

A dummy's guide to receptor modelling

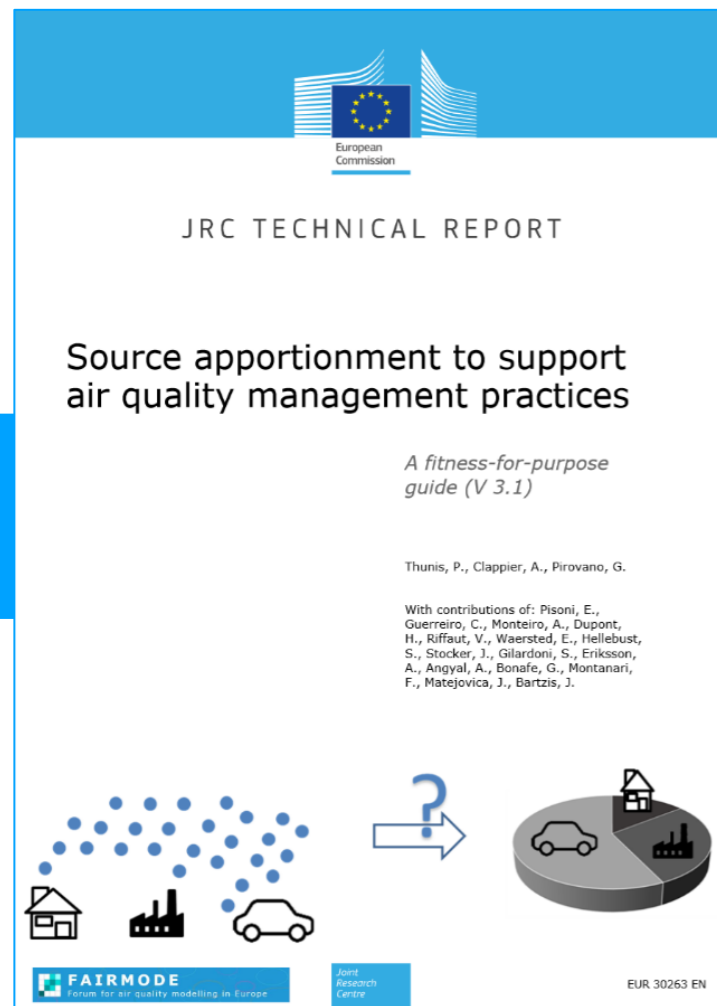
CT1 - Source apportionment

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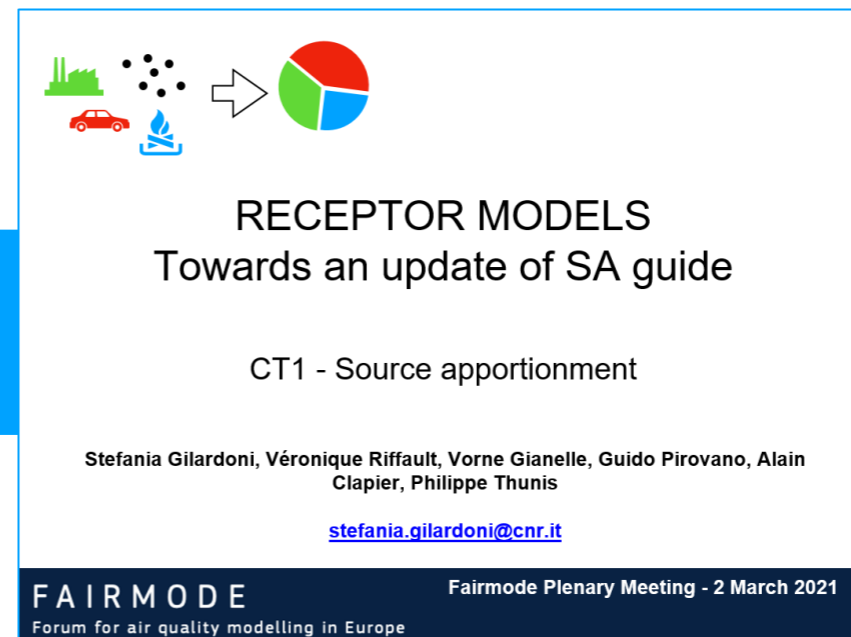
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MOTIVATION

Need to update the latest JRC guide with more details on receptor models, with a framework similar to the one used for source-oriented models



*Thunis, Clappier, Pirovano et al.
June 2020*



*Gilardoni et al.
March 2021*

RECEPTOR MODELS: PRINCIPLES

“Receptor models use the chemical and physical characteristics of gases and particles measured at source and receptor to both **identify the presence** of and to **quantify source contributions** to receptor concentrations.” (US EPA)

Based on 3 fundamental assumptions:

- ➊ A source emission has a **constant composition** over time
- ➋ The species do not react with each other but add linearly
- ➌ A number of p user-defined sources contribute to the receptor observations

If these assumptions are met:

$$C = a \times E \times D$$

Concentration matrix = Fractional amount in the emission × Emission rates × Atmospheric dispersion

J. G. Watson (1984) Overview of Receptor Model Principles, Journal of the Air Pollution Control Association, 34:6, 619-623, DOI: 10.1080/00022470.1984.10465780

RECEPTOR MODELS: PRINCIPLES

$$C = a \times E \times D$$

Concentration matrix = Fractional amount in the emission × Emission rates × Atmospheric dispersion

In a source model:

- C is **calculated**
- $a \times E$ is known
- D is known

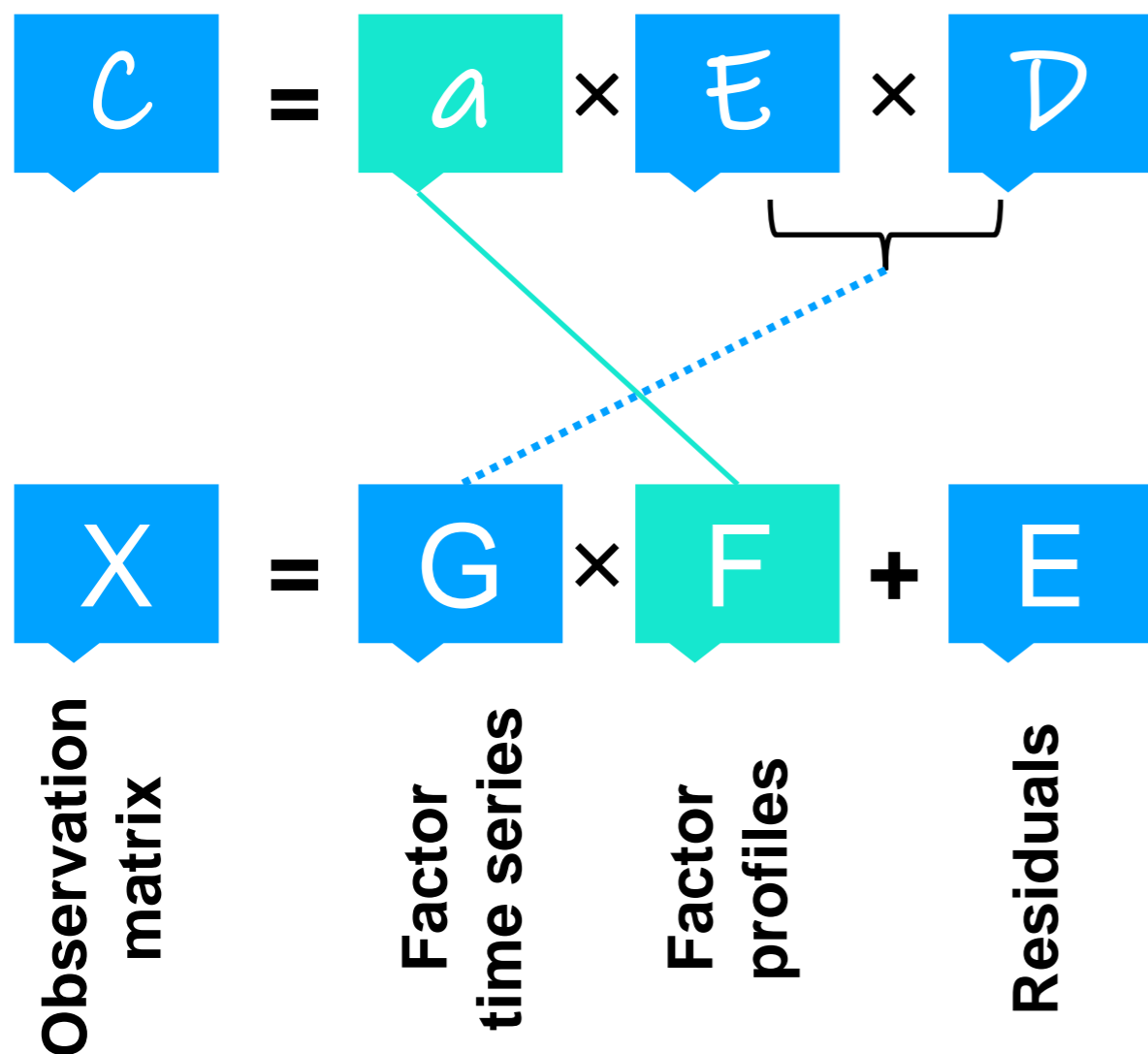
In a receptor model:

- C is known
- a is known (*)
- $E \times D$ is **calculated**

(*) qualitatively or quantitatively

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RECEPTOR MODELS: PRINCIPLES



Mass balance equation

$$X_{ij} = \sum_{k=1}^p g_{ik} f_{kj} + e_{ij}$$

Where

$i = 1, \dots, n$ samples

$j = 1, \dots, m$ species

$k = 1, \dots, p$ factors

Can be solved by a linear least-square fit

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RECEPTOR MODELS: PRINCIPLES

Mass balance equation

New assumptions arise to solve this equation:

- ④ p , the number of sources (factors), $\leq m$, the number of species
- ⑤ Source compositions are linearly independent from each other

$$X_{ij} = \sum_{k=1}^p g_{ik} f_{kj} + e_{ij}$$

Where

$i = 1, \dots, n$ samples

$j = 1, \dots, m$ species

$k = 1, \dots, p$ factors

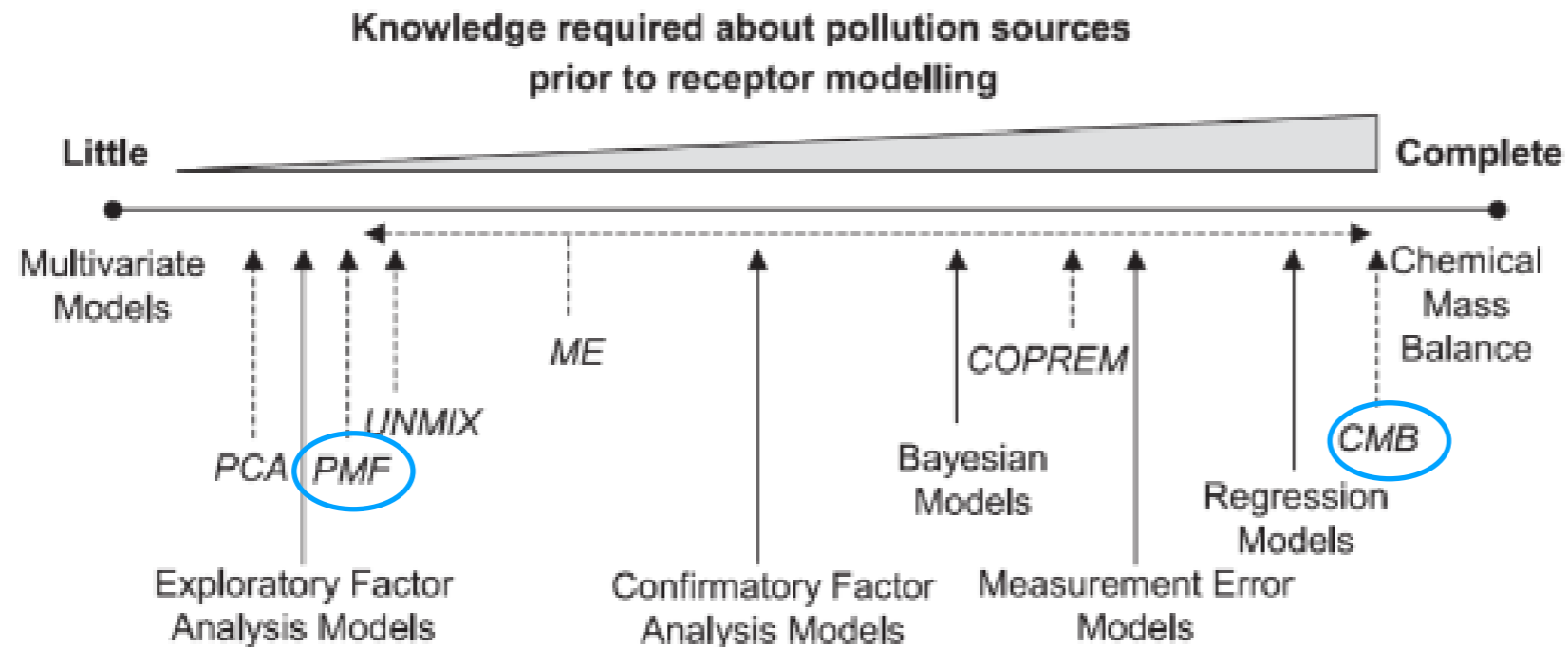
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RECEPTOR MODELS: TYPES of MODELS



What knowledge of the sources **at the receptor site?**



Viana et al. (2008)
Source apportionment of particulate matter in Europe: A review of methods and results, *Journal of the Aerosol Science*, 39, 827-849, DOI: 10.1016/j.jaerosci.2008.05.007

Positive Matrix Factorization (PMF)

- Number of sources (p) explored by the user
- Computed source profiles (f_{kj})
- Computed source contributions (g_{ik})
- Equations solved numerically

Chemical Mass Balance (CMB)

- Known number of sources (p)
- Known source profiles (f_{kj})
- Computed source contributions (g_{ik})
- Equations solved analytically

RECEPTOR MODELS: TYPES of MODELS

Positive Matrix Factorization (PMF)

- Number of sources (p) explored by the user
- **Computed** source profiles (f_{kj})
- **Computed** source contributions (g_{ik})
- Equations solved numerically



$$N_t \geq \frac{N_{sp} \times N_{sr}}{N_{sp} - N_{sr}}$$

Minimization of:

$$Q = \sum_{sp} \sum_t \left(\frac{C^{sp}(t) - \sum_{sr} C_{sr}^{sp}(t) f_{sr}^{sp}}{U^{sp}(t)} \right)^2$$

Technical requirements

Number of samples?

Use of uncertainties?

Chemical Mass Balance (CMB)

- **Known** number of sources (p)
- **Known** source profiles (f_{kj})
- **Computed** source contributions (g_{ik})
- Equations solved analytically



$N_t = 1$ sample
is enough to solve the equation

Variables are weighted in the least-square solution so that less precise measurements have less influence than more precise ones

RECEPTOR MODELS: TYPES of MODELS

Positive Matrix Factorization (PMF)

- Number of sources (p) explored by the user
- **Computed** source profiles (f_{kj})
- **Computed** source contributions (g_{ik})
- Equations solved numerically



No

Can appear as 1 or 2 factors

How to choose
the best solution
with PMF?

Chemical Mass Balance (CMB)

- **Known** number of sources (p)
- **Known** source profiles (f_{kj})
- **Computed** source contributions (g_{ik})
- Equations solved analytically



~Yes

Should stay negligible

Results

**Unicity of
the solution?**

Background?

Results need to make sense environmentally.
No structure left in the residuals.

SUMMARY of POSSIBLE CASES? (ongoing discussion ...)

Type of pollutant	Spatial variability (from source to receptor)	Temporal variability (at the receptor site)	Example of identified factors	Example of identified sources
Primary	Profile constant	Profile constant	Hydrocarbon-like organic aerosol (HOA)	Primary traffic exhaust emissions
Factor = source = emission profile				
Primary	Profile not constant	Profile constant	Fresh marine aerosols Aged marine aerosol	Sea spray emissions Sea spray emissions + other(s)
Secondary	Profile not constant	Profile can be assumed constant over time (diffuse sources)	Secondary organic aerosol (SOA) Secondary inorganic aerosol (SIA)	Sources are precursor gases
Secondary	Profile not constant	Profile changes over time	IEPOX-SOA	Biogenic SOA

Thank you for your attention

Any questions/comments?