SPECIEUROPE

The European data base for PM sources' profiles

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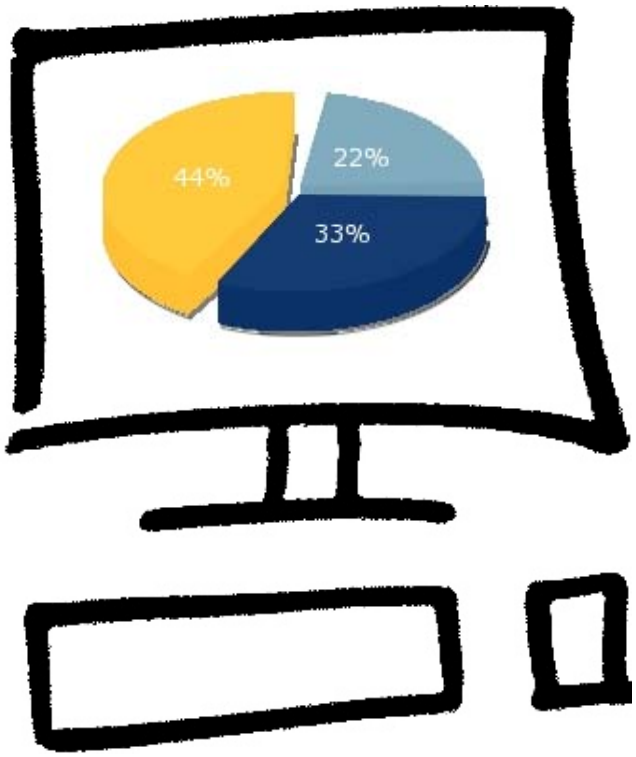
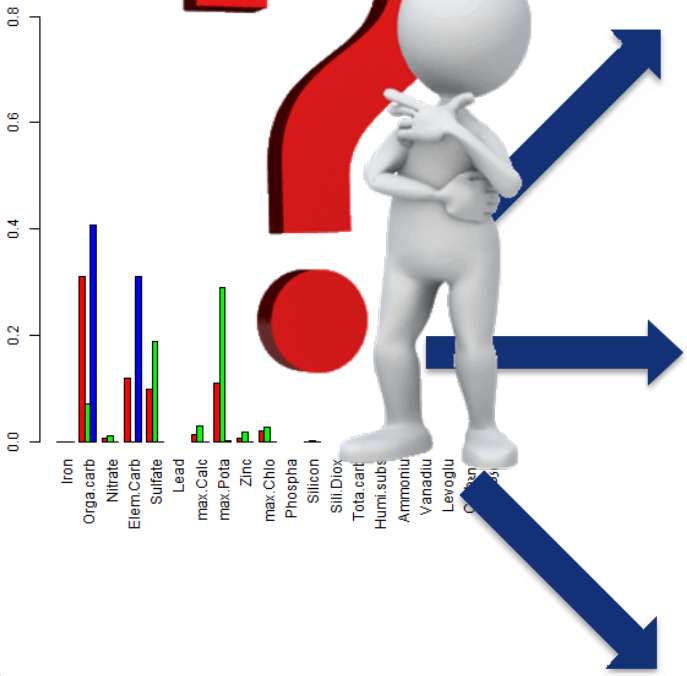
Outline

- **Motivations**
- **Content**
  - database architecture
  - overview on source categories
- **Usage examples**
  - clustering
  - ranking
- **Conclusions**

Motivations





source apportionment
multivariate factor
analytical approach

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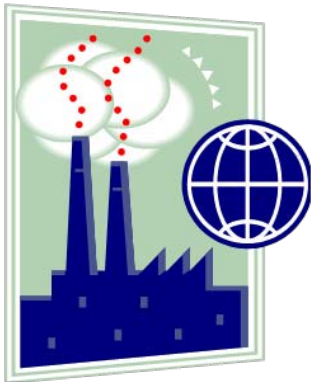
Motivations



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Source profiles for Europe Database

http://source-apportionment.jrc.ec.europa.eu/Specieurope

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Database architecture

***Principal table**:*

1. *Profiles' species relative concentrations, their uncertainties and the analytical technique used.*

***Metadata tables**:*

1. *Single profile name and description.*
2. *Publication information (each publication normally contains more than one profile).*
3. *Information on source categories (next slide).*

→ ***Ancillary tables** store the codification system used for uncertainty methods, chemical families, chemical species, chemical analytical methods and source categories' description.*

→ *Each species is generally corresponding to the one reported in SPECIATE*

→ *The source profiles are identified by a unique ID, which should be reported*

Most frequent species

Calc.ion
Potass.ion
Zinc
Copper
Manganese
Nickel
Iron
Lead
Chromium
Vanadium
Sodium.ion
Cadmium
Magnes.ion
Aluminum
Barium
Strontium
Chlo.ion
Sulfate
Nitrate
Antimony
Arsenic
Ammonium
Titanium
Cobalt
Silicon
Bromine
Tin

Organic carbon
Elemental Carbon
Selenium
Zirconium
Sulfur
Scandium
Thallium
Gallium
PAH
Benzo(ghi)perylene
Rubidium
Molybdenum
Carbonate
Indeno[1,2,3-cd]pyrene
Benzo[b]fluoranthene
Benzo[a]pyrene
Benzo[k]fluoranthene
Benzo[e]pyrene
Coronene

Src ID	SOURCE	PARENT_ID	Src ID	SOURCE	PARENT_ID
999	All sources		**33**	Natural gas burning	999
1	Traffic	999	**34**	Boiler	20
2	Exhaust	1	**35**	Petrochemical	20
3	Diesel exhaust	2	**36**	Fugitive	20
4	Gasoline exhaust	2	**37**	Ship exhaust	999
5	Road dust	1	**40**	Biomass burning	999
6	Tyre wear	5	**41**	Wood burning	40
7	Brake dust	5	**42**	Pine burning	41
10	Soil dust	999	**43**	Pellet burning	41
11	Desert dust	999	**44**	Beech burning	41
12	Marine aerosol	999	**45**	Grape wine burning	41
13	Construction dust	999	**46**	Leaves burning	40
14	Volcanic dust	999	**47**	Closed fireplace	41
20	Industrial	999	**48**	Open fireplace	41
21	Iron and steel production	20	**49**	Olive oil burning	40
22	Foundries	20	**50**	Oak burning	41
23	Refineries	20	**51**	Spruce burning	41
24	Metal smelting	20	**52**	Larch burning (sw)	41
25	Cement	20	**53**	Soft wood burning	41
26	Incinerator	20	**54**	Hard wood burning	41
27	Ceramic	20	**55**	Open burning	40
28	Powerplant	20	**60**	Secondary inorganic aerosol	999
29	Fertilizer production	20	**61**	Ammonium nitrate	60
30	Fuel oil burning	20	**62**	Ammonium sulfate	60
31	Coal burning	999	**65**	Secondary organic aerosol	999
32	Coke burning	999	**66**	Deicing salt	999

Source categories

*Each profiles is associated to one or more **source category**, which are **hierarchically organized** (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**.*

src ID	Source category name	#prof	#spec	#pub	src ID	Source category name	#prof	#spec	#pub
1	**Traffic**	**28**	14.3	9	24	Metal smelting	4	18.5	2
5	Road dust	15	14.2	8	54	Hard wood burning	4	34.0	2
20	**Industrial**	**77**	17.0	7	33	Natural gas burning	3	15.3	2
40	**Biomass burning**	**24**	20.8	6	43	Pellet burning	3	19.7	2
10	Soil dust	20	14.8	6	53	Soft wood burning	3	26.3	2
41	Wood burning	18	23.8	6	44	Beech burning	2	15	2
30	Fuel oil burning	11	28.2	5	46	Leaves burning	2	13	2
47	Closed fireplace	16	25.7	4	55	Open burning	2	13	2
37	Ship exhaust	14	21.7	4	14	Volcanic dust	2	16	1
2	Exhaust	12	17.6	4	35	Petrochemical	2	38	1
25	Cement	11	15.1	4	49	Olive oil burning	2	16	1
28	Power plant	10	19.5	4	60	Second. inorg. Aer.	2	1	1
34	Boiler	8	18.0	4	6	Tyre wear	1	8	1
66	Deicing salt	6	2.2	4	7	Brake dust	1	17	1
31	Coal burning	12	20.5	3	23	Refineries	1	22	1
21	Iron & steel prod.	7	16.0	3	26	Incinerator	1	23	1
32	Coke burning	6	24.9	3	42	Pine burning	1	23	1
12	Marine aerosol	3	5.7	3	50	Oak burning	1	41	1
29	Fertilizer prod.	9	29.3	2	51	Spruce burning	1	77	1
22	Foundries	6	14.2	2	52	Larch burning	1	41	1
27	Ceramic	6	27.1	2	61	Ammonium nitrate	1	2	1
3	Diesel exhaust	5	19.3	2	62	Ammonium sulfate	1	2	1
4	Gasoline exhaust	4	20.0	2					

Source categories population

209 profiles:

- **150 original,**
- **13 composite**

- **39 derived,**
- **6 calculated theoretically**

following elaborations refer to **163 profiles** (original and composite)

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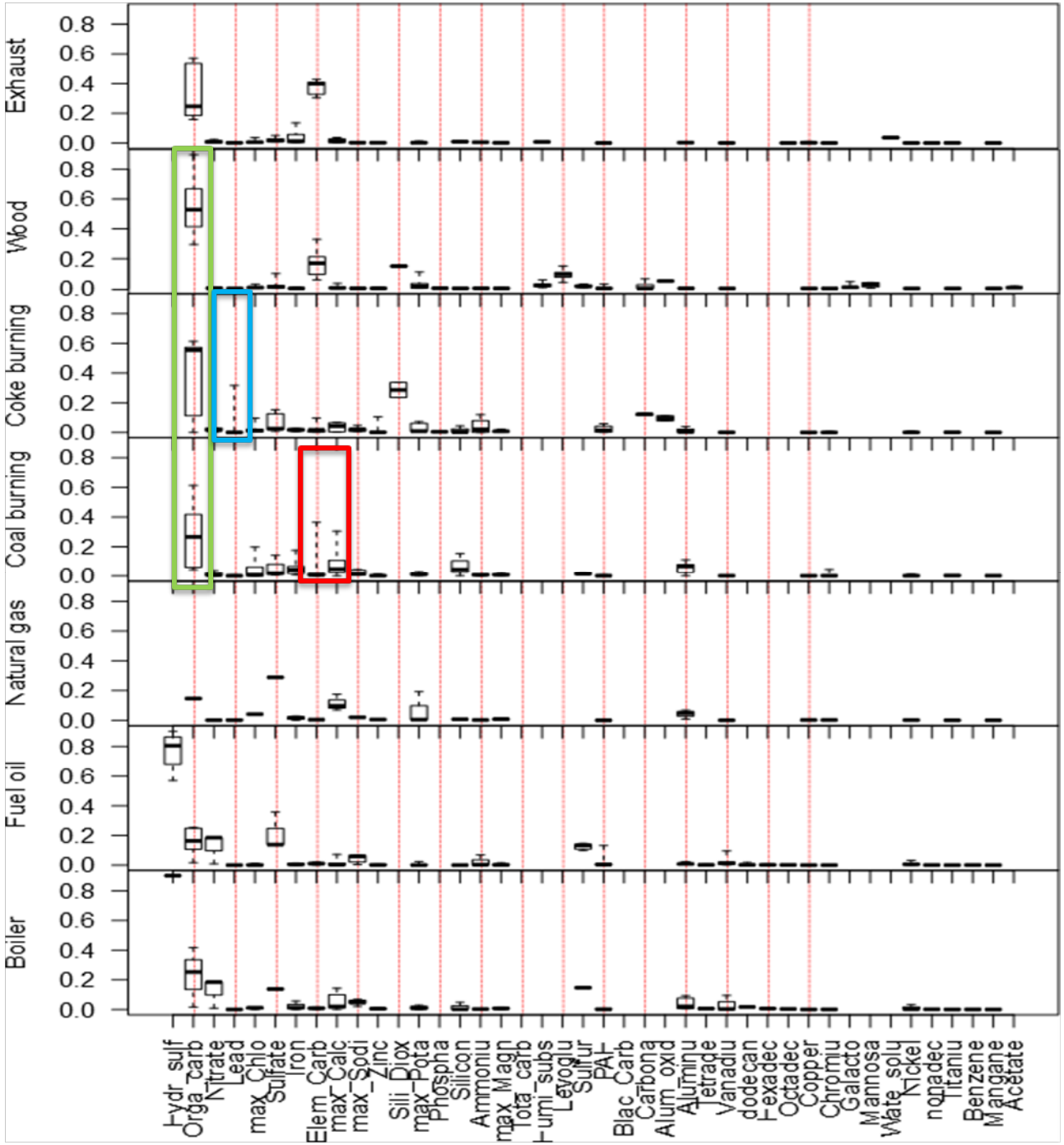

combustion processes

Boxplots represent the statistical distribution of the *42 most abundant chemical species* in the profiles attributed to the same category.

considerable variability:

- **organic carbon** especially in coke, coal and wood burning;
- **lead** in coke burning
- **EC and calcium** in coal burning

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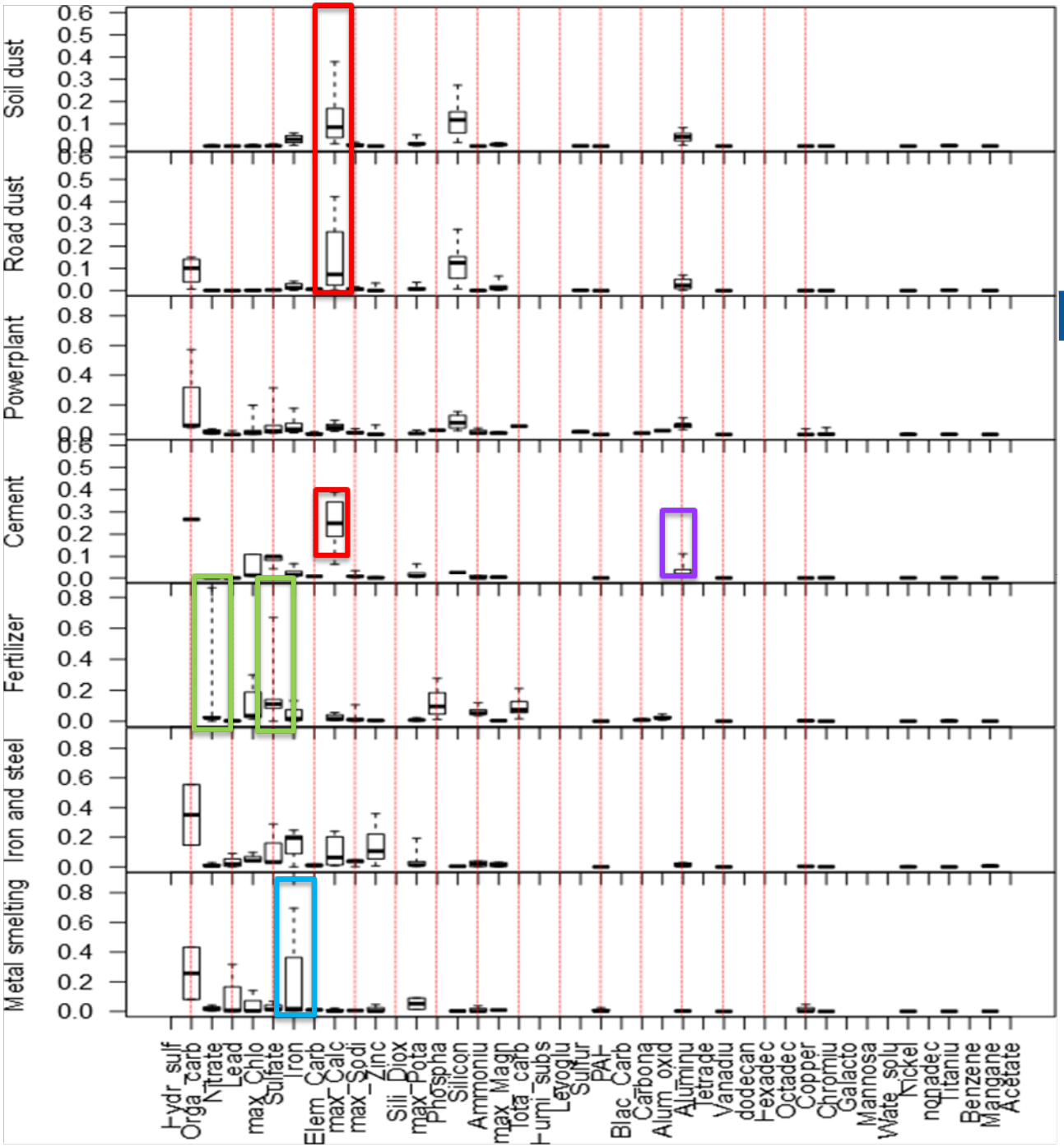

dust and industrial production

considerable variability:

- the **nitrate** and **sulfate** relative abundances in Fertilizer
- the **calcium** in Road, Cement and Soil dust
- the **aluminum** in Cement
- the **iron** in metal smelting

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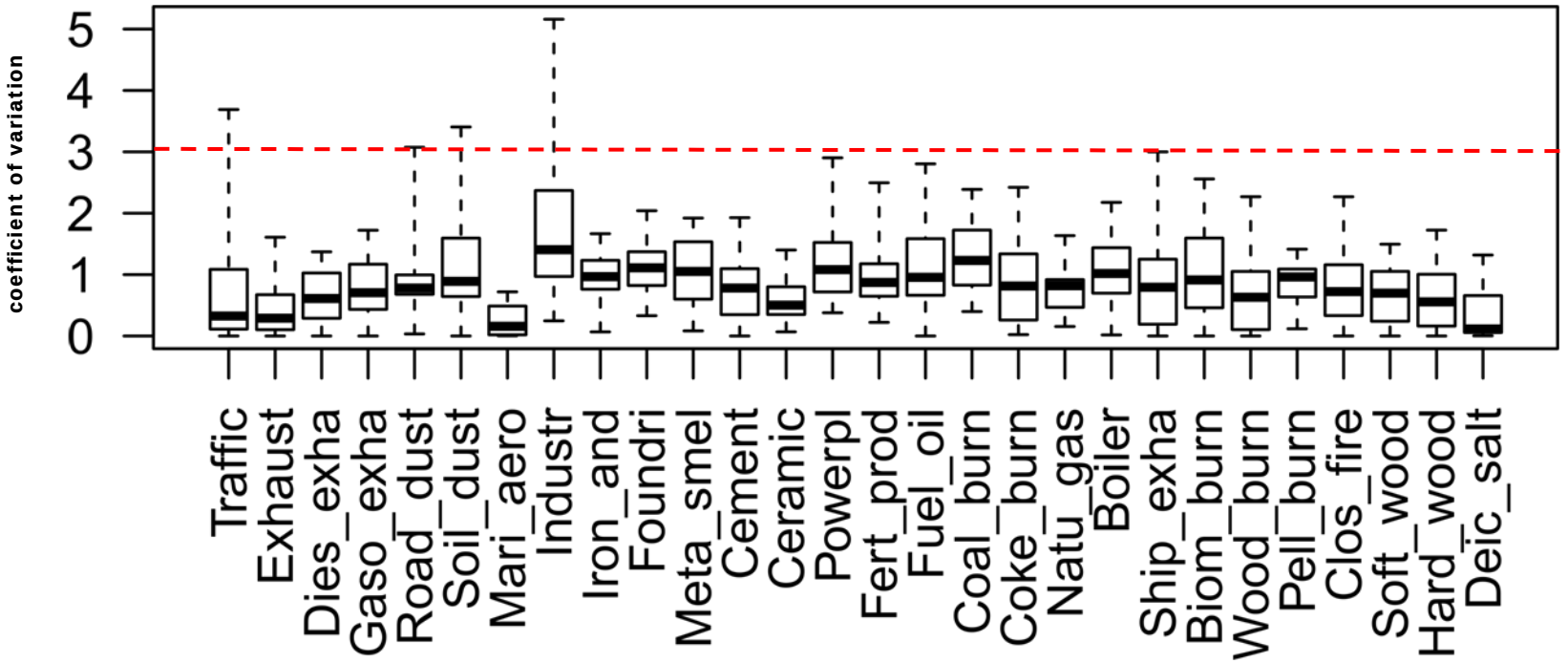
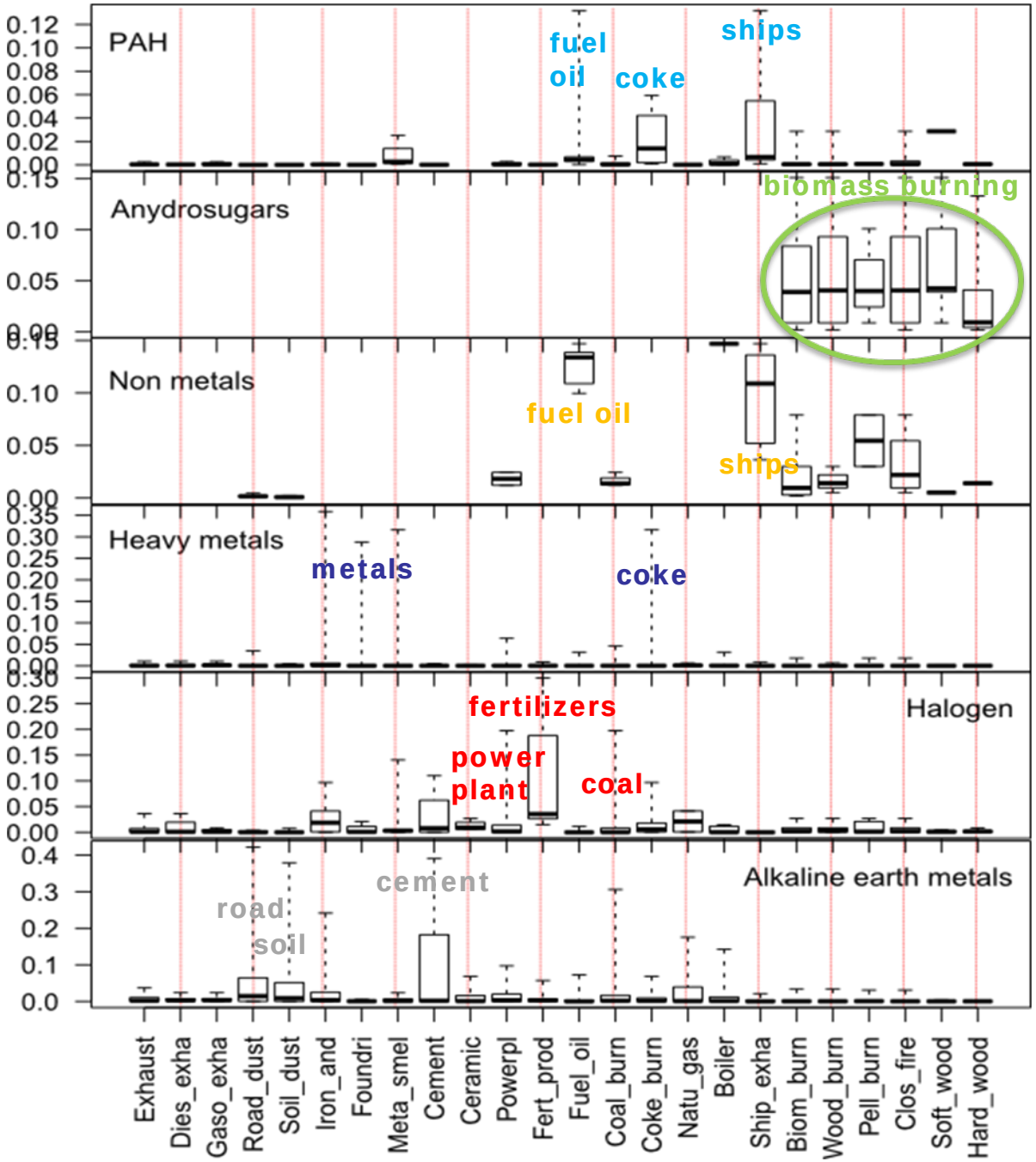
Variability within source categories



The coefficient of variation among all species within a source category is higher for more generalist categories: industrial, traffic, soil and road dust



species families
abundances

- **PAH** in Ship exhaust followed by Coke, and wood burning (in particular soft wood).
- **Anhydrosugars** (mostly Levoglucosan) are *only measured* in biomass burning and related sources.
- **Non-metals** (Sulfur) in Boiler, fuel oil and ship exhaust.
- **Heavy metals** in some of the metal related activities and coke burning,
- **Halogens** in fertilizer production, power plants and coal burning.
- **Alkaline earth metals** in road and soil dust, and in cement production.

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Application 1: Clustering

R pvclust :hierarchic clustering resampling the data via bootstrap (10000 replications) and assigning to each cluster an approximated unbiased (AU) p-value, using SID proportional indicator as distance (divide by 110)

http://bioinformatics.oxfordjournals.org/content/22/12/1540.full

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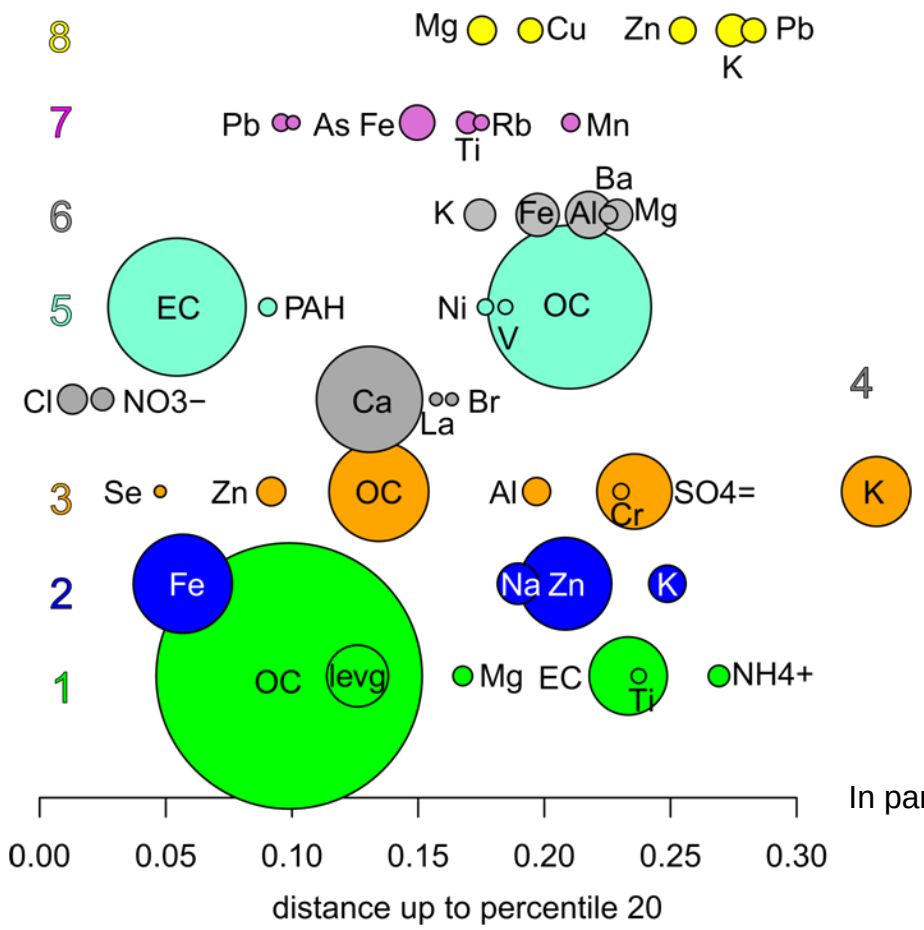
Clusters' markers



8. industrial (11)

7. industrial (5)

6. soil dust (20)

5. exhaust (8)

4. cement (6)

3. combustion (6)

2. industrial (steel,3)

1.wood burn. (16+3)

In parenthesis the number of 'independent' profiles within the cluster

within cluster species distances from species mean
(circle area proportional to relative mass)

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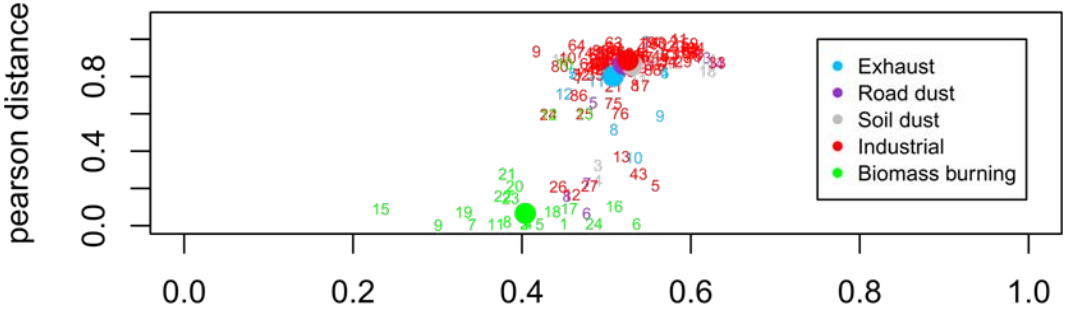
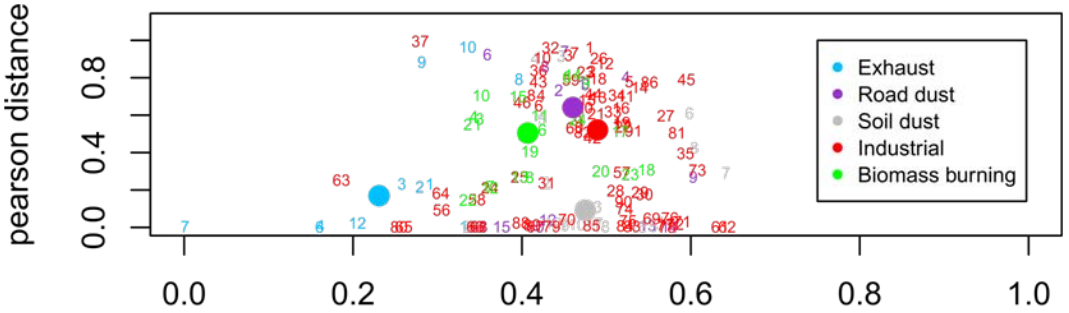
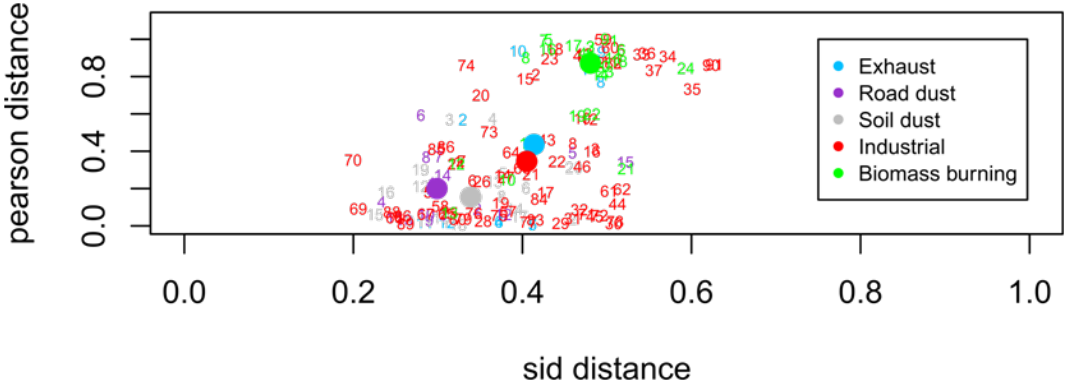
Profile 118: Wood burning



Profile 44: Exhaust



Profile 17: Soil Dust Composite Rural



Application2: Ranking

Some distances can be used in order to rank the **proximity of a single profile against all the profiles** present in SPECIEUROPE.

For some profiles these distances seem to give a good result (profiles that are correctly clustered by hpvclust)

Big colored point is the median on the distances of the given profiles from all profiles of that source category.

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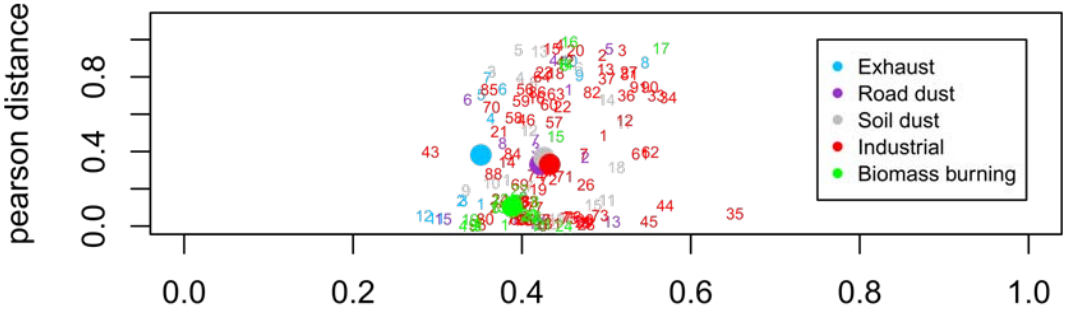
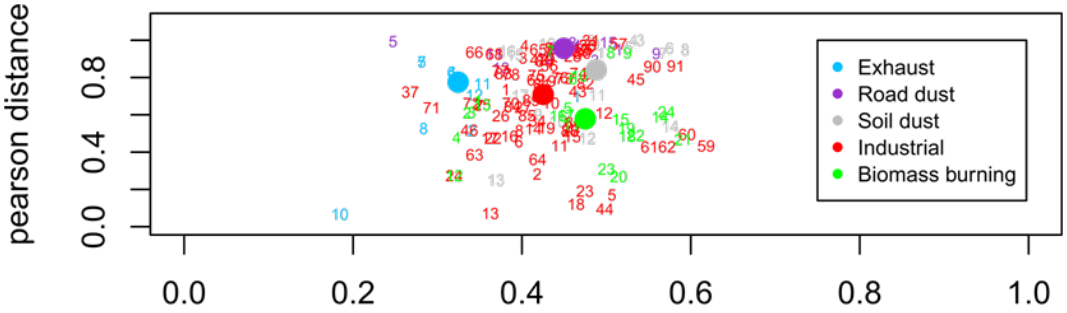
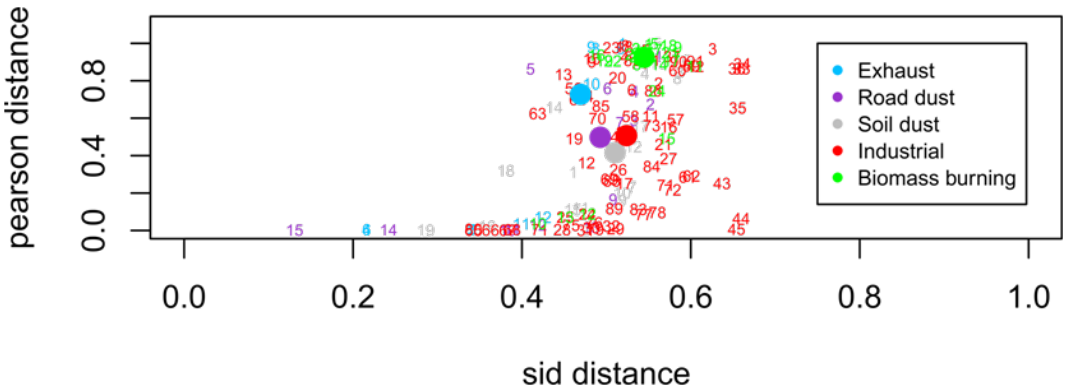
Profile 24: Open burning Leaves of chestnut and oak Combustion



Profile 88: Exhaust diesel taxi



Profile 182: Travertine rock



Big colored point is the median on the distances of the given profiles from all profiles of that source category.

Usage: Ranking

For other profiles (unclassified in cluster analysis) the **result is not so clear**.

More work needed in order to:

- check authors' classification
- identify the source category

Conclusions

- reference chemical composition of the PM sources for source apportionment applications in Europe.
- *common reference* → better definition of the sources
- *more measurements* → needed to better characterize sources form the chemical and geographical point of view
- *cluster analysis* → checking data quality and finding good source category markers
- *ranking* → need of a good source characterization and optimization of the metrics

Web site:

http://sourceapportionment.jrc.ec.europa.eu/Specieurope/index.aspx

Welcome to SPECIEUROPE

SPECIEUROPE is a repository of source profiles developed by the JRC in the framework of FAIRMODE WG3. The target users are source apportionment and emission systems, the encoding of species in SPECIEUROPE is coherent with the one of the well-known US-EPA SPECIATE repository for north-American sources.

SPECIEUROPE contains particulate chemical profiles including organic and inorganic species deriving from both measurements of European sources and source appor in studies, 39 derived from source apportionment studies and 6 theoretical (from stoichiometric ratios). The profiles bibliography is available in the DB, so that original very much welcomed (the list of collaborators is available in the credits section). The data distributed via this service can be used provided the source is mentioned.

For further information contact us at http://source-apportionment.jrc.ec.europa.eu/contact.aspx

For citation, we recommend the following sentence:

SPECIEUROPE
European Commission – Joint Research Centre
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http://source-apportionment.jrc.ec.europa.eu/
Contacts: Claudio Belis and Denise Pernigotti

European Commission

Contribute welcome!

Contribution of source profile data is very much welcomed and will be acknowledged in the dedicated page of the website.

http://source-apportionment.jrc.ec.europa.eu/Specieurope/howtoContribute.aspx

European Commission

Thanks

Laurent Y. Alleman, Andrés Alastuey Urós, Fulvio Amato,Vera Bernardoni, Imad El Haddad, Jorge Pey Betran, Adriana Pietrodangelo , Gianluigi Valli, Roberta Vecchi, Peter Wåhlin and Sinan Yatkin

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