Recent Air Quality Developments: Management, Assessment, and Modeling

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A Brief Introduction

- 40+ years of scientific research, publishing, consulting, editing, and teaching, including 2 years at KISR, Kuwait
- Author of the most comprehensive books on air pollution modeling
- Specialist in modeling of accidental releases
  - http://www.envirocomp.com/zcv/L.10.pdf
- Litigation expert in complex legal disputes related to industrial, transportation, and agricultural activities (ExxonMobil, Vulcan Materials, Marathon, Tosco, IBM, Chevron, Monsanto, Ciba Chemicals, Zen-Noh Grain, Dow Chemical, Dupont, KBR, CalPortland, Teck Metals, etc.)
  - http://www.envirocomp.com/zcv/P.49.pdf
- Full CV: http://www.envirocomp.com/zcv/zannetti.pdf

Chemical Releases → Air Pollution

- Anthropogenic ("man-made"), e.g., power plants
  - Industrial activities, e.g., from stacks
  - Urban activities, e.g., heating
  - Transportation, e.g., cars and trucks
- Natural, e.g., volcanoes

- Planned, e.g., regular industrial production
- Unplanned, e.g., accidental releases

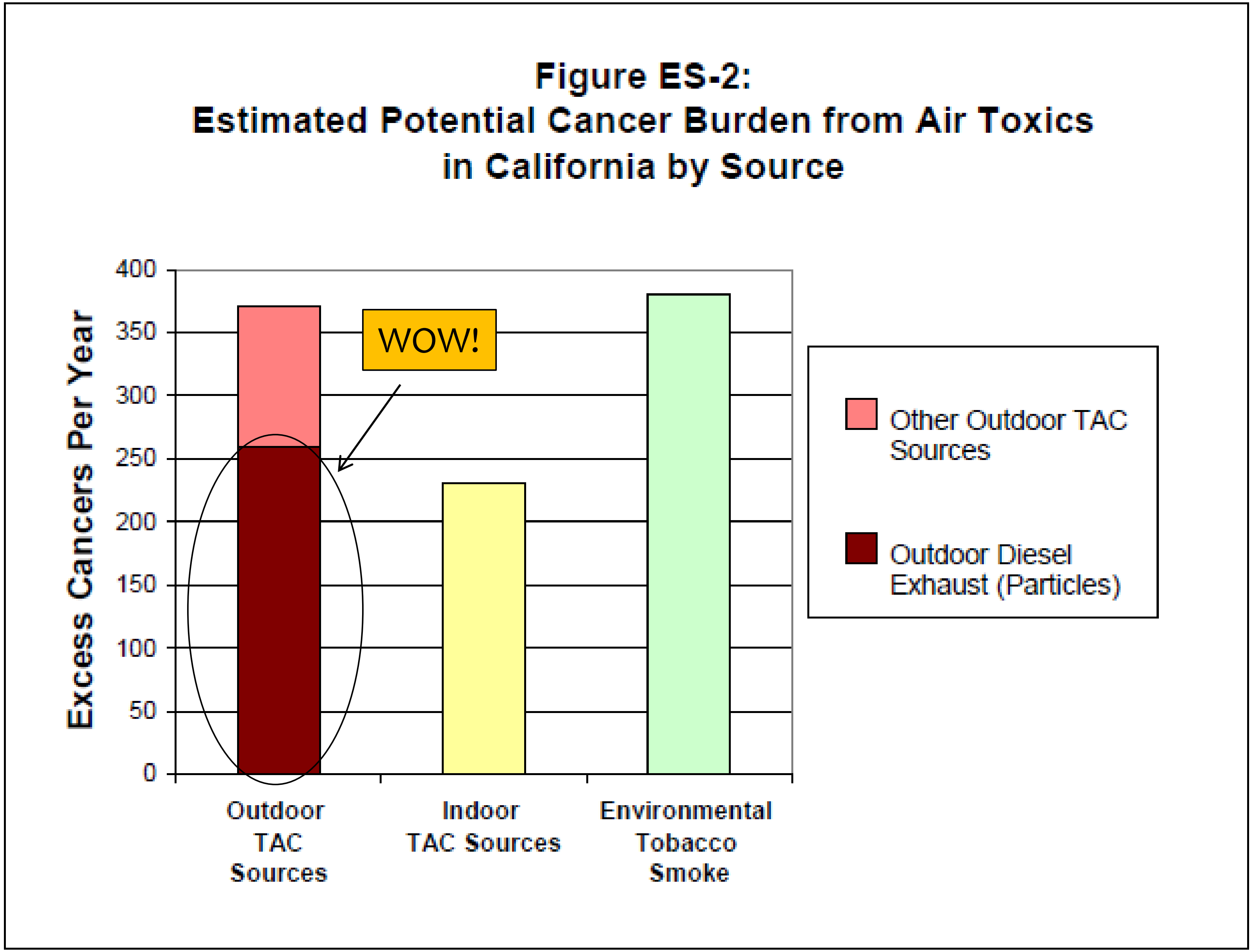
- Traditional ("criteria") chemicals, e.g., SO_2, CO
- Air Toxics, e.g., benzene

- Primary emissions (e.g., NO, CO)
- Secondary chemicals (e.g., NO_2, O_3 and a fraction of $PM_{2.5}$)

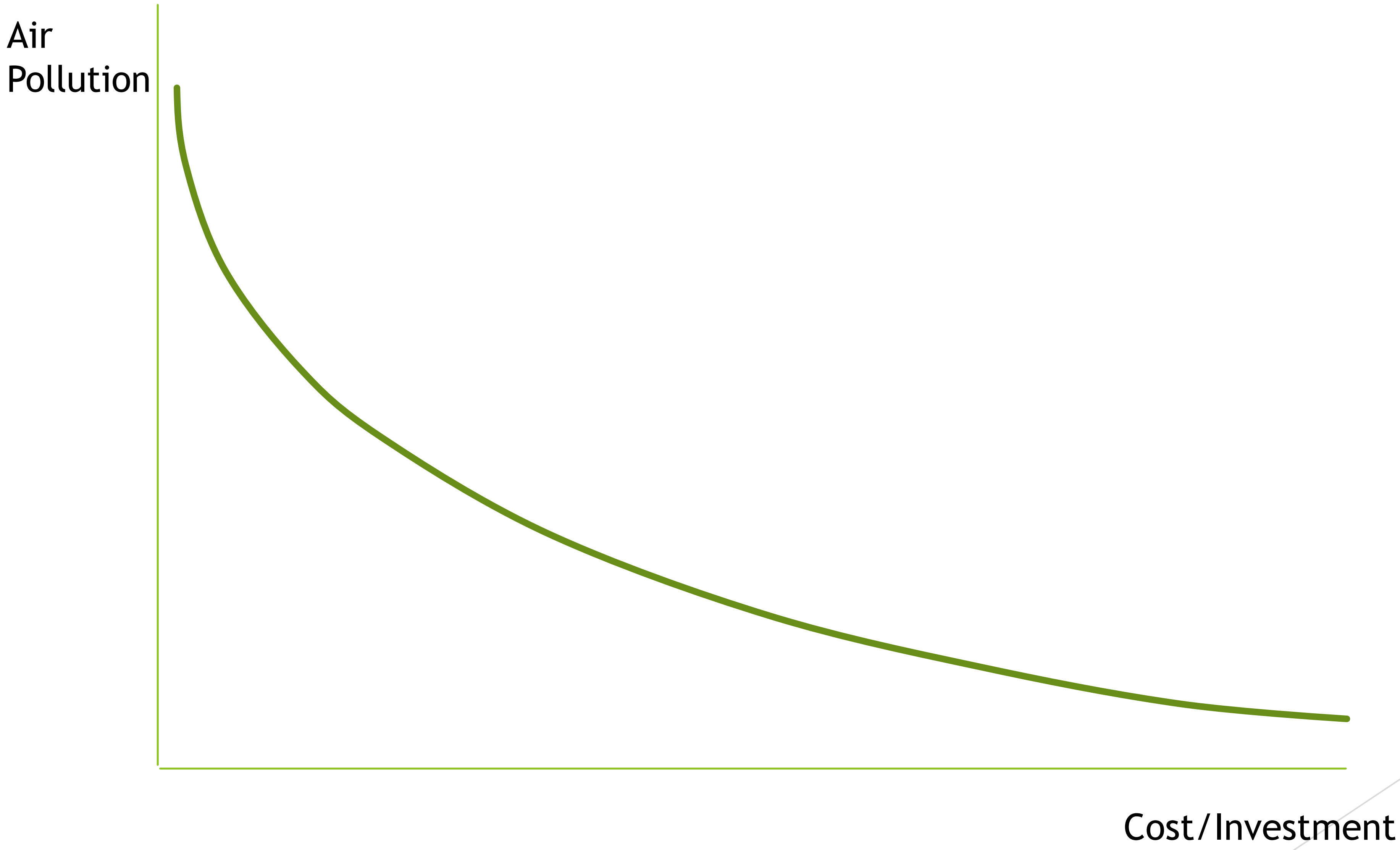
Air Quality: What is New?

- California → US → Europe → Rest of the World
- What is new in California?
  - Success in decreasing air toxics (e.g., benzene)
    - Unique monitoring/analysis of toxic pollutants:

      https://www.arb.ca.gov/toxics/toxics.htm
    - Identification of diesel emissions as dominant factor for health risks
  - Complete success against ETS
  - Yet … some regulatory excesses, and often, a lack of **cost-benefit** justifications
- For more: http://www.envirocomp.com/zcv/L.9.pdf



Note: TAC = "Toxic Air Contaminant", which is comprised of many air pollutants that are toxic
http://www.arb.ca.gov/research/apr/reports/l3041.pdf


Air
Pollution
Cost/Investment

Cost-Effectiveness - Optimization

- Cost-effectiveness should be the constant, dominant factor for all regulations, especially environmental regulations
- … But it is not
- Optimization can be expressed in two forms:
  1. **To achieve the max benefits with a fixed cost**
  2. To achieve a pre-defined benefit with a minimum cost
- But, in practical situations, only the first form is applied
- Optimization remains a difficult concept for politicians and decision makers
  - Important decisions are delegated to a computer program

It is a Fact! Let’s Admit it!

- Advanced computer simulation/optimization techniques have never been used so far to guide the actions of governments and agencies toward a well organized
  - maximization of benefits (with fixed costs) or
  - minimization of costs (with fixed benefits)
- The actions of governments have focused instead on
  1. air quality standards (that should not be exceeded, but often are) verified by air quality measurements, even though air monitoring is costly and we cannot of course measure all pollutants in all locations;
  2. emission standards, that again are not always easy to control;
  3. enforcement, often partial and selective.

An Effort to Include Cost-Benefit Optimization into Air Quality Management

- A conceptual model (CAMOS): http://www.camos.co/
- This site describes our preliminary design of a Comprehensive Air Modeling/Optimization System (CAMOS). Our goal is to provide a simulation system to guide and assist decision makers in developing cost-effective emission reduction strategies to improve air quality in a region.
- Presentation ➔ http://www.camos.co/material/Hamilton%20Conf-FINAL%2024Feb2014.pdf

Management Issues

- “Routine” management al local level
  - To achieve pre-defined air quality goals
  - To protect human health and the environment
- Emergency management
  - Emergency preparedness
  - Emergency response
- Large scale issues
  - Long-range pollution within a country
  - Trans-boundary pollution
  - Global issues
- Computer modeling is the key tool, e.g., in the US …

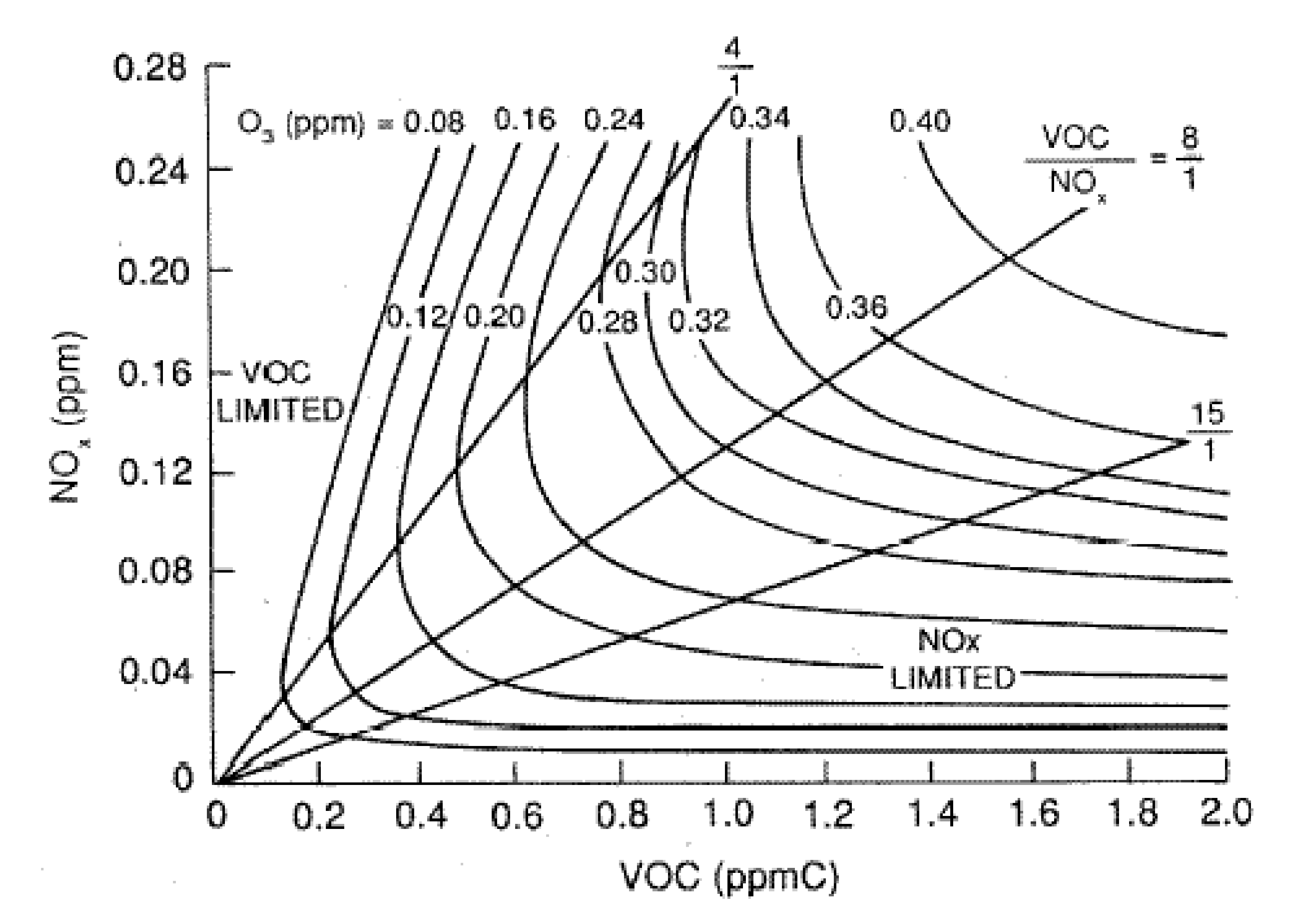
Air Quality Management

- How do we manage?
- How do we (scientists) assist government decision makers in managing air quality? How do we convince decision makers to make science-based, optimized decisions?
- We cannot manage without a deterministic assessment of cause ➔ effect, i.e., emissions ➔ concentrations
- This assessment can only be made with computer models – PERIOD!
- Air quality measurements are important but do not provide cause-effect information (except somehow when using receptor models: https://www3.epa.gov/scram001/receptorindex.htm)

Basic Air Quality Management Logic

- To “manage” air quality we need to be able to assess/estimate:
  - Emission rates of pollutants from all sources
  - Meteorological parameters
  - Atmospheric chemical reactions
  - Air pollution impact: concentrations and depositions
  - Air pollution adverse effects on human health and environment
- All these relationship are complex and often **non-linear (➔)**
- Main goal: to decrease adverse effects (ΔA) by decreasing emissions (ΔE) with a cost (Δ$)
  - **Computer simulation modeling is indispensable**

Challenge: Non-Linearity (e.g. Ozone)



Empirical kinetic modeling approach (EKMA) diagram. SOURCE: NRC 1991, adapted from Dodge 1977.

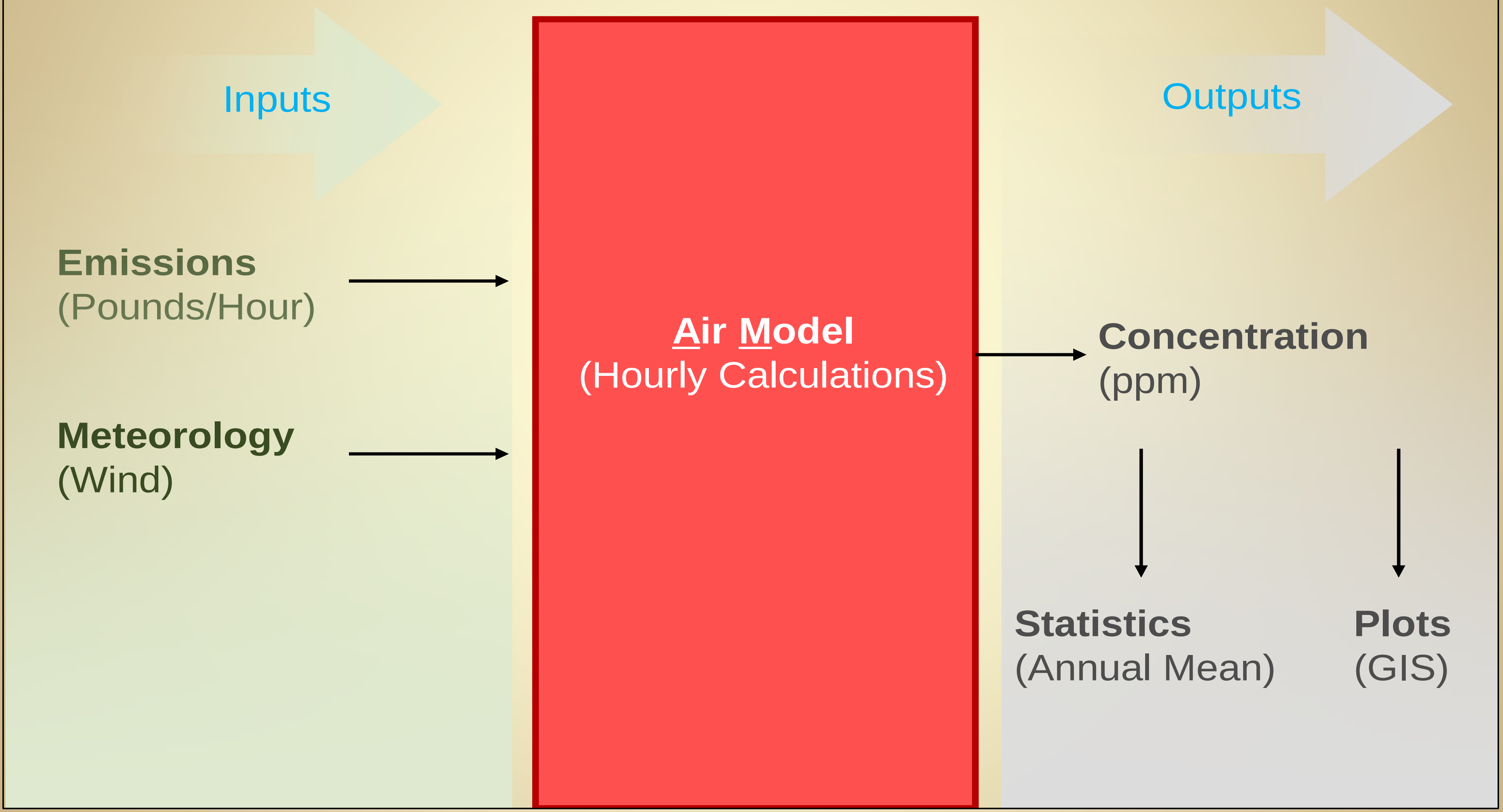
About Measurements…

- Air quality is now monitored all over the world (with data often available online and real-time)
  - However, doubts remain about the **representativeness** (spatial and temporal) of collected data
- PM used to be measured as 24-h averages. Now new monitoring equipment allows continuous measurements of PM1, PM2.5, and PM10 and others, e.g.:
  - https://www.tsi.com/dust-monitors/
- Remote sensing technology is improving, e.g.: Nasa projects:
  - https://earthobservatory.nasa.gov/features/AirQuality

What do we Recommend to Emerging Countries?

- We expect emerging countries eventually to follow the historical pattern of the West (e.g., Europe and North America),
  - after major industrial developments ➔ development of environmental protection regulations
  - major investments in remediation and emission control
  - positive results that can be measured and verified in most (but certainly not all) regions.
- But is this historical path the best, today, especially for emerging countries that need fast solutions at minimum costs?
- We believe that any country today investing funds for air quality improvement/protection can benefit from planning through computer simulation modeling and optimization techniques

Air Modeling Methodology



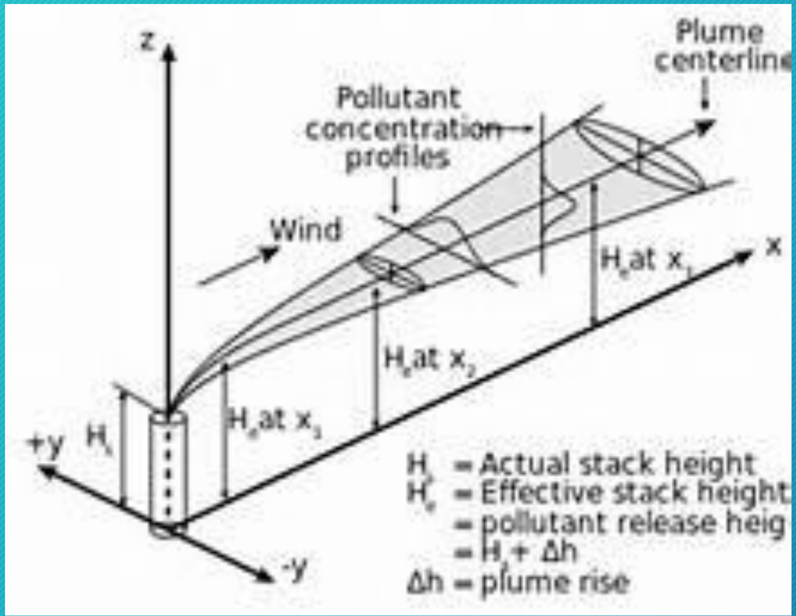
New Air Modeling Trends in the US

Modeling Approaches

- Gaussian Plume models (e.g., AERMOD)
  - Hourly, stationary, straight line plume
- Gaussian Puff models (e.g., CALPUFF)
  - Allow plume dynamics, calm conditions, accumulation, bending of the plume
- Lagrangian Particle Models (e.g., LAPMOD)
  - Allow highest degree of spatial/temporal resolution
  - http://www.envirocomp.com/zcv/L.16.DynamicSimulationsUsingParticleModels.pdf
- Other Models
  - Photochemical smog (O3), secondary particles (SO4), etc.

Mathematical Methods

- Either very simple …
  - Empirical engineering formula (simple algebraic formulas)
  - E.g.: the Gaussian Plume Equation



$$C(x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \times \left[\exp - \left(\frac{y^2}{2\sigma_y^2}\right)\right]\left\{\exp\left(\frac{-(z-H)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z+H)^2}{2\sigma_z^2}\right)\right\}$$

C = Concentration of the chemical in air. $[M/L^3]$
Q = Rate of chemical emission. $[M/T]$
u = Wind speed in x direction. $[L/T]$
σ_y = Standard deviation in y direction. $[L]$
σ_z = Standard deviation in z direction. $[L]$
y = Distance along a horizontal axis perpendicular to the wind. $[L]$
z = Distance along a vertical axis. $[L]$
H = Effective stack height. $[L]$

Mathematical Methods (cont.)

- … Or very complex
  - Numerical solutions of partial differential equations
  - E.g.: the Navier-Stokes equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0 \quad (1)$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2)}{\partial x} + \frac{\partial (\rho uv)}{\partial y} + \frac{\partial (\rho uw)}{\partial z} = -\frac{\partial p}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) \quad (2)$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial (\rho uv)}{\partial x} + \frac{\partial (\rho v^2)}{\partial y} + \frac{\partial (\rho vw)}{\partial z} = -\frac{\partial p}{\partial y} + \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) \quad (3)$$

$$\frac{\partial \rho w}{\partial t} + \frac{\partial (\rho uw)}{\partial x} + \frac{\partial (\rho vw)}{\partial y} + \frac{\partial (\rho w^2)}{\partial z} = -\frac{\partial p}{\partial z} + \nu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) \quad (4)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho uE)}{\partial x} + \frac{\partial (\rho vE)}{\partial y} + \frac{\partial (\rho wE)}{\partial z} = -\frac{\partial pu}{\partial x} - \frac{\partial pv}{\partial y} - \frac{\partial pw}{\partial z} + S \quad (5)$$

where ρ is the air density, u, v, w are the components of the air's velocity, E is measure of the air's internal energy (which allows us to compute its temperature) and p is the air pressure.

EPA Guideline on Air Quality Models (Federal)

- Enhancements to the **preferred near-field** (up to 50 km) dispersion model, **AERMOD**
- To provide more flexibility and improve the meteorological inputs used for regulatory modeling, the EPA is finalizing the use of **projected meteorological data** **(!)** in AERMOD where there is no representative National Weather Service (NWS) station and it is prohibitive or not feasible to collect adequately representative site-specific data
- For **long-range**, beyond 50 km from an emissions source, air quality assessments, the EPA is **removing CALPUFF** as a preferred model and now will consider it as a screening technique, along with **other Lagrangian models**, to be used in consultation with the appropriate reviewing authority

2017 Appendix W Final Rule (https://www3.epa.gov/ttn/scram/appendix_w-2016.htm)

Projected Meteorological Data

- Appendix W now allows the use of **projected meteorological data** derived from meteorological models.
- Data derived from meteorological models are very useful when:
  - Lack of representative meteorological measurements
  - Available meteorological measurements do not meet quality standards (e.g., poor treatment of calms, many missing data, insufficient number of data)
  - Meteorological stations not ideally suited for specific purposes
    - Represent instantaneous readings and we need time averages
    - Vertical profiles not available
    - Some variables not available (e.g., solar radiation, cloud cover)

AERMOD ("Traditional" Use)

- **AERMOD** is the US-EPA preferred model for near-field applications
  - https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models#aermod
- It requires surface meteorological data from a single station, and upper air data that are typically obtained from a different station
- Meteorological data derived from the closer station (or the more representative one) are elaborated by the **AERMET** processor, which also includes information about geophysical parameters (roughness length, albedo and Bowen ratio) obtained from the AERSURFACE processor
- The meteorological station may be several km away from the source(s) of interest, **therefore the meteorological data might not always be representative**

AERMOD (New Option)

- The meteorological data very close to the sources, or over them, can be obtained from complex meteorological grid models and their processors.
- It is possible for example to use the **WRF** (Weather Research and Forecasting) model to get the hourly meteorological fields for one or more years over a location, then extract specific variables and format them as needed by AERMOD though the **MMIF** (Mesoscale Model Interface) program.

WRF: https://www.mmm.ucar.edu/weather-research-and-forecasting-model
MMIF: https://www.epa.gov/scram/air-quality-dispersion-modeling-related-model-support-programs#mmif

CALMET/CALPUFF ("Traditional" Use)

- The **CALMET/CALPUFF** modeling system (http://www.src.com/) may be used for atmospheric dispersion over complex orography, where the single point meteorology and straight-plume of AERMOD are not enough to fully describe the circulation pattern
- CALMET is the diagnostic meteorological model associated to CALPUFF. It requires in input the **geophysical parameters** of the domain (at least terrain elevation and land use), hourly **surface meteorological data** from several stations within its domain, and one or more **vertical profiles** (at least one every 12 hours).
- CALMET calculates the **3D, non-stationary, meteorological fields** over the whole simulation domain, plus the micro-meteorological variables related to **turbulence** (Monin-Obukhov length, friction velocity, convective velocity, mixing height, etc.).
- This output is used to feed CALPUFF (and other dispersion models).

CALMET/CALPUFF (New WRF Option)

- The preparation of the meteorological data is a very long and delicate process. Many **subjective decisions** may enter in the data preparation
- The output data of complex prognostic meteorological models, such as WRF may be used to prepare the input of CALMET, or directly of CALPUFF
- The output of **WRF** may be entered in the **CALWRF** processor in order to prepare data to be used in CALMET in place of, or together with, the observations
- The output of **WRF** may also be processed by **MMIF** to get directly the meteorological input file of CALPUFF.

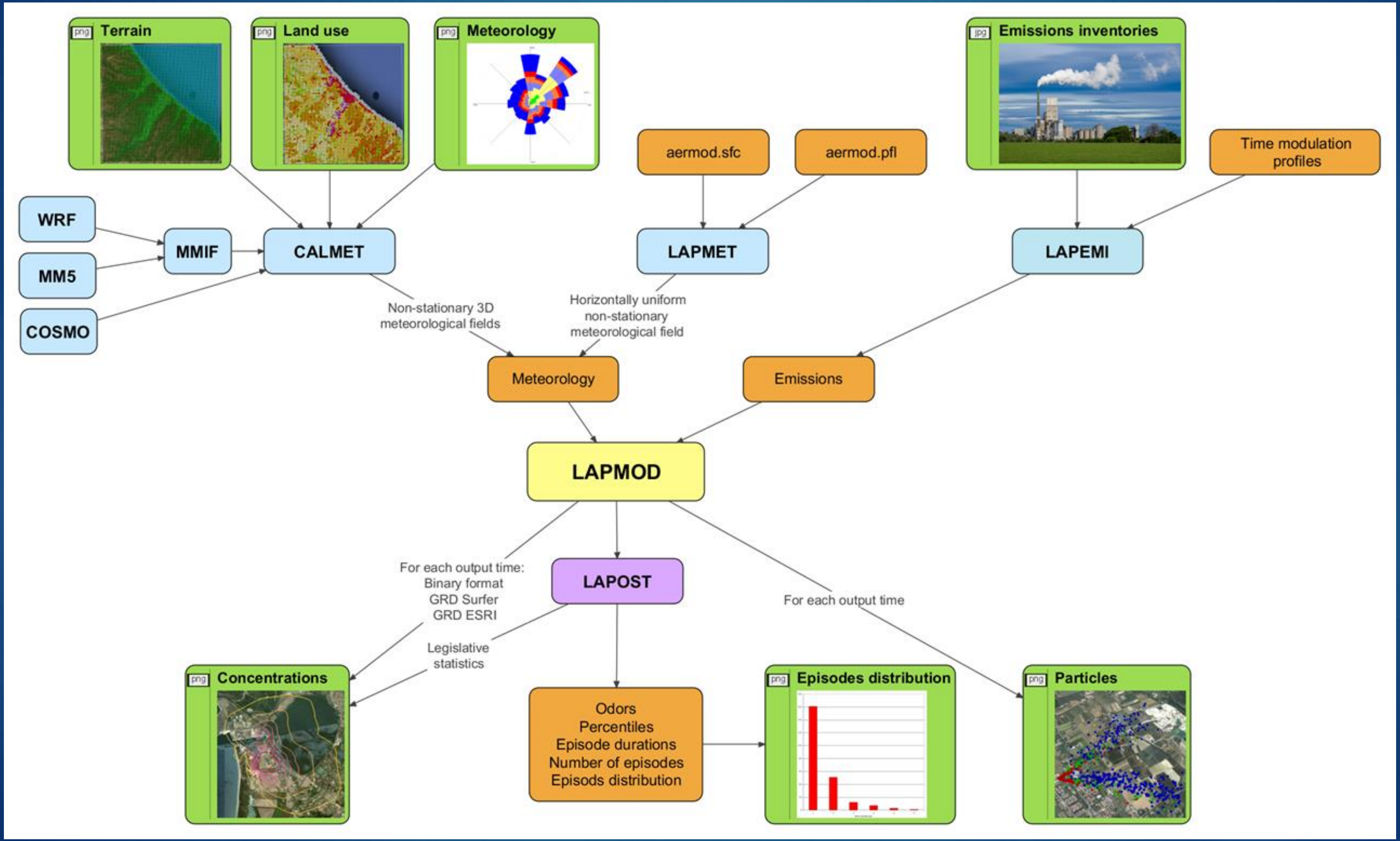
Lagrangian Particle Models (LPMs)

- Lagrangian Particle Models are relatively complex tools:
  - N computational particles are released from the sources
  - Each particle represents a portion of mass of each pollutant
  - Each particles moves according to the mean wind and to the local turbulence (plume rise can be included)
  - The mass associated to a particle may vary due to deposition and/or to radioactive decay
  - The concentration may be calculated by the “counting method” (counting the mass of the particles within a specific volume), or by kernel methods
- LPMs were research tools up to few years ago.
- Nowadays they are **operating tools** thanks to modern computers, the introduction of parallel calculation and cloud computing.

LAPMOD

- LAPMOD is an **open source** Lagrangian Particle Model available at
  - https://www.enviroware.com/lapmod/
- LAPMOD is **interfaced to CALMET**, that is used to prepare its meteorological and turbulence fields.
- LAPMOD has been **validated** both in **rural environment** (Kincaid data) and in **urban environment** (Indianapolis data)

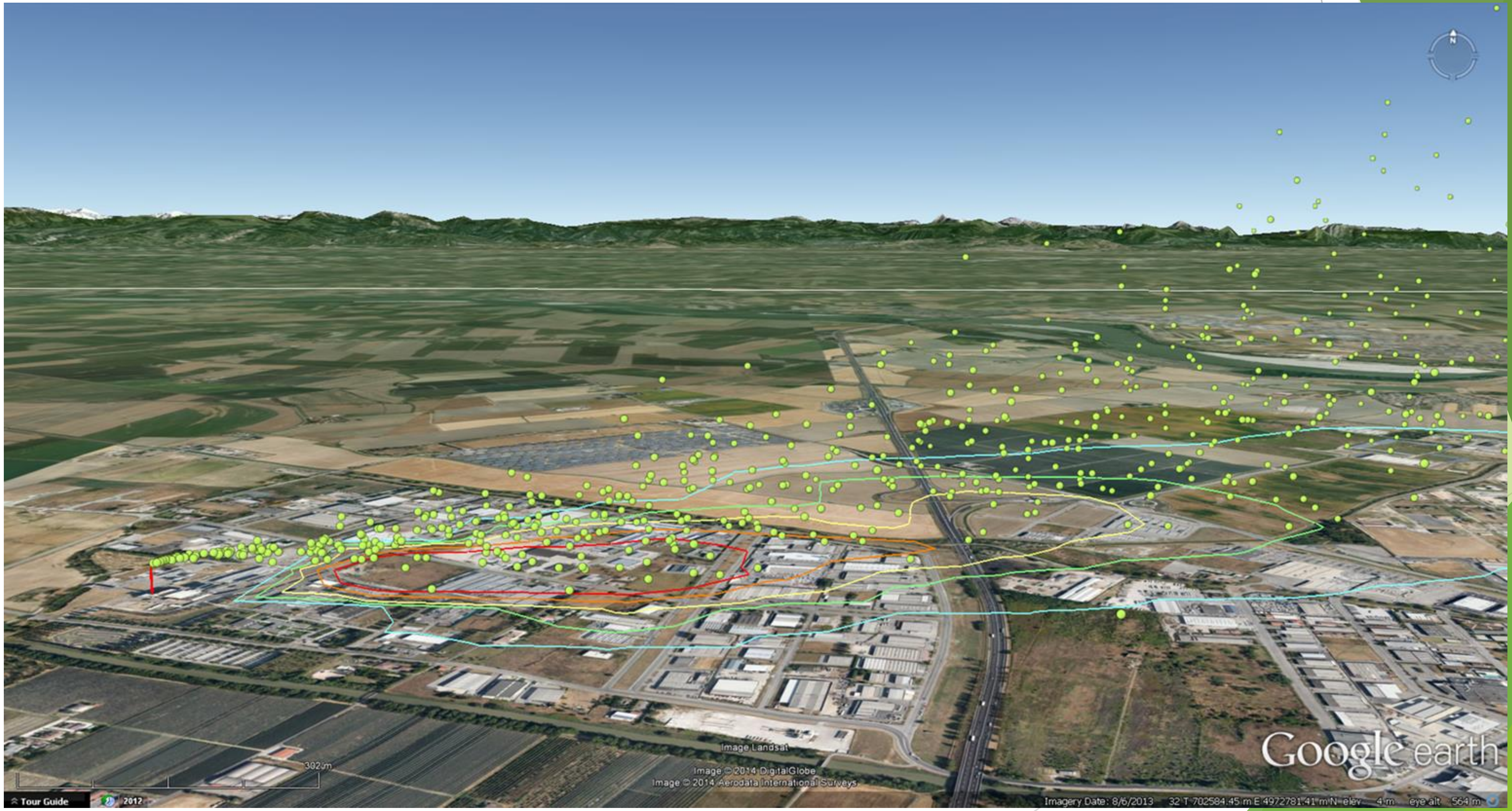
LAPMOD



png Terrain
png Land use
png Meteorology
jpg Emissions inventories
aermod.sfc
aermod.pfl
Time modulation profiles
WRF
MM5
COSMO
MMIF
CALMET
LAPMET
LAPEMI
Non-stationary 3D meteorological fields
Horizontally uniform non-stationary meteorological field
Meteorology
Emissions
LAPMOD
For each output time: Binary format GRD Surfer GRD ESRI
LAPOST
For each output time
Legislative statistics
png Concentrations
Odors Percentiles Episode durations Number of episodes Episods distribution
png Episodes distribution
png Particles

LAPMOD

LAPMOD example



WRF

- The use of WRF is very complex, it requires:
  - **Knowledge** of the model and of the physics behind it (including complex calculation options, geophysical dataset to download for each domain, meteorological dataset to download, …)
  - **Powerful computational resources** (typically used in Linux OS, powerful CPUs, parallel computation, …)
- Concerning the computational resources, sometimes it might be useful to use **cloud computing services** such as those offered by **Amazon Web Services** (AWS https://aws.amazon.com), **Google Cloud Platform** (GCP https://cloud.google.com/) and others.
- These services are scalable and allow to use (and pay) computational resources when needed

- The alternative to cloud computing services is to buy a powerful server and to install and run WRF on it.
- There are companies that provide the output of WRF formatted for specific models (AERMOD, CALMET, CALPUFF) as a **commercial service:**
  - **Lakes Environmental** https://www.weblakes.com/index.html
  - **Trinity Consultants** https://www.trinityconsultants.com/
  - **EnviroComp Consulting** http://envirocomp.com/

Thank you!

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