



Source Apportionment (SA) Guide: present status

European Guide on Air Pollution Source Apportionment (SA) for estimating particulate matter source contributions with source oriented models (SM) and receptor models (RM)

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Appendix 1: Applications of AQ/CTM and RM models for estimating particulate matter source contributions in Europe



Source Apportionment (SA) Guide: Introduction

SA techniques provide information useful for the reduction of pollution levels by combating the “emissions of pollutants at source”

Which is the added value of SM with respect to SR?

- evaluate the contributions of sources in the absence of measurements or as a complement of them
- allow to estimate the contribution to secondary pollutants
- allow to estimate the contribution of transported pollutants
- is directly linked to estimation of emissions
- can be used for any time period, not only for measurement campaigns
- allow to distinguish the individual contribution of meteorology
- allow knowing variability in time and space of source contributions
- modelling of specific sources???

Which is the added value of using simultaneous SM and SR?

- additional validation for SM. Required or desirable?

Target Audience

- support to the organizations, companies, institutions, etc which carry out source apportionment studies in support to authorities responsible for developing, implementing and evaluating official air quality plans under Directive 2008/50/EC
- assist the authorities in the interpretation of the modelling results for source apportionment purposes
- help the air quality modellers, independent of the level of experience, to approach the source apportionment issues



Source Apportionment (SA) Guide: Introduction

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Source oriented models (SM)

- Gaussian and non-Gaussian parametrized models;
- Lagrangian puff and particle models;
- Eulerian chemical transport models.

Source-oriented modelling techniques

- sensitivity analysis and source apportionment approaches? Or sensitivity analysis and tracer approaches ?
- Sensitivity analysis: brut force method, zero-out method, decoupled direct method, ...
- Tracer approaches: PSAT, labelling routine, ...

European SA studies with SM and with SM-RM: survey results

- Fragkou et al. (2012) published a review of SA methodologies for PM used by Member States for the preparation of their extension reports regarding compliance with PM10 limit values at 1 January 2005
- more recent review on the use of models for source apportionment carried out in the frame of the project APPRAISAL (Belis et al 2017)
- the survey carried out in 2017, in the framework of WG3 FAIRMODE, regarding the SA methodologies used in the last years, the number of SM studies is 11 while SR studies were more than 150. Only 2 studies are shown results for SM-SR.

Open question: how to choose the proper SA technique?

Other suggestions?



Source Apportionment (SA) Guide: PM modelling – base case

All PM modelling aspects were extensively addressed by ETC/ACM Technical Paper (2013) and issues related to its validation can be found in air quality modelling guide (EEA, 2011)

Domain, time period and spatial resolution

The configuration of the modelling domain has to take into account several aspects such as:

- to ensure the maximum possible spatial resolution in the area with PM exceedances;
- to have as much as possible measurements in the domain;
- to have details on anthropogenic emissions at source category level.

Boundary conditions: linking model outputs over different domains

- the boundary conditions has to be provided with a relative high time frequency, at least every 3 hours at regional scale, in order to capture the intensity and the occurrence of high PM concentrations due to transport through the boundaries
- dynamic boundary conditions from other simulations are preferable to the static ones, derived from long term series of measurements

Meteorological data

- recommend to use meteorological data provided by meteorological services, reanalysis when possible, or to perform a validation of the output of the meteorological model before performing air quality simulations
- recommended to use meteorological data produced on a grid resolution close to the one used for air quality simulation, on the same projection if possible, in order to avoid uncertainties introduced by interpolation methods

Emissions: anthropogenic and natural

- the activities are classified using three sets for source categories: SNAP97, EMEP/NFR and UNFCCC/CRF. There are reasons to suggest one of this set? ..
- how to have emissions inventory with enhanced source classification detailing some macrosectors? May suggest sources or methodologies?
- similar problems with spatial proxies and temporal profiles for source categories. The most used proxies are population, land-use and, recently bottom-up emission inventory. More discussion about proxies can be found in Trombetti et al. (2018) and about temporal profiles in Menut et al. (2012)....
- emission evaluation with Delta Emission Tool?
- the spatial resolution of proxy data has to be higher or equal to that of the finer grid.??? General and particular cases? Minimum emissions resolutions? Chemical speciation: minimum requirements?
- how to deal with Dust emissions, Sea salt emissions, Biogenic emissions?



Source Apportionment (SA) Guide: PM modelling – base case

2.2 Model evaluation/validation-MQO

- model performance evaluation of main aerosol compounds or just PM mass concentration?
- model evaluation time period: year, season, week vs weekend days? Multiannual model evaluation?
- model performance evaluation with particular emphasis on “marker” species?
- model evaluation on hourly basis or on daily averages?
- model evaluation on episode and non-episode conditions? How to define episodes?

Core set of statistical indicators (Guidance Document on Modelling Quality Objectives and Benchmarking, v2.1) for PM10 and PM2.5 considered in Delta Tool:

- Includes: Root Mean Square Error, Correlation, Normalised Mean Bias, Normalized Mean Standard Deviation
- Serves as a basis for the definition of the main model quality indicator MQI (linked to RMSE) and additional Model Performance Indicators (MPI), linked to the remaining core statistical indicators.

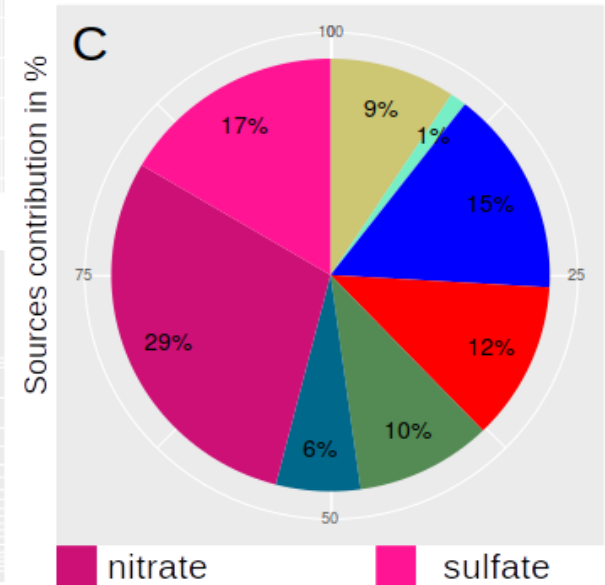
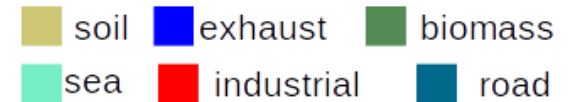
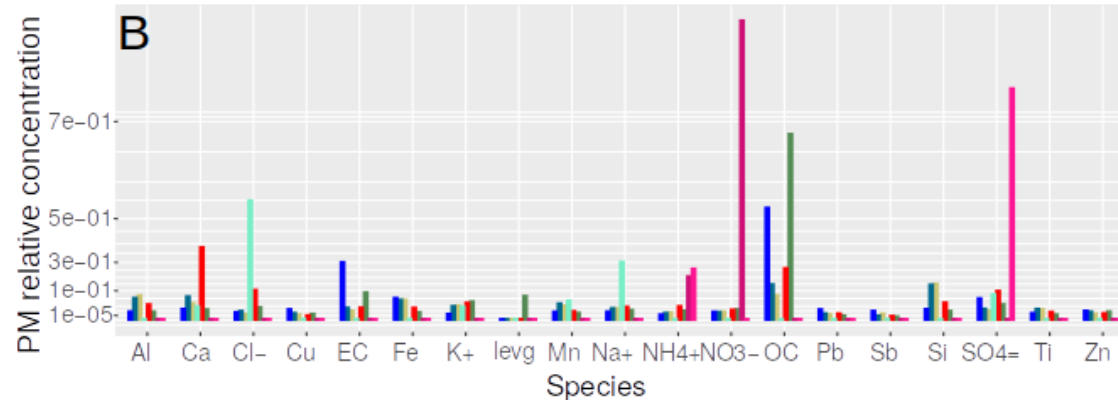
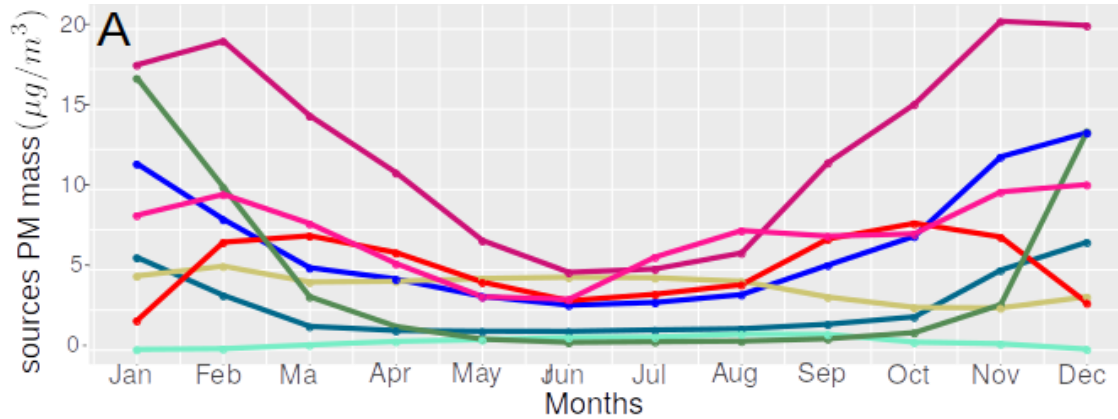
Has Delta Tool to be extended for main aerosol compounds (elemental carbon (EC), organic carbon (OC), nitrate (NH₃), sulphate (SO₄), ammonium (NH₄) and other primary aerosol (OPA))? Which one?

Is target diagram enough for validation?

How relevant is “space” validation shown in summary report?

Source Apportionment (SA) Guide: Estimation of source contributions with SM

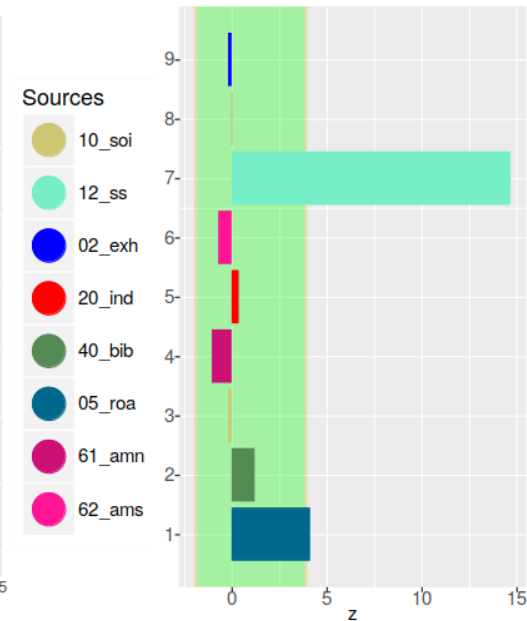
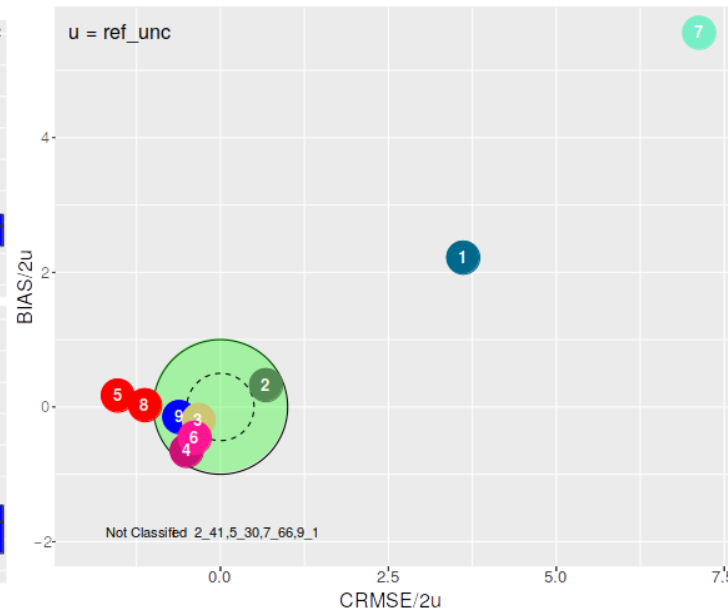
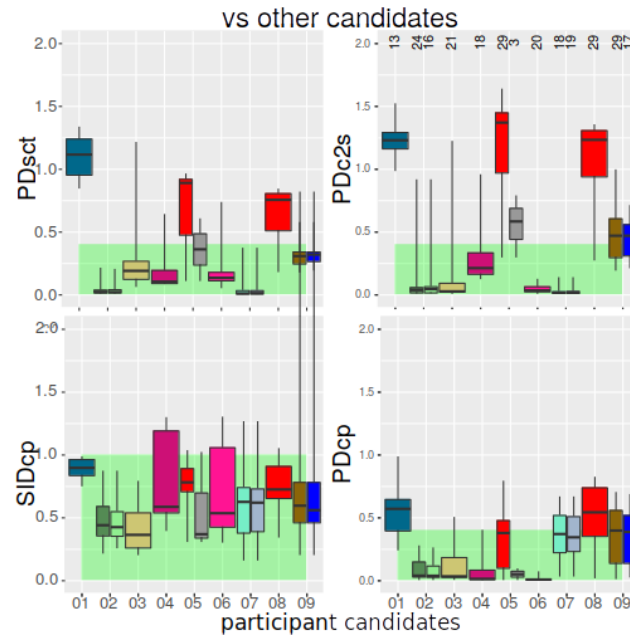
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Sources of the synthetic dataset used as reference: soil, marine, exhaust, industry, biomass burning, road dust, ammonium nitrate and ammonium sulphate. On panel B the chemical profiles in relative mass (CP), on panel A the seasonal trend of SCT in $\mu\text{g}/\text{m}^3$, on panel C the SCE as % of total PM mass

Source Apportionment (SA) Guide: Estimation of source contributions with SM

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Example of boxplots for one synthetic participant displaying distances of the user candidates to the other candidates (four boxplots on the left); scatter plot of SID_norm and PD distances between the user candidates and DeltaSA set of measured profiles (right)

Example of performance plot for one participant against the reference. On the left is shown the target plot (RMSEu) and the z-score is displayed in the right panel.



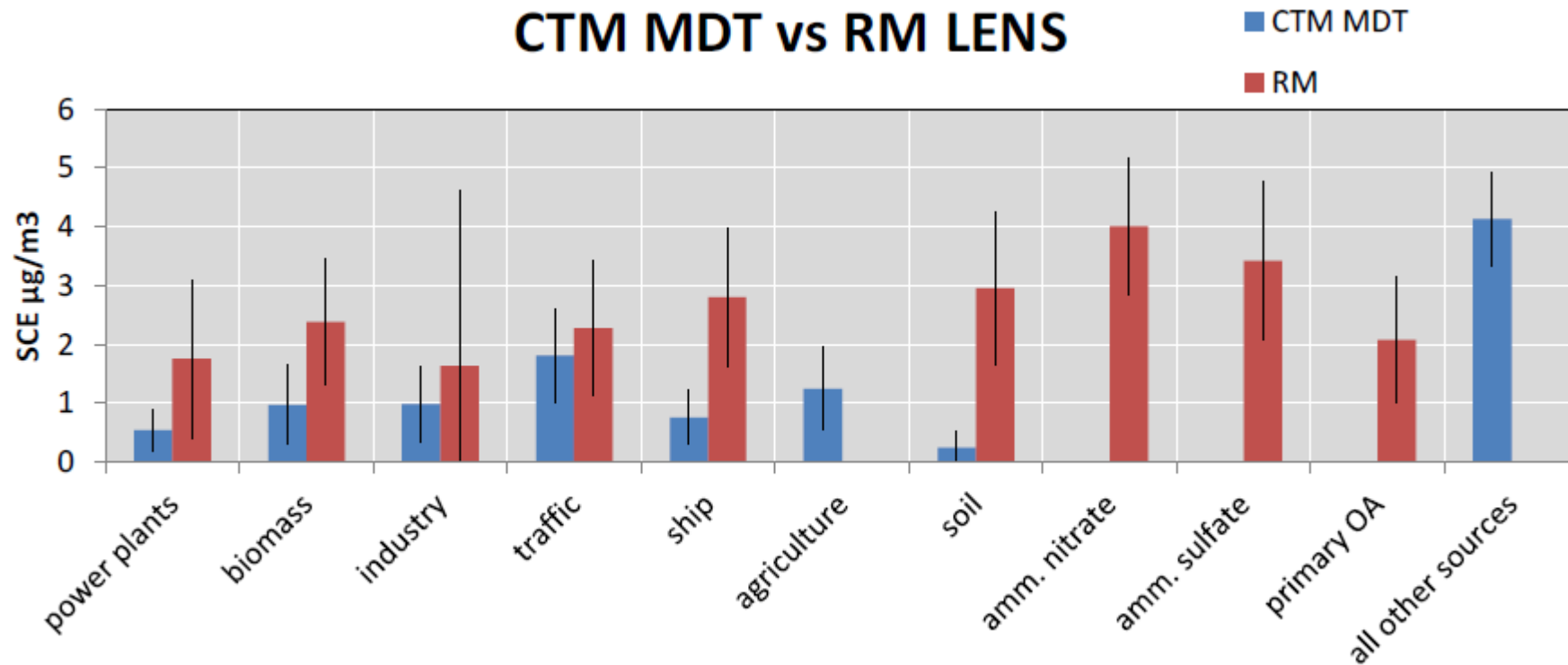
Source Apportionment (SA) Guide: Combined use of SM and RM

4.1 Estimation of source contributions with RM

4.2 Source categories association, emissions changes for brute force? other issues?

4.3 Comparison of source contributions from SM and RM

CTM MDT vs RM LENS



Source Apportionment (SA) Guide: Combined use of SM and RM – Reference data

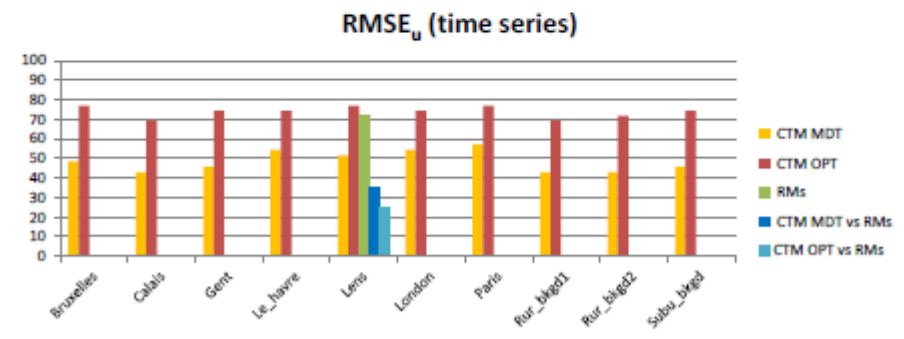
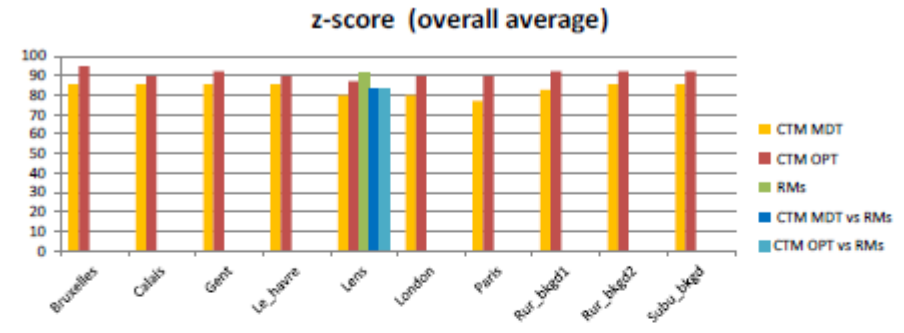
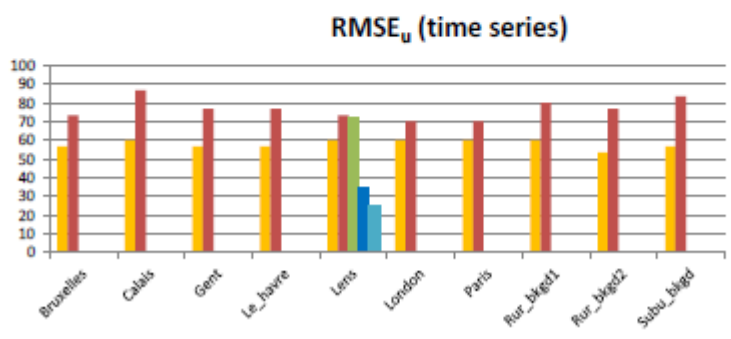
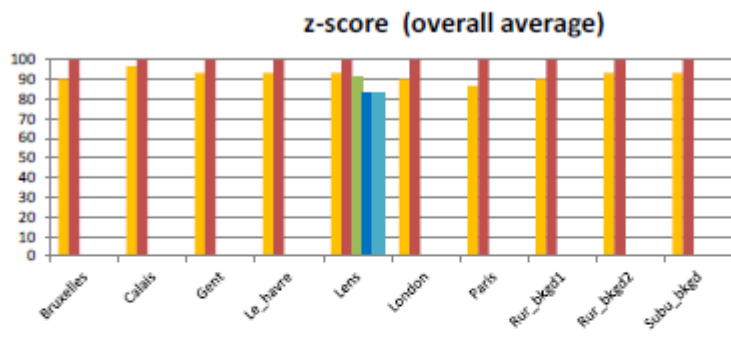


Figure 30. Synthesis of the intercomparison performance tests. a) and b) with all CTMs in the reference, c) and d) with only tagged species CTMs in the reference.



Table 12. Correspondence between CTM sources (SNAP) and RM sources (SPECIEUROPE) defined for this intercomparison

CTM Mandatory	RM corresp. Mandatory	CTM Optional	RM corresp. Optional
01_ENI	30 fuel oil combustion or 28 power plant	01_ENI	30 fuel oil combustion or 28 power plant
99_OTH		02_OTH	
02_BIO	40 biomass burn.	02_BIO	40 biomass burn.
34_IND	20 industry	34_IND	20 industry
07_RTR	1 traffic	71_RTG	2 exhaust
		72_RTD	
		07_RTR (OTH)	
		07_RTR (OTH)	
		75_RTW	5 road dust
08_SHP	37 ship	08_SHP	37 ship
99_OTH		99_OTH	
10_AGR	NH4 sum	10_AGR	NH4 sum
11_DST	10 dust	11_DST	10 dust
99_OTH		11_SLT	12 marine, 71 aged sea salt
99_OTH		11_BSO	
99_OTH		99_OTH	

Belis et al., 2018 Results of the first European Source Apportionment intercomparison for Receptor and Chemical Transport Models, EUR 29254 EN, Publications Office of the European Union, Luxembourg, 2018, ISBN 978-92-79-86573-2, doi: 10.2760/41815, JRC 111887.