



Modeling the atmospheric concentrations of pesticides with an air quality model: toward the determination of population exposure at a regional/national scale

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Introduction

Necessity to have high-resolution maps of pesticide concentrations for epidemiologists in order to study the impact of pesticides on human health

⇒ a prediction tool is therefore necessary to better assess atmospheric contamination by pesticides and population exposure

Air quality models could be used to simulate maps of pesticide concentrations at the regional or national scale



Air quality modeling with CHIMERE

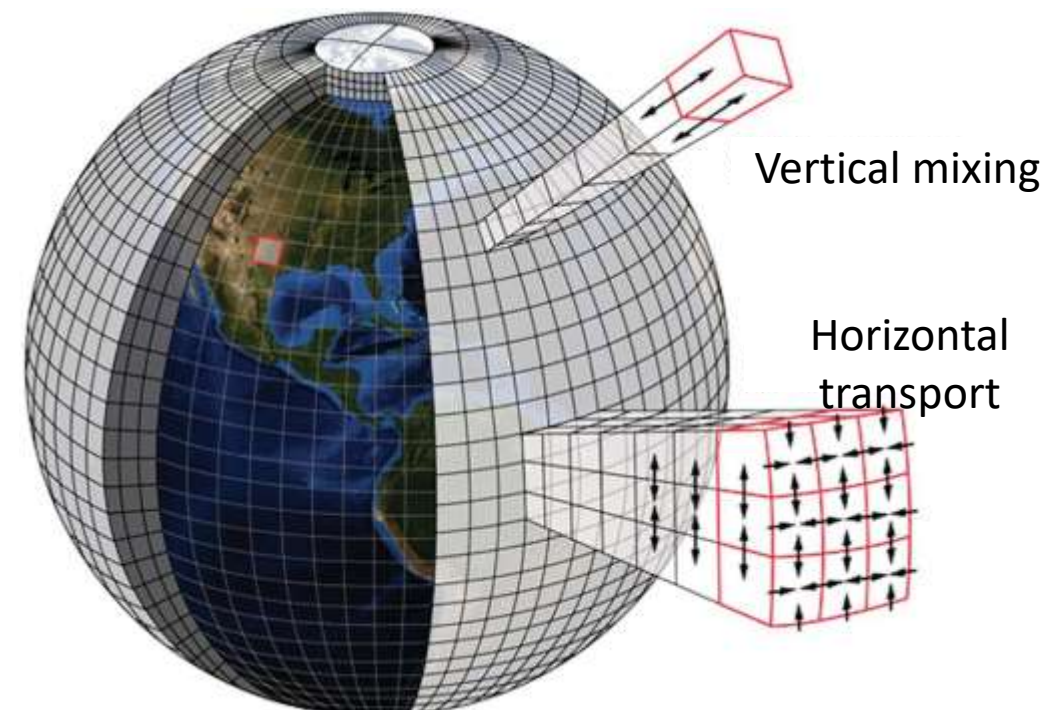
- Chemical-Transport Models are deterministic models aiming at representing the physicochemical processes occurring in the atmosphere
- Objective: simulating concentrations over a geographical domain
- CHIMERE is an eulerian model. The domain is dividing into several cells covering the whole domain.
- Typical resolution with CHIMERE: from a few kilometers to 100 of kilometers depending on the size of domain



<https://www.lmd.polytechnique.fr/chimere/>

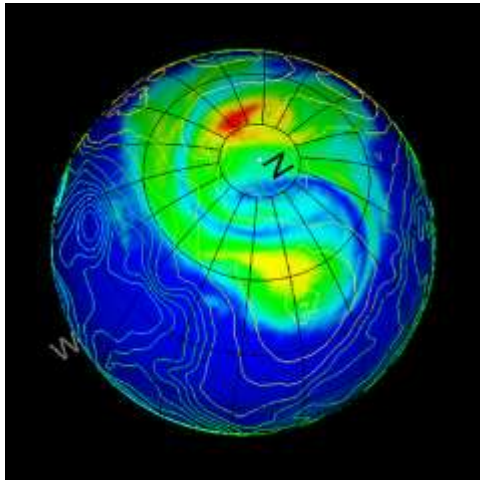
Modèle Open-Source codéveloppé
par le CNRS (LMD, LISA) et l'Ineris

Representation of a Chemical Transport Model

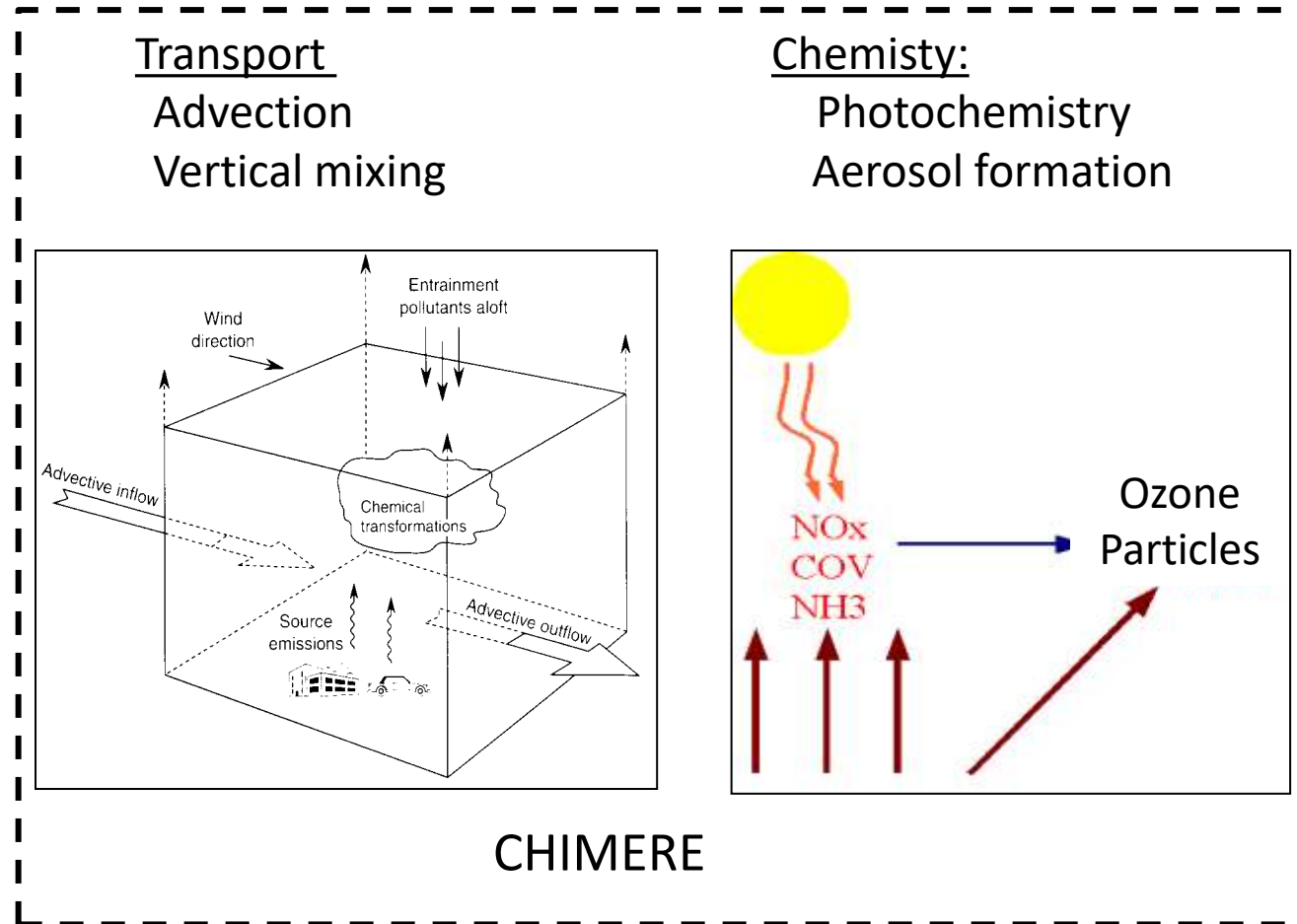
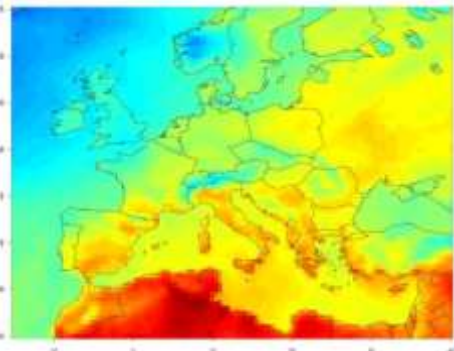




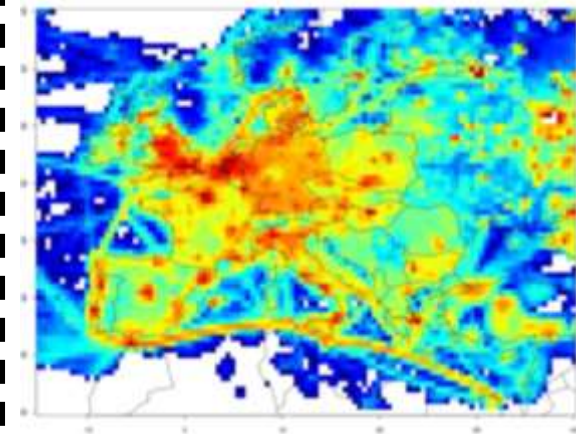
Long-range transport



Meteorology

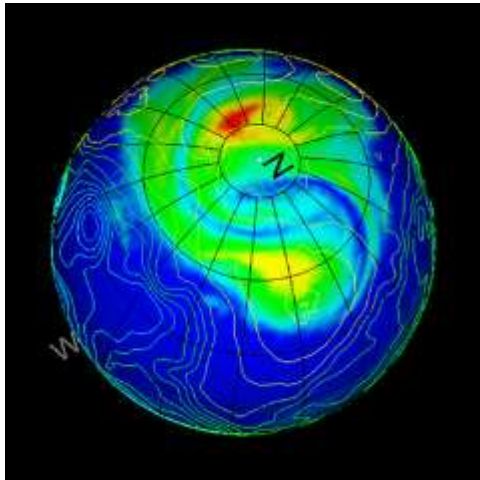


Emissions

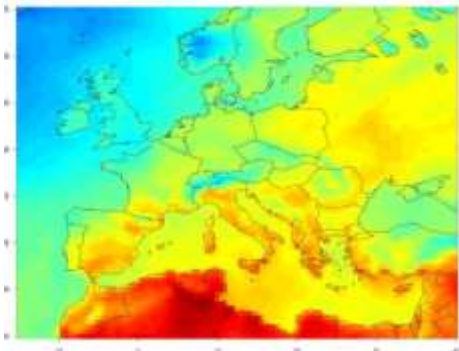




Long-range transport



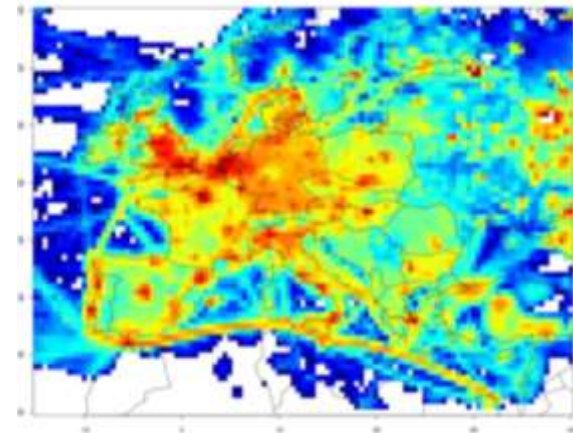
Meteorology



Exemple de résultats:
- Maps of PM2.5 concentrations over the Northern Hemisphere

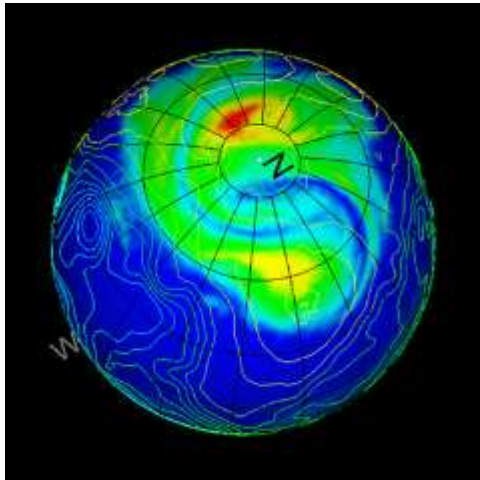


Emissions

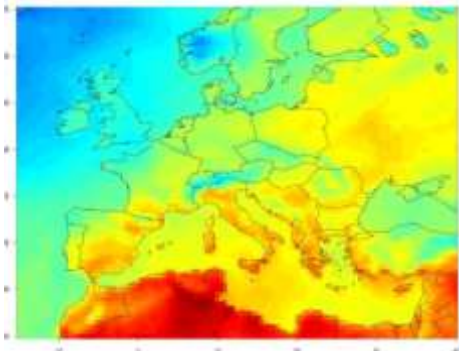




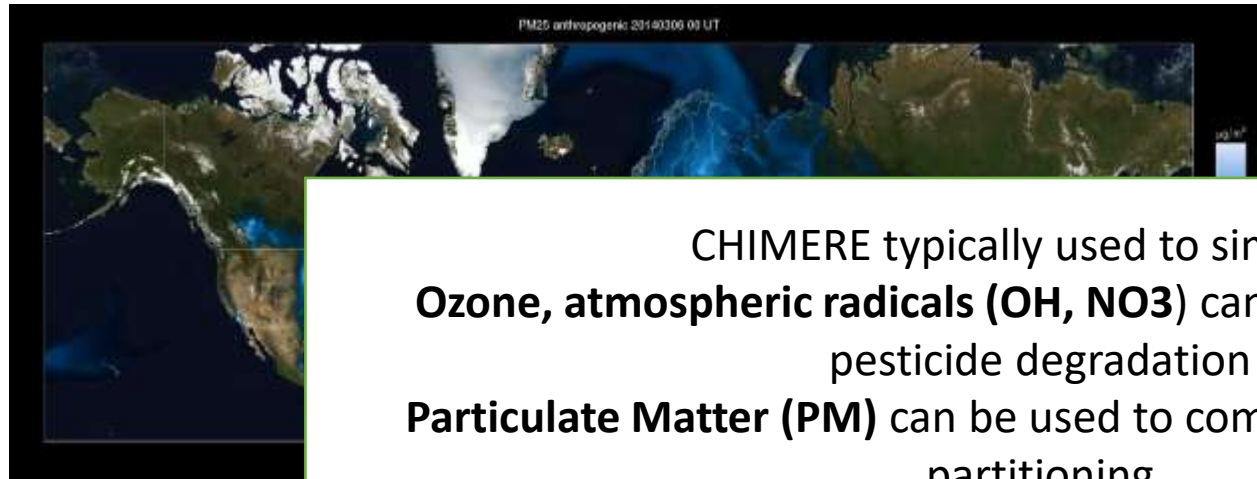
Long-range transport



Meteorology

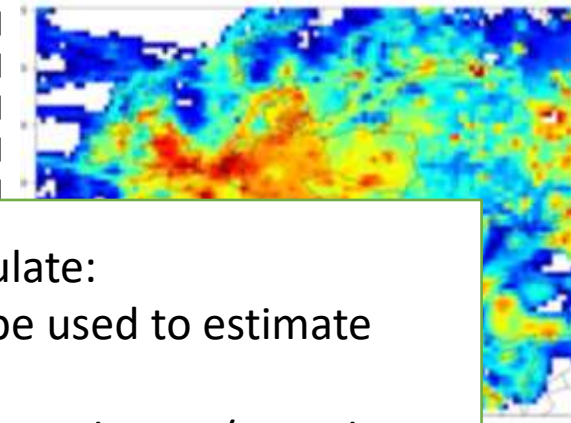


Exemple de résultats:
- Maps of PM2.5 concentrations over the Northern Hemisphere



CHIMERE typically used to simulate:
Ozone, atmospheric radicals (OH, NO₃) can be used to estimate pesticide degradation
Particulate Matter (PM) can be used to compute the gas/particle partitioning
Deposition
Other atmospheric pollutants (NO₂, sometimes POPs)

Emissions





Using CHIMERE

- CHIMERE is a CPU time consuming model
- A supercomputer must be used (example Topaze at CCRT)
- Simulating a year of concentrations (with a resolution around 0.2-0.5° over Europe) with CHIMERE can take several days of computation with between 100 and 200 processors
- CHIMERE typically works with a resolution of a few kilometers
- Medium-range/Long-range transport: Resolution not adapted to the exposure of residents
- Case study: Simulation of S-metolachlor and Folpet atmospheric concentrations over France



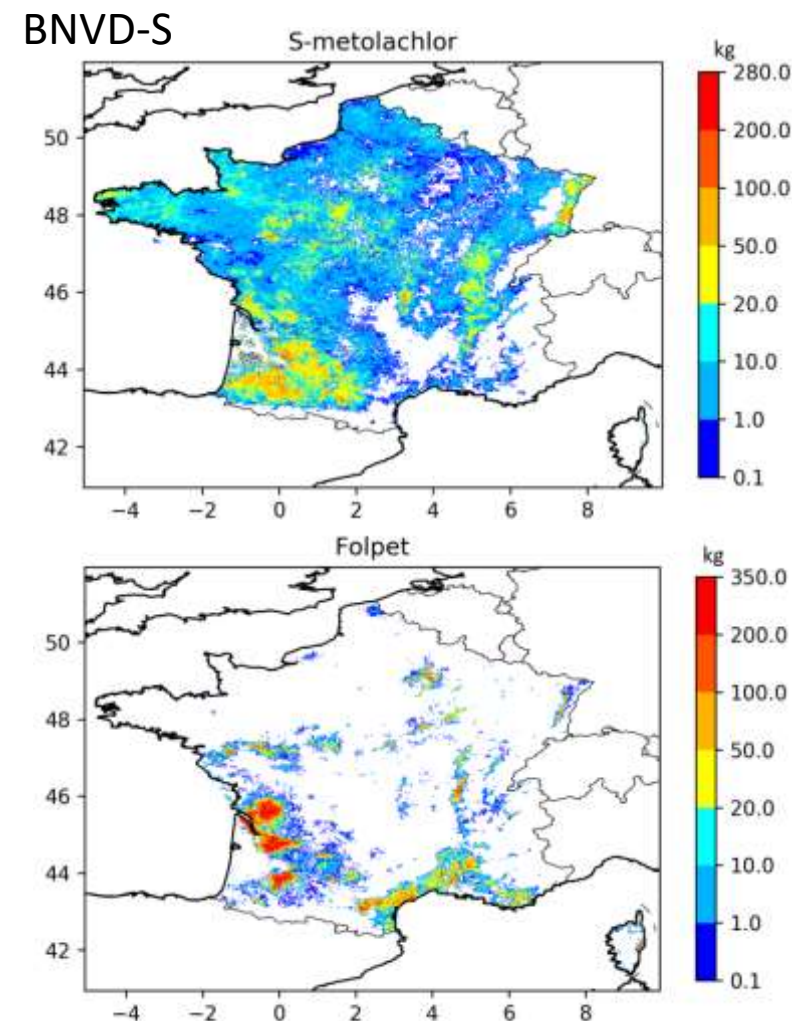
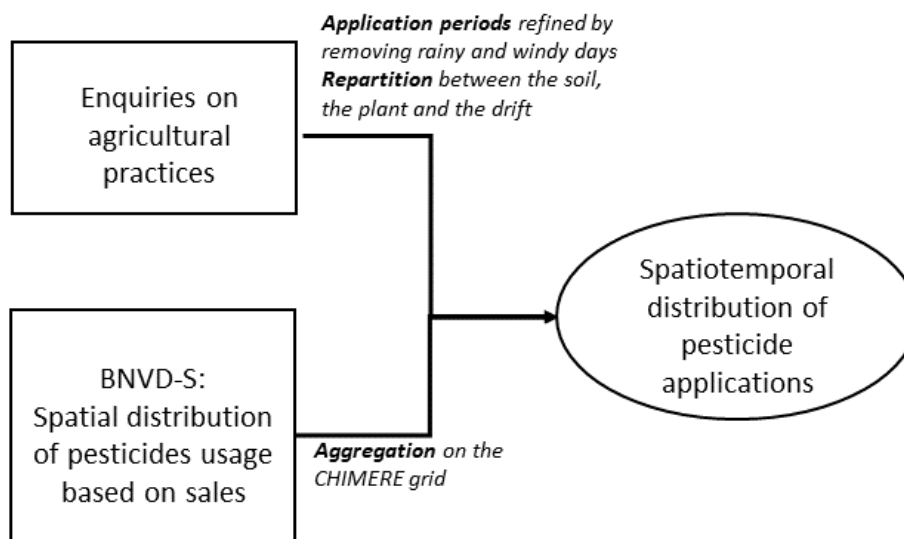


Simulating pesticide concentrations with CHIMERE

First step: Estimating the spatiotemporal distribution of pesticide applications

Over France, the BNVD-S database provide a good estimation of pesticide usages (methodology based on sales and provided ZIP code)

Temporal distribution determined based on expert enquiries for the southeastern region of France (applied for the whole country)

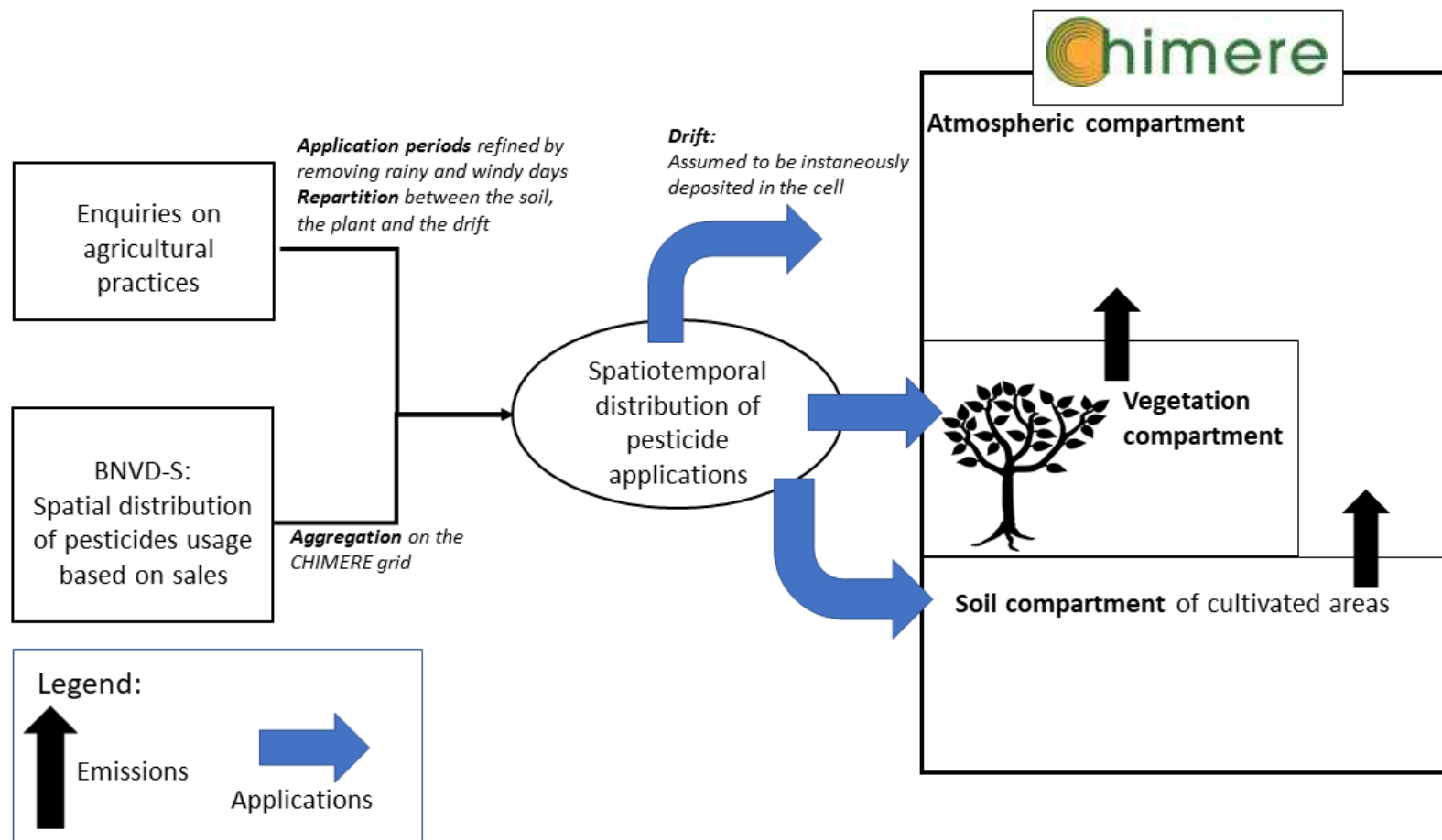




Simulating pesticide concentrations with CHIMERE

Second step: Distributing pesticide usages on the different compartments

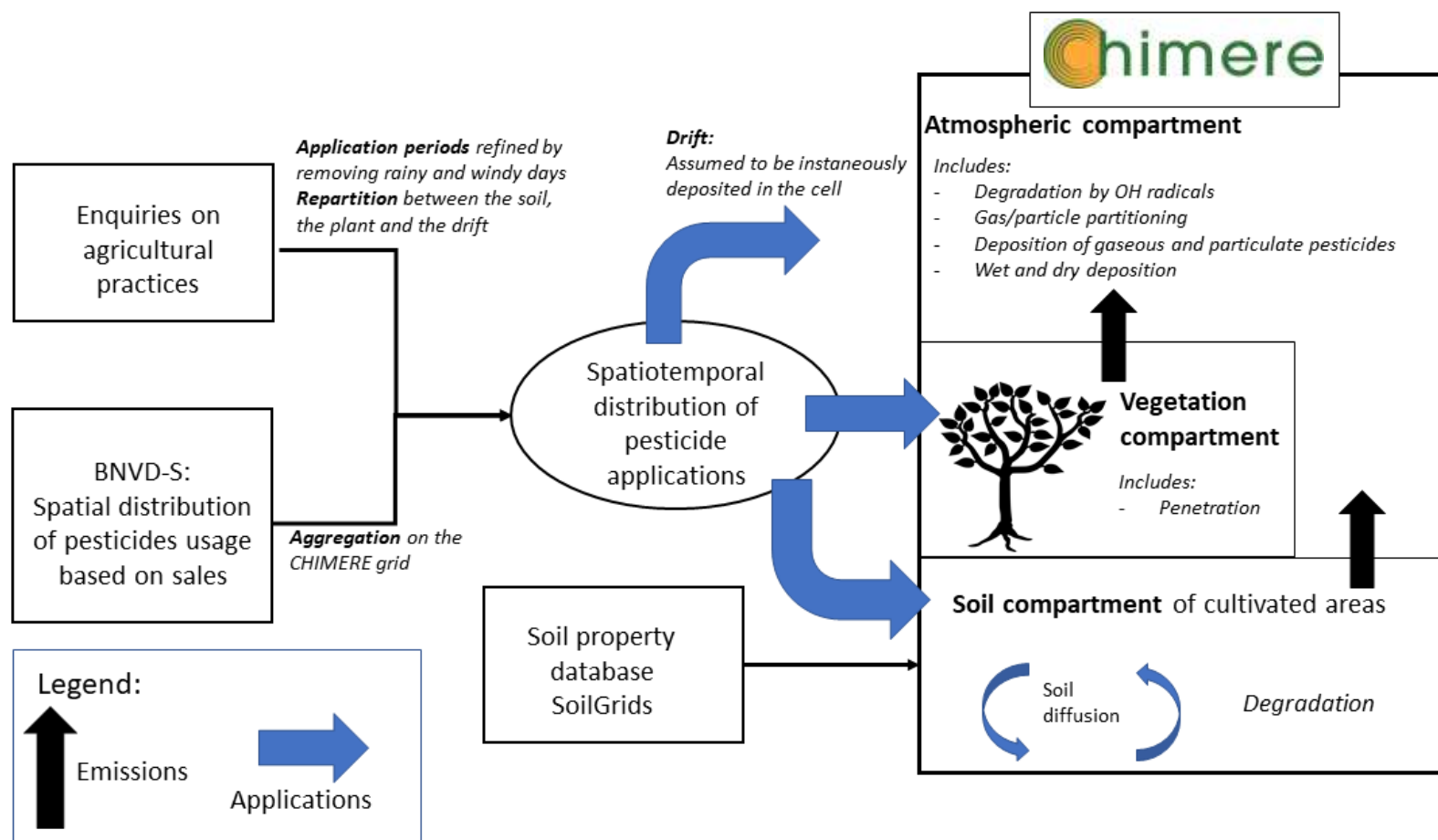
Estimation based on the type of materials used





Simulating pesticide concentrations with CHIMERE

Third step: representing the different processes into CHIMERE

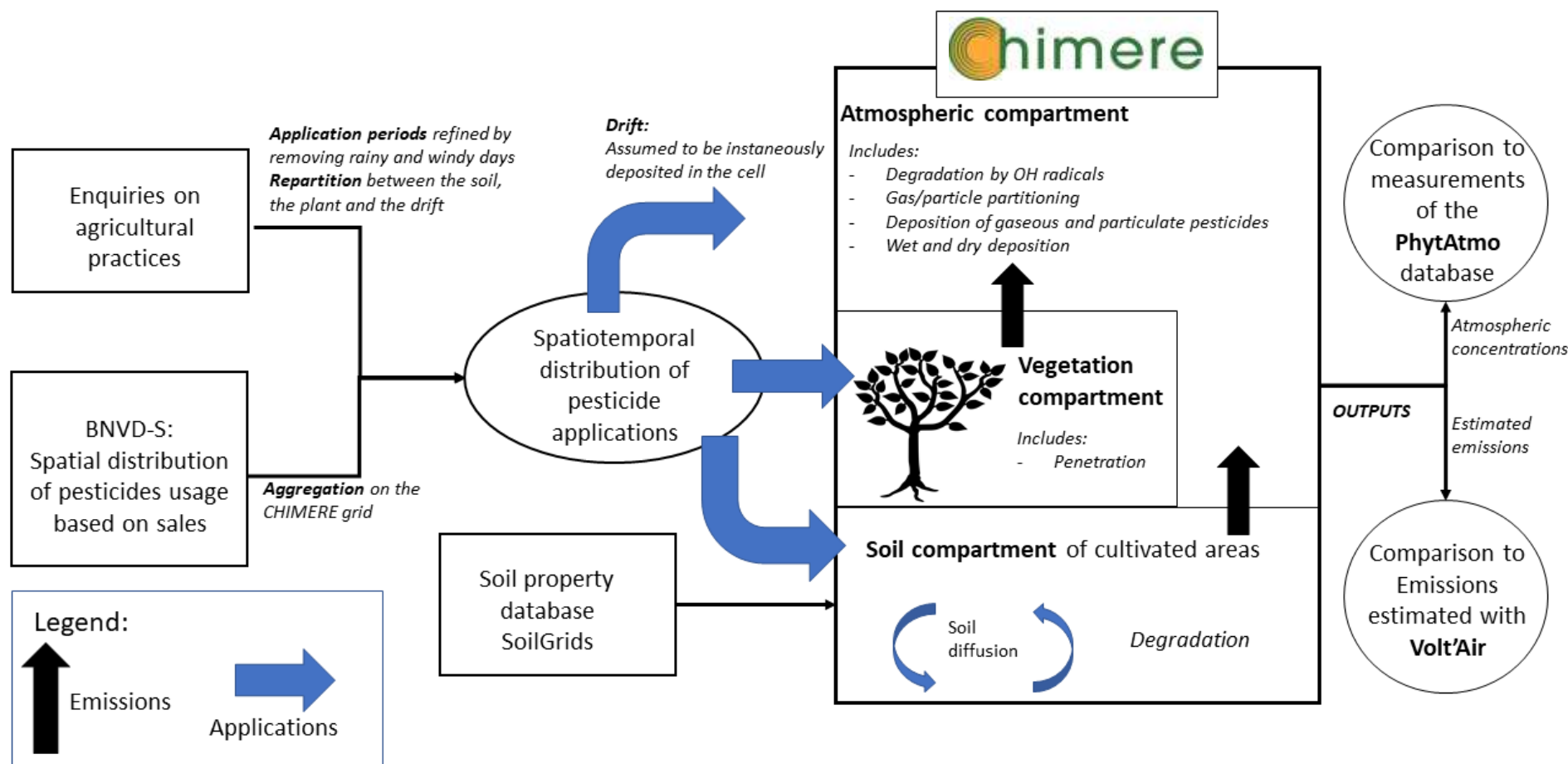




Simulating pesticide concentrations with CHIMERE

Fourth step: Validation

Comparison of model results to measurements (ambient concentrations and volatilization fluxes) and/or other model results (Volt'Air for volatilization fluxes)

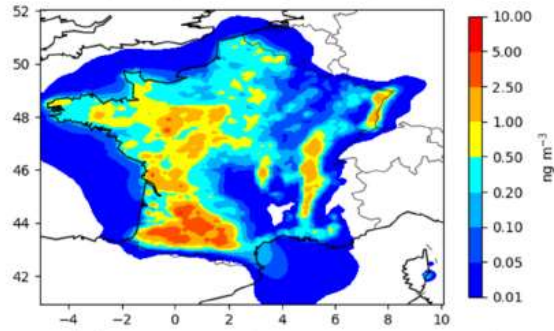




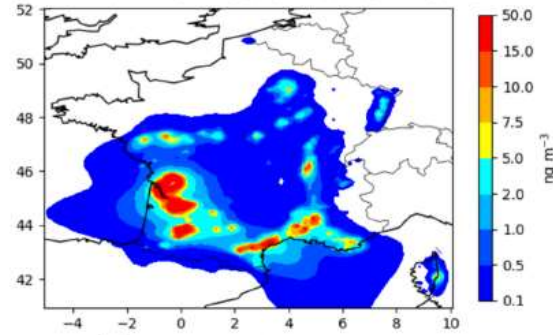
Main results

Concentrations in ng/m³

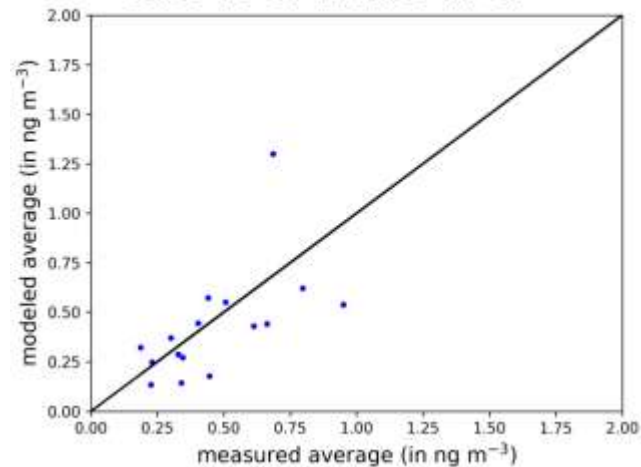
(a) simulated concentrations of S-metolachlor over France from 2014-04-15 to 2014-05-15



(b) simulated concentrations of Folpet over France from 2014-05-01 to 2014-07-01



(a) S-metolachlor
2014-04-15 to 2014-05-15

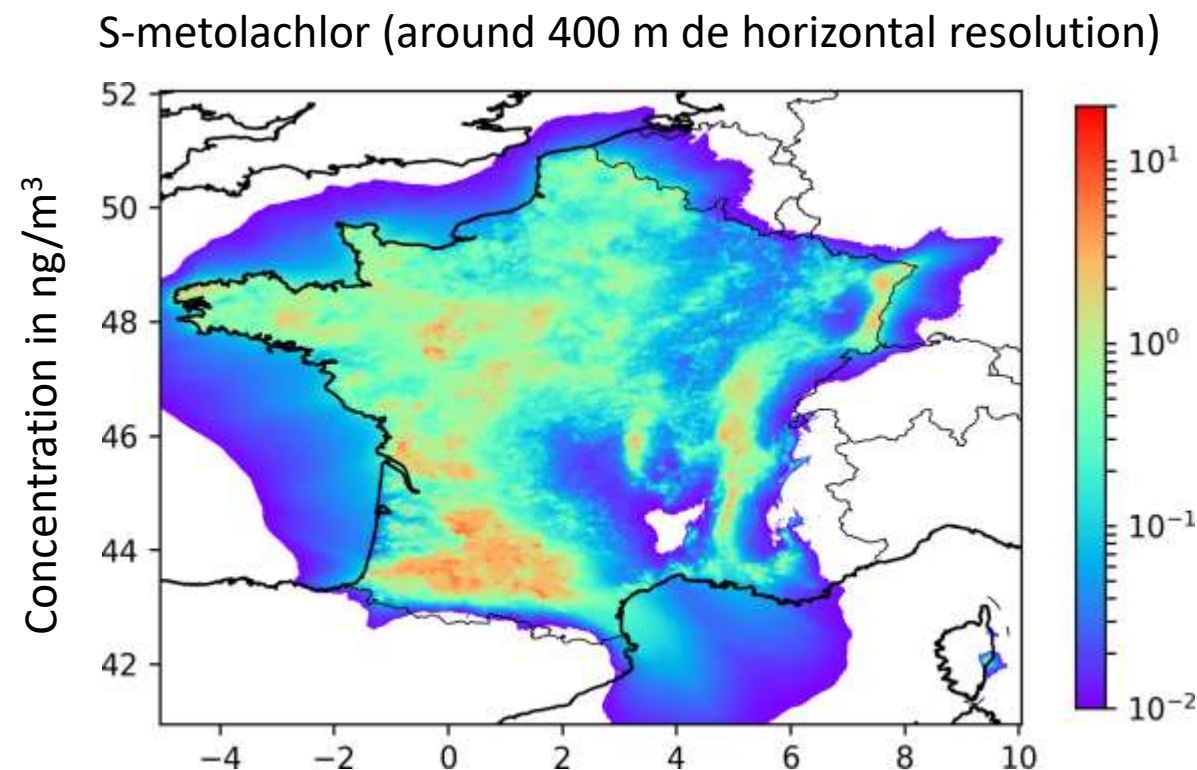


- The model can reproduce the order of magnitude of pesticide atmospheric concentrations
 - ✓ S-metolachlor and folpel
- Can reproduce the spatial distribution of concentrations over France
 - ✓ S-metolachlor – spatial correlation of 0.79 (correlation between measured and modeled temporal average)
 - ✓ Folpet : high detection limit – few exploitable data



Downscaling

- The resolution of CHIMERE simulations can be a limit to their use for exposure calculations
- A downscaling method has been implemented in CHIMERE (Couvidat et al., in prep)
- Resolution still insufficient to calculate exposure to drift droplets
- Possibility to combine CHIMERE with models dedicated to drift dispersion





Conclusions

- CHIMERE-pesticides : methodological barriers were removed. Could be used as a basis for epidemiological studies.
- The model should be improved by improving emission calculation
 - Improving representation of surface conditions
 - For each pesticide, modeled emission fluxes should be compared to multiple flux measurements performed under different conditions. Need of data to evaluate the long-term emissions of pesticides (several days/weeks after the application)
- The model could be used to study the atmospheric concentrations of degradation products
- Process occurring in the atmosphere (degradation, gas/particle partitioning, wet and dry deposition) should be investigated and evaluated



Limits to the use of CHIMERE-pesticides

- The lack of information is currently the primary barrier to the use of CHIMERE-pesticides for exposure determination. Lack of:
 - Accurate spatio-temporal data on pesticide application
 - BNVD-S provides information on spatial distribution of applications
 - Need information on treatment schedules
 - Pesticide volatilization data to adjust some model parameters
 - Observations to validate the model and statistically correct the model results. Many results were provided by the French national campaign
- Specific cases of certain substances such as lindane, which would require the reconstruction of concentrations on a global scale over several decades because of its long lifespan



Thank you for your attention

2014-04-15 at 00



Simulating the impact of volatilization on atmospheric concentrations of pesticides with the 3D chemistry-transport model CHIMERE: Method development and application to S-metolachlor and folpet

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S-metolachlor
ng/m³

