Air Quality Modeling and Simulation

A Few Issues for HPCN

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INRIA/ENPC CLIME project

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Motivations

Atmospheric Chemical Composition

- The atmosphere as a chemical reactor
- Trace species: from ng m^{-3} to μg m^{-3}

Applications

- Risk assessment (NBC)
- Photochemistry (ozone, nitrogen oxides, volatile organic compounds)
- Transboundary pollution (heavy metals, acid rains)
- Oxidizing power of the atmosphere and lifetime
- Greenhouse gases and radiative effects
- Stratospheric ozone (halogen compounds)
- ...

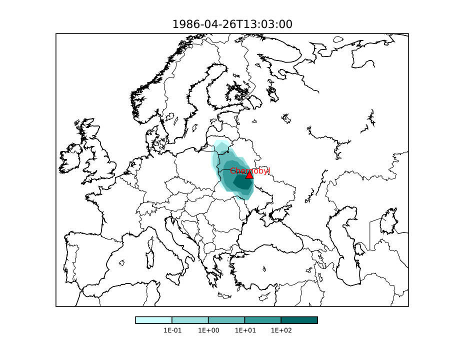
Model Uses

- Process studies
- Forecast (e.g. accidental release)
- Impact studies

Forecast and Risk Assessment

Chernobyl Accidental Release, 25 April-5 May 1986

POLYPHEMUS run, Forecast Emergency Center IRSN/CEREA

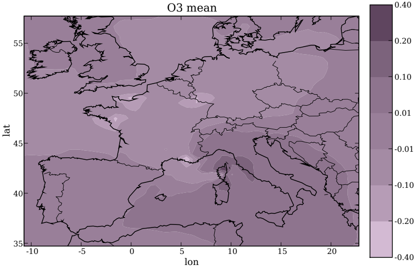


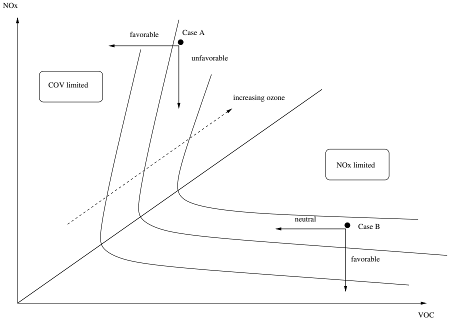
D. Quélo, M. Krysta, M. Bocquet, O. Isnard, Y. Minier, and B. Sportisse. Validation of the POLYPHEMUS system: the ETEX, Chernobyl and Algeciras cases. *Atmos. Env.*, 2007

Impact Studies

POLYPHEMUS Run for the Impact of French Emission of Power Plants for the Year 2001 (NEC/CAFE Round)

Credit: Yelva Roustan (CEREA)



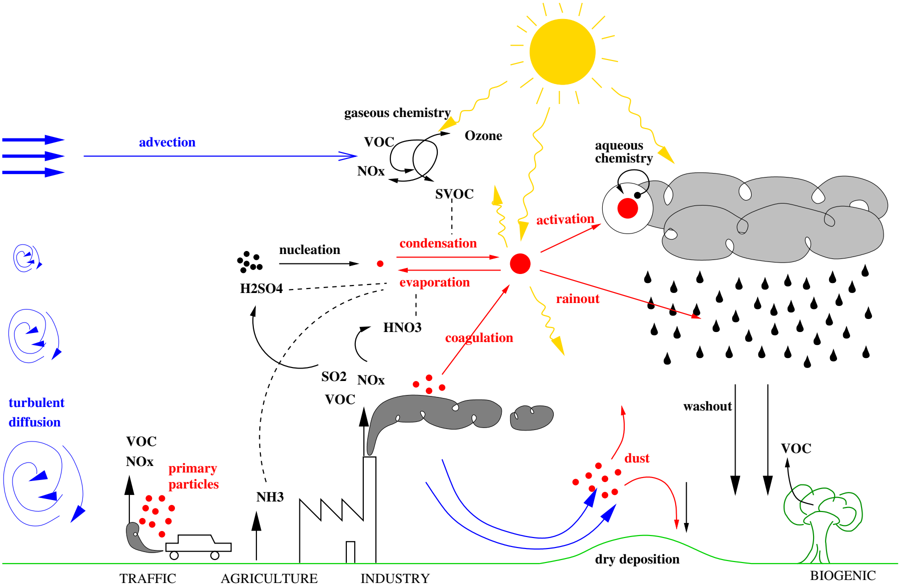


Expertise for Disbenefit Effects and Dilemma

Three Case Studies

- NO_x disbenefit
- Reduction of *emitted* mass versus increase of number for *secondary* particles
- Climate change versus air pollution (e.g.: impact of E85 flexfuel or sulfate aerosols)

Processes


gaseous chemistry
advection
VOC
Ozone
NOx
SVOC
aqueous chemistry
activation
nucleation
condensation
H2SO4
evaporation
rainout
HNO3
coagulation
SO2
NOx
VOC
turbulent diffusion
washout
VOC
NOx
primary particles
dust
VOC
NH3
dry deposition
TRAFFIC
AGRICULTURE
INDUSTRY
BIOGENIC

The Arms Race

- Air Quality Models (Chemistry-Transport Models) rely on subgrid parameterizations.
- The resulting equations generate high-dimensional numerical issues.
- Both issues (modeling & numerics) are much more challenging for aerosol dynamics, based on more and more detailed models.
- Yet, even after having tackled these problems, models have to be carefully used, because of uncertainties. Ensemble modeling is one possible answer.
- Coupling together observational data and numerical models is carried out with data assimilation methods. Advanced issues are related to network design.
- For impact assessment, integrated modeling relies on look-up tables, to be computed with detailed models.

Outline

Scales

Microphysics

- Aerosols: 1 nm - 10 μm
- Cloud droplets: 1 - 100 μm
- Rain droplets: 0.01 - 0.1 mm

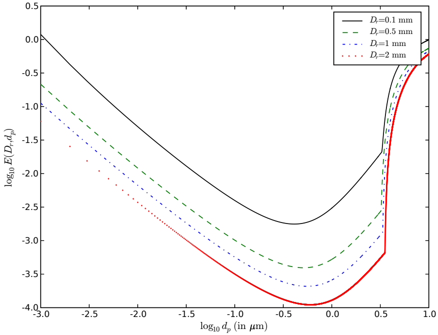
Numerics (Grid Cell)

- Short-range (CFD): 1 - 10 m
- Regional: 1 km
- Continental: 10-100 km

Scavenging of Radionuclides

Gas-Phase or Particle-Bound Radionuclides

- Detailed microphysics versus tailored parameterizations
- Uncertainties: rain parameters and size distribution



Size distribution of the aerosol collision efficiency

Towards Micro/Macro Models

- Based on stochastic micro models

Segregation Effect

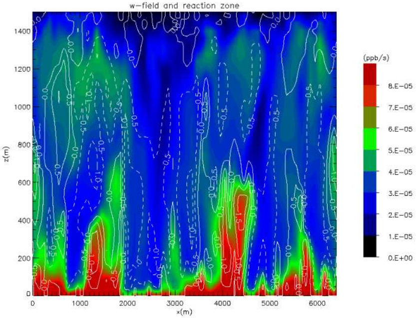
Downdraft O_3/Updraft NO

- Rate of the titration reaction $NO + O_3 \rightarrow NO_2$:

$$\omega = k \langle NO \rangle \langle O_3 \rangle \left(1 + \underbrace{\frac{\langle NO' O_3' \rangle}{\langle NO \rangle \langle O_3 \rangle}}_{I_s} \right)$$

Closure Scheme

- State-of-the-art in 3D models: $I_s = 0$!
- Towards Large Eddy Simulation ?



Reaction rate (DNS computation; credit: J.F. Vinuesa, JRC)

Outline

Time Integration of High-Dimensional Stiff Systems

Model Dimension (State Vector per Grid Cell)

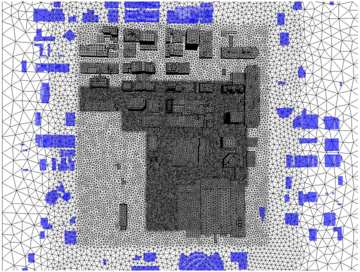
- Passive tracer: 1 tracer
- Gas-phase: 50-100 *surrogate* species
- Diphasic: 10-50 dissolved species
- Aerosols: 20 species $\times$ 10 bins (size) $\times$ 1 family (internal mixing)

Wide Range of Timescales (Stiffness)

- From radical ($\tau = 10^{-10}$s) to inert species

Towards Highly Resolved Model

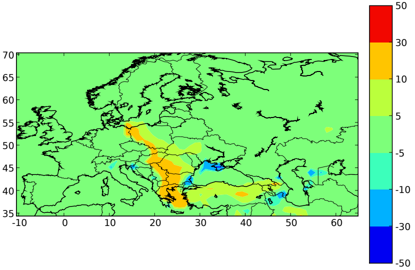
- Next-generation mesoscale model: 1-3 km grid
- Unstructured meshes near sources ?



Towards on-line Coupling

Many Motivations

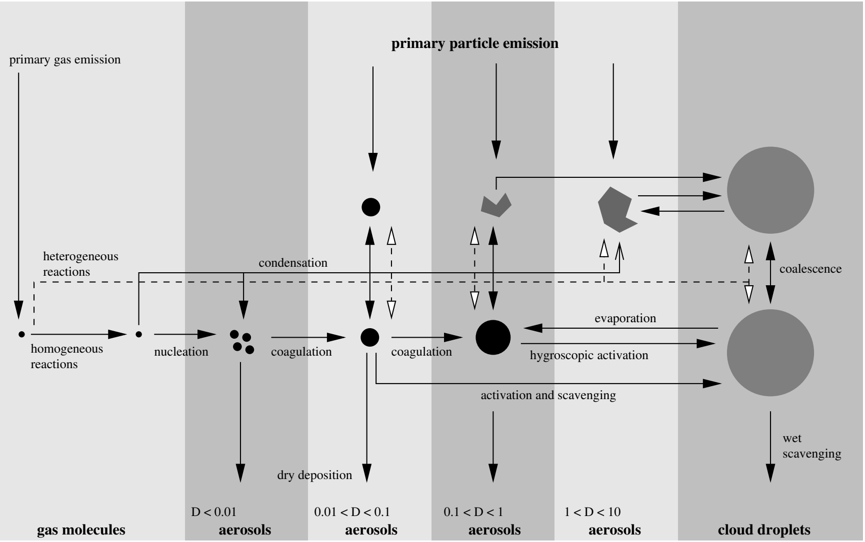
- Physics: conservation of homogeneous mixing ratio for a passive tracer (mass consistency error)
- Numerics: discrepancies in the wind fields for ρ and c
- Convective episodes



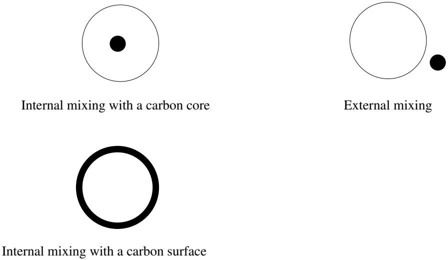
Relative difference for the Chernobyl release (fitted w)

Outline

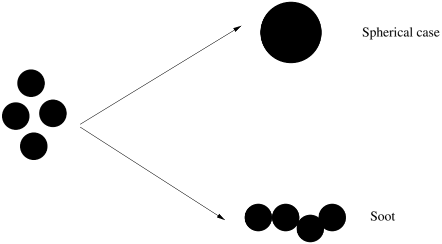
Aerosol Dynamics



Towards External Mixing of Fractal Particles



Mixing state and radiative properties



Geometrical configuration of soot

Outline

Model Reduction

Arms Race versus Robustness

- Impact studies over many (meteorological) years (Long Range Transport Air Pollution/Clean Air For Europe)
- "Integrated" modeling:

$$\min_e \; F_{\text{impact}} \circ F_{\text{CTM}} \circ F_{\text{economic activity}}(e)$$

  where e stands for emissions
- 4D distributed systems with a few observations versus low-dimensional models

Many strategies

- Source-Receptor matrices ($2500 \times 5 \times 5 \times 5$ runs of one meteorological year)
- Look-up tables (HDMR, chaos expansion)

In Models We Trust

Outline

Uncertainties in CTM

Major Uncertainties

- Input data: emissions, met. data
- Parameterizations and physics
- Numerics
- Bugs

Data	Uncertainties
Cloud attenuation	$\pm 30\%$
Dry deposition (O_3 and NO_2)	$\pm 30\%$
Boundary Conditions (O_3)	$\pm 20\%$
Anthropogenic emissions	$\pm 50\%$
Biogenic emissions	$\pm 100\%$
Photolytic rate	$\pm 30\%$

In Models We Trust: the Overtuning Issue

- Too few observational data (chemical, vertical, time)
- Key target: ozone peak (impact study versus forecast)

Some strategies

- Sensitivity analysis
- Monte Carlo simulations on the basis of Probability Density Functions (PDF)
- Ensemble meteorological forecasts
- Multi-configuration/multi-model runs

Ensemble Forecast

Ensemble (Set) of Models $\mathcal{E} = \{M_m(\cdot)\}_m$

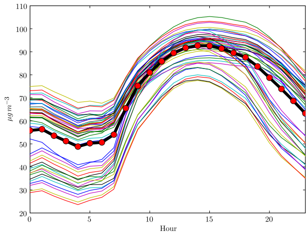
- Ensemble mean:

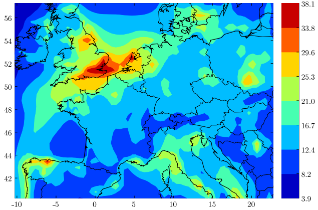
$$\text{EM}(\cdot) = \frac{1}{|\mathcal{E}|} \sum_{M \in \mathcal{E}} M_m(\cdot)$$

- Super-ensemble:

$$\text{ELS}(\cdot) = \sum_m \alpha_m M_m(\cdot)$$

with weights α_m to forecast on the basis of past observations





Ensemble & relative uncertainties (POLYPHEMUS run for ozone)

Outline

Background

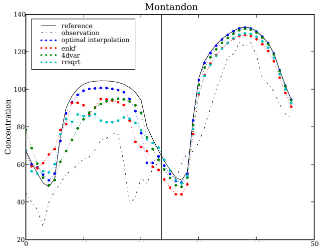
Monitoring Networks

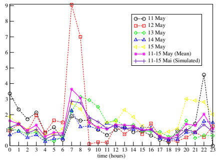
- Terrestrial sensors
- Satellite data

Key Features

- Variational and sequential methods
- Inverse modeling of emissions
- High-dimensional systems
- Second-order sensitivity

Data assimilation for ozone (Credit: Lin Wu/CLIME/CEREA)





Inverse modeling of NO_x emissions

Forecast and Risk Assessment

Source Localization and Operational Forecast of a Release

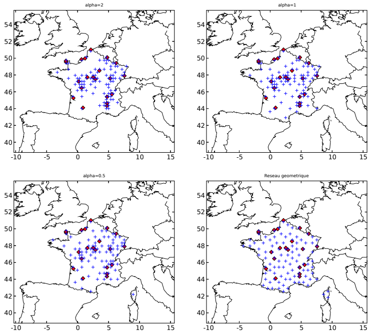
- Pre-operational case
- Maximum Entropy technique
- POLYPHEMUS run, credit: Marc Bocquet (CEREA)

See
movie

Network Design

IRSN Descartes monitoring network design over France

- to monitor potential radionuclides releases accidents (Credit: Marc Bocquet, CEREA)
- ≃20000 simulated releases



Many Challenging Issues for HPCN

An Increasing Spatial Resolution

- Towards 1-kilometer grid
- Parameterization, adaptive unstructured meshes ?

An Increasing Chemical Resolution

- From *surrogate species* to *chemical species*
- Secondary Organic Aerosol, external mixing, . . .

An Increasing Complexity: Coupling Models and Scales

- Towards multi-media integrated modeling
- From off-line coupling to on-line coupling

From Deterministic to Probabilistic Models

- CTM are not deterministic models.
- From all-in-one models to a new generation of modeling systems (ensemble modeling)