

Status of WG3

*C.A. Belis,
European Commission - JRC*

G. Pirovano
RSE SpA







**Fairmode Plenary meeting
Utrecht, 14-15 February 2017**

Outline

- Activities of WG3 in 2014-2016
- Lessons learned from the intercomparison exercise
- Road map for WG3 in 2017-2019

Activities carried out in the cycle 2014-2016

- Publications about the methodology for performance evaluation and RMIE results
- Organisation and evaluation of an ambitious IE for RM and CTM
- Developed recommendations to the e-reporting community (report feb/2016)
- Contribute to the creation the TC264 WG44 on the SA applications performance evaluation 
- Development of an online database for chemical source profiles of PM SPECIEUROPE  (<http://source-apportionment.jrc.ec.europa.eu/Specieurope/index.aspx>)
- Development of the online tool for SA model performance evaluation DELTASA  (<https://delta-sa.jrc.ec.europa.eu/sadelta/html/public/login.jsf>)
- Training activities in collaboration with IAEA 

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

The intercomparison was 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,
- Cross-validating results (to overcome the lack of SA observed data)
- Providing insights to understand the behavior of models:
 - ✓ *influence of specific factors (e.g. type of site, type of source, spatial resolution, vertical dispersion, etc...)*
 - ✓ *sensitivity to modelling approaches (e.g. RMs vs CTMs; brute force vs tagged)*
- Generating reference datasets for future tests (a posteriori)

Participants



RM: 33 participants – 38 results

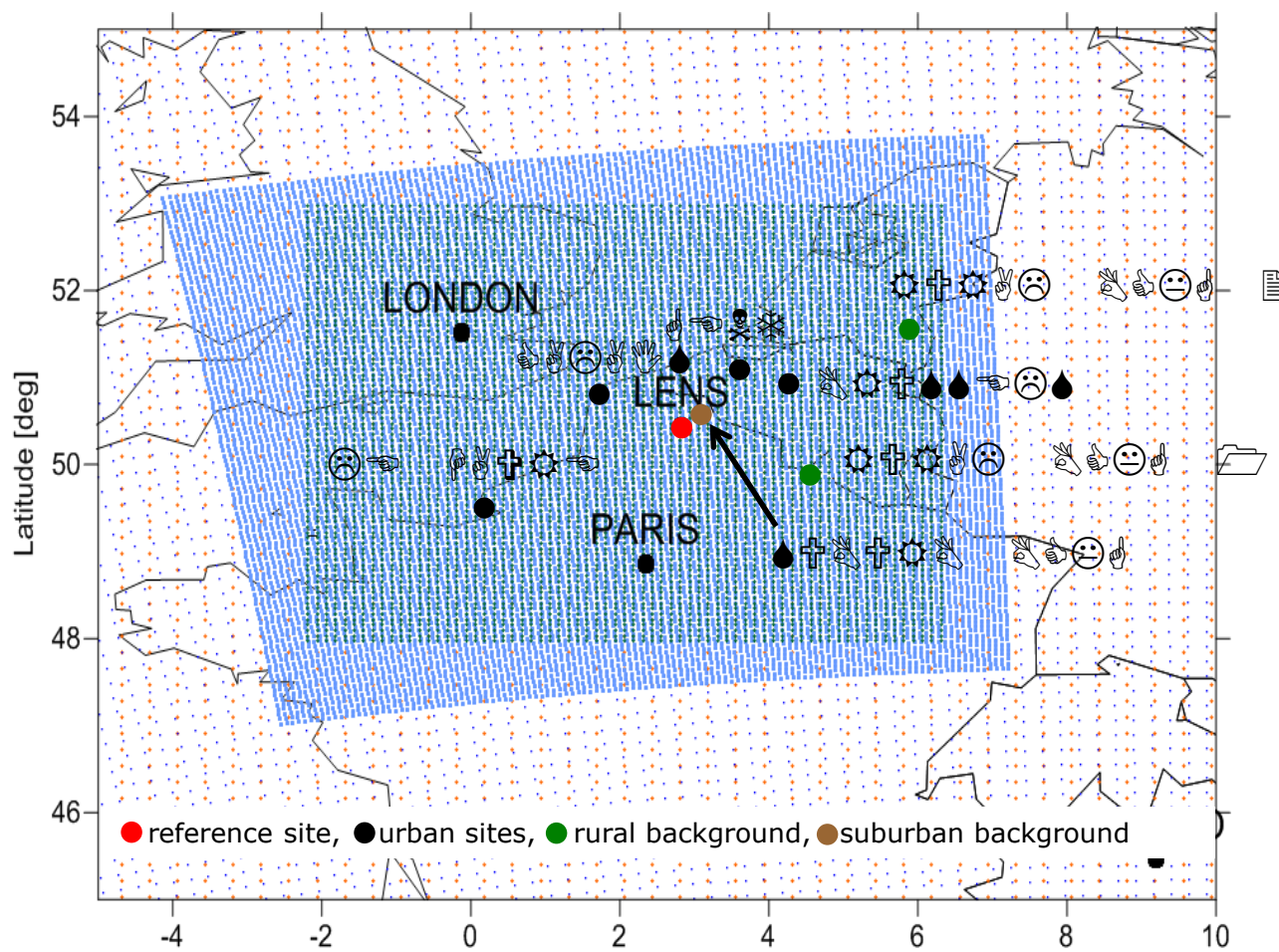
AGH-UST	ISAC LE	RIVM
APPATN	FMI	SAGE
ARPA ER	IDAEA_T	UCC
ARPA LO	IDAEA_A	UMH
ARPA PU	IMROH	UNIBO
ARSO	ISSeP	UNIHE
AUTH	IST	UNIMI
CARES	LGGE+	UNMIB
CNR IIA	NCSR	UNIFI
ENEA	PSI	UNIGE
ISAC BO	PUC	WUT

CTM: 7 participants – 11 results

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

Special thanks to: M.T. Pay (BSC), M. Rezler (WTU), O. Favez (INERIS), J.L. Jaffrezo (LGGE), J. Kuenen and H. Denier van Der Gon (TNO)

Domains and Receptors

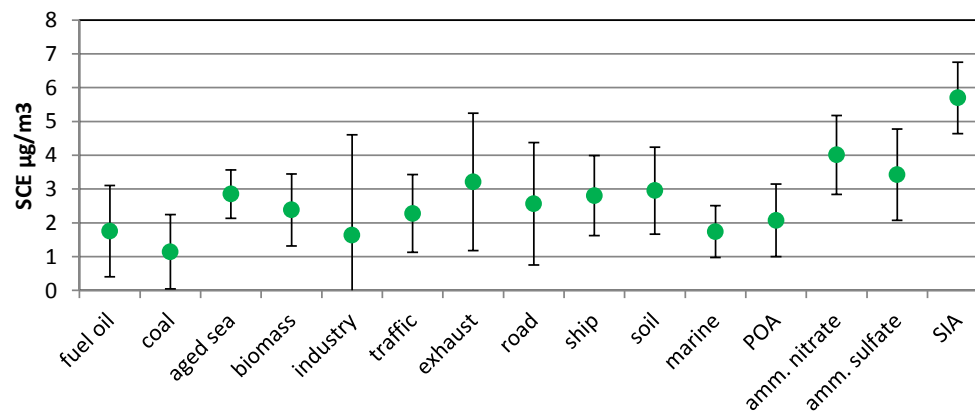


Special thanks to: M.T. Pay (BSC), M. Rezler (WTU), O. Favez (INERIS), J.L. Jaffrezo (LGGE), J. Kuenen and H. Denier van Der Gon (TNO)

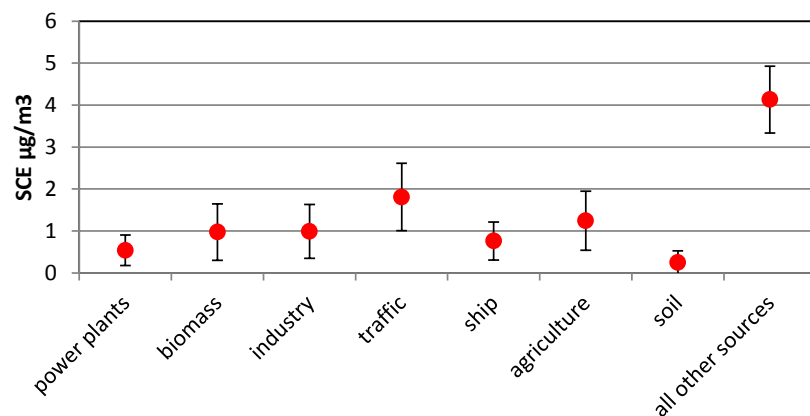
Source Contributions



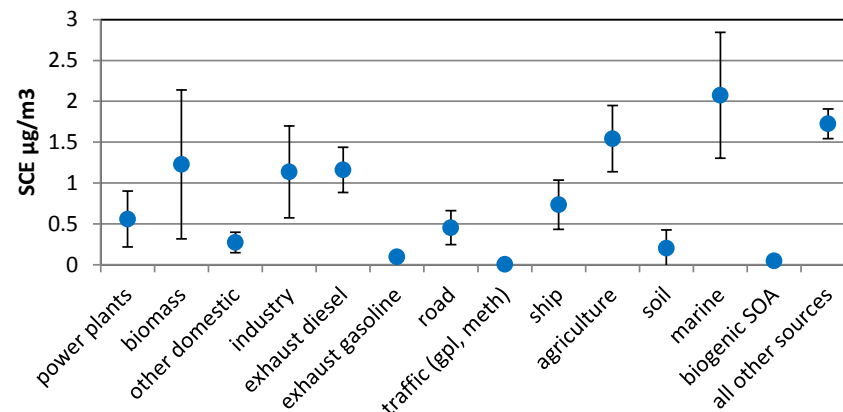
RM LENS



CTM mdt LENS



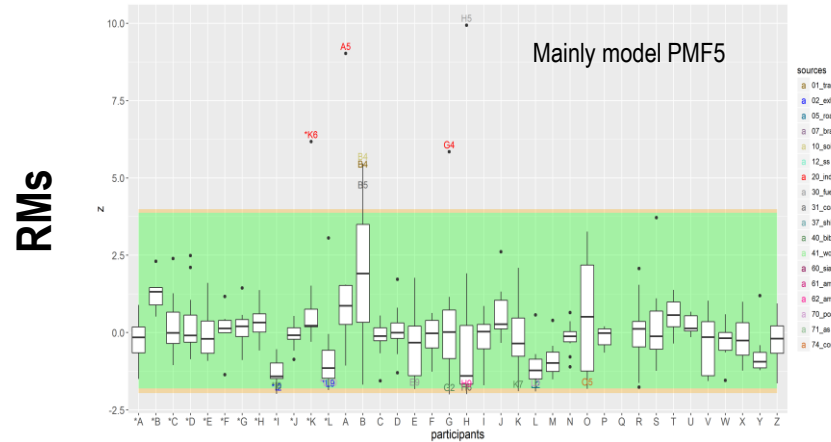
CTM opt LENS



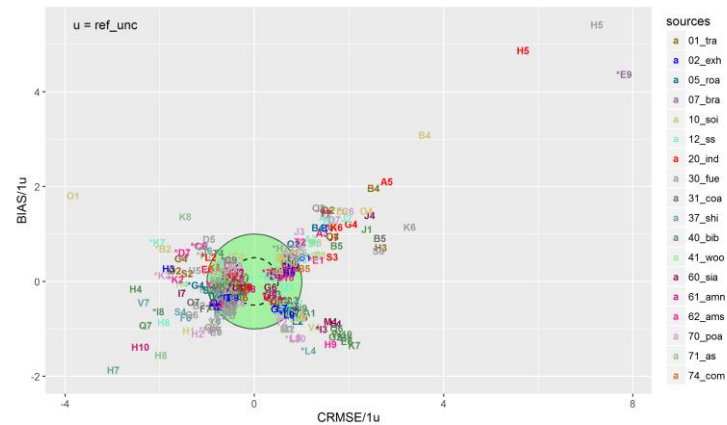
SA performance



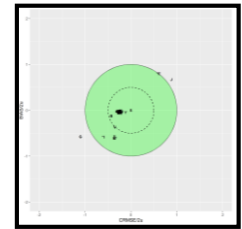
z-score (overall average)



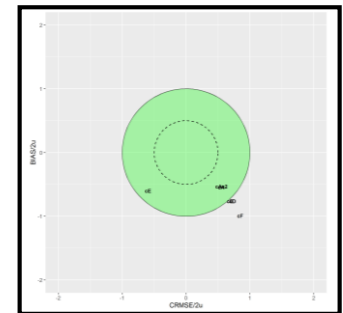
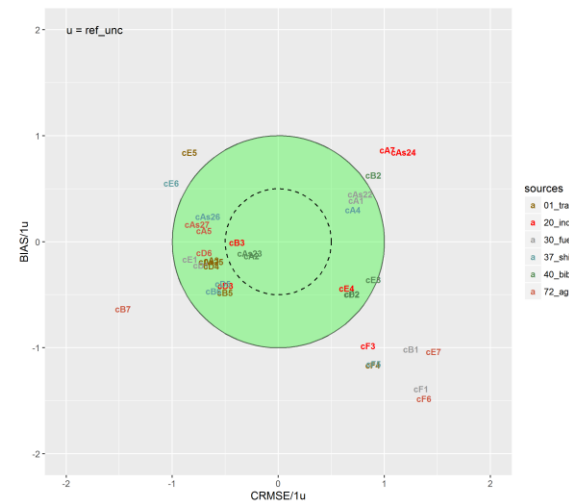
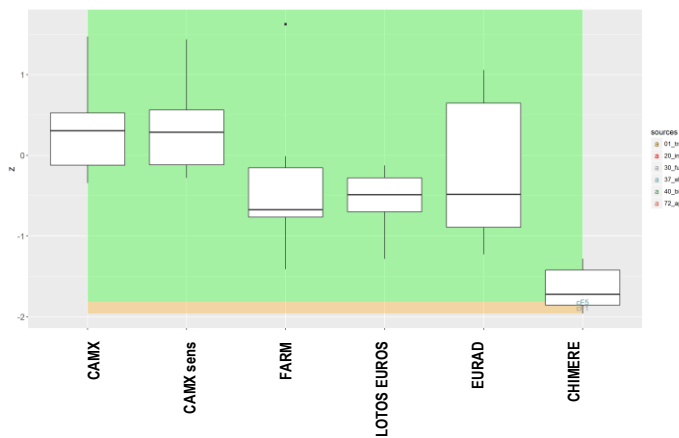
Target plot (time series)



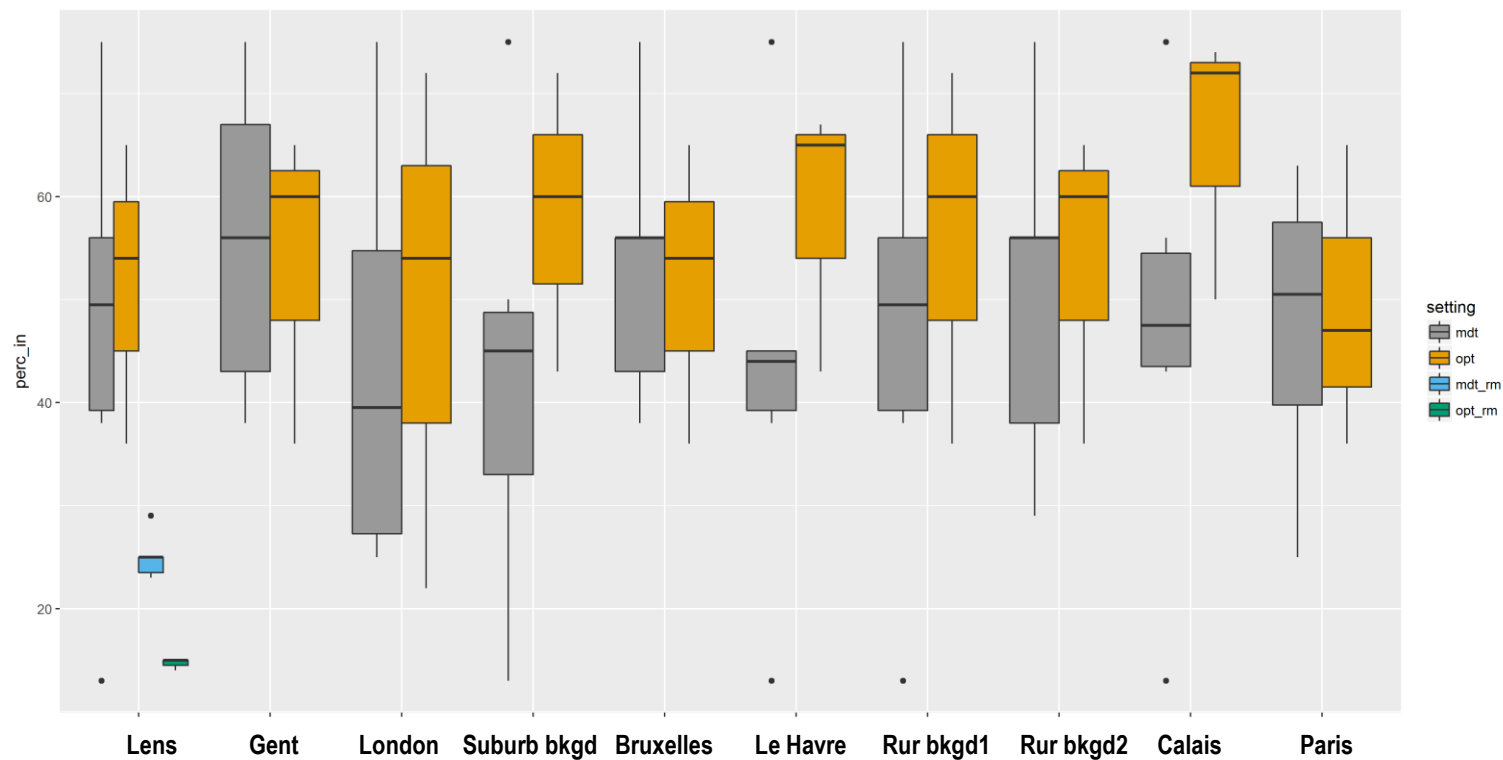
total mass test



CTMs

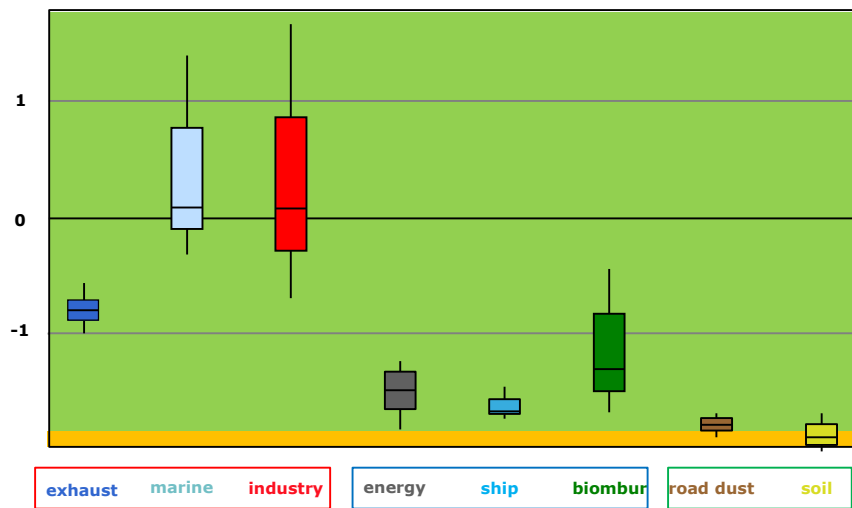


CTM percentage of successful scores (crsme) in different sites

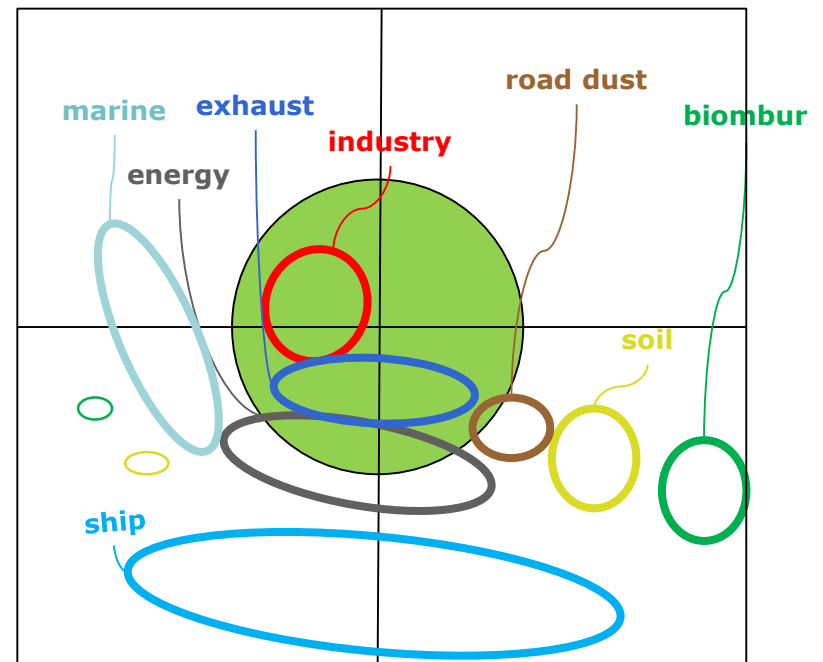


CTMs vs RMs Lens

z-score (overall average)



Target plot (time series)

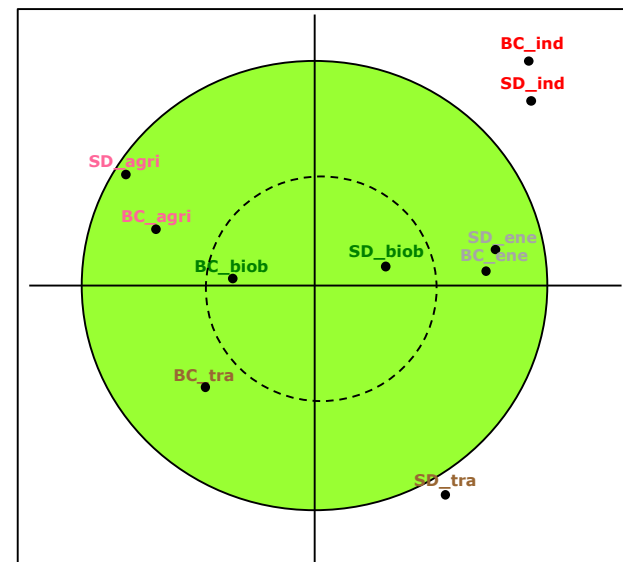
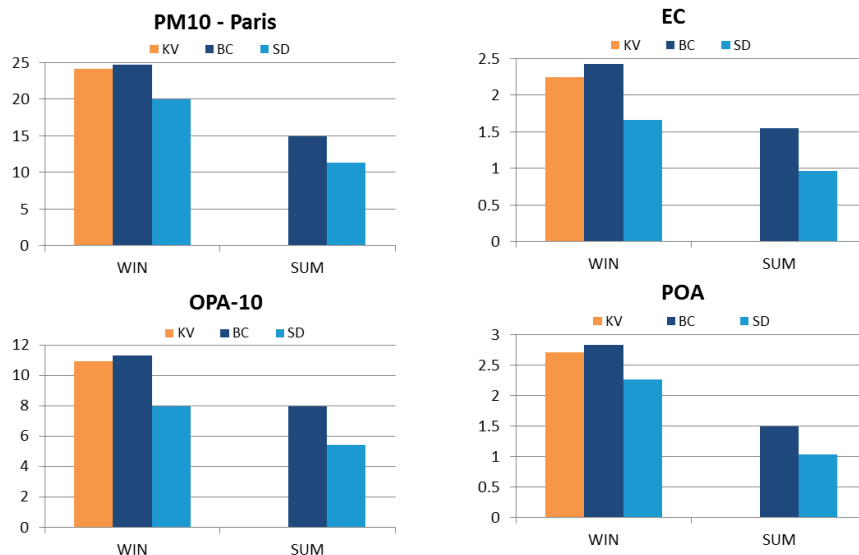


The comparability between RMs and CTMs
varies among sources

Sensitivity tests

The goal of the sensitivity test was to evaluate the influence of the reduced horizontal resolution on the CAMX output.

To that end, CAMx run were performed with two different grid steps 7 km (BC) and 20 km (SD). The reduced cell dimension in an area close to primary emissions (traffic) was expected to cause a reduction in the concentrations of pollutants associated with that source.



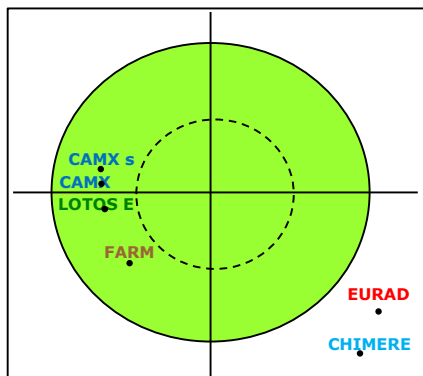
A PM10 concentration decrease for SD matched a decrease in Elemental Carbon (EC), Primary Organic Aerosol (POA) and other Primary Anthropogenic Aerosol (OPA-10) compared to the base case.

When comparing the performances of PSAT using two different grid steps it was also observed that the contribution of traffic was underestimated when using low spatial resolution. No significant changes were observed in the other tested sources (industry, energy production, biomass burning and agriculture).

Agriculture



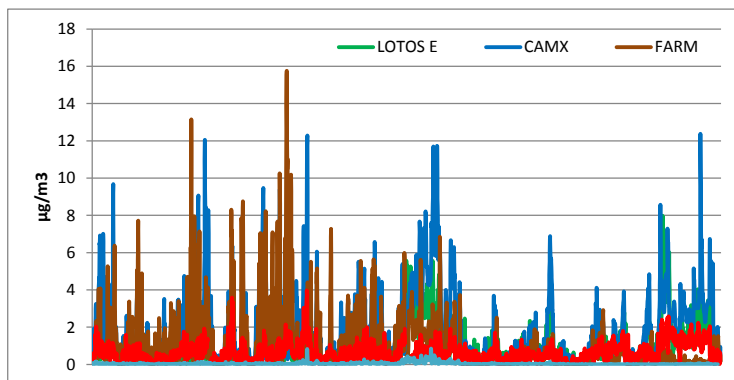
Performance of CTMs for Agriculture



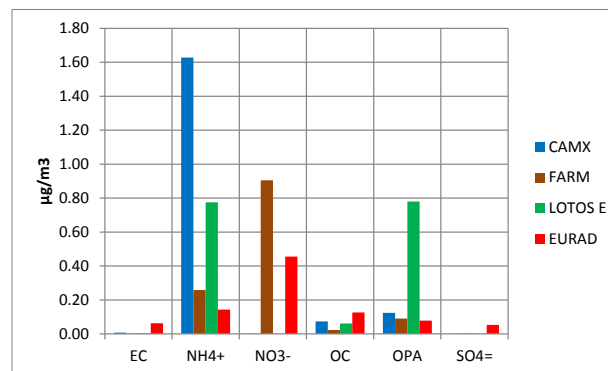
whole period	LOTOS E	CAMX	FARM	EURAD	CHIMERE
average ($\mu\text{g}/\text{m}^3$)	0.91	1.78	0.95	0.64	0.04
sd ($\mu\text{g}/\text{m}^3$)	1.09	1.87	1.51	0.49	0.06

R	LOTOS E	CAMX	FARM	EURAD	CHIMERE
LOTOS E	1	0.60	0.26	0.50	0.37
CAMX	0.60	1	0.42	0.52	0.49
FARM	0.26	0.42	1	0.27	0.24
EURAD	0.50	0.52	0.27	1	0.25
CHIMERE	0.37	0.49	0.24	0.25	1

Time trends for Agriculture



Chemical profiles for Agriculture



The contributions to PM_{2.5} from agriculture, a complex source, were analysed more into detail. CAMx presents the highest contributions on average.



The time trends of CAMx and LOTOS E were the most correlated among each other.

FARM presents highest levels in summer while LOTOS E shows highest ones in winter.

The chemical components associated with this source provide evidence about the underlying assumptions of the different types of models.

Different CTM SA approaches



	Tagged	Brute force
Description	Tagged species are used to track the contributions of sources in every grid cell by mass balance. $\text{Conc.} = (\text{emission} + \text{import} + \text{formation}) - (\text{export} + \text{degradation} + \text{deposition})$	Estimate the contribution of sources by comparing the BC with a run where the source of interest has been reduced by a given % over the whole domain.
Kind of approach	Static  Depicts the situation corresponding to the input dataset	Dynamic  It is actually a sensitivity analysis. Estimations are obtained by altering the input dataset.
Underlying question	What is the actual contribution of sources in the studied area/time window?	What would be the reduction in concentrations corresponding to a given reduction in emissions?
Runs	Accomplishes the apportionment in one single run	Requires a number of runs equal to the number of sources to apportion plus base case
Mass conservation	The total mass is conserved	The total mass of the different sources is obtained from independent runs. The mass is not conserved. Post processing is needed to re-normalize the sources.
Uncertainties	Uncertainties of the model (e.g. processes,), uncertainties of the input data (EIs, meteo data, BC)	Same as previous, plus the uncertainty of the sensitivity coefficients. In addition, it sums up the uncertainties of every run
Advantages	Reflects the current situation	Respond to the question of interest for the policy maker
Disadvantages	The actual contribution of source is not necessarily what can be abated	Require many runs More assumptions and uncertainties

Conclusions of the IE (1)

GENERAL

- In general models show better performances in estimating the average source contribution for the entire period than the contributions for single time steps (time series).

RMS

- RMs present comparable results which are also coherent with measured PM.
- There is a convergence towards one particular model: PMF5.
- Industry source category in RM needs better definition because too generic.
- Care is required in defining the conditions for the comparison between RMs and CTMs.
- The comparability between RMs and CTMs varies for the different sources.

Conclusions of the IE (2)

CTMs

- CTMs show good performances when tested using an ensemble reference.
- No significant differences in performance between source categories.
- The sensitivity analysis for CTM demonstrates the influence of the spatial resolution on the SA performance of model in densely populated areas.
- More effort is needed to improve the estimation of **soil and road dust** sources, in particular in the emission inventories.
- More work is needed to understand the implications of the different CTM approaches (tagged, brute force) and the information about the sources they provide.

Road Map 2017-2019 (1)

- Develop comprehensive **guidelines** for RM and CTM approaches on the basis on the inter-comparison exercise and other scientific evidence.
- Develop methodologies to support the evaluation of CTM models, with a particular focus on **spatial issues**.
- Promote the **integration** between RM and CTM in order to take advantages of the strengths of both approaches.
- Support to the **e-reporting** process (built-in SHERPA report facility)
- Support **pilot regions/cities** in their source-apportionment estimates (first stage of an air quality plan)

Road Map 2017-2019 (2)

- Interact with **CEN** to take advantage of synergies and contribute to standardization
- Continue improving the **DeltaSA** on line tool for testing SA applications
- Extend the activities to pollutants for which there are already available tools (**ozone, nitrogen oxides**, etc.)
- Perform **training** activities to disseminate harmonized best practices

In collaboration with IAEA regional projects on source apportionment and the newly created Task Force on Air Quality of the EU Strategy on Danube Region.

Thank you for your attention!

Intercomparison exercise: what's next

- Extend evaluation to identification of geographical origin of pollutants
- Better understanding of the differences between brute force and tagged approaches
- More work is needed to improve estimation of critical sources (involving complex processes: i.e. secondary) such as agriculture
- Verification if the acceptability thresholds are appropriate
- Evaluation of other pollutants (specific PM components: BC, PAHs)
- On the basis of the performance of the different models develop a strategy combining RM and CTM to take advantage of the advantages of both
- Continue development of state-of-the-art SA CTM models and use RM for validation purposes

Guidance on the use of air quality models for estimating particulate matter source contributions (thanks to M. Mircea – ENEA)

Contents

1 Introduction

- 1.1 Aims – link with WG4
- 1.2 Audience
- 1.3 Why use an air quality (AQ)/chemical transport model(CTM)?

2 Air quality models -link with WG1

- 2.1 Primary aerosol: Gaussian steady-state and Lagrangian puff models
- 2.2 Primary and secondary aerosol: Eulerian photochemical grid models

3 PM source attribution in grid models

- 3.1 Sensitivity analysis methods
- 3.2 Reactive tracer methods

4 Modelling source impacts

- 4.1 Source categories and/or source regions -link with WG2
- 4.2 Representativeness of the domain and time period-link with CCA1 - Spatial representativeness
- 4.3 Spatial and temporal resolutions of simulations
- 4.3 Emission inventories-link with WG2
- 4.4 Natural emissions
- 4.5 Boundary conditions
- 4.6 Meteorology
- 4.7 Model evaluation-MQO -link with WG1
- 4.8 Estimate modelled source contributions

5 Evaluation of estimated source contributions

- 5.1 Impact of input data uncertainties on source contributions from AQ/CTM
- 5.2 Comparison of source contributions from AQ/CTM and receptor modelling (RM) approaches -link with previous work in WG3
- 5.2 Combined use of AQ/CTM and RM source contributions: hybrid approaches-link with previous work in WG3

References

Appendix 1: Applications of AQ models for estimating particulate matter source contributions in Europe

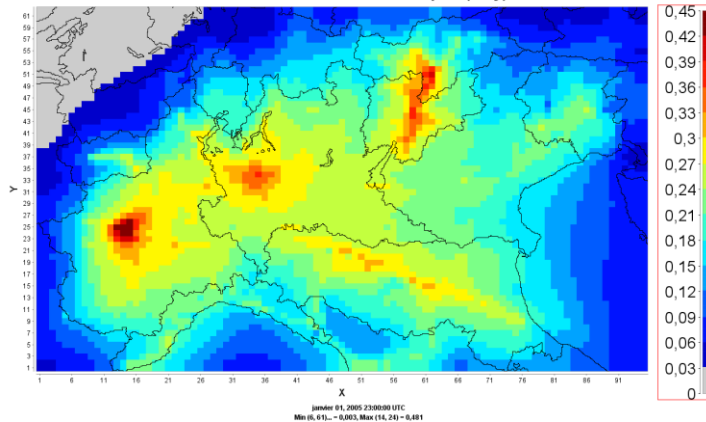
Geographical Source Apportionment (Contribution Estimate from Source Regions)



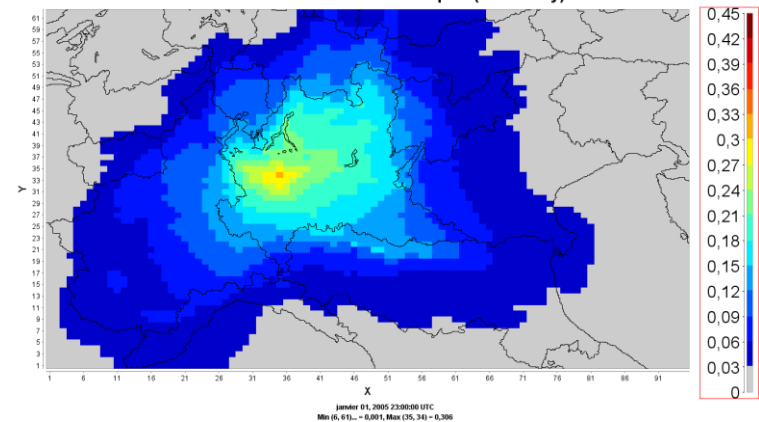
PM_{2.5}

(Emission sectors – Po valley vs Lombardy)

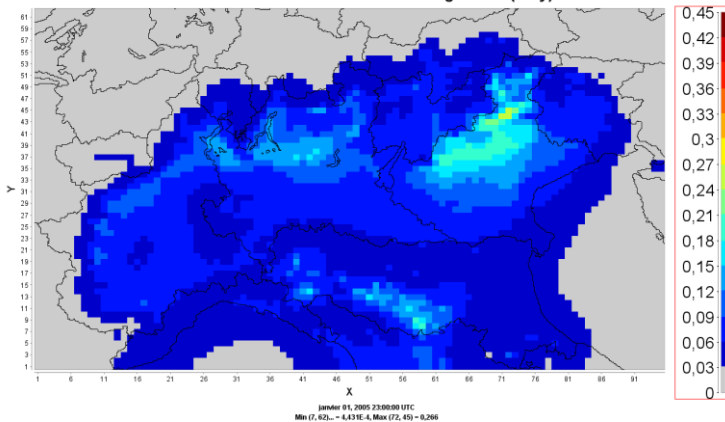
PM2.5 Yearly Mean concentration
Contribution from Road transport (Italy)



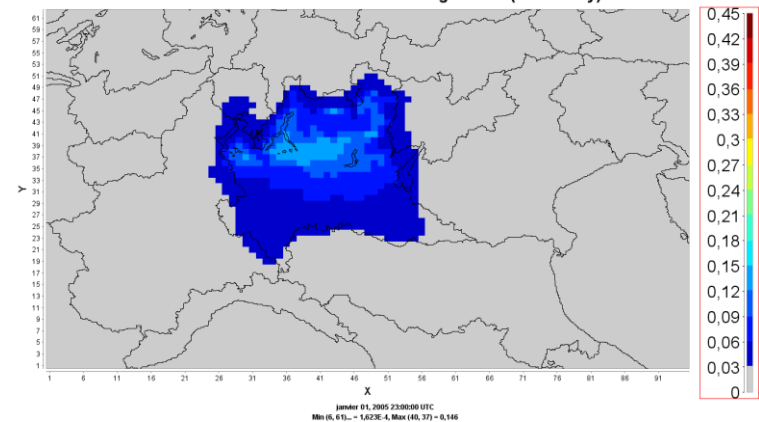
PM2.5 Yearly Mean concentration
Contribution from Road transport (Lombardy)



PM2.5 Yearly Mean concentration
Contribution from Biomass burning in DH (Italy)



PM2.5 Yearly Mean concentration
Contribution from Biomass burning in D.H. (Lombardy)

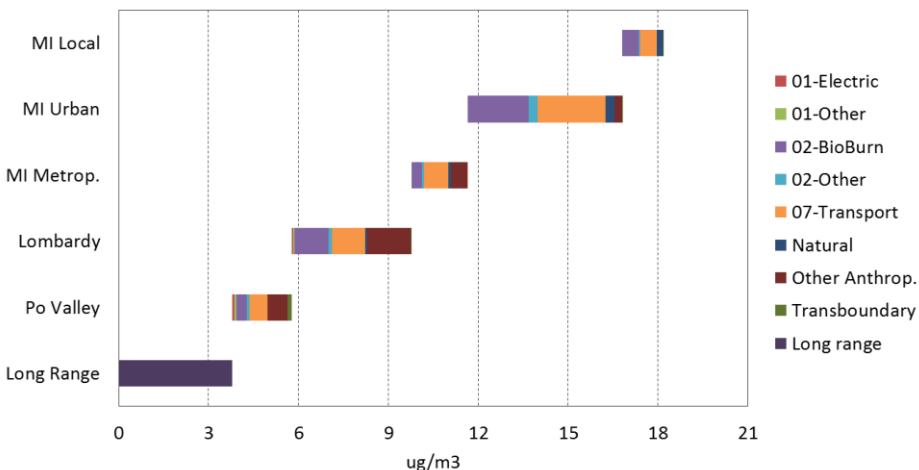


Geographical Source Apportionment (Contribution Estimate from Source Regions)

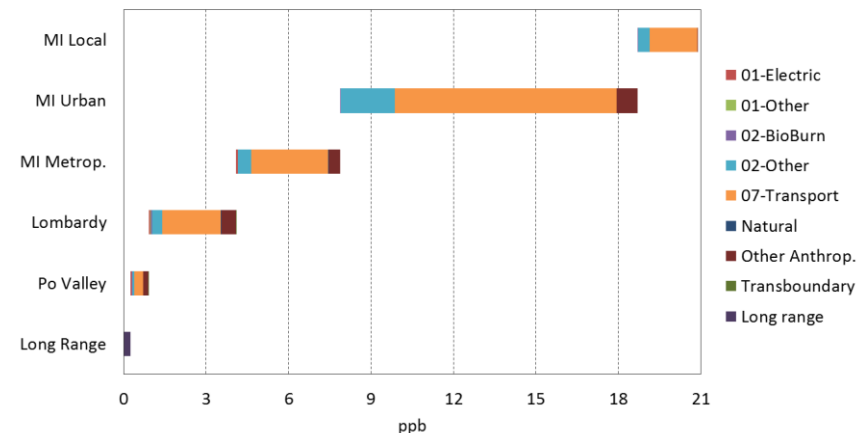


Milan Receptor

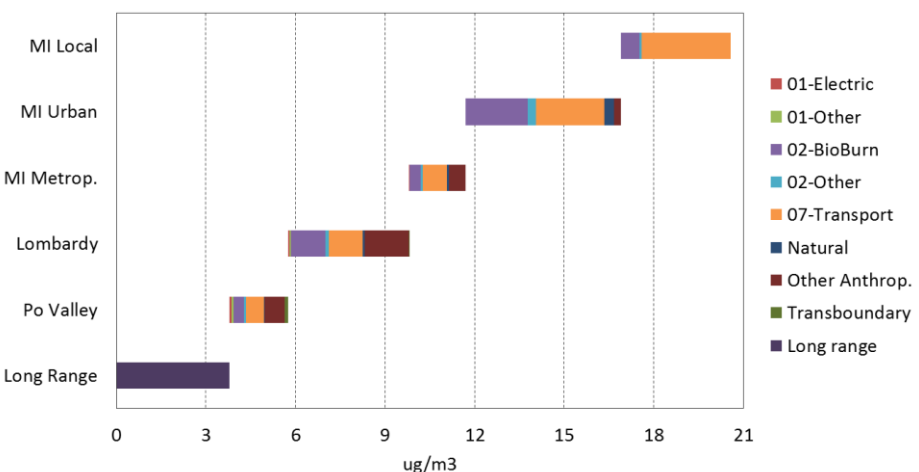
PM2.5 - Duomo (CAMx)



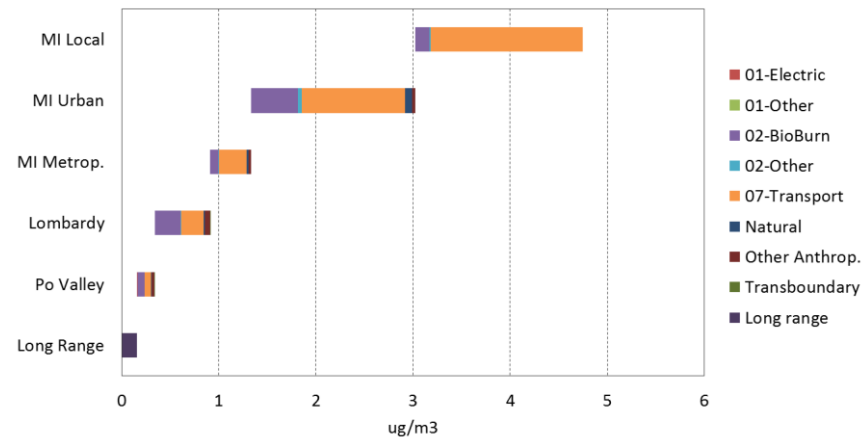
NO2 - Duomo (CAMx)



PM2.5 - Traffico (CAMx-HMS)



EC - Traffico (CAMx-HMS)





Consider an ideal situation with only two sectors: **Transport** and **Agriculture**

Suppose **Transport** emits just NO_x and **Agriculture** just NH_3
...suppose also they emit the same rate and there are no limiting effects.

Therefore the same amount of NO_x moves to NO_3^- and NH_3 to NH_4^+

Brute Force (BF) computes source contribution removing it:

If I remove **agriculture** I remove NH_4^+ but also NO_3^- $\rightarrow \Delta\text{PM}_{\text{AG}} = \text{PM}_{\text{tot}}$

If I remove **Transport** I remove NO_3^- but also NH_4^+ $\rightarrow \Delta\text{PM}_{\text{RT}} = \text{PM}_{\text{tot}}$

...? $\Delta\text{PM} = 2 * \text{PM}_{\text{tot}}$??

After normalization...

$$\text{PM}_{\text{RT}} = \text{NO}_3^-/2 + \text{NH}_4^+/2 = \text{PM}_{\text{AG}} = \text{NO}_3^-/2 + \text{NH}_4^+/2 = \text{PM}_{\text{tot}}/2$$

(Apportionment of Source Effects)

Tagged (TAG) computes source contribution according to precursors:

Agriculture emits just NH_3 $\rightarrow \text{PM}_{\text{AG}} = \text{NH}_4^+$

Transport emits just NO_x $\rightarrow \text{PM}_{\text{RT}} = \text{NO}_3^-$

$$\text{PM}_{\text{RT}} = \text{PM}_{\text{AG}} = \text{PM}_{\text{tot}}/2$$

(Apportionment of Source Precursors)

Scenario Analysis

If I remove **agriculture** I remove NH_4^+ but also NO_3^- $\rightarrow \Delta\text{PM}_{\text{AG}} = \text{PM}_{\text{tot}}$

If I remove **Transport** I remove NO_3^- but also NH_4^+ $\rightarrow \Delta\text{PM}_{\text{RT}} = \text{PM}_{\text{tot}}$

$$\Delta\text{PM}_{\text{AG}} = \Delta\text{PM}_{\text{RT}} = \text{PM}_{\text{tot}} = 2 * \text{PM}_{\text{RT}} = 2 * \text{PM}_{\text{AG}}$$

On-line Delta SA tool

User : jrc1

Home | Glossary | Logout

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.

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 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.

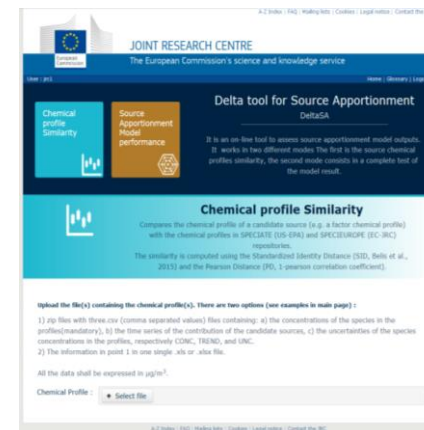
The output of the source apportionment models are Source Contribution Estimates (sce), in other words, the estimation of the contribution from source categories ("candidate sources" or simply "candidates") to the total mass of the studied pollutant(s). In the present release of the tool, are only available 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 (µg/m³) of every species, plus the mass concentration (µg/m³) 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 (µg/m³), b) the time series of source contribution (µg/m³) for each candidate source, c) the uncertainty of the chemical profiles (µg/m³) 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.

Download CPS

Download MP

A-Z Index | FAQ | Mailing lists | Cookies | Legal notice | Contact the JRC



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)