smelting	4
5	Road dust	15	54	Hard wood burning	4
20	Industrial	77	33	Natural gas burning	3
40	Biomass burning	24	43	Pellet burning	3
10	Soil dust	20	53	Soft wood burning	3
41	Wood burning	18	44	Beech burning	2
30	Fuel oil burning	11	46	Leaves burning	2
47	Closed fireplace	16	55	Open burning	2
37	Ship exhaust	14	14	Volcanic dust	2
2	Exhaust	12	35	Petrochemical	2
25	Cement	11	49	Olive oil burning	2
28	Power plant	10	60	Second. inorg. Aer.	2
34	Boiler	8	6	Tyre wear	1
66	Deicing salt	6	7	Brake dust	1
31	Coal burning	12	23	Refineries	1
21	Iron & steel prod.	7	26	Incinerator	1
32	Coke burning	6	42	Pine burning	1
12	Marine aerosol	3	50	Oak burning	1
29	Fertilizer prod.	9	51	Spruce burning	1
22	Foundries	6	52	Larch burning	1
27	Ceramic	6	61	Ammonium nitrate	1
3	Diesel exhaust	5	62	Ammonium sulfate	1
4	Gasoline exhaust	4			

Each profiles is associated to one or more **source category**, which are **hierarchically organised** (see table).


For example if a fingerprint is attributed to the source category **gasoline**, it is **also** attributed to the source categories **exhaust** and **traffic**.



SPECIEUROPE
 Source profiles for Europe database

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Available source categories

Name
All sources (209)
Ammonium nitrate (4)
Ammonium sulfate (3)
Beech burning (2)
Biomass burning (25)
Boiler (8)
Brake dust (3)
Cement (11)
Ceramic (6)
Closed fireplace (16)
Coal burning (12)
Coke burning (7)
Construction dust (1)
Densin salt (6)
Densin salt (6)


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SPECIEUROPE
 Source profiles for Europe database


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Available species

Name	Symbol
1,2,3-Benzenetricarboxylic Acid (4)	C9H6O6
1,2,4-Benzenetricarboxylic Acid (4)	C9H6O6
1,2-Benzenedicarboxylic acid, 4-methyl- (4)	C9H8O4
1,3,5-Benzenetricarboxylic Acid (4)	C9H6O6
1,3-butadiene (9)	BUD113
17a(H),21b(H)-30-Norhopane , also noted as 'ab30nh' (4)	C29H50
17a(H),21b(H)-Hopane , also noted as 'ab_hop' (4)	
17a(H)-22,29,30-Triannorhopane (4)	
18a(H)-22,29,30- trisnormeohopane (4)	C27H46
20R&S-5a(H),14R(H),17B(H)-ergostane (4)	
20R-13B(H),17a(H)-diacholestane (4)	
20S-13B(H),17a(H)-diacholestane (4)	C27H48
22R-17a(H),21b(H)-homohopane (4)	C31H54
22S-17a(H),21b(H)-homohopane (4)	C31H54
2-Ethylhexanoic acid (4)	C8H16O2

On-line Delta SA tool



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Delta tool for Source Apportionment

DeltaSA

Chemical profile Similarity

Source Apportionment Model performance

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.

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 PM₁₀/PM_{2.5} source measured chemical profiles from the online SPECIATE (US-EPA) and SPECIEUROPE (EC-JRC) 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. PM₁₀ or 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.

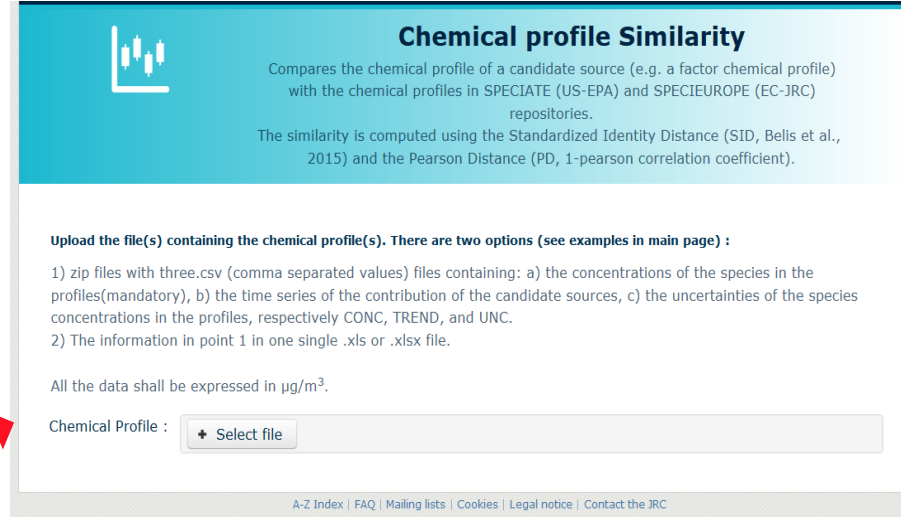
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On-line tool to test SA model performance using existing testing datasets developed by JRC.

<https://delta-sa.jrc.ec.europa.eu/sadelta/html/public/login.jsf>



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, Belis et al., 2015) and the Pearson Distance (PD, 1-pearson correlation coefficient).

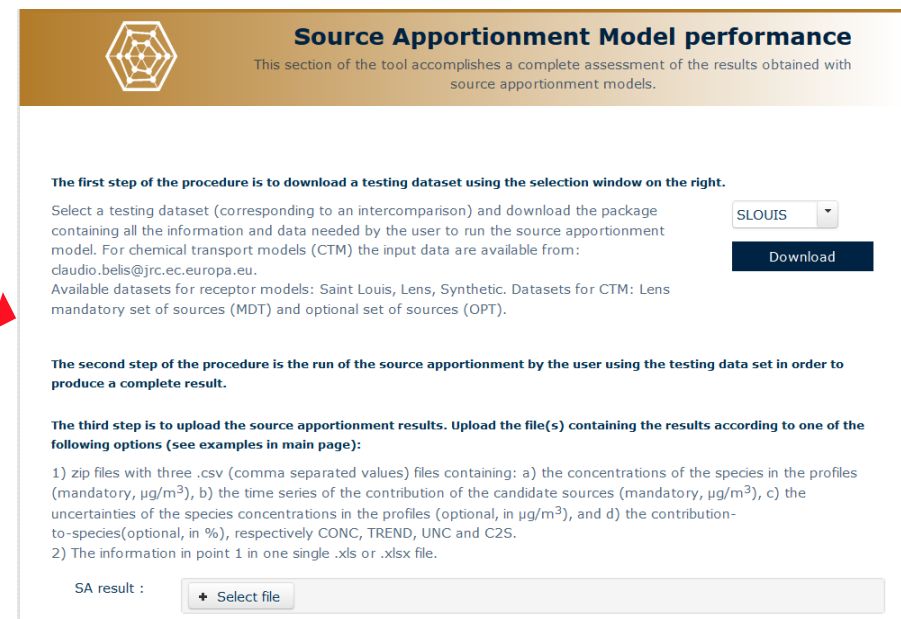
Upload the file(s) containing the chemical profile(s). There are two options (see examples in main page) :

- 1) zip files 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 CONC, TREND, and UNC.
- 2) The information in point 1 in one single .xls or .xlsx file.

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

Chemical Profile :

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Source Apportionment Model performance

This section of the tool accomplishes a complete assessment 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 all the information and data needed by the user to run the source apportionment model. For chemical transport models (CTM) the input data are available from: claudio.belis@jrc.ec.europa.eu.

Available datasets for receptor models: Saint Louis, Lens, Synthetic. Datasets for CTM: Lens mandatory set of sources (MDT) 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 files 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-species(optional, in %), respectively CONC, TREND, UNC and C2S.
- 2) The information in point 1 in one single .xls or .xlsx file.

SA result :

DELTASA: the online tool for the evaluation of SA models

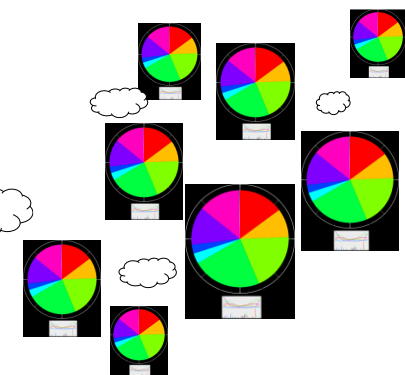
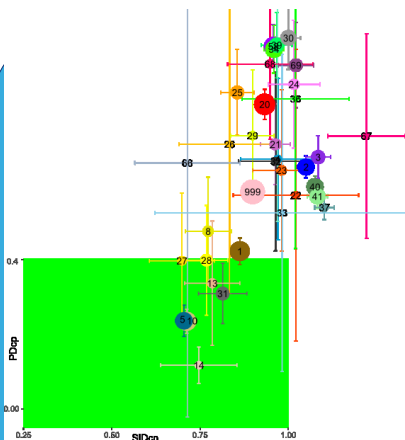
Chemical profiles similarity test (CPS)

Any registered user can upload to the server his/her chemical profile (s) in relative mass on the total PM.

The similarity test is performed with more than one thousand PM₁₀/PM_{2.5} source measured chemical profiles from the online SPECIATE (US-EPA) and PECIEUROPE repositories using as distances:

- Pearson Distance (PD=1-R)
- Standard Identity Distance (SID).

A report is generated to support the identification of factors



Chemical Profile Similarity

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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 performance (MP).

<https://delta-sa.jrc.ec.europa.eu/sadelta>

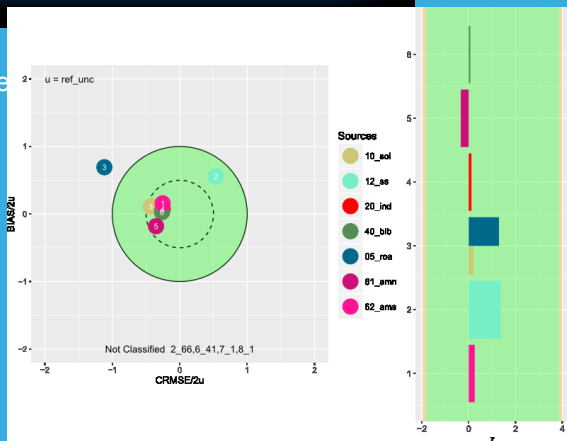
Model Performance (MP)

On-line calculation of the performances using one of the three preloaded intercomparison (IE) dataset.

The user downloads a dataset, run its model and uploads his/her results (CP, SCE, CP see methodology), attributing each candidate to one or more predefined sources.

The tool calculates for each candidate-source a measure of the performances.

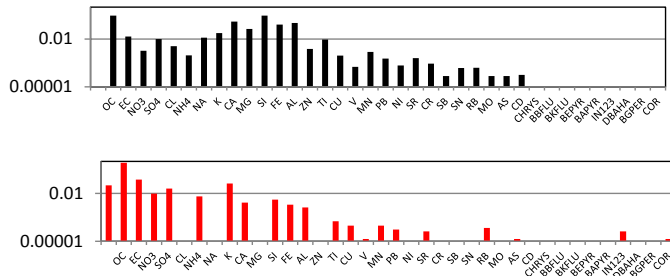
→ a report is generated with a summary of the performances



The performance criteria used are:
 Target ← SCT SCE → z-score

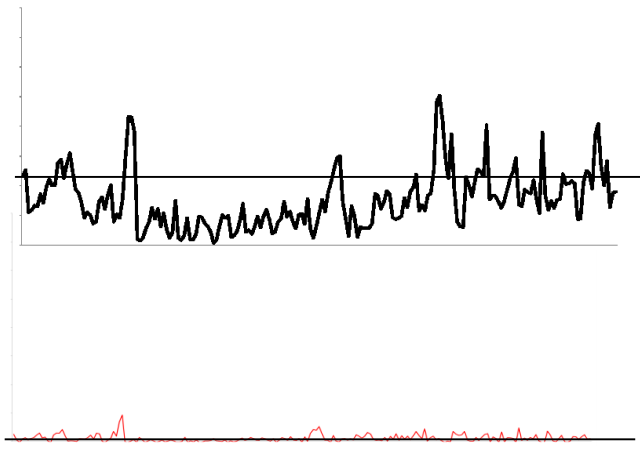
Belis et al., 2015

Performance indicators are based on both chemical profiles and time trends



p_{ref} $p_{ref}(u)$
 p_1 $p_1(u)$

Chemical profiles (ID)



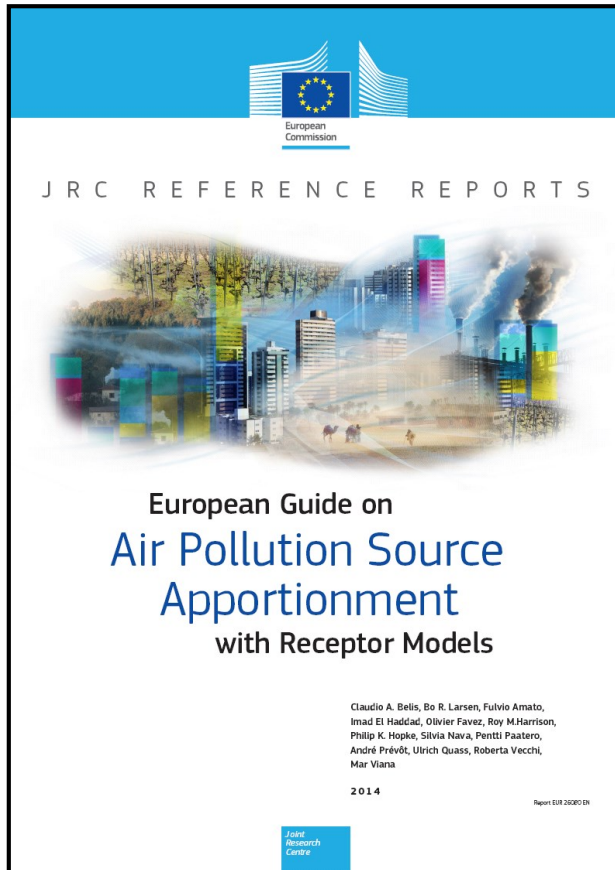
$\bullet \bar{x}_{ref}$ } $sd t_{ref}$
 $\bullet \bar{x}_1$ } $sd t_1$

Time trend (behaviour)



Guide on SA with RMs: Driving elements

UNDER REVISION



- The main objective is to promote the best available operating procedures and to harmonise their application across Europe.
- Promote implementation of quality assurance steps
- Establish a common reporting of results
- Collect the experience of European leading teams in the subject

C.A. Belis, B. R. Larsen, F. Amato, O. Favez, I. El Haddad, R.M. Harrison,
A.S.H. Prévôt, S. Nava, U. Quass, R. Vecchi, M. Viana, P. Paatero

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New report available for download:
"A comparative analysis of the causes of air pollution in three cities of the Danube region"
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DeltaSA
The new online tool to assess source apportionment model outputs. It works in two different modes:
(1) the source chemical profiles similarity,
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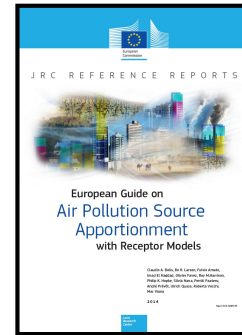
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Delta tool for Source Apportionment
DeltaSA

Chemical profile Similarity

Source Apportionment Model performance

<https://source-apportionment.jrc.ec.europa.eu/>

How these tools can be useful for you?

SPECIEUROPE:

- *definition of sources based on real-world measurements*
- *run and validation of RM and validation of SM results*
- *common reference for all SA studies in Europe*

DELTA SA

- *automatic test of user source profiles*
- *assess single user capabilities using existing datasets (training)*

GUIDE on SA with RMs:

- *harmonised procedures -> comparability of results,*
- *best practices (quality assurance),*
- *bibliographic references*

Thank you for your attention

