The importance of inter-comparison exercises for the development of source apportionment tools

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Presentation overview

- Source apportionment approaches
- Main goals and information that can be obtained from an intercomparison
- How is the intercomparison organized?
- What is the evaluation approach?
- State of play of IE
- Future work

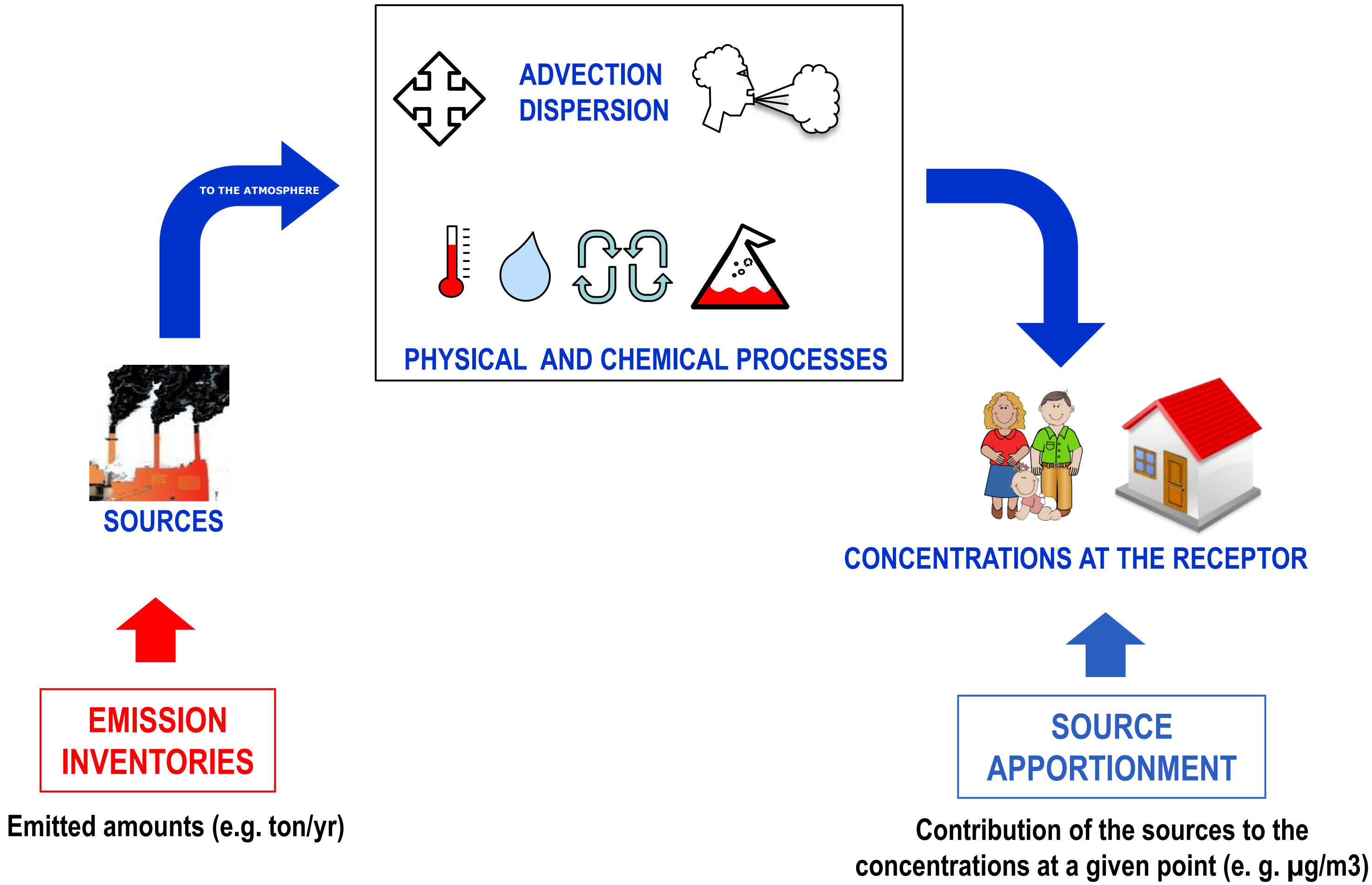
What is source apportionment?

Source Apportionment (SA) is the practice of deriving quantitative information about the contribution of sources to the concentration of pollutants at a given receptor or area.

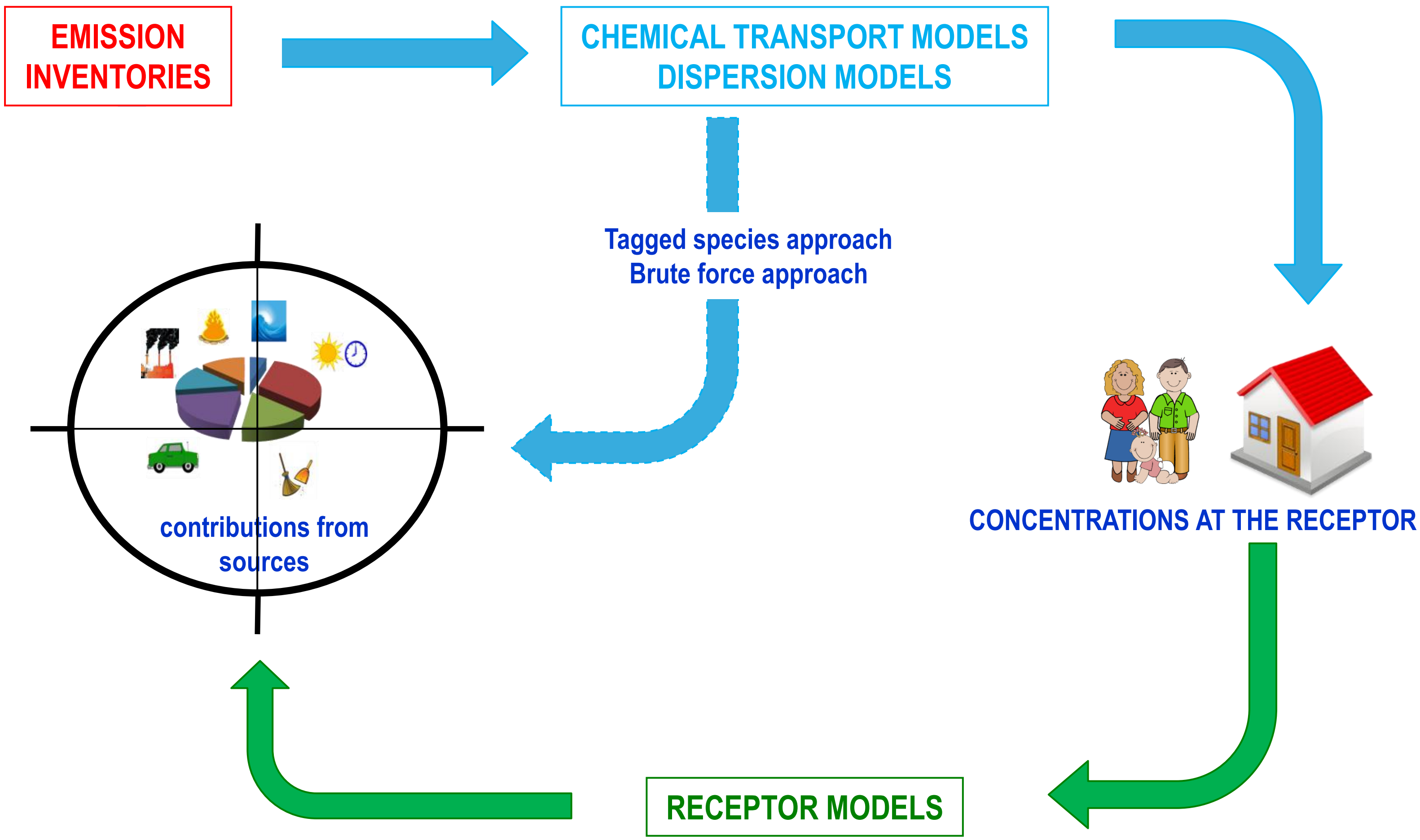
The fundamental limiting factor for source apportionment is that the actual contribution of sources to the concentration of a pollutant at a given cannot be directly observed.

Source apportionment is needed for the air quality management to fulfil MS obligations under the AQD and the IPR.

Source apportionment and emission inventories: similar but different



Source apportionment approaches



Main goals

- Contributing to the **harmonization** of Source Apportionment methods and tools

  (development and sharing of Best Practices)

- Contributing to the **integration** of Source and Receptor oriented techniques

  (to provide more robust and complete Source Apportionment information)

- Favoring the **connection** between Source Apportionment and Planning

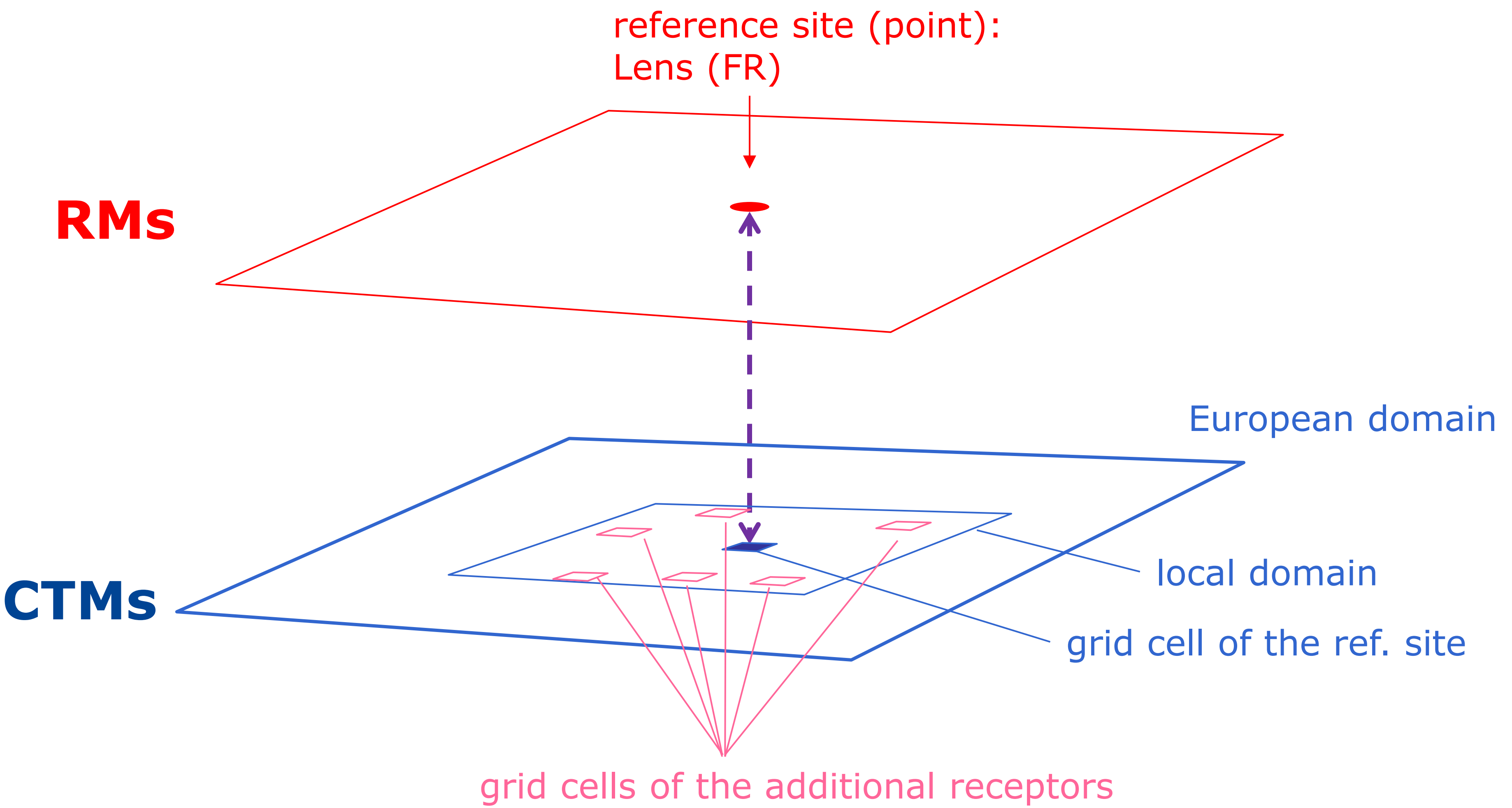
  (e.g. use of common indicators, orienting the choice of effective plans)

Information that can be obtained from this IE

- Overall model performance on the basis of pre-established criteria,
  - ✓ *for the purposes of air quality management (AQM)*
- Indirect measure of the overall output uncertainty,
- More robust SA results (from a single outcome to an ensemble)
- Cross-validation of obtained results (to overcome the lack in observed data)
- Provide 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 SMs) and assumptions*

- Additional details about SMs performance
- Integration of RMs outcomes (e.g. Apportionment of secondary pollutants, source-regions apportionment,…)

How is the intercomparison organized?



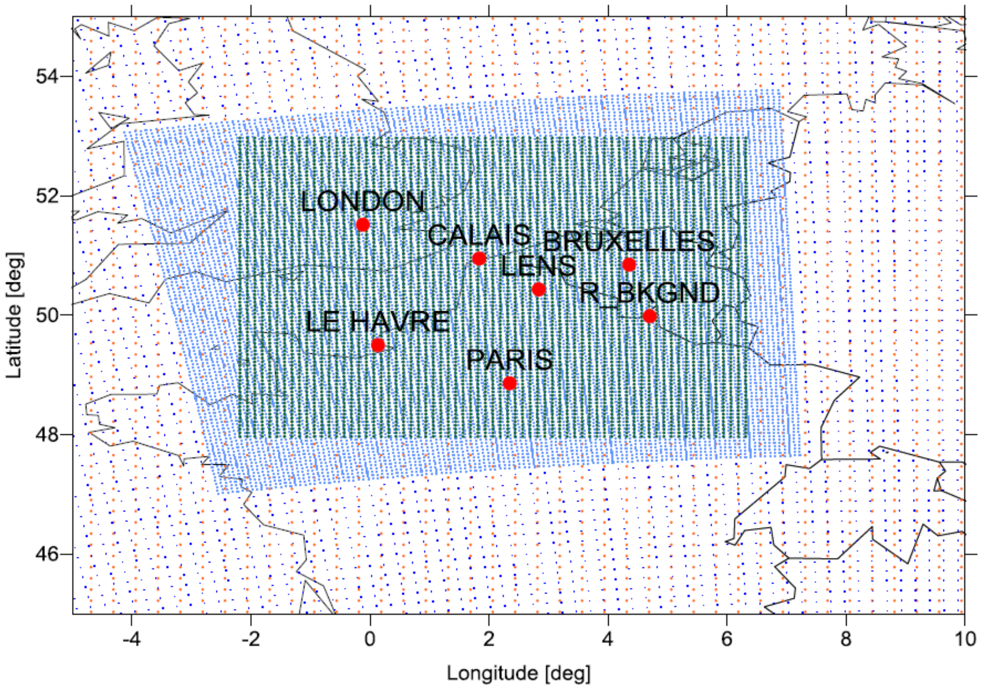
Intercomparison outline – Receptor oriented models

DATA SET WITH SPECIATED PM (including organic markers)

COUNTRY	France
PERIOD	03.2011 to 03.2012
TIME RES.	every 3 days
DURATION OF SAMPLING	24 hours
TYPE OF SITE	Urban background
	PM10
N SAMPLES	116
IONS	ok (8 species)
EC/OC	ok
TRACE ELEMENTS	ok (25 species)
PAHs	ok (15 species)
LEVO/MANN	ok + galacto
HOPANES	ok (10 species)
N-ALKANES	ok (29 species)
CHOLESTEROL	
SOA MARKERS	ok
OTHER	Pristane, Phytane, Glucose

Intercomparison outline – Source oriented Models

- **Common input dataset**
  - **ECMWF meteorology**
  - **TNO emissions**
  - **MACC chemical fields**
- **Centralized MPE**
  - **LENS dataset**
  - **AIRBASE sites**
  - **Local networks**
- **Set of receptors (10)**
  - **Lens**
  - **Urban sites**
  - **Coastal sites**
  - **Background sites**



8 - 14 source categories
3 + 3 summer/winter months
Hourly concentrations
Primary and secondary PM
PM precursors

European Commission

Evaluation Methodology (RM)

Complementary tests: provide ancillary information about the solutions' performance

- Mass apportionment
- Number of factor/sources

Preliminary tests: test if source/factors belong to a given source category

- Chemical profiles → Pearson, Pearson (log-transformed), SID, WD
- Time-trends → Pearson
- Contribution-to-species (%) → Pearson

= % of species total matrix (EPA PMF v3) = explained variation (PMF 2) = contribution by species (CMB 8.2)

Performance tests Evaluate if source/factor SCEs fall within an established quality objective

- Z-scores → test solution bias coherence with the quality objective (σ_p)
- Z'-scores → test SCE reported uncertainty coherence with the one of the reference
- RMSD* → test the bias, amplitude and phase of the SCE time trends

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A new methodology to assess the performance and uncertainty of source apportionment models in intercomparison exercises

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A new methodology to assess the performance and uncertainty of source apportionment models II: The results of two European intercomparison exercises

C.A. Belis [a,*], F. Karagulian [a], F. Amato [b], M. Almeida [c], P. Artaxo [d], D.C.S. Beddows [e], V. Bernardoni [f], M.C. Bove [g], S. Carbone [h], D. Cesari [i], D. Contini [i], E. Cuccia [g], E. Diapouli [j], K. Eleftheriadis [j], O. Favez [k], I. El Haddad [l], R.M. Harrison [e,m], S. Hellebust [n], J. Hovorka [o], E. Jang [e], H. Jorquera [p], T. Kammermeier [q], M. Karl [r], F. Lucarelli [s], D. Mooibroek [t], S. Nava [s], J.K. Nøjgaard [u], P. Paatero [v], M. Pandolfi [b], M.G. Perrone [w], J.E. Petit [l,z], A. Pietrodangelo [x], P. Pokorná [o], P. Prati [h], A.S.H. Prevot [m], U. Quass [q], X. Querol [b], D. Saraga [y], J. Sciare [z], A. Sfetsos [y], G. Valli [g], R. Vecchi [g], M. Vestenius [i], E. Yubero [aa], P.K. Hopke [ab]

RSE Ricerca Sistema Energetico

Joint Research Centre

European Commission

Evaluation in this IE

RM

SINGLE SITE

Complementary tests:

Mass apportionment

Number of factor/sources

Preliminary tests:

Chemical profiles

Contribution-to-species (all)

Time-trends

Performance tests

Z-scores

Z'-scores

RMSD*

BOTH

SINGLE SITE

Complementary tests:

~~Mass apportionment~~

~~Number of factor/sources~~

Preliminary tests:

Chemical profiles

Contribution-to-species (selected ones)

Time-trends

Performance tests:

Z-scores

Z'-scores

RMSD*

CTM

MULTI SITE

Complementary tests:

~~Mass apportionment~~

~~Number of factor/sources~~

Preliminary tests:

Chemical profiles

Contribution-to-species (seleted ones)

Time-trends

Performance tests:

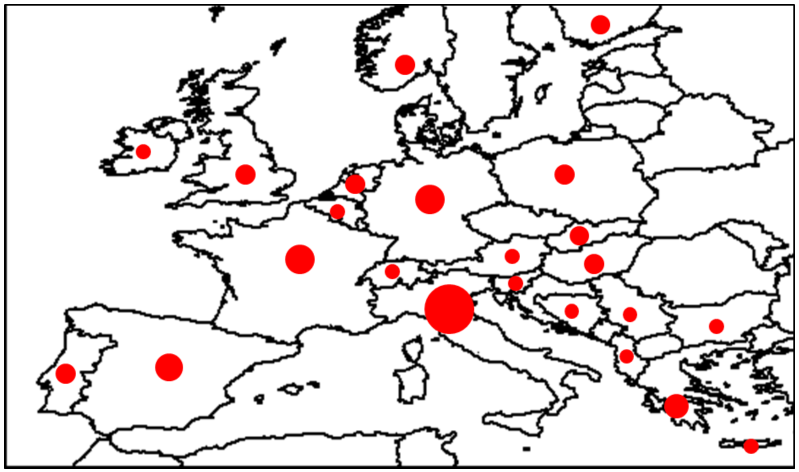
Z-scores

Z'-scores

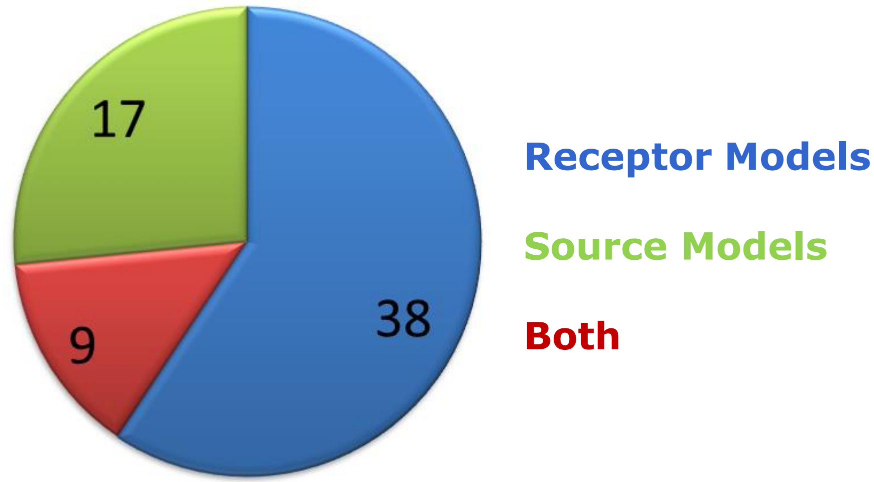
RMSD*

State of play of IE

Applications: 79
Withrawed: 15
Expected to deliver: 64



21 EU countries + USA, Brasil, Chile, India



- **RM results reported 32 teams**
- **Modeled SA report in progress**
- **Analysis of results → first half 2016**
- **Discussion → Technical meeting Zagreb (June 2016)**

Future work

- Update SA technical guidance
- Extension to:
  - ✓Other receptors/areas, e.g. Western vs Eastern Europe
  - ✓Primary vs Secondary pollutants
  - ✓Anthropogenic vs Natural sources
- Harmonization and testing of geographical origin of pollutants (transboundary, long-range transport vs local)
- Development of combined RM and SM techniques
- Extension to other pollutants (e.g. NO_X, O_3, VOCs)
- Connection with Planning
- Test the overall approach in pilot areas

Thank you for your attention

Receptor models

Strengths

- **Derive from real-world measurements on one or more sites.**
- **Appropriate for urban areas and source-oriented sites, but also for regional scale.**
- **Good output uncertainty estimation.**
- **Can be used to identify main source categories even when there is poor information about source chemistry and location.**
- **Mainly used for PM, but also for VOC, PAH and gaseous pollutants.**
- **Combination with trajectories or wind analysis makes it possible to track the geographic origin of pollution.**

Limitations

- **Time series of pollution measurements and chemical characterization are needed.**
- **Not appropriate for reactive species.**
- **Provide limited information on secondary inorganic aerosol sources.**
- **Need for harmonization of methodological steps like estimation of the number and definition of source categories.**

Eulerian models

Strengths

- Reproduce complex physical and chemical atmospheric processes in a simplified manner.
- Provide estimation for every cell in the grid with hourly time resolution.
- Deal with reactive species and, therefore, are suitable to estimate the sources of secondary pollutants.

Limitations

- The complexity of the model makes it difficult to estimate the uncertainty of the output.
- The output depends on the quality and resolution of the emission inventories.
- Current versions do not focus much on the contribution of species that have a small share of the total pollution mass (e.g. heavy metals, PAHs).
- Models using brute force (BFM) or zero out (ZO) methods to identify sources have high computational intensity, and the smaller concentration changes between the simulations may be strongly influenced by numerical errors (Koo et al., 2009). In addition, model response may be nonlinear or non-additive making difficult to compare the base case and the scenario case.