# Receptor source modeling of particulate and organic pollutants


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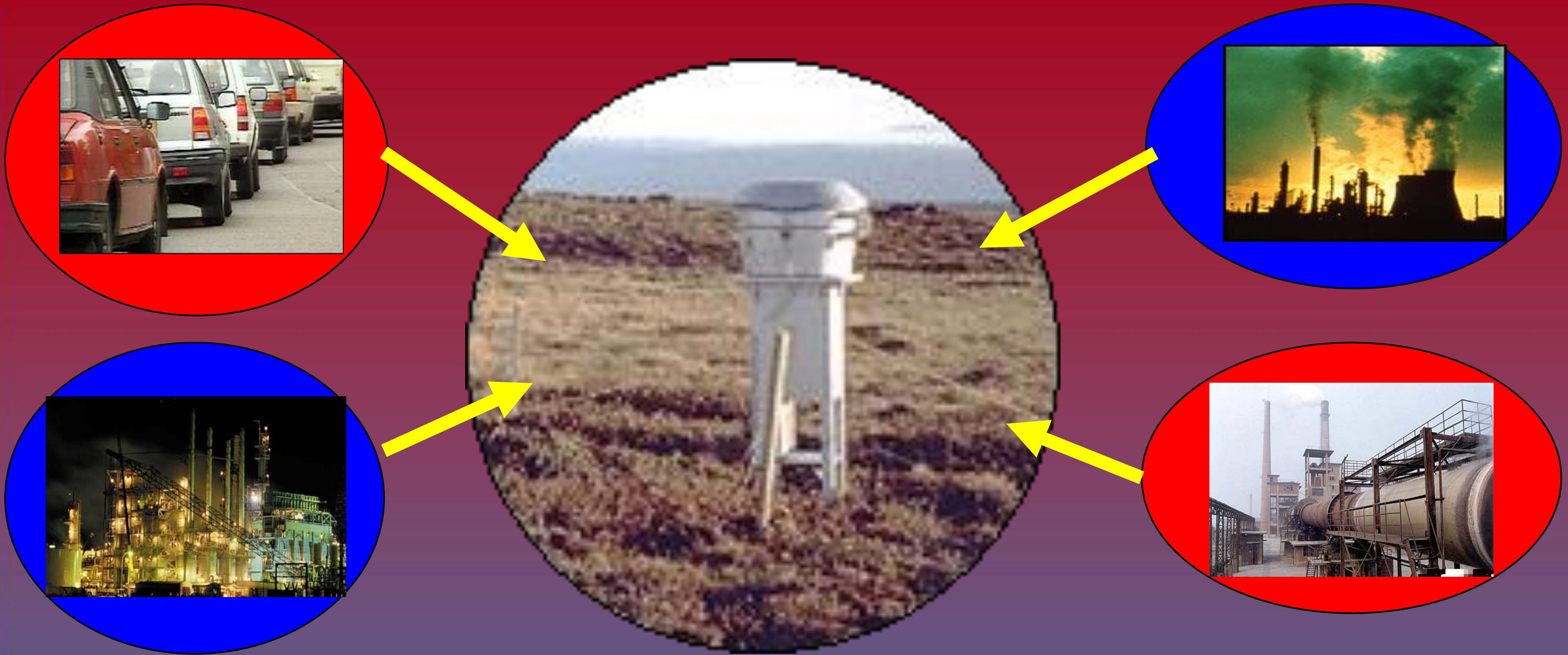


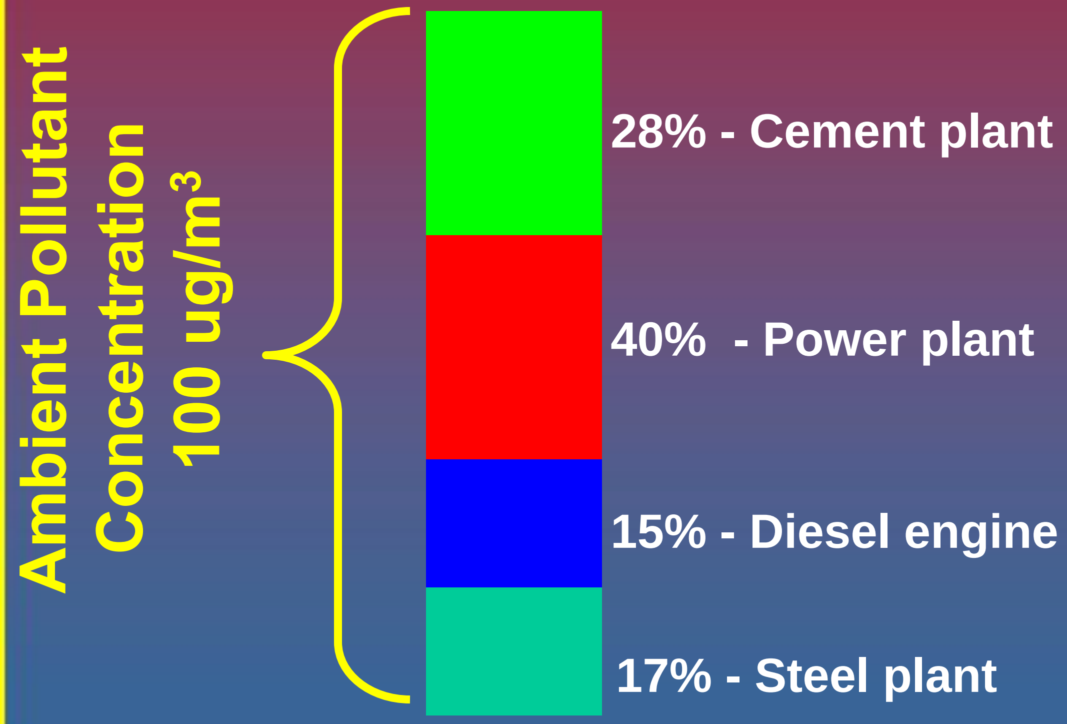
**Apportioning the contributions to monitored Ambient Levels of pollutants among various sources**

# Basic Requirements to Assess Air Pollution Source/Receptor Relationships

- Understand the chemical and physical characteristics of air pollutants.
- Understand transport from sources to receptors.
- Estimate the contribution of each source to air pollutant concentrations measured at receptors.

# Capabilities

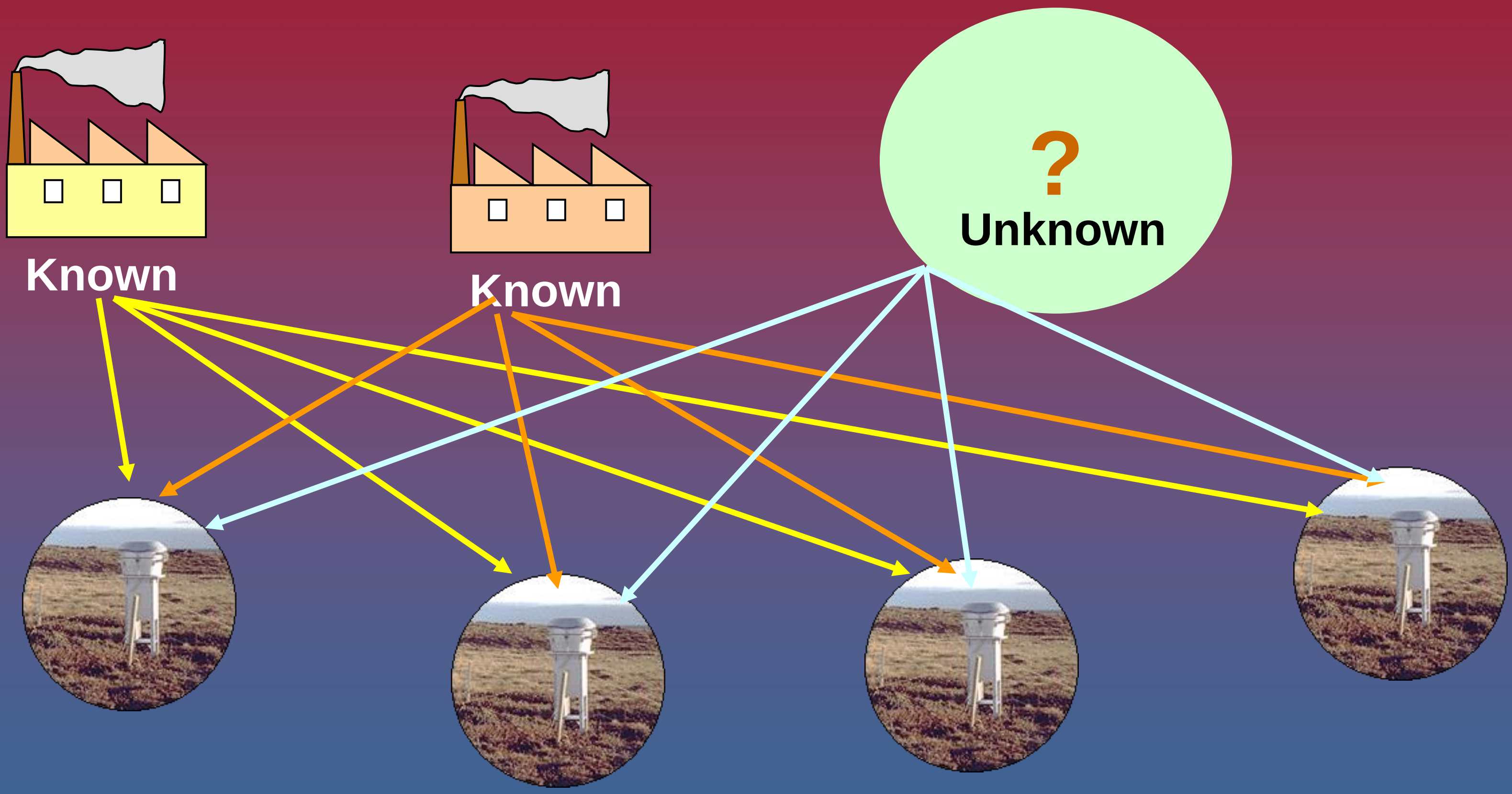
## Identification of pollutant contribution due to several sources




**Back calculate impacts due to specific sources**

# Capabilities

## Identification of unknown sources

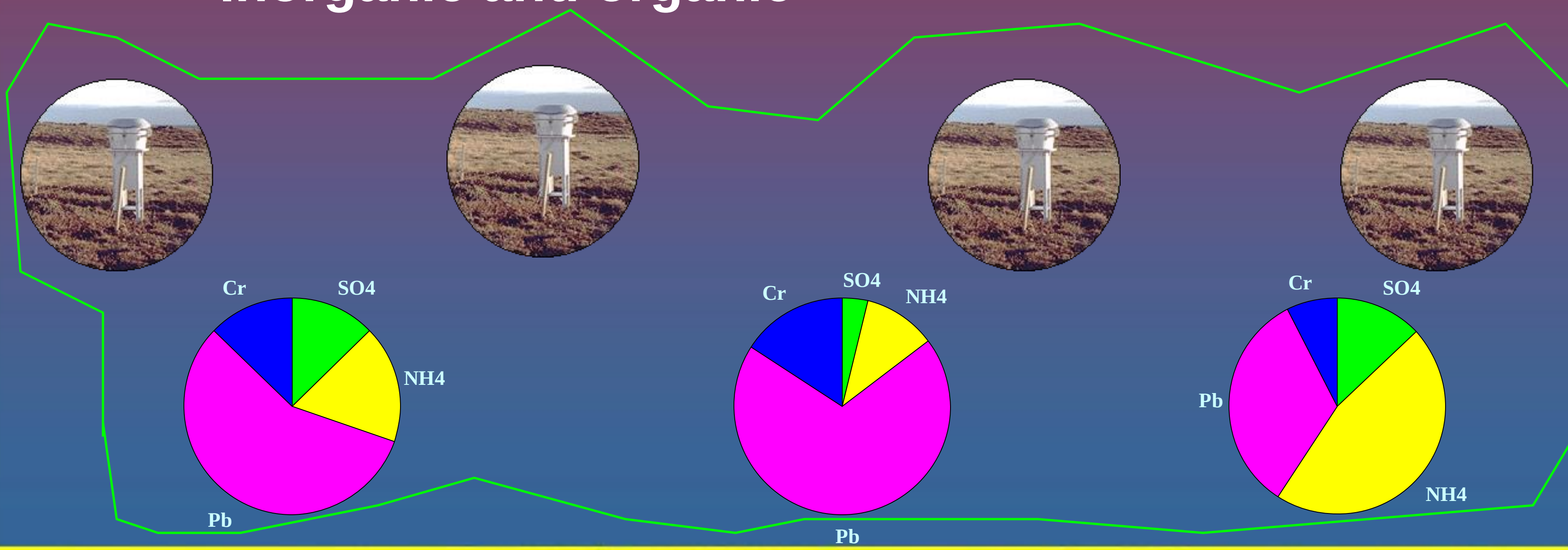



## Emission inventory of unknown sources

# Basic Data Requirement

## Complete speciation of particulate matter

- Physical (size distribution)
- Elements (Heavy metals)
- Inorganic and organic

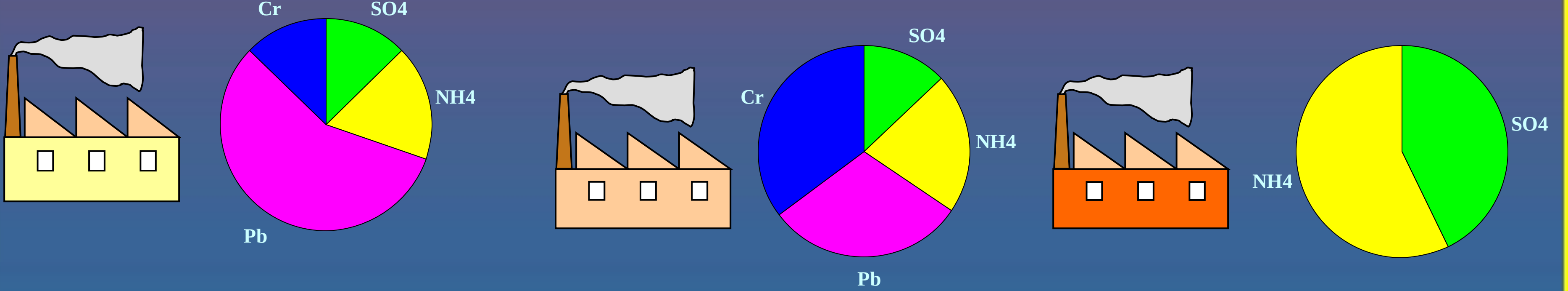



# Basic Data Requirement

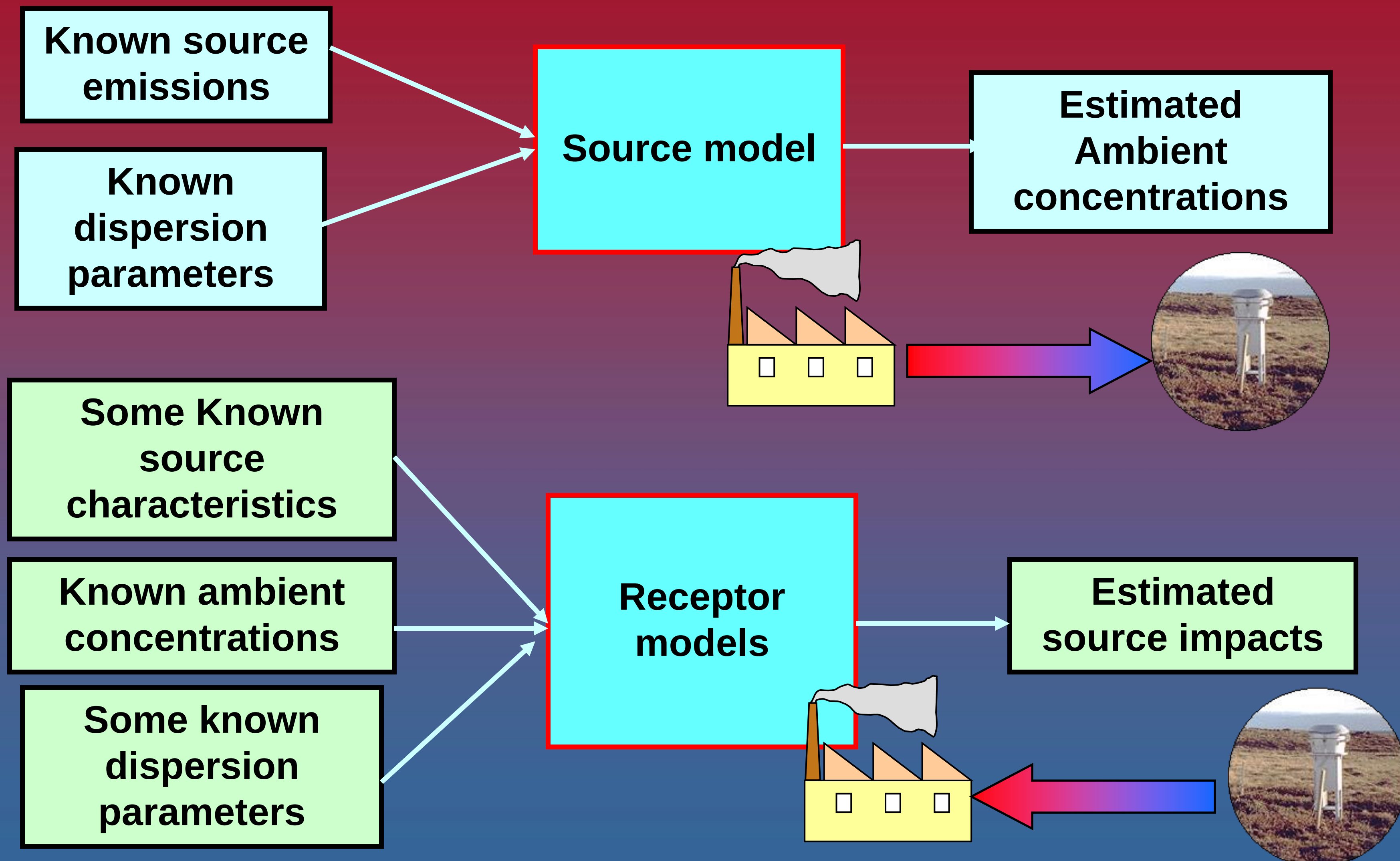
## Characterization of source emissions

- Physical (size distribution)
- Elements (Heavy metals)
- Inorganic and organic

## Maximum possible known sources




# Source Models vs. Receptor Models




# Limitations

**Receptor models cannot replace the dispersion models for the following cases**

- **For future predictions**
- **No contribution from proposed installations**
- **Simulations for the change in stack flue gas parameters**
- **Stack height determination**
- **Source contribution to formation of secondary aerosols such as sulfate etc.**

# Source Models vs. Receptor Models

## Dispersion models

- Predictions of future air quality
- Analysis of alternative control strategies
- Identification of secondary aerosols
- Impact predictions with change stack height and flue gas parameters
- Identification from single, group source with similar characteristics

## Receptor models

- Fugitive emission impacts
- Analysis of actual and worst case impacts
- Identification of new sources
- Also suitable for complex terrain and meteorology
- Regional scale air quality impacts

# Definitions

## Model

- Based on a scientific understanding of physical interactions.
- A set of mathematical relationships between variables.
- Values are provided to some variables to calculate others.
- Input values are obtained from measurements.
- Each model is an imperfect representation of reality.

# Definitions (continued)

**Measurement Process:**

- Observables measured.
- Range of values of observables.
- Frequency and duration of sampling.
- Spatial density of samples.
- Validity, precision, and accuracy of measurements.
- Each measurement process is an imperfect representation of reality.

# Source Apportionment Models

- **Conceptual model.** Describes the relevant physical and chemical processes in an area. No mathematics
- **Emissions model.** Estimates temporal and spatial emission rates based on activity level, emission rate per unit of activity, and meteorology
- **Meteorological model.** Describes transport, dispersion, vertical mixing, and moisture in time and space

# Source Apportionment Models

- **Air quality model.** Estimates concentrations at receptors based on emissions, transport, and transformation
- **Chemical model.** Describes transformation of gases to particles and equilibrium between gas and particle phases
- **Chemical mass balance receptor model.** Infers source contributions from chemical fingerprints of source emissions and receptor concentrations
- **Multivariate receptor models.** Infer source profiles from ambient data

# Source Apportionment Methods

- Source models
  - Dispersion models
- Receptor models
  - Microscopic methods
  - Chemical methods
  - Physical methods
- Emission inventory models
  - Micro scale analysis

## Receptor models

### Microscopy techniques

### Chemical

**Technique**

Measurement of particle size, shape, light scattering properties

Compare with reference library for known emission sources

**Disadvantages**

Limited to particle size

Operator skill/Bias

Very costly and needs large sample size

## Source Apportionment Models - Chemical Methods

| Method | Advantages | Disadvantages |
|---|---|---|
| Enrichment factor | Provides evidence of source impact by change in aerosol composition | Semi-quantitative method, requires source composition data |
| Time series analysis | Provides clues to sources | Does not provide specific source impact |
| Chemical mass balance | Quantitative estimates based on real time data, impact uncertainties | Source composition shall be known and chemical non descriptive sources cannot be evaluated |
| Multivariate analysis | No prior knowledge of sources is required. Composition needed to identify sources by common natures | Large data sets are required |

**Widely Used by USEPA**

## Basic Steps in Receptor modeling

- **Measure PM at maximum possible locations in the study area**
- **Speciation of PM samples for**

  **Inorganic/ Organic/Elemental carbon**

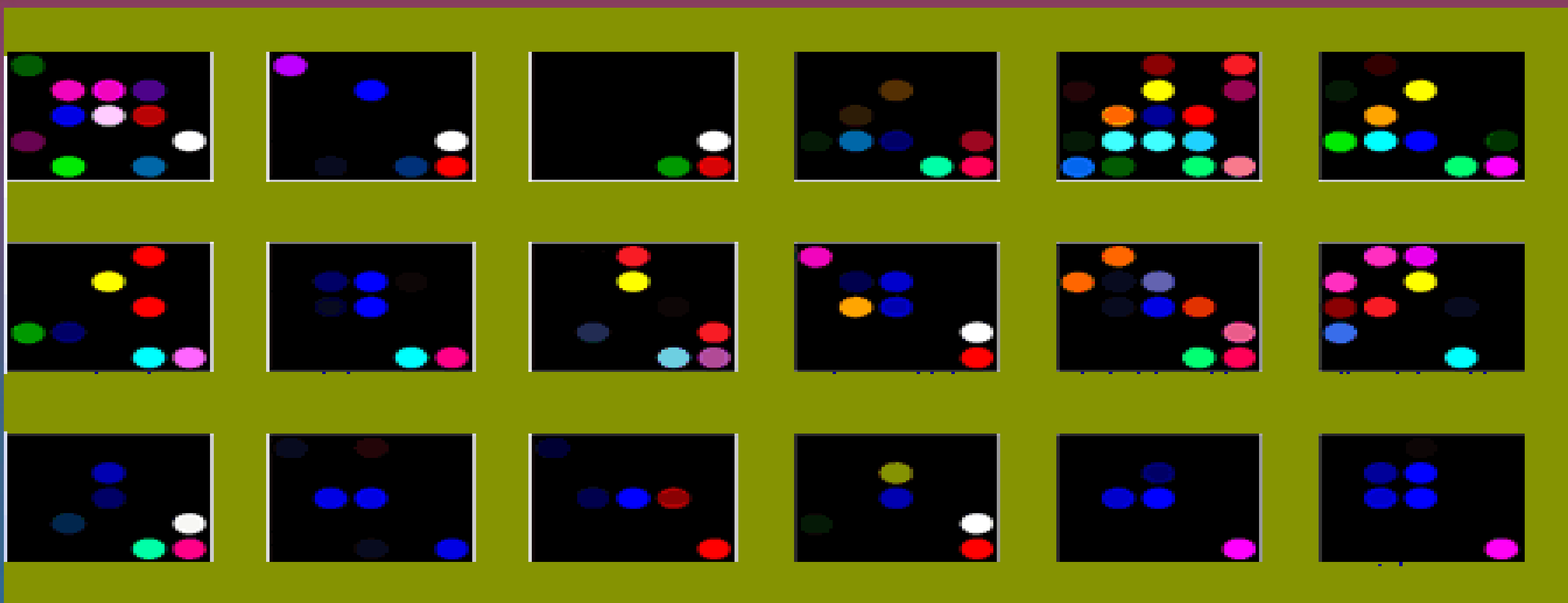
- **Source characterization (library)**

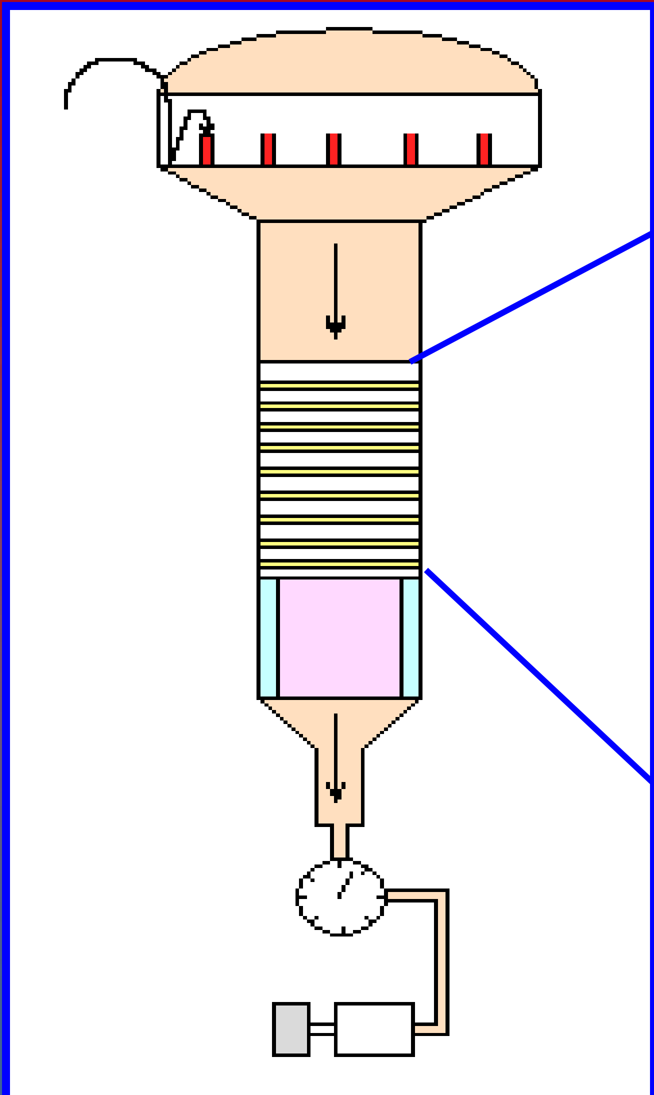
# Source Composition

Each source may possess unique

- Chemical composition or
- Size distributed species
- Unique tracer compound

Finger prints





>10

7.2-10

7.2-3.0

3.0-1.5

1.5-0.95

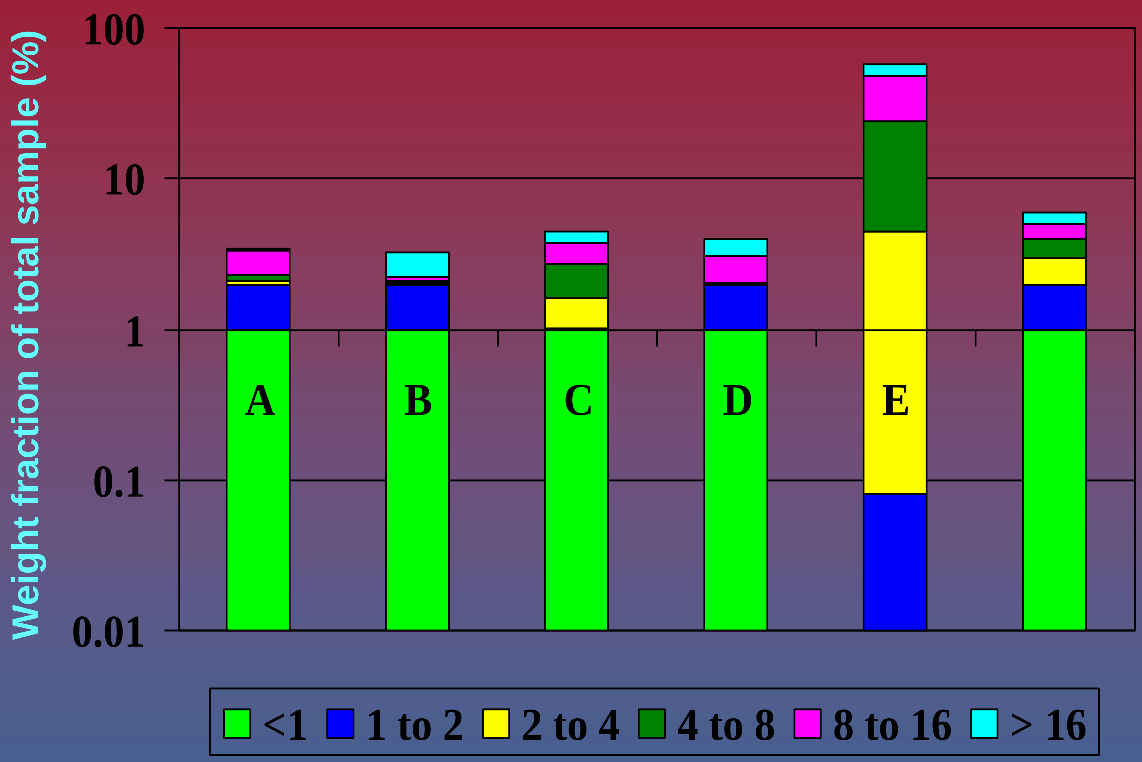
0.95-0.45

0.45-0.25

<0.25

**Each fraction subjected to chemical analysis**

# Particle Size – A Key Indicator




A: Soil

B: Wood combustion

C: Auto exhaust

D: Fuel oil combustion

E: Coal fly ash

Source: USEPA, Emission Factors Guide Book

# Heavy Metals in Fuels

Source: Robert E. Lee, USEPA, JAPCA, 1973

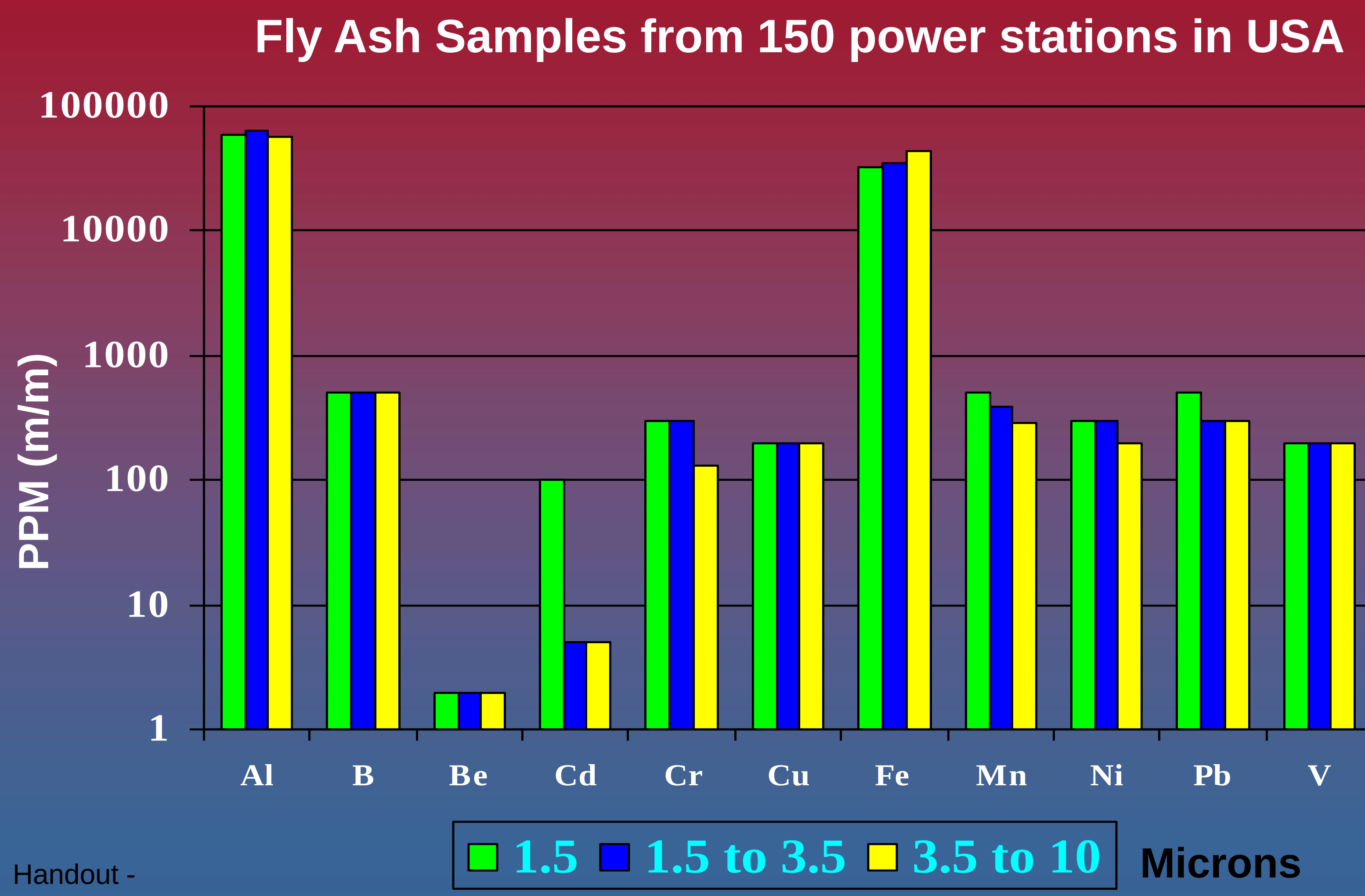
**Coal**

| Element | 0.01 | 0.1 | 1 | 10 | 100 | 1,000 | 10,000 |
|---|---|---|---|---|---|---|---|
| Al | | | | | | ■ | ■ |
| Co | | | ■ | ■ | | | |
| Cr | | | ■ | ■ | ■ | | |
| Cu | | | ■ | ■ | | | |
| Fe | | | | | ■ | ■ | ■ |
| Mn | | | ■ | ■ | | | |
| Sb | | ■ | ■ | ■ | | | |
| Se | | ■ | ■ | | | | |
| Ti | | | | | ■ | | |

**Fuel oil**

| Element | 0.01 | 0.1 | 1 | 10 | 100 | 1,000 | 10,000 |
|---|---|---|---|---|---|---|---|
| Al | | ■ | ■ | ■ | | | |
| Co | | | | | | | |
| Cr | | ■ | ■ | ■ | ■ | | |
| Cu | | | | | | | |
| Fe | | | | | | | |
| Mn | ■ | ■ | | | | | |
| Sb | | | | | | | |
| Ni | | | ■ | ■ | ■ | | |
| V | ■ | ■ | ■ | ■ | | | |

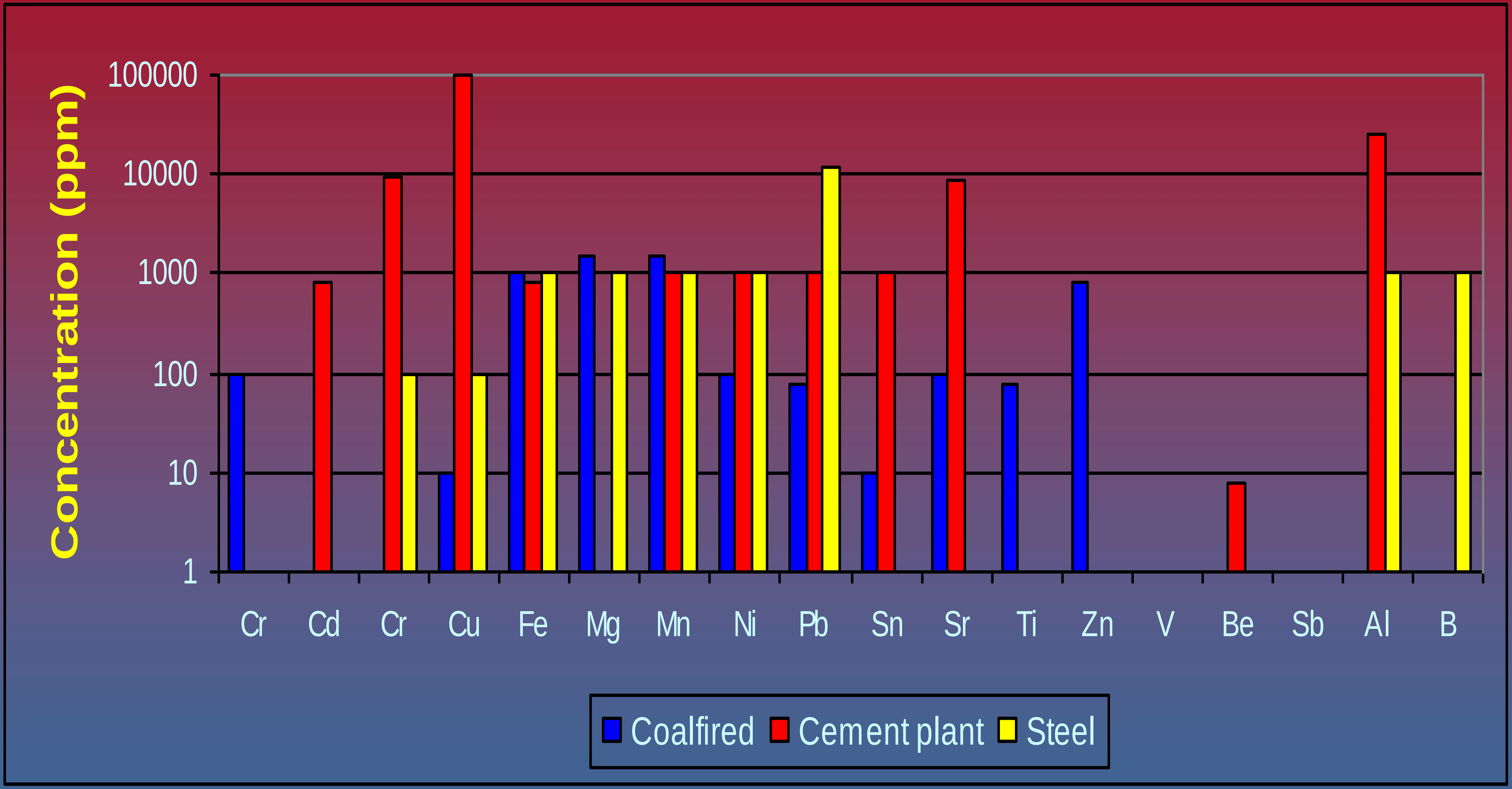
# Distribution of Species – Size Fractions




Handout -

Source: USEPA, 1984

# Signature Compounds




**Source: Robert E. Lee, USEPA, JAPCA, 1973**

# Signature Compounds

| Source | Indicator | Size Fraction |
|---|---|---|
| Motor vehicles | Pb, Br | Fine |
| Soil and road dust | Si, Al | Coarse |
| Fuel oil combustion | Ni, V | Fine |
| Limestone cement | Ca | Coarse |
| Paint and pigment | Ti/Fe <0.3 | Fine |
| Diesel emissions | Ba/Pb | Fine |
| Marine aerosols | Na, Cl | Coarse |
| Fly ash | Se, As | Total |

# Basic Models

## Source Models

$$C_{ik} = \sum_{j=1}^{J} a_{ij} D_{jk} E_{jk}$$

$C_{ik}$ = Concentration of component “i” in the “k” sample

$a_{ij}$ = Fraction amount of component “I” in source “j”

$D_{jk}$ = Dispersion parameter for source “j”

$E_{jk}$ = Total emission rate of all components from source “J”

**Assumptions:**

- Composition of source emissions are constant
- Components do not under go any reaction I.e add linearly
- Pollutant identified sources contribute to the receptor

# Basic Models

## Receptor Models

$$C_{ik} = \sum_{j=1}^{j} a_{ij} S_{jk} \quad for\ i = 1, n$$

$C_{ik}$ = Concentration of component “i” in the “k” sample

$a_{ij}$ = Fractional amount of component “i” in source “j”

$S_{jk}$ = Total contribution from source “J”

n = Total number of components measured

**Assumptions:**

- Number of sources “j” is less than or equal to number of components “I”
- The composition of all sources is linearly independent of each other

# Chemical Balance Model (CMB)

Cement | Power | DG sets | Vehicles

Pb | C | Al | $SO_4$ | Mn | Cr

**Measure signature species both in air and source emissions**




**Receptor concentrations**



# Example

Weight Fraction of source composition

| | Steel | Cement | Vehicle | Soil |
|---|---|---|---|---|
| Fe | 57 | 0.38 | 0.1 | 4.7 |
| Al | 0.7 | 2.4 | 0 | 8 |
| Pb | 0 | 0 | 14.8 | 0.002 |
| Ca | 1.2 | 30.2 | 0 | 2.21 |

**Ambient Particulate Matter concentration: 33.4 ug/$m^3$**

**Concentration of "Fe" = 0.015 ug/$m^3$**

**"Al" = 0.074 ug/$m^3$**

**"Pb" = 0.660 ug/$m^3$**

**"Ca" = 0.100 ug/$m^3$**

**Handout**

$$C_{Fe} = F_{Fe}*E_{Steel} + F_{Fe}*E_{Cement} + F_{Fe}*E_{Vehicle} + F_{Fe}*E_{soil}$$

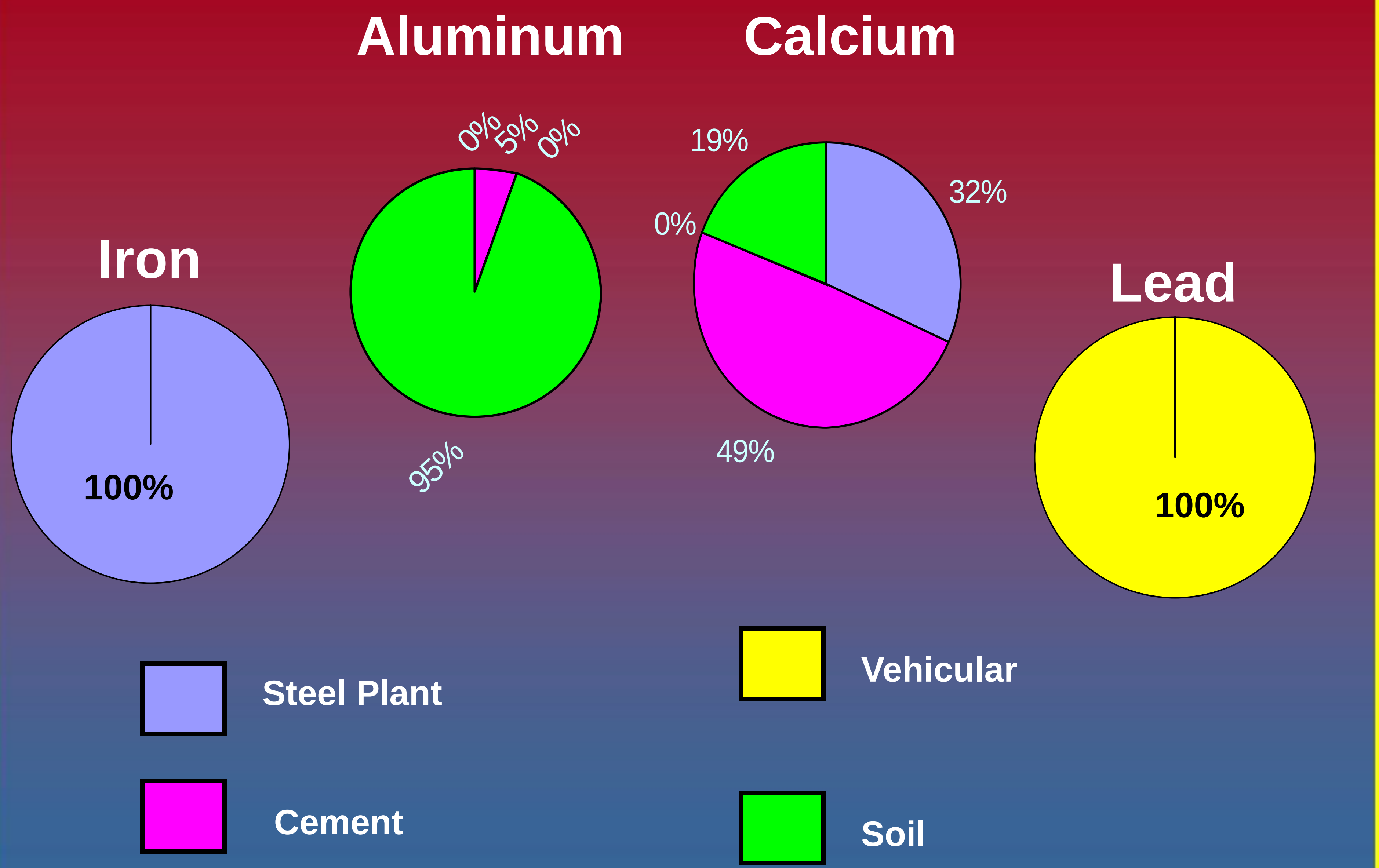
$$C_{Al} = F_{AL}*E_{Steel} + F_{AL}\,E_{Cement} + F_{AL}*E_{Vehicle} + F_{AL}*E_{soi}$$

$$C_{pb} = F_{pb}*E_{Steel} + F_{pb}*E_{Cement} + F_{pb}*E_{Vehicle} + F_{pb}*E_{Soil}$$

$$C_{Ca} = F_{Ca}*E_{Steel} + F_{Ca}*E_{Cement} + F_{Ca}*E_{Vehicle} + F_{Ca}*E_{Soil}$$

**Solving the simultaneous equations for "E"**

**Number of target Elements should be not less than number of sources**



Aluminum
Calcium
Iron
Lead
0%
5%
0%
95%
19%
32%
0%
49%
100%
100%
Steel Plant
Cement
Vehicular
Soil


# Comparisons of Measurement: Source and Receptor Model Components to Reality on an Urban Scale

| | Reality | Measurement | Source Model | Receptor Model |
|---|---|---|---|---|
| Air Volume ($m^3$) | $10^{11}$ | $10^3$ | $10^7$ | $10^3$ |
| No. of Variables | $10^3$ | 50 | 50 | 50 |
| Range of Pollutant Concentrations (g) | $10^{-15}$ to $10^{-3}$ | $10^{-9}$ to $10^{-3}$ | $10^{-6}$ to $10^{-3}$ | $10^{-9}$ to $10^{-3}$ |
| No. of Variable Interactions | $10^4$ | 0 | 10 | 0 |
| No. of Pollutant Sources | $10^3$ | 10 | $10^2$ | 10 |
| Range of Pollutant Emissions (g/sec) | $10^{-2}$ to $10^3$ | 1 to $10^3$ | 1 to $10^3$ | 1 to $10^3$ |
| Emissions Time Scale (sec) | $10^2$ | $10^7$ | $10^7$ | $10^7$ |
| Emissions Spatial Scale (m) | vert. 10<br>horiz. 100 | 10<br>100 | 10<br>100 | 10<br>100 |
| Dispersion Time Scale (sec) | $10^2$ | $10^2$ | $10^3$ | $10^4$ |
| Dispersion Spatial Scale (m) | vert. 0 to 1,000<br>horiz. 100, micro<br>$10^4$, meso<br>$10^6$, macro | 10, 100<br>1,000<br>few<br>few | 10<br>1,000<br>none<br>none | 10<br>1,000<br>none<br>none |

Source: Johan, G. Watson, JAPCA, 1984