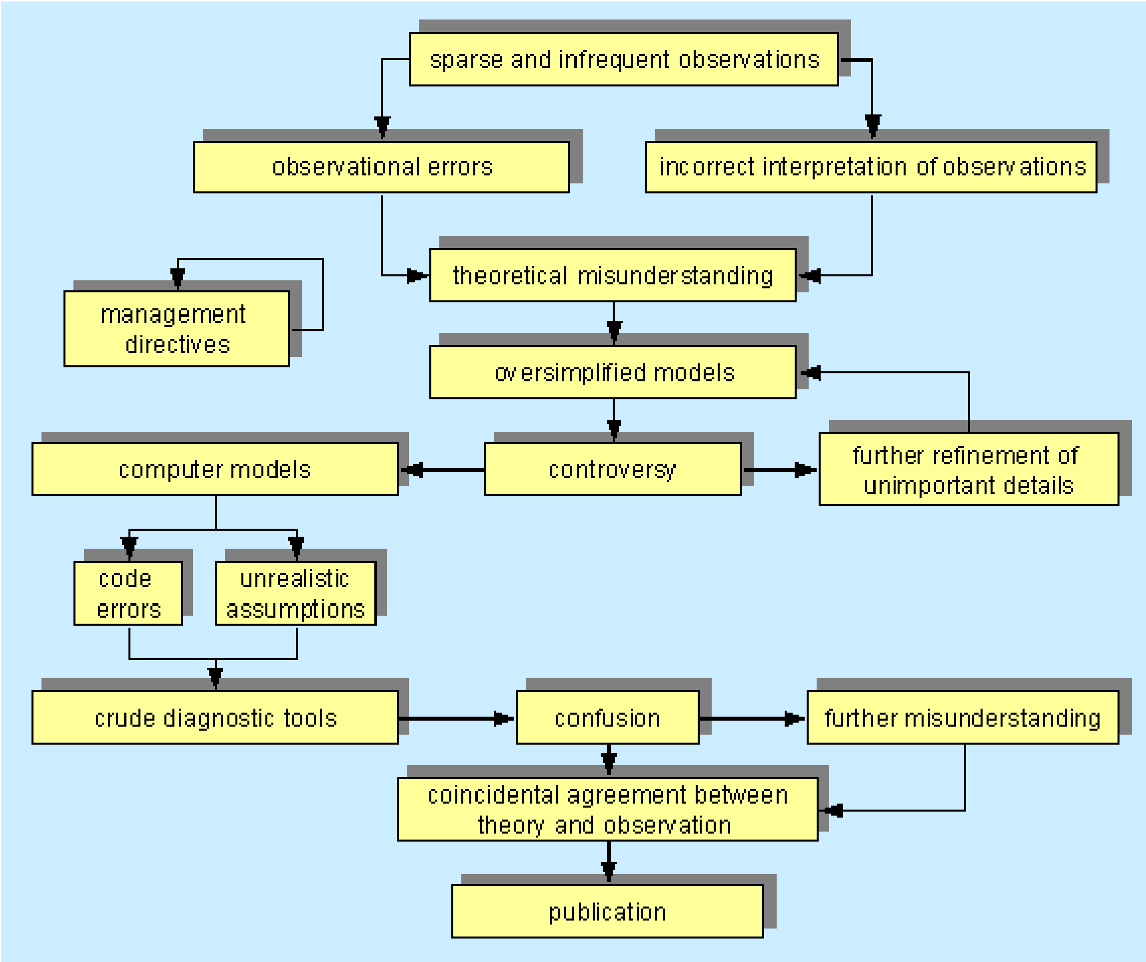
Atmospheric transport modelling concepts Source oriented / receptor oriented approaches

Questions? Write delia.arnold-arias@zamg.ac.at

ATM background

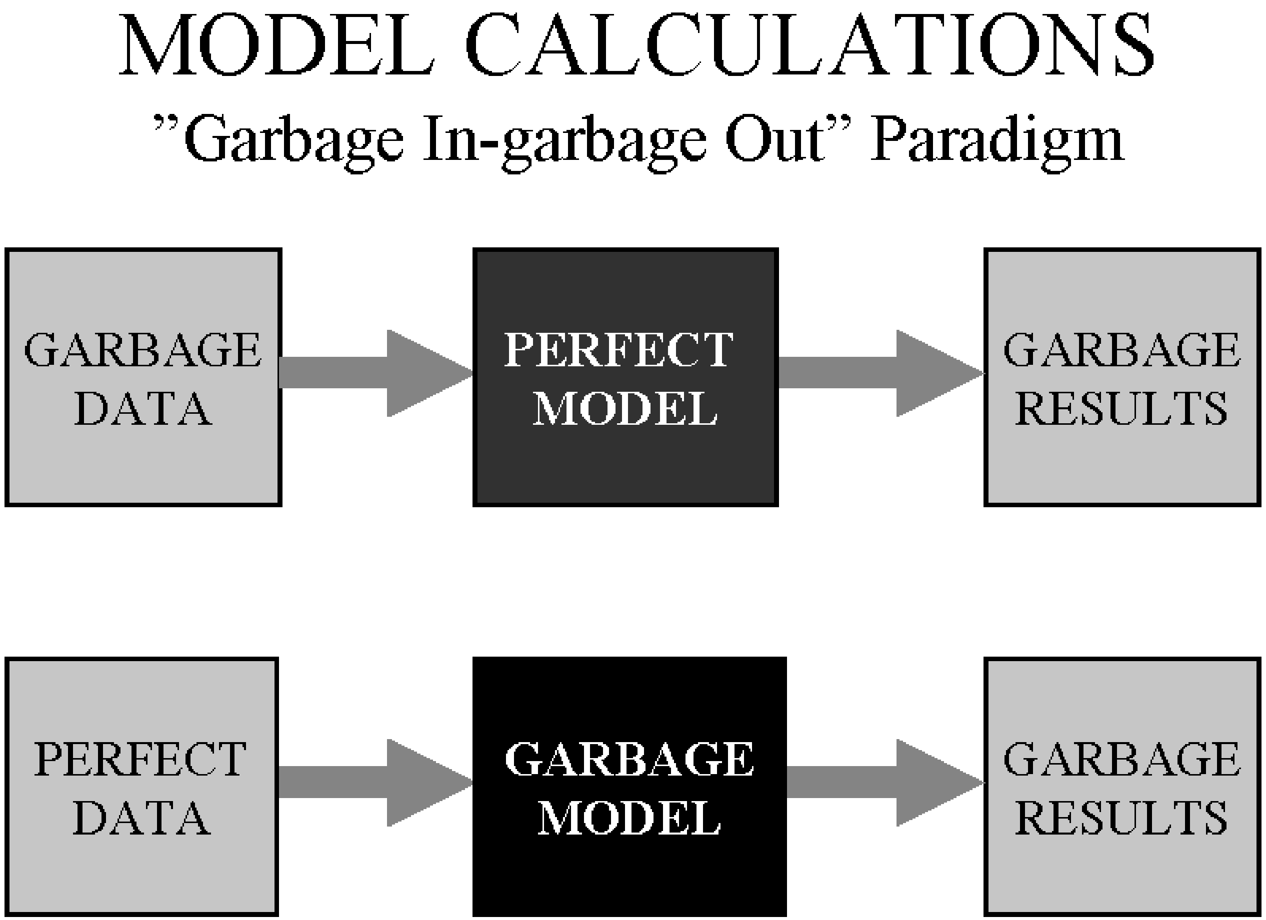
All about computer modelling … http://biocycle.atmos.colostate.edu/~marek/research/mod.htm



"All models are wrong but some are useful" G.E.P. Box *Robustness in the Strategy of Scientific Model Building*

… and continues "**For such a model there is no need to ask the question "Is the model true?". If "truth" is to be the "whole truth" the answer must be "No". The only question of interest is "Is the model illuminating and useful?**".

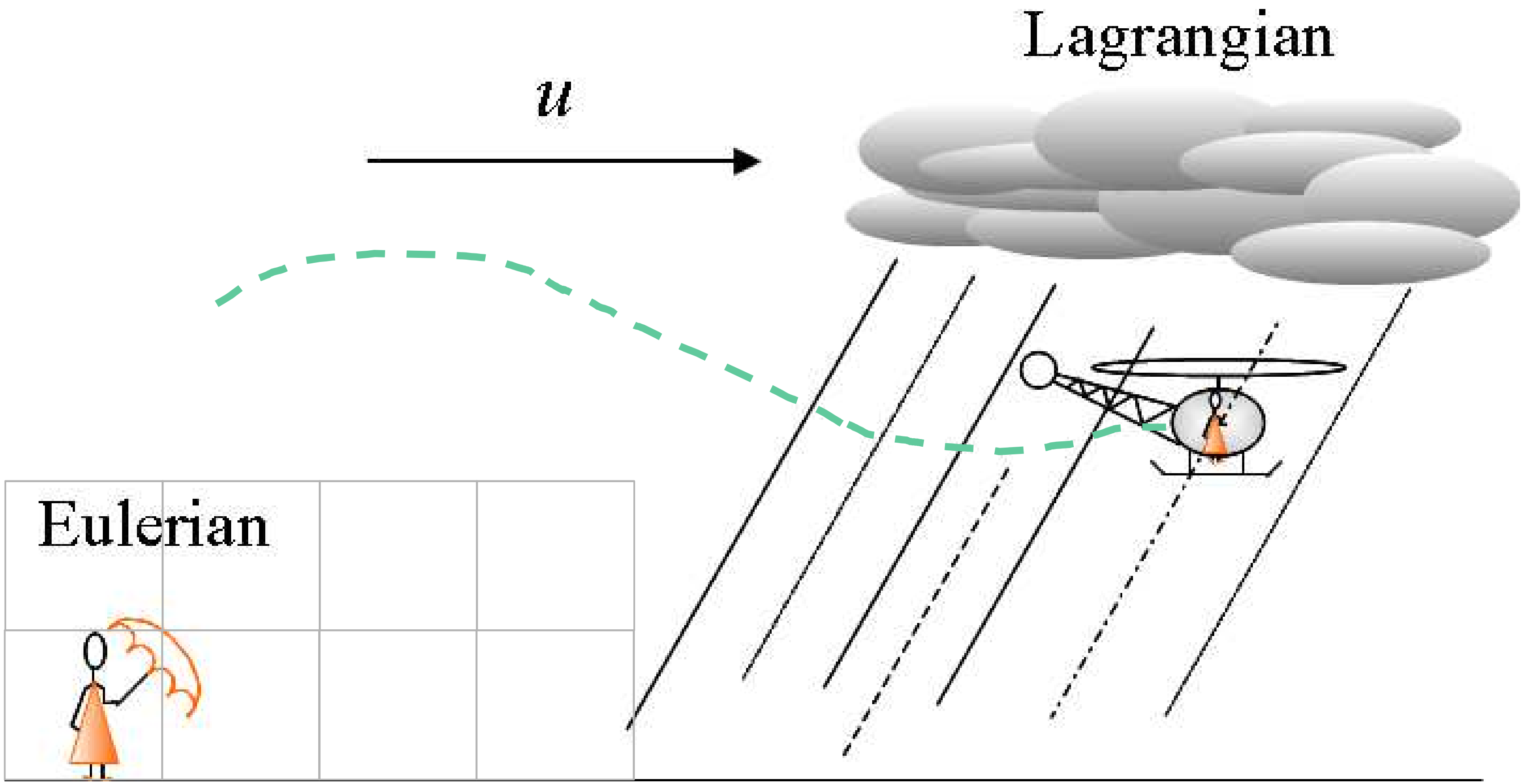
https://www.cfact.org/2017/02/27/gigo-based-energy-and-climate-policies/



Neither perfect model nor perfect data exist.

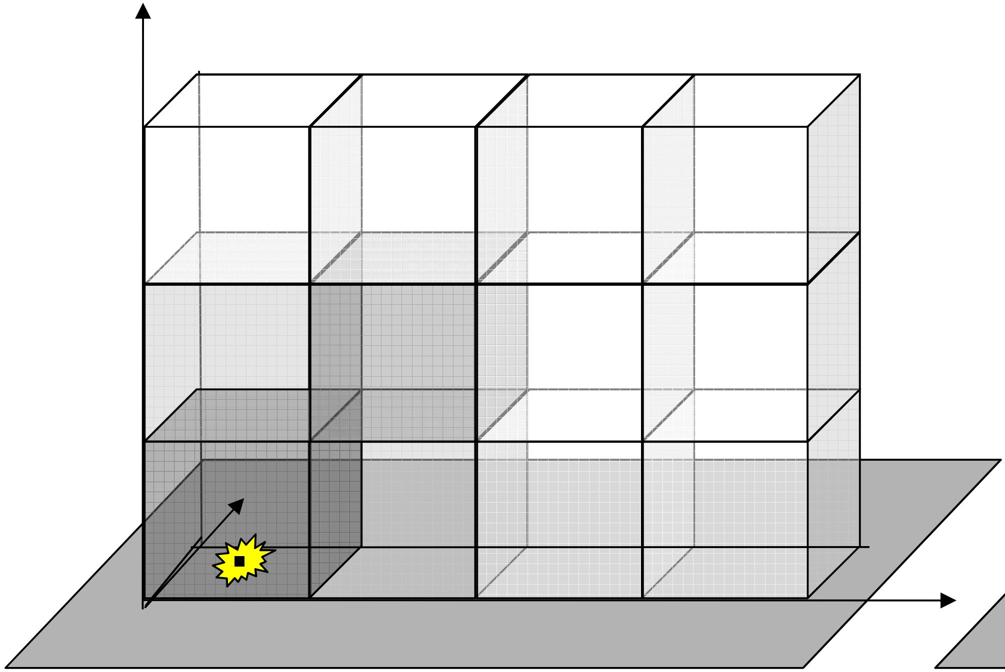
ATM background

- Two basic types of reference frames to model atmospheric flows:



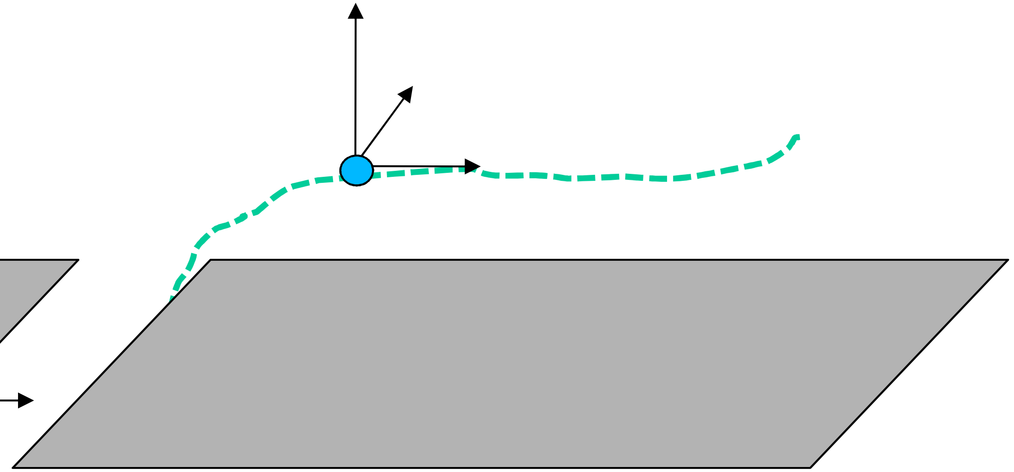
Fixed gridded system   Following an air parcel

Eulerian



Lagrangian

Trajectories consistent with pre-defined Eulerian probability functions in physical and velocity space – trajectory differential equation



$$\frac{\partial c_i}{\partial t} + \boxed{u_x \frac{\partial c_i}{\partial x} + u_y \frac{\partial c_i}{\partial y} + u_z \frac{\partial c_i}{\partial z}}$$

Divergence of the advected flux

$$= \frac{\partial}{\partial x}\left(K_{xx}\frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial c_i}{\partial z}\right) + R_i(c_1, c_2 \cdots, c_n) + E_i(x, y, z, t) - S_i(x, y, z, t)$$

Chemical reactions

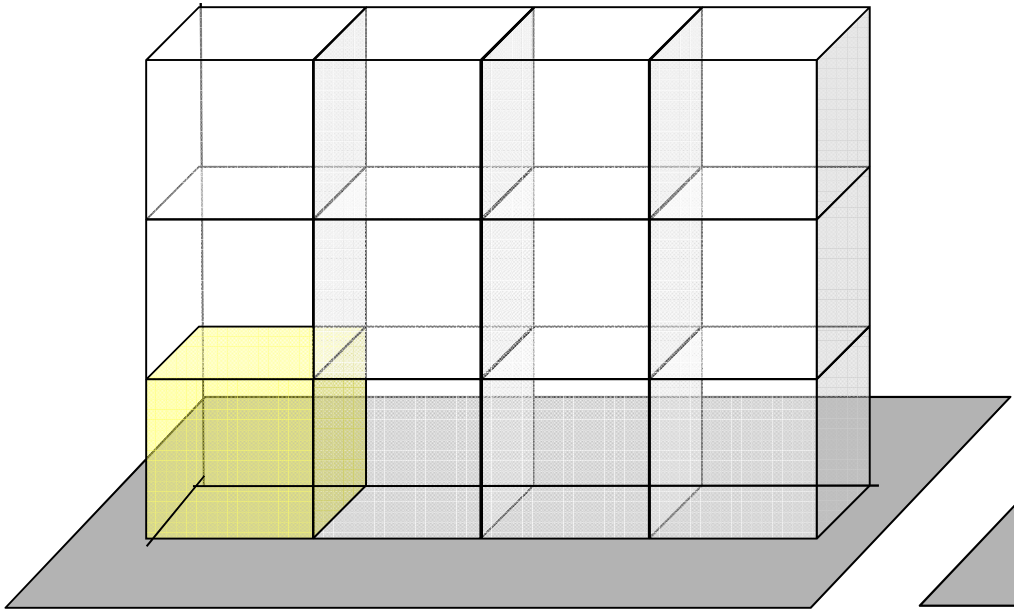
Sinks

Divergence of the turbulent fluxes

Emissions

ATM background

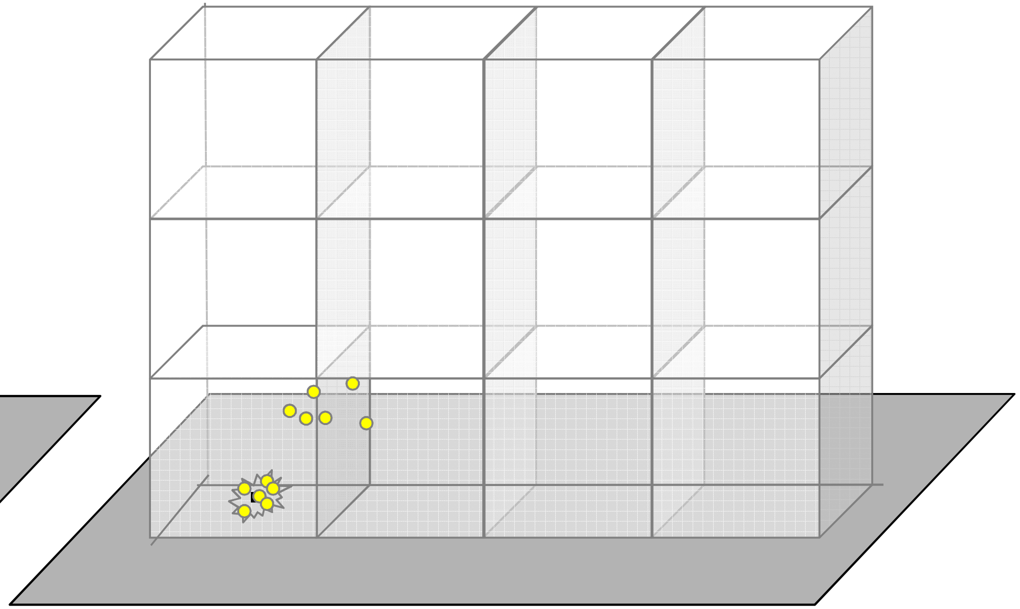
Eulerian



Immediate dilution in the grid cell

Point source sub-model then needed

Lagrangian

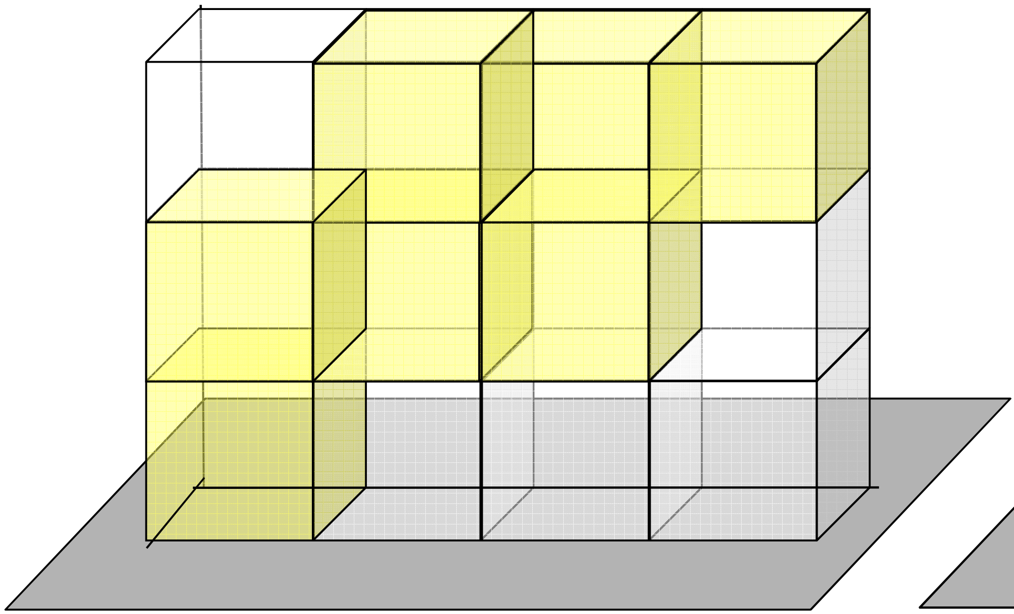


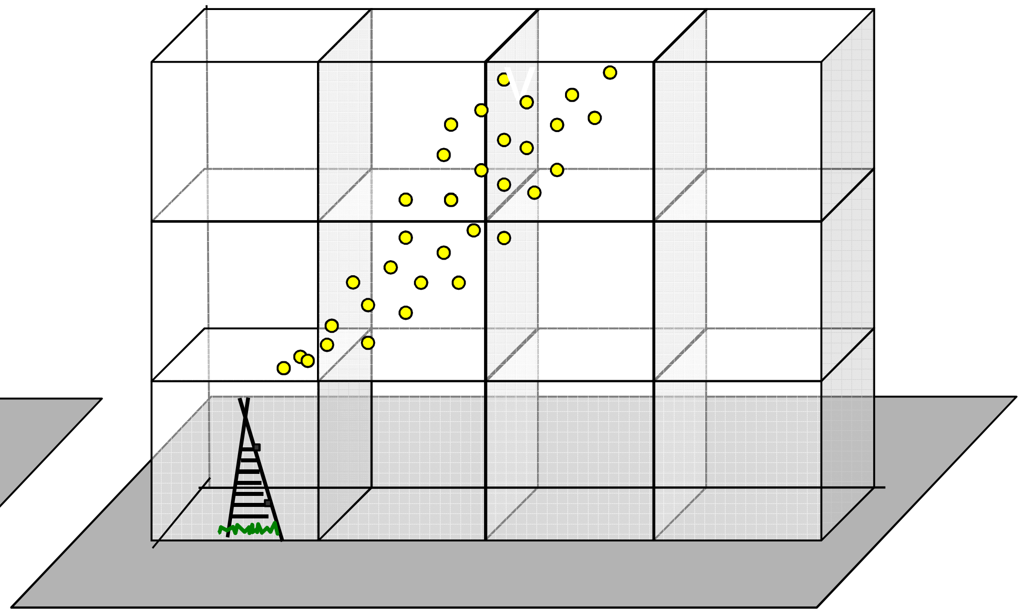
LPDM can deal naturally with point sources

The grid is only applied to output fields

Eulerian

Lagrangian





Problems with representing narrow plumes

ATM background

Eulerian

Fig. 10a Initial isolated puff

MSC-W Note 2/92, August 1992.EMEP "An Evaluation of Eulerian Advection Methods for the Modelling of Long Range Transport of Air Pollution". By Erik Berge and Leonor Tarrasón. EMEP_1992_N2.pdf

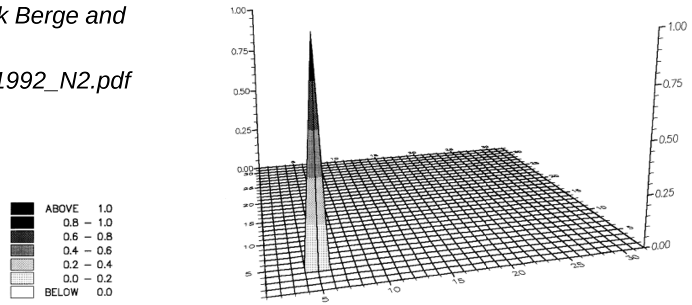


Fig. 10d BOS: Diagonal puff

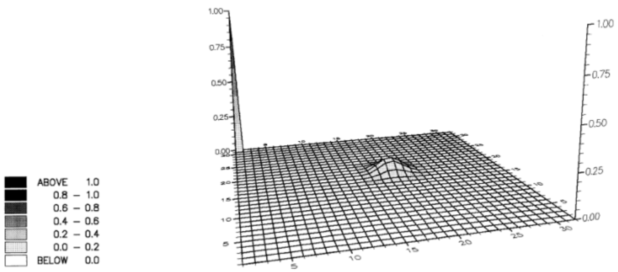
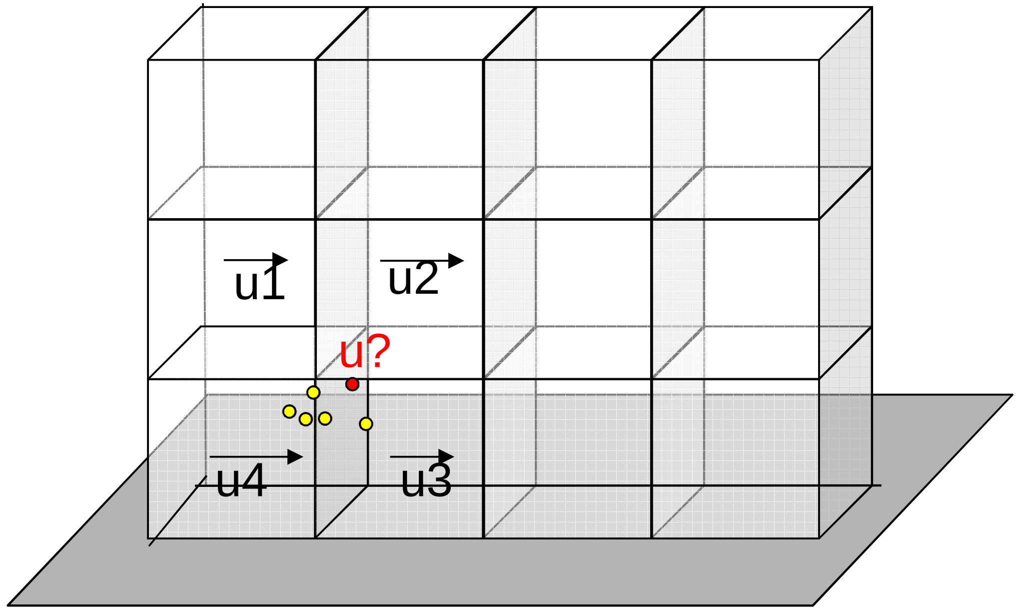


Fig. 10e PSS: Diagonal puff

Numerical diffusion in the advection

Lagrangian



Interpolation errors (of all variables to particle position) and discretization of differential equations

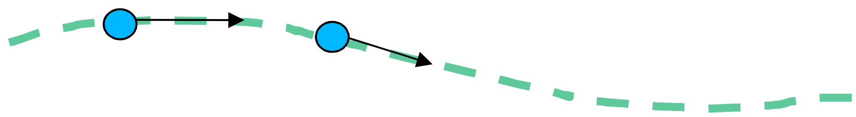
Why Lagrangian?

- Can be **computationally very efficient** (depending on size of plume): only the fraction covered with particles is simulated. Computational cost depending on particle numbers BUT LPDM are easily parallelized.
- **Turbulent processes** are included in a more natural way unlike Eulerian models
- Capacity to describing **non-diffusive near-field** to sources.
- There is **no numerical diffusion** due to a computational grid
- Grid and/or kernels are used only for output purpose therefore **no artificial diffusion** is due to the averaging process
- Model is **"self-adjoint**" – can run backward in time, too. Important for RO modelling
- Many **first order processes** can be easily included with a prescribed rate: radioactive decay, dry deposition, washout, etc.
- One particle can carry more than one species
- Gravitational settling is easily included (as long as particles carry a single species)

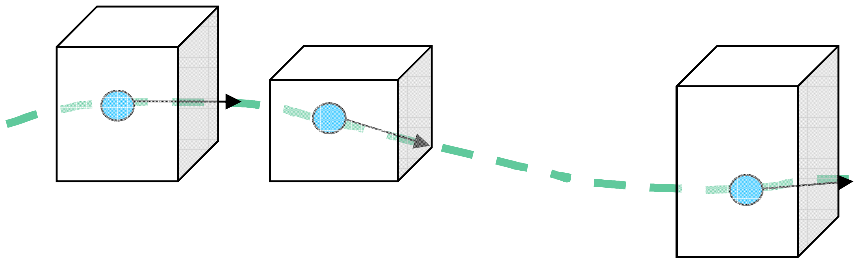
However: *it is quite difficult and computationally expensive to include* ***non-linear chemical reactions*** *and the process of* ***gridding the output*** *make as well loose some of the advantages of Lagrangian modelling.*

Main types of Lagrangian models

- Mean Trajectories – it assumes that the air parcel does not have the identity modified and that one single line represents its motion defined solely by the mean wind.
  - No diffusion is considered
  - No turbulence is considered
  - Very simple, very fast and visually appealing (*by some*)
  - More valid for laminar or little turbulent flows such in the stratosphere

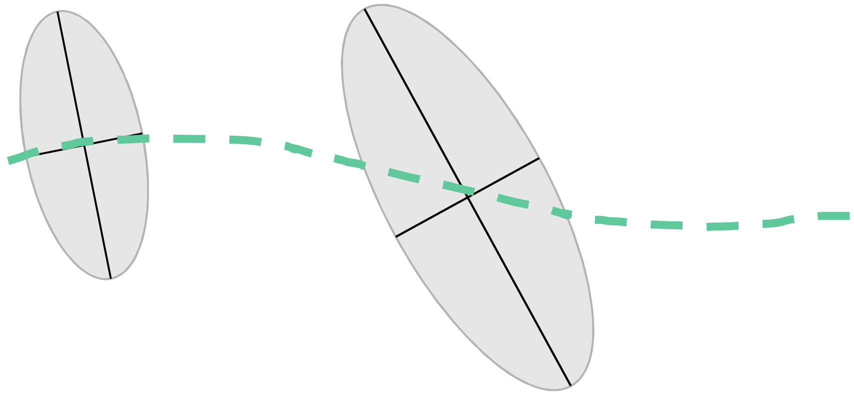


- Box models – a box that stretches or compresses along a trajectory defined, once more, by the mean wind. The box may be re-presented by one or more trajectories.
  - No diffusion is considered
  - No turbulence is considered
  - Good for chemistry
  - Strong wind shear deforms the boxes



Main types of Lagrangian models

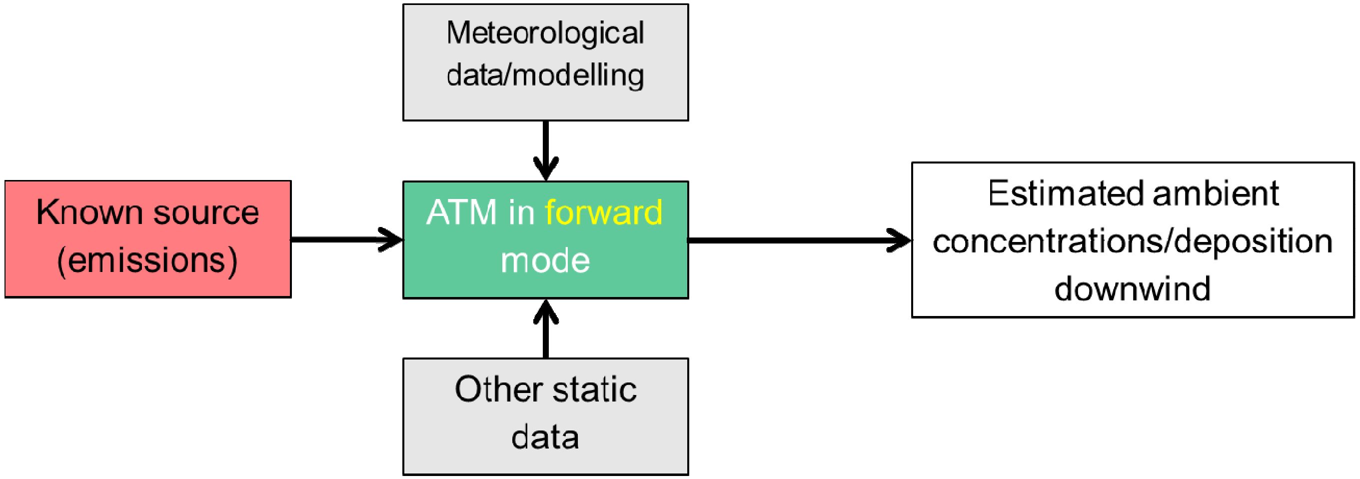
- Gaussian Puff model – it uses puffs moving along with the mean wind and with puffs growing in size (usually following a Gaussian) according to turbulence.
  - Good for constant winds and turbulence
  - Problems in strong wind shears
  - Handling merging of puffs



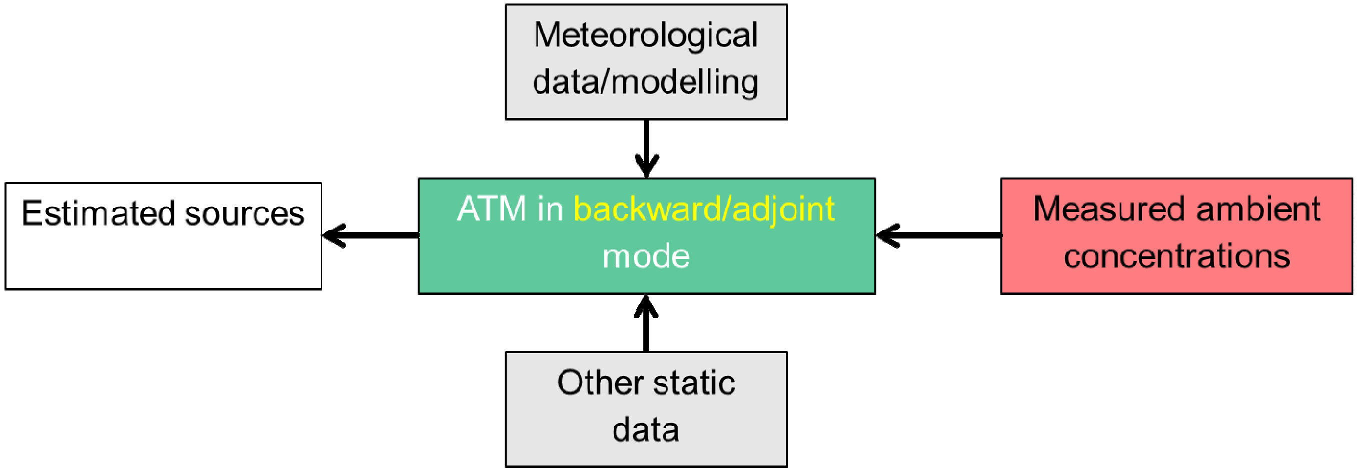
- Lagrangian particle dispersion models (LPDM) – particles are released with a certain amount of mass and species and are moved by the mean wind but also by turbulent contributions to the velocity.
  - Particles follow the eddies and are not “deformed”
  - Many particles are needed to properly represent a plume (more computational costs than previous models)
  - Possibility to treat heterogeneous turbulence

SO ATM / RO ATM

- **Source (emission) oriented ATM** aims at estimating the concentrations downwind given a known emission (location, time, strength, type).



- **Receptor (measurement) oriented ATM** aims at using physical and chemical measurements to infer some knowledge on the potential/probable sources and usually quantify their contributions (source attribution, source apportionment).



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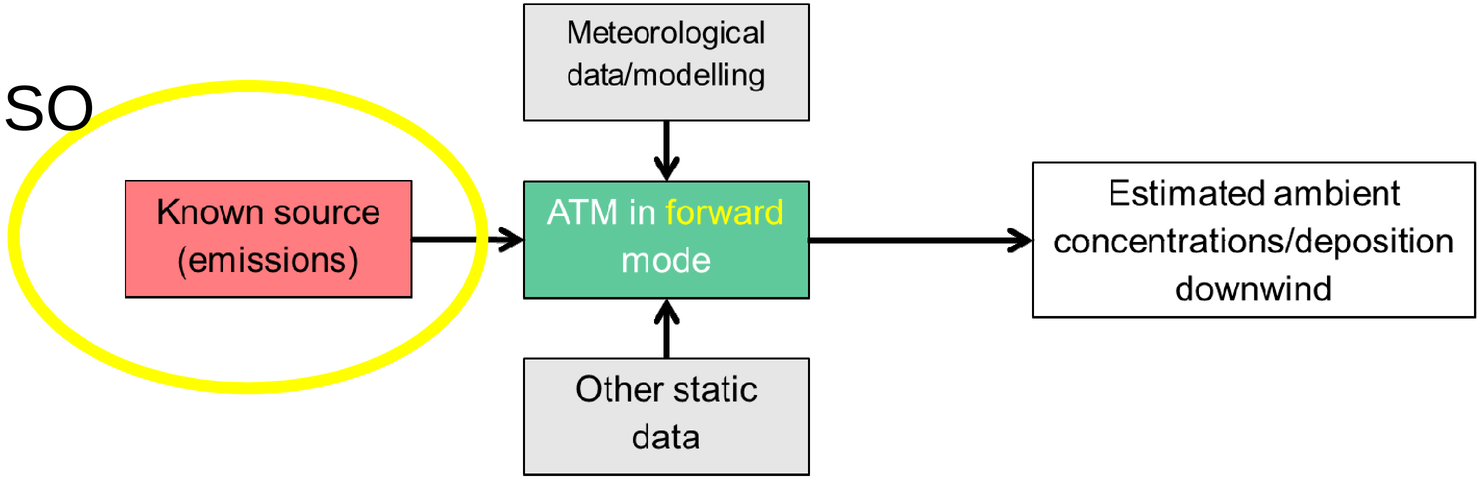

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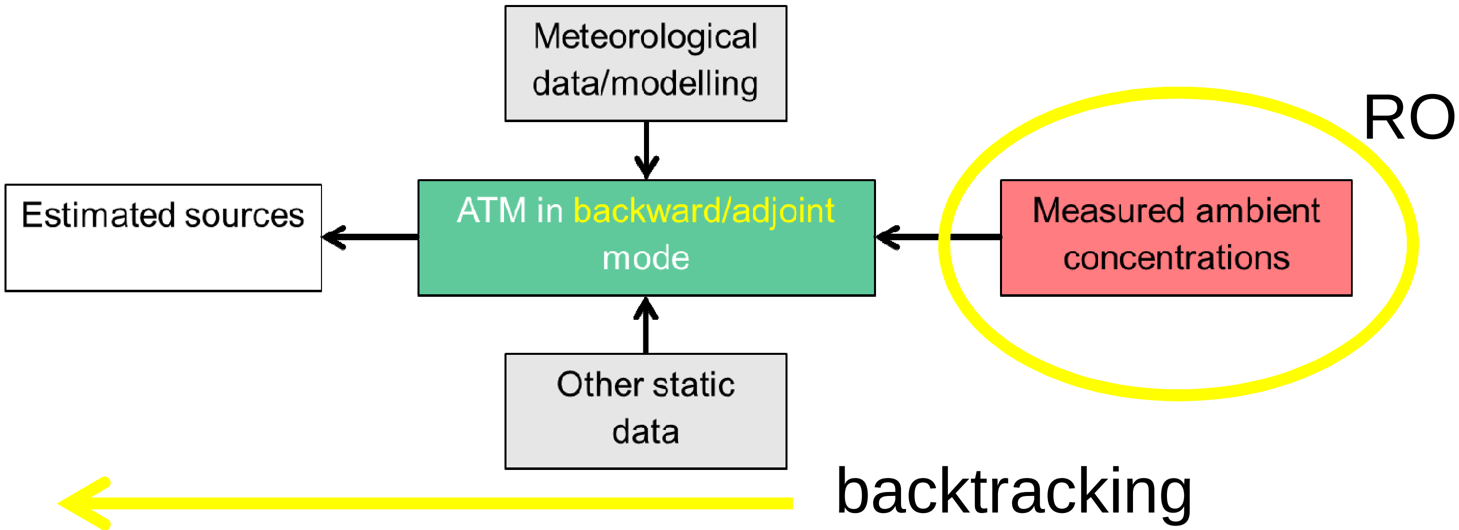
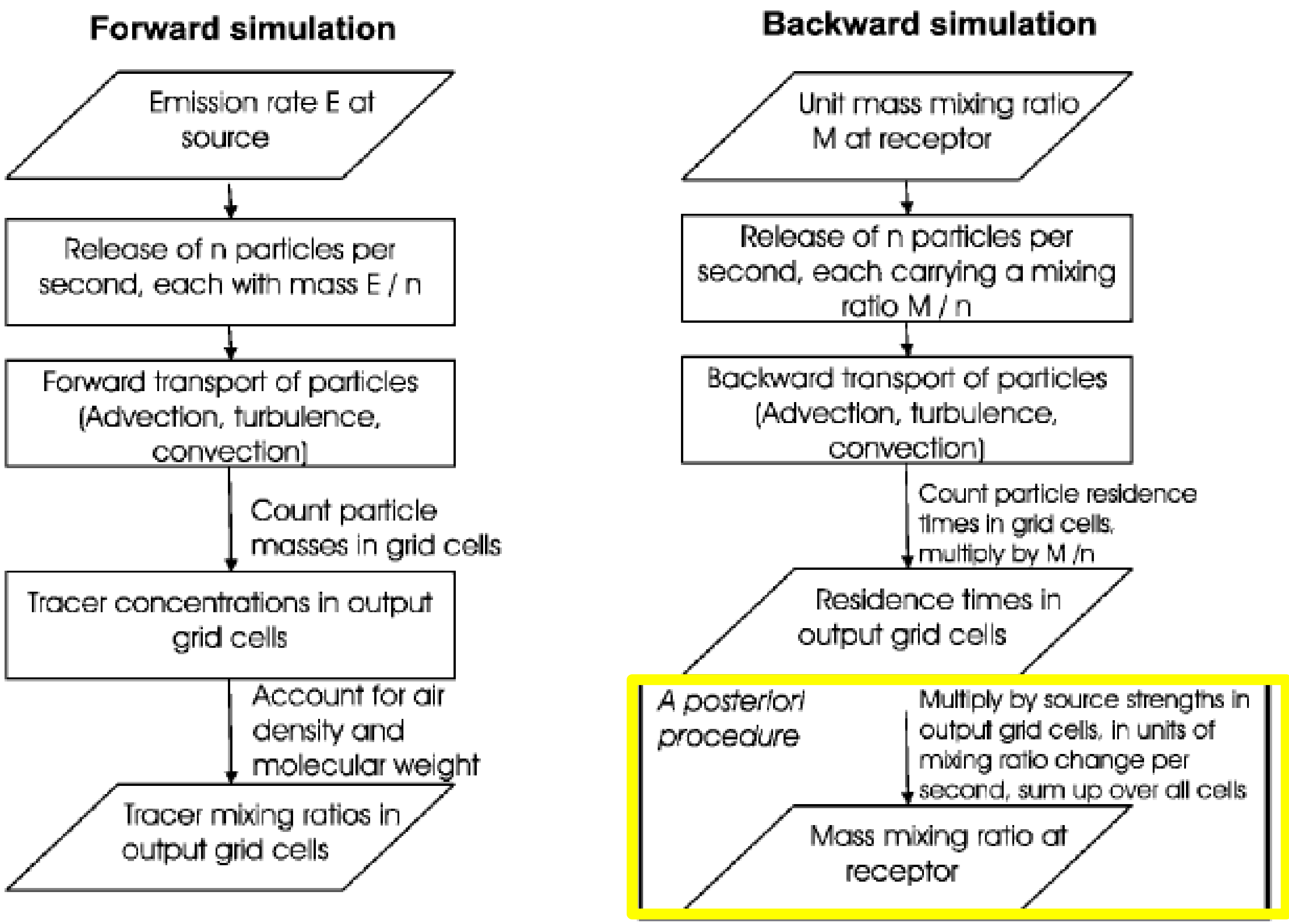


SO ATM / RO ATM



Once the residence times (model sensitivities, source receptor sensitivities) are obtained, additional processing to get estimates

SO ATM / RO ATM - fwd/bwd calculations

- From Lin (“Lagrangian Modeling of the Atmosphere: An Introduction”, 2012), examples of questions that can be addressed by fwd vs bwd Lagrangian simulations:

Forward	**Backward**
Where does the air go?	Where does the air come from?
What is the downwind impact of a source?	What are the upwind influences on the receptor?
Where do tracers get transported?	Where are the source regions of tracers?
How much is the concentration of the tracer at downwind locations affected by a unit emission of the source?	How strong is the sensitivity of the receptor to a particular upwind source region? *** this can be done either fwd or bwd, bwd is more efficient*

SRS definition

Definition – SRS Source Receptor Sensitivity

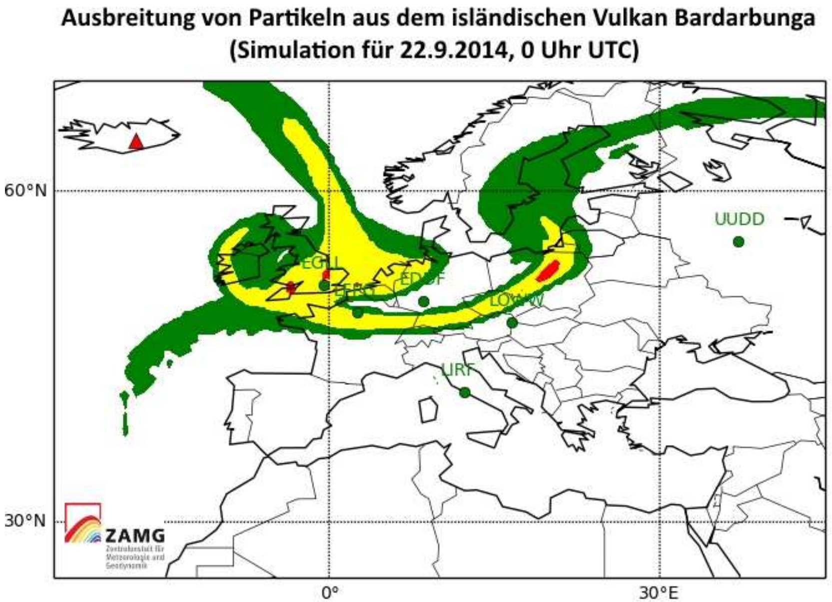
A Source Receptor Sensitivity Field is a 3-dimensional (2 spatial, 1 temporal) array *M* pertaining to one single measurement *k*, providing a multiplication factor [m^{-3}] which translates each element of a source cell at position (*i,j*) and time step *t* (duration: Δt) in a resulting concentration value *c* [kgm^{-3}/Bqm^{-3}]:

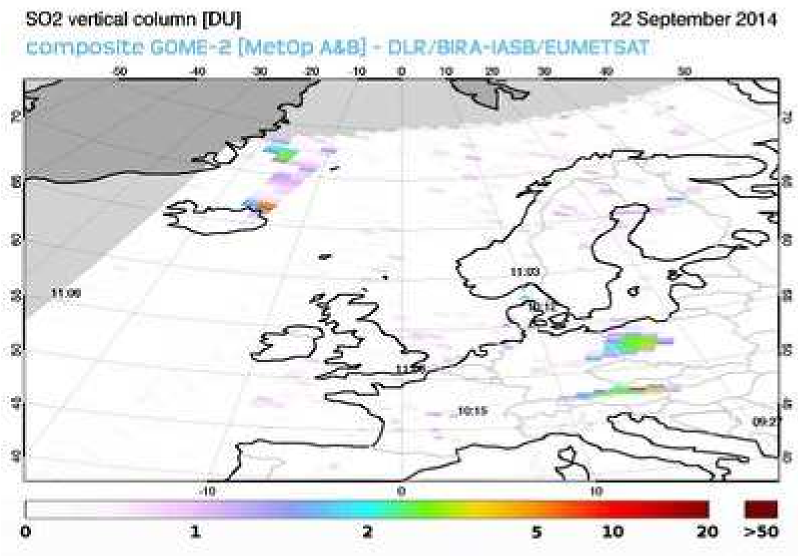
$$c_k = M_{k\,ijt} \cdot S_{ijt}$$

M are the SRS fields or also called model sensitivities or Transfer Coefficient Matrices (TCM) – these are obtained by the atmospheric transport model calculations – either forward or backward (often more efficient)

VAST

- Volcanic Ash Strategic initiative Team (VAST) – vast.nilu.no - The ESA project VAST has been established involving teams from four European countries to improve the quality and use of EO based observations in numerical atmospheric dispersion models for the purpose of assisting global aviation.

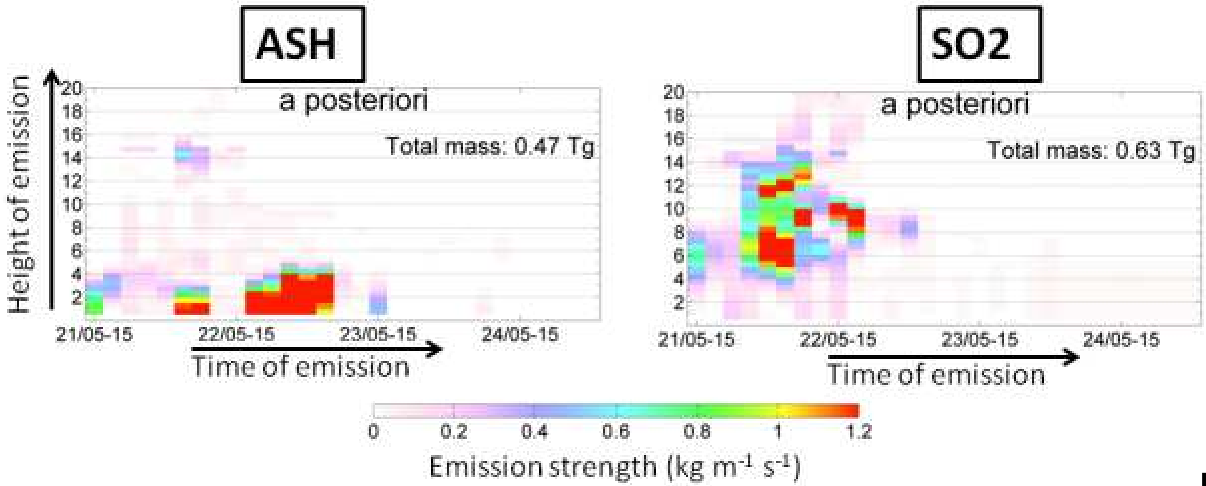




Bardarbunga SO2 emissions – clearly measured in Austria (Sonnblick mountain station) and leading to exceedances of regulatory levels.

Starting point : emission of 1Tg of SO2, in a column, during one day → the source

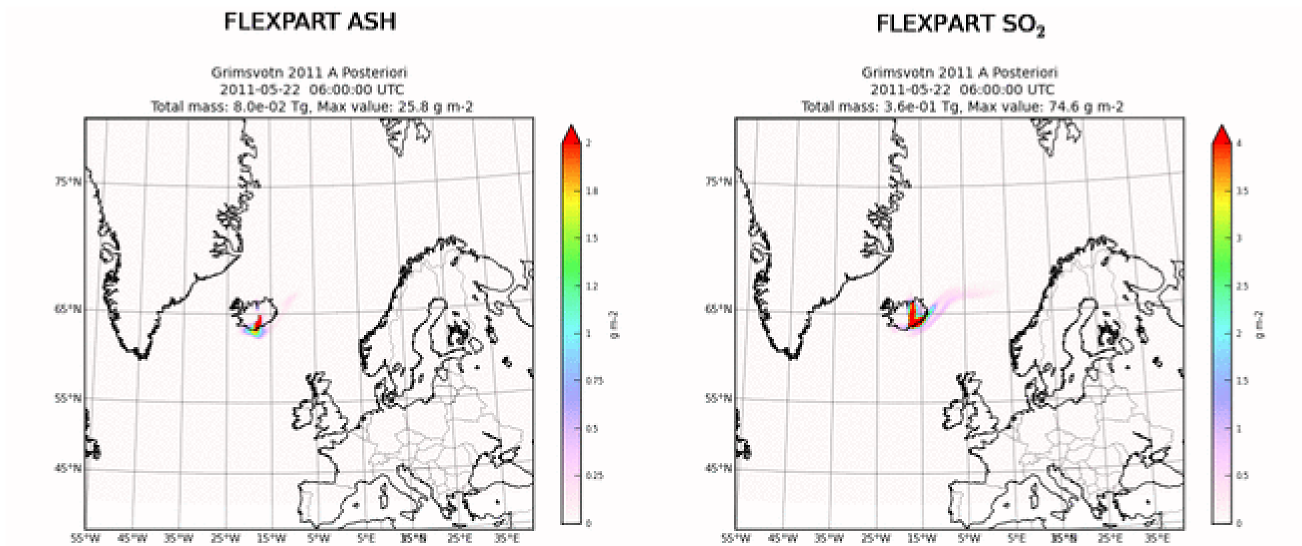
VAST



Source term "forensics":

- Ash /SO2 emission (vertical profile with time)

Forecast with the estimated ST

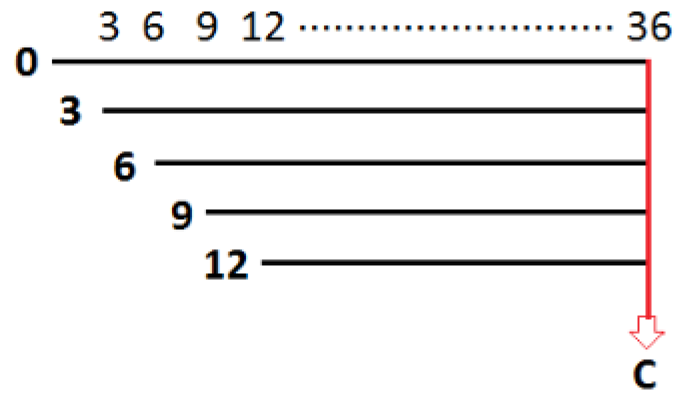


From N. I. Kristiansen, vast.nilu.no

Fukushima

- Releases every 3-h from 11-31 March
- 168 simulations of duration of 72 h
- 601 by 401 grid cells
- 0.05° horizontal resolution (about 5 km)
- 3-h averaged air concentrations
- 3-hour deposition totals
- Output layer: ground to 100 m
- 3 surrogate radionuclides
- gas with no wet or dry scavenging (noble)
- gas with a relatively large dry deposition velocity and wet removal (I-131)
- particle with wet removal and a small dry deposition velocity

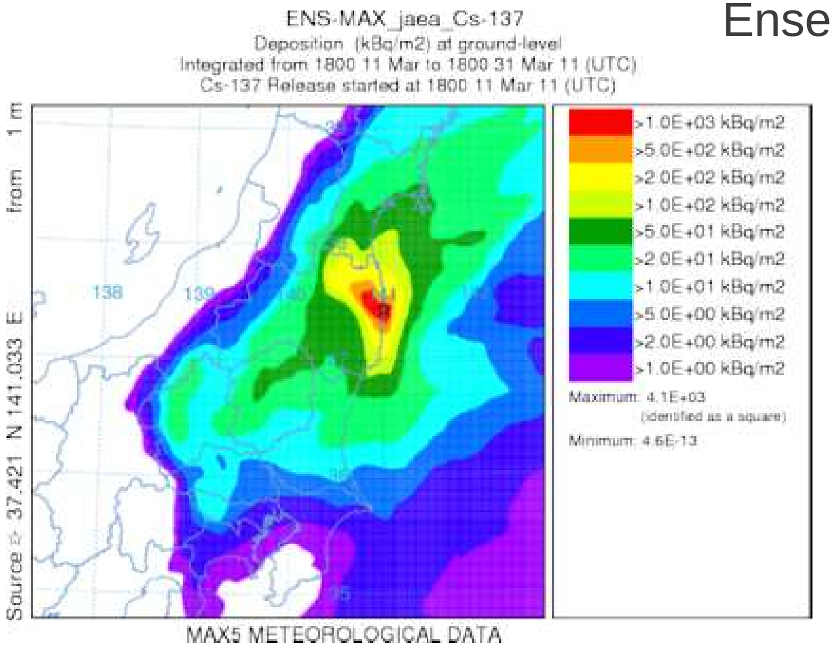
- $C_{j,k,m} = \sum Q_{i,m} D_m TCM_{i,j,k,m}$
- Q is the emission rate for release (i) and species (m)
- D is the species (m) dependent radioactive decay factor
- i represents the number of time varying releases
- j represents the number of sampling periods
- Concentration and deposition are available over k grid points
- with each new release (i), there will be one less output period (j)
- Computations are made with a unit emission
- TCM is computed for each computational species (scavenging dependent)
- The emission (Q) and decay (D) are applied in a post-processing step



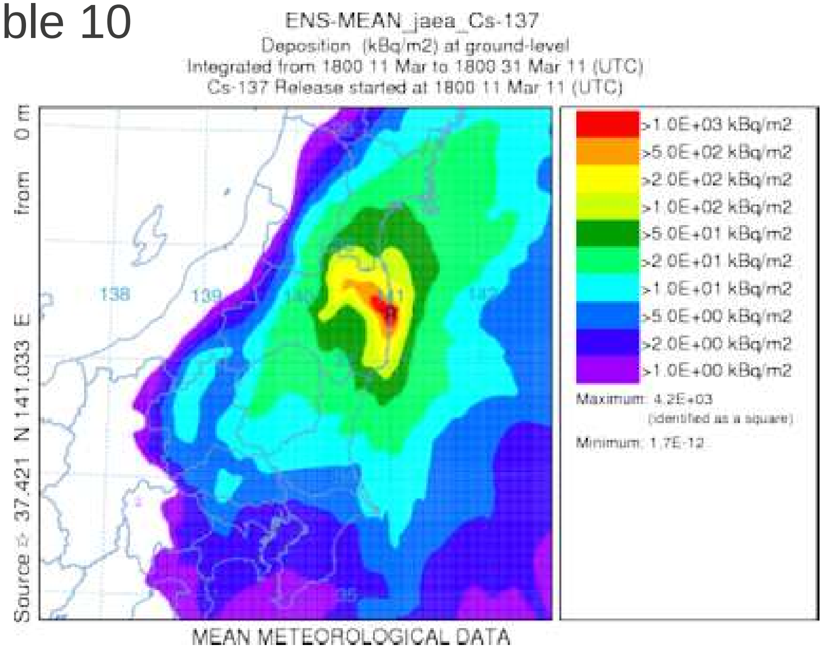
SO ATM - Nuclear applications

- CMC's **MLDP0** - Modèle Lagrangien de Dispersion de Particules d'ordre 0
- NOAA's **HYSPLIT** - the Hybrid Single-Particle Lagrangian Integrated Trajectory
- UKMET's **NAME** - Numerical Atmospheric-dispersion Modelling Environment
- JMA's **RATM** - Regional Atmospheric Transport Model
- ZAMG's **FLEXPART** - Lagrangian Particle Dispersion Model

Ensemble 5



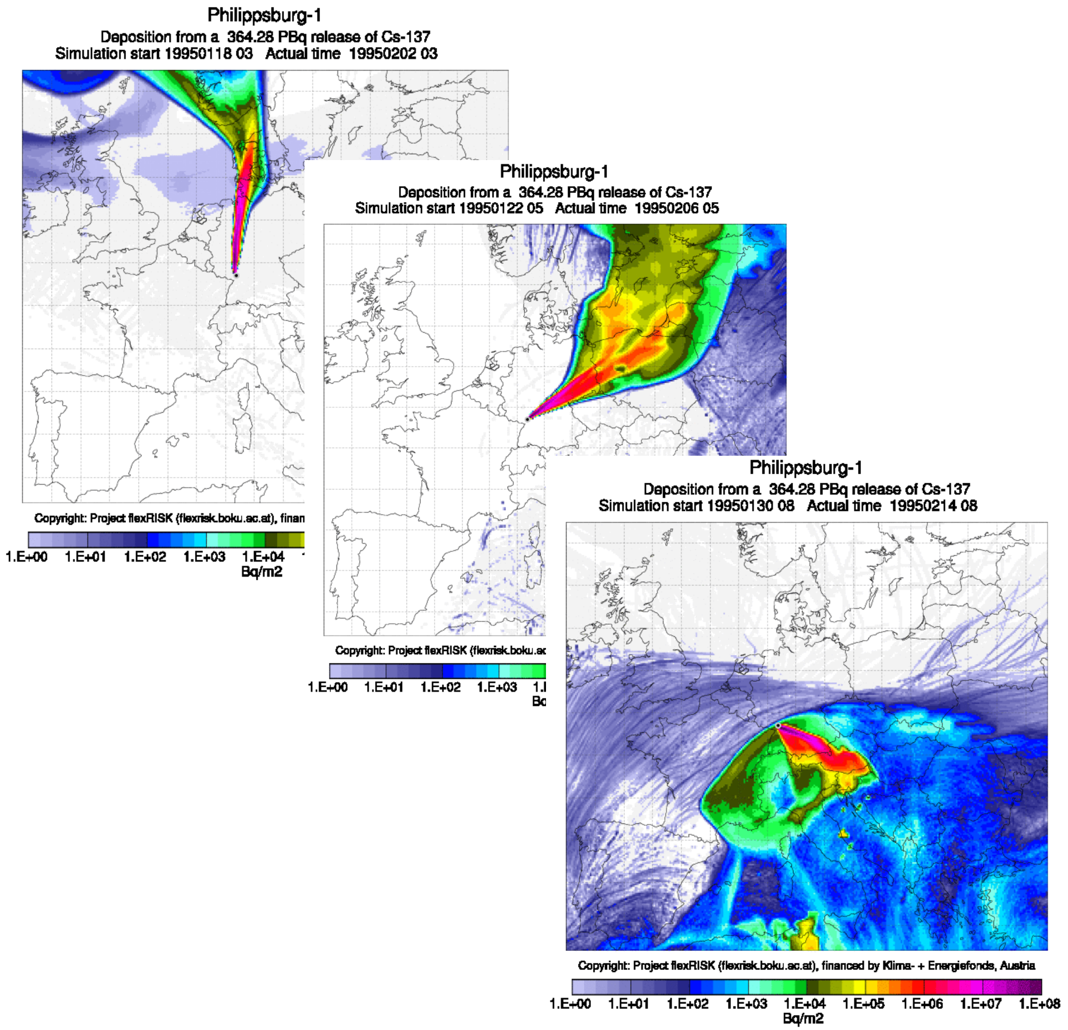
Ensemble 10

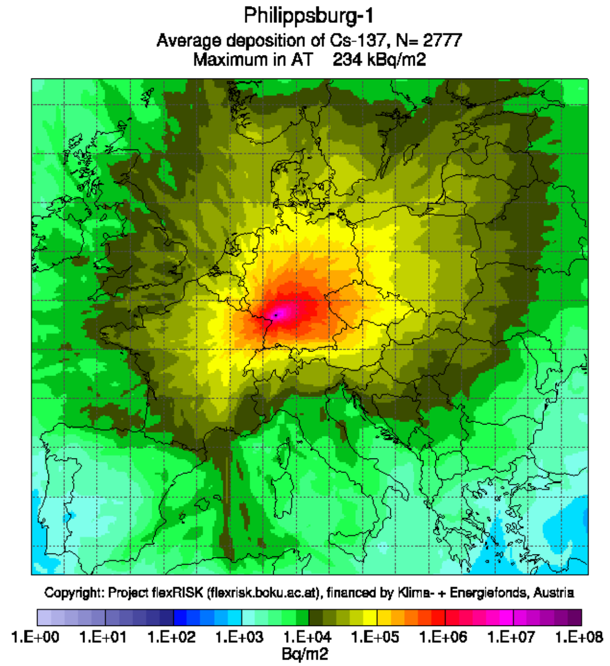


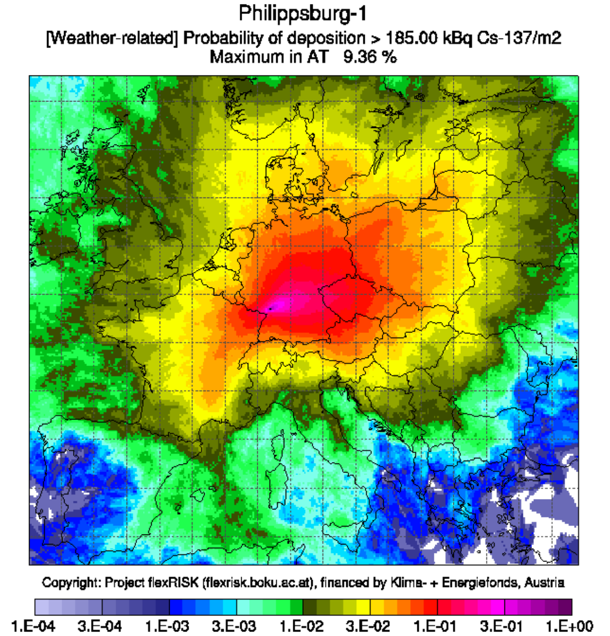
FLEXRISK

- Flexrisk.boku.ac.at - flexible tools for assessment of nuclear risk in Europe
  - Database of European NPP with two information on type, start up and shutdown, safety measures, thermal power and accident and release frequencies. – grouped into similar characteristics
  - Definition of two release scenarios per type but analysis focused on one (plausible but with significant activity released)
  - Fwd ATM calculations (different times of year and day) for all the scenarios the 10-year-period 2000-2009 + 1995– climatological representativeness.
  - For selected radionuclides – calculation of dosimetric endpoints
  - Risk import-export

FLEXRISK - Philippsburg-1





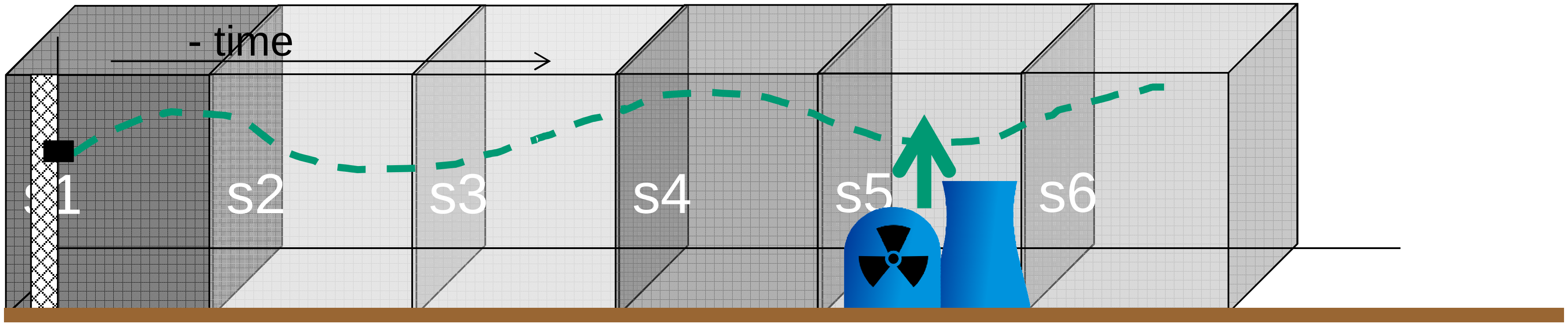


SO ATM - Applications

- Advantages of this approach:
  - *Multiple sources can be used since they are simply multiplied by the source receptor sensitivities*
  - *Additional runs can be easily added without having to redo the already existing ones*
  - *It can be operationally very efficient and fast.*
- Disadvantages of this approach:
  - *Some a priori knowledge of the source is needed:*
    - *Location*
    - *Emission heights (release shape)*
    - *“Species” (aerosol, gas, noble gas)*

RO ATM – ideal example

Relation between measurement and emission? Very simple example: 1 point measurement, 1 D transport, 1 single emission at one single time and place



Measurement: Y (Bq/m^3)

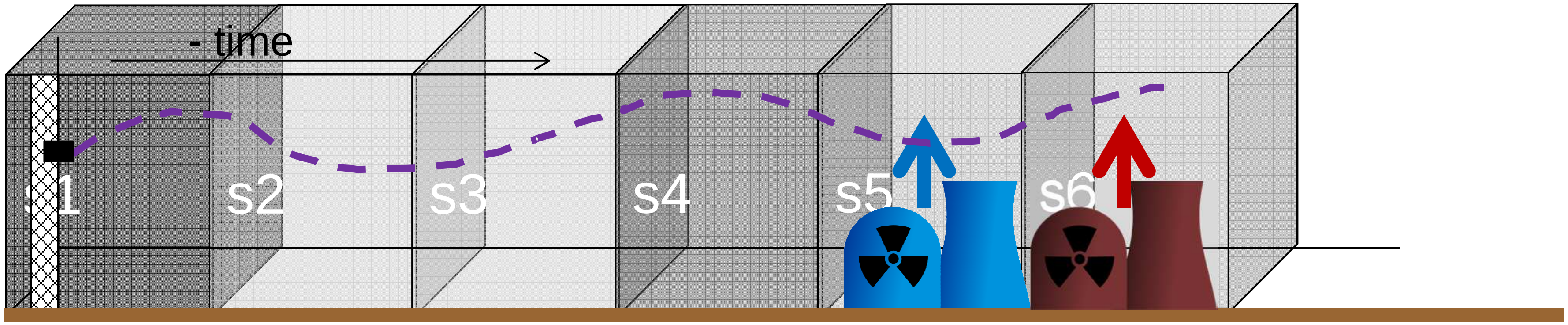
FLEXPART sensitivities: sx (s)

Emission flux: X Bq/m^2 s dilluted in a layer (m) --- (Bq/m^2 sm)

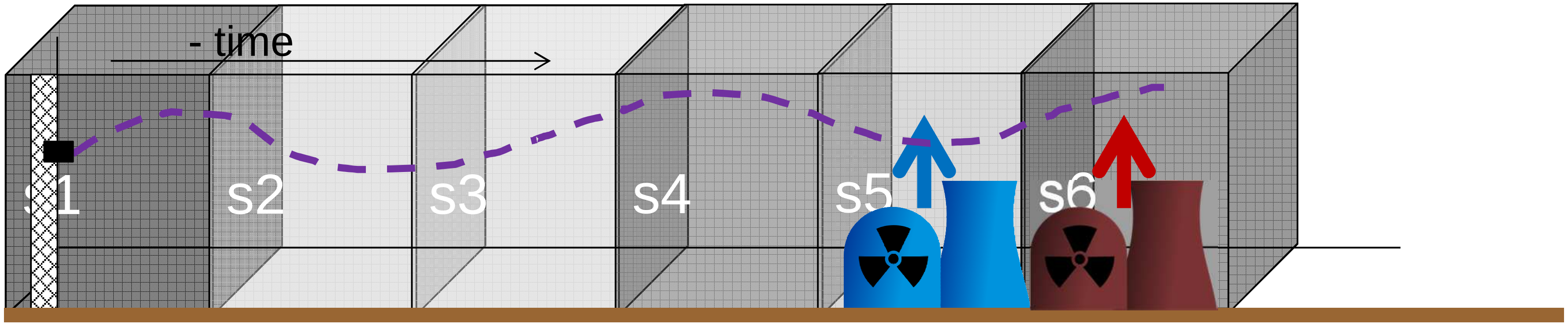
$$Y(t_o) = s1\ X1(t_{e1}) + s2\ X2(t_{e2}) + s3\ X3(t_{e3}) + S4\ X4(t_{e4}) + s5\ X5(t_{e5}) + s6\ X6(t_{e6})$$

In this ideal case, only X5 is non-zero at time t_{e5} → $Y(t_o) = s5\ X5(t_{e5})$ Easy!!

RO ATM – ideal example



Is it the red or the blue emitting or both? $Y(t_o) = s5\ X5(t_{e5}) + s6\ X6(t_{e6})$

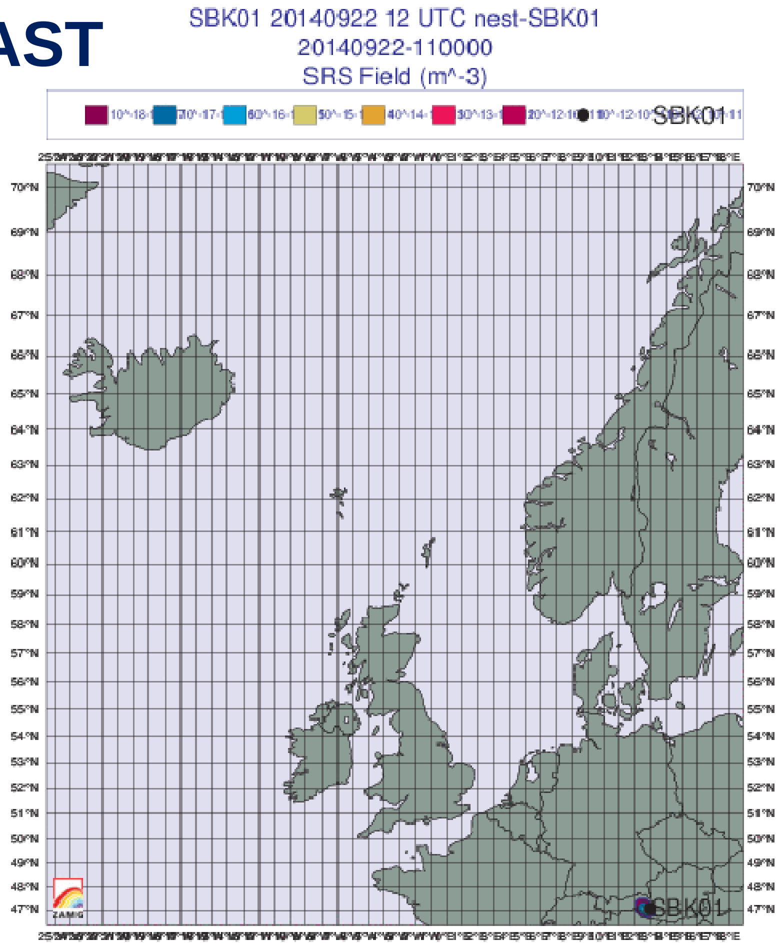


s6 is now much larger than s5. This means that actually even if emission X6 is smaller, it will contribute more to the measurement!

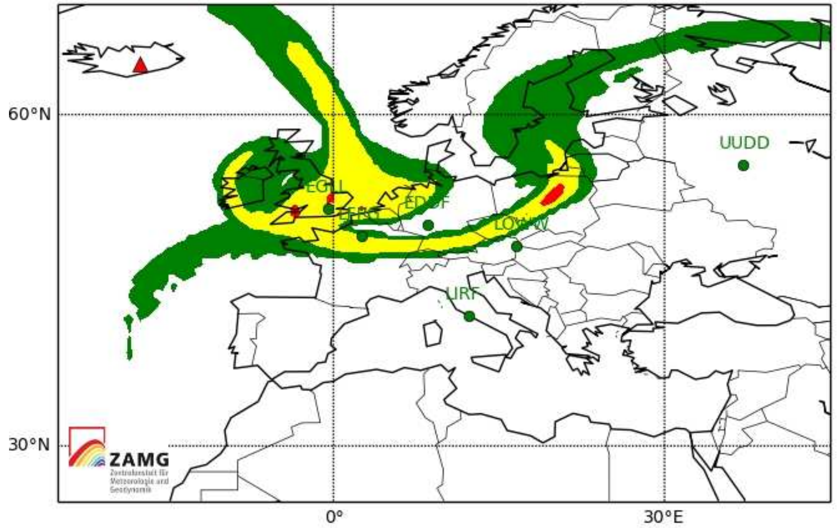
$Y(t_o) = s5\ X5(t_{e5}) + s6\ X6(t_{e6})$

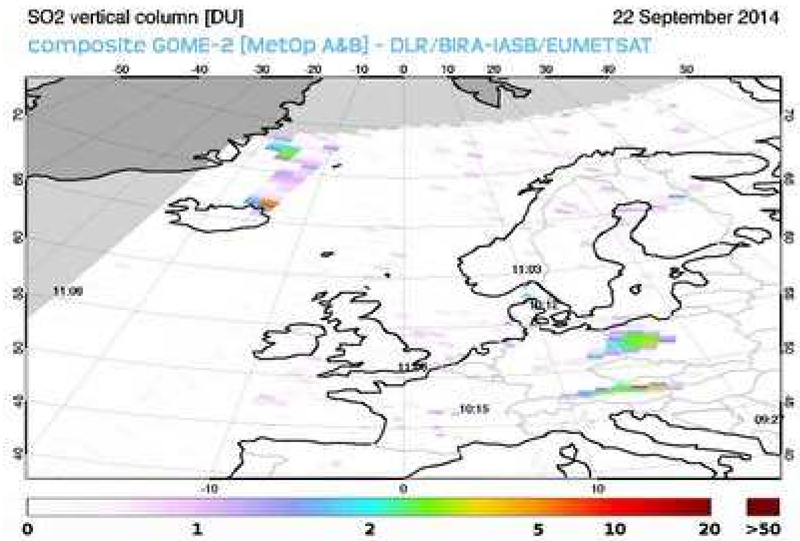
Not so easy

VAST



Ausbreitung von Partikeln aus dem isländischen Vulkan Bardarbunga
(Simulation für 22.9.2014, 0 Uhr UTC)





We do not have longh enough backtracking (therefore limitted SRS). The highest measurement in Sonnblick was of 250 ug/m3 and we assume that the SRS on the emission grid was in the order of 2x10**12 m-3, then we have a first guess of an emission (for that emission time) of 5x10**14 ug in one hour which means about **140 kg/s**. http://en.vedur.is/earthquakes-and-volcanism/articles/nr/2947#sep18 suggests **200 -600 kg/s**

RO ATM – Radon time series

Let's try to understand the concept and application

Land-sea mask (1/0)
x
^{222}Rn inventory ($Bqm^{-2}h^{-1}$)

t_1

0	0	0	1
0	0	1	1
0	1	1	1
1	1	1	1

x

FLEXPART output
SRS (h^{-1})

1,1	1,2	1,3	1,4
2,1	2,2	2,3	2,4
3,1	3,2	3,3	3,4
4,1	4,2	4,3	4,4

$$C_{t1} = 50 \sum_i \sum_j LSM_{ij} \times SRS_{ij}$$

RO ATM – Radon time series

Let's try to understand the concept and application

Land-sea mask (1/0)
x
^{222}Rn inventory (Bqm^{-2}h^{-1})

FLEXPART output
SRS (h^{-1})

t_1

0	0	0	1
0	0	1	1
0	1	1	1
1	1	1	1

x

1,1	1,2	1,3	1,4
2,1	2,2	2,3	2,4
3,1	3,2	3,3	3,4
4,1	4,2	4,3	4,4

$$C_{t1} = 50 \sum_i \sum_j LSM_{ij} \times SRS_{ij}$$

t_2

0	0	0	1
0	0	1	1
0	1	1	1
1	1	1	1

x

1,1	1,2	1,3	1,4
2,1	2,2	2,3	2,4
3,1	3,2	3,3	3,4
4,1	4,2	4,3	4,4

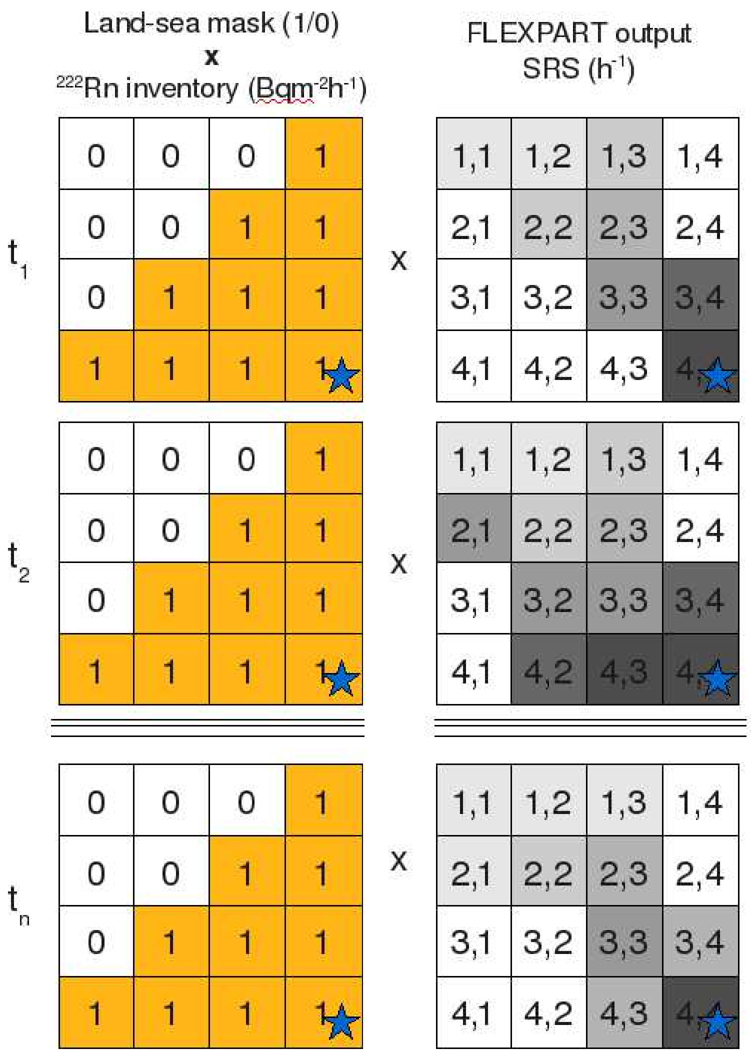
$$C_{t2} = 50 \sum_i \sum_j LSM_{ij} \times SRS_{ij}$$

RO ATM – Radon time series

Let's try to understand the concept and application

	Land-sea mask (1/0) **x** ^{222}Rn inventory (Bqm^{-2}h^{-1})					FLEXPART output SRS (h^{-1})				
t_1	0	0	0	1	x	1,1	1,2	1,3	1,4	$C_{t1} = 50 \sum_i \sum_j LSM_{ij} \times SRS_{ij}$
	0	0	1	1		2,1	2,2	2,3	2,4	
	0	1	1	1		3,1	3,2	3,3	3,4	
	1	1	1	1★		4,1	4,2	4,3	4,★	
t_2	0	0	0	1	x	1,1	1,2	1,3	1,4	$C_{t2} = 50 \sum_i \sum_j LSM_{ij} \times SRS_{ij}$
	0	0	1	1		2,1	2,2	2,3	2,4	
	0	1	1	1		3,1	3,2	3,3	3,4	
	1	1	1	1★		4,1	4,2	4,3	4,★	
t_n	0	0	0	1	x	1,1	1,2	1,3	1,4	$C_{tn} = 50 \sum_i \sum_j LSM_{ij} \times SRS_{ij}$
	0	0	1	1		2,1	2,2	2,3	2,4	
	0	1	1	1		3,1	3,2	3,3	3,4	
	1	1	1	1★		4,1	4,2	4,3	4,★	

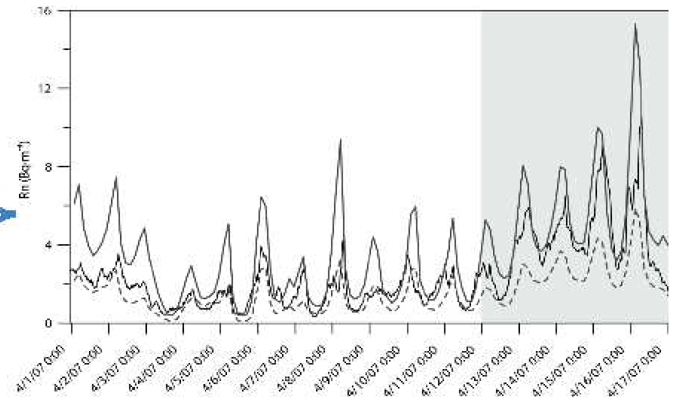
Let's try to understand the concept and application



$$C_{t1} = 50 \sum_i \sum_j LSM_{ij} \times SRS_{ij}$$

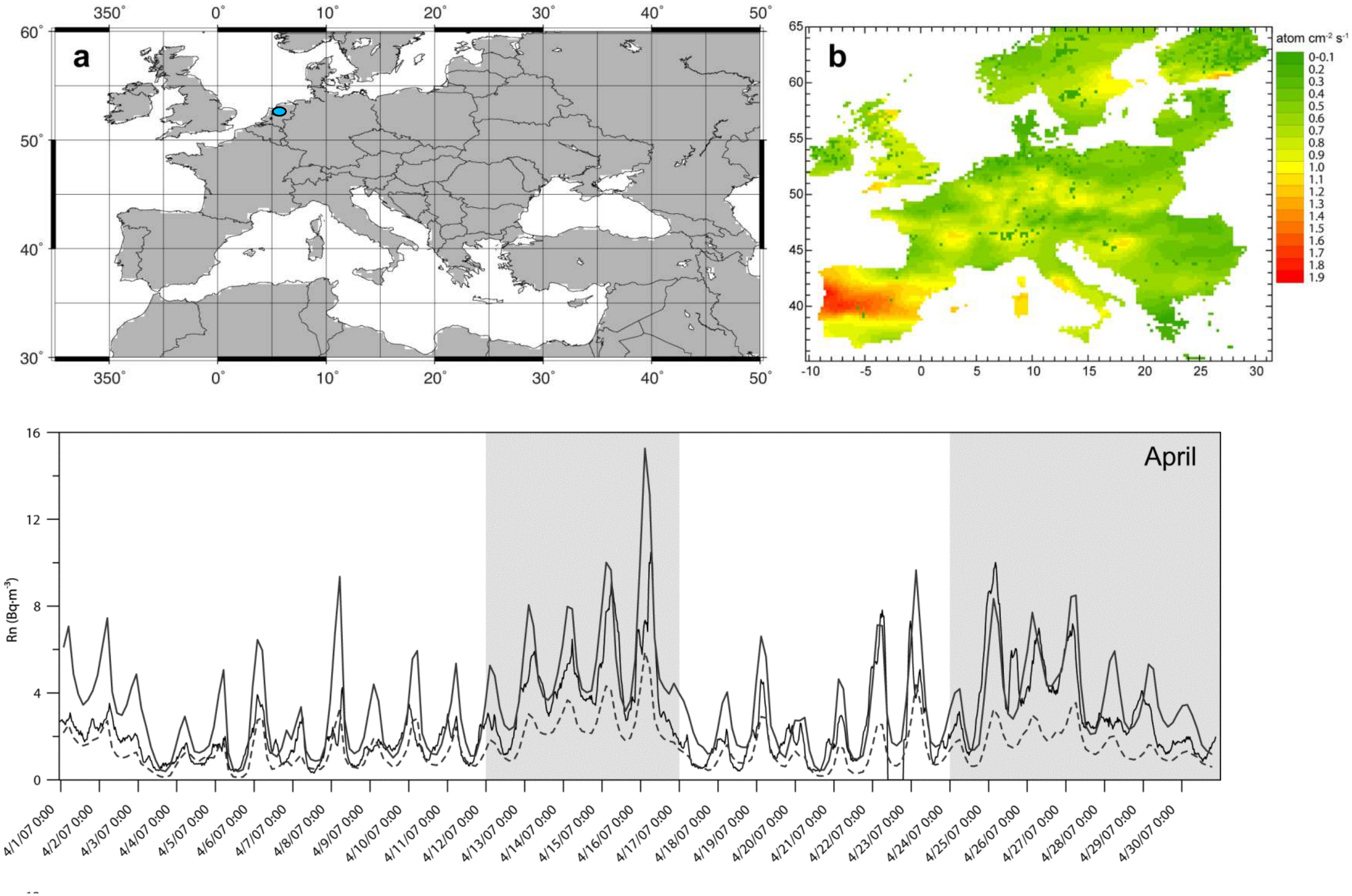
$$C_{t2} = 50 \sum_i \sum_j LSM_{ij} \times SRS_{ij}$$

$$C_{tn} = 50 \sum_i \sum_j LSM_{ij} \times SRS_{ij}$$



RO ATM – Radon time series

Example to reproduce the measurements of Rn in Cabaw (Arnold et al. 2009 Atm. Env.)



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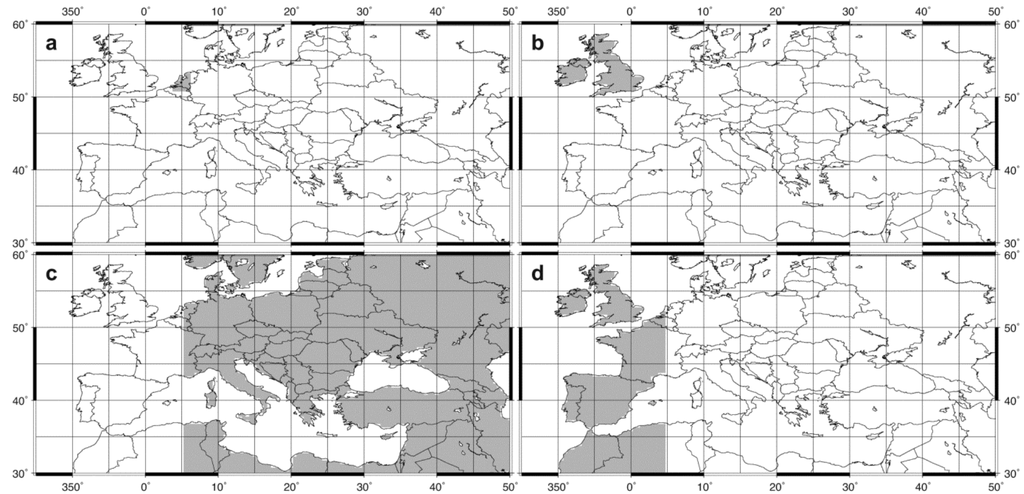
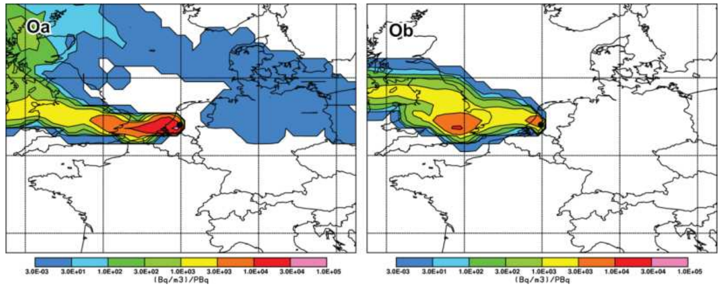
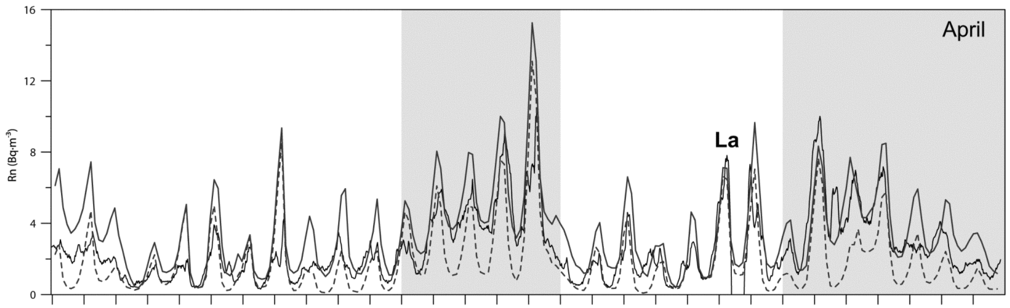
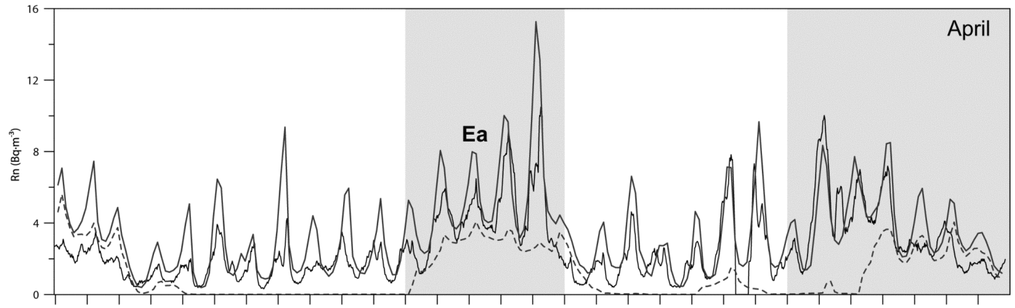
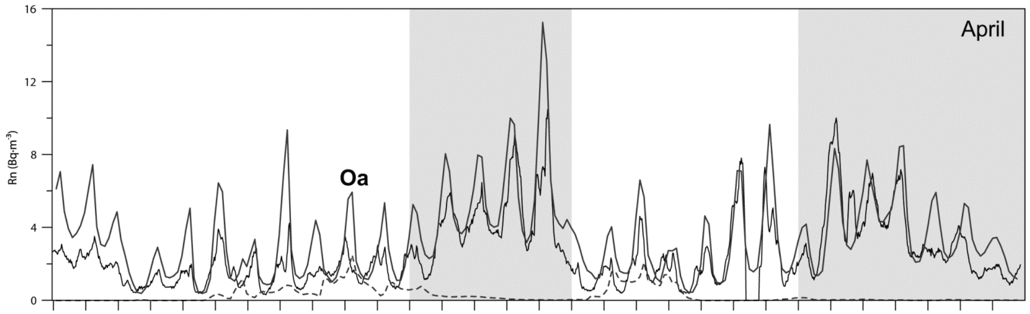


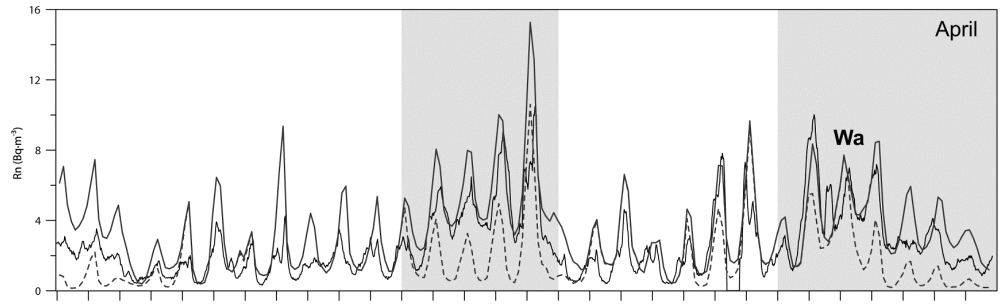
X











CTBTO – where/when nuclear test?

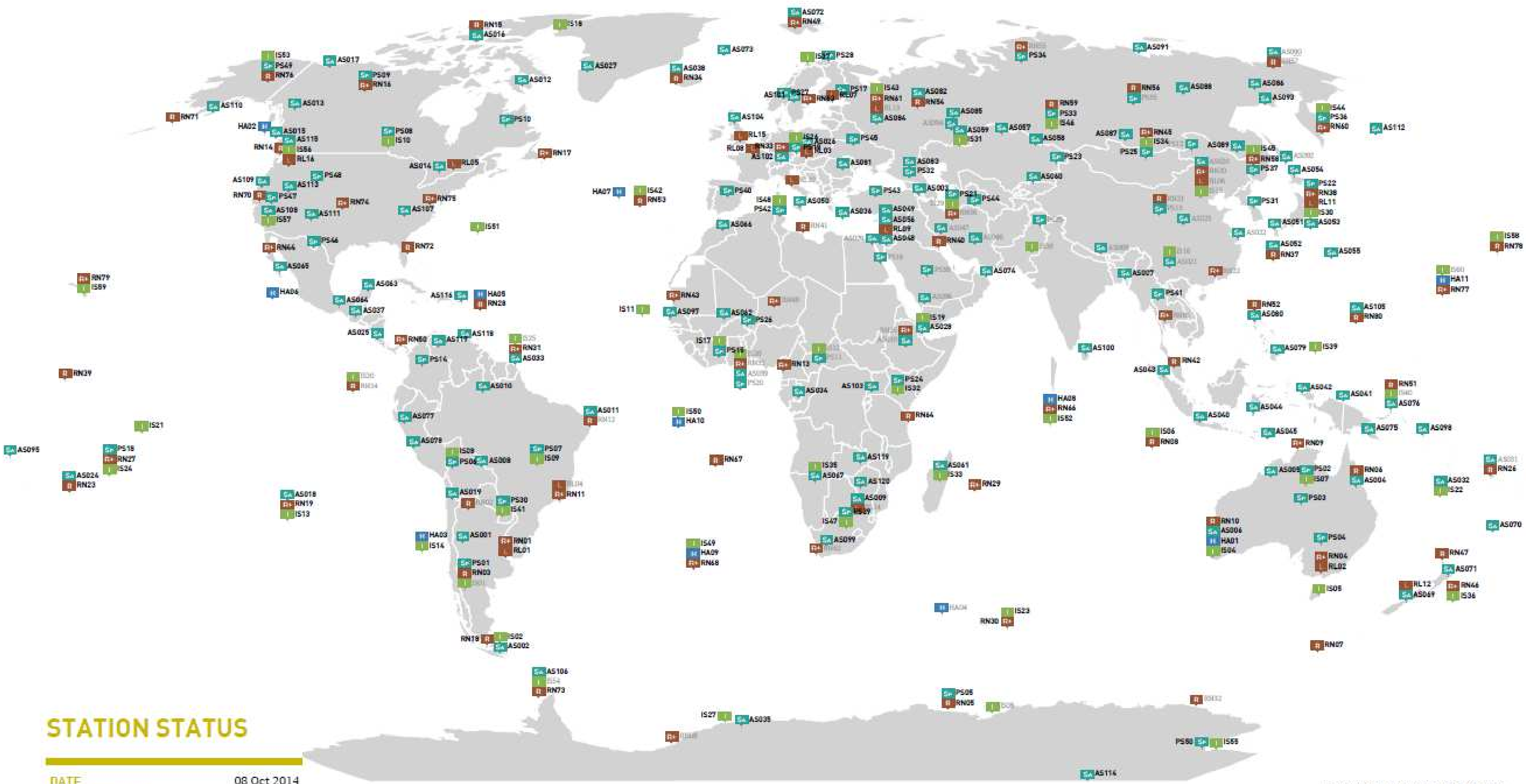
FLEXPART

INTERNATIONAL MONITORING SYSTEM

GLOBAL OVERVIEW - CERTIFIED STATIONS AND NON-CERTIFIED STATIONS

08 OCTOBER 2014

preparatory commission for the comprehensive nuclear-test-ban treaty organization



STATION STATUS

DATE	08 Oct 2014
TOTAL STATIONS	337
PLANNING	19
UNDER CONSTRUCTION	19
INSTALLED	21
CERTIFIED	278

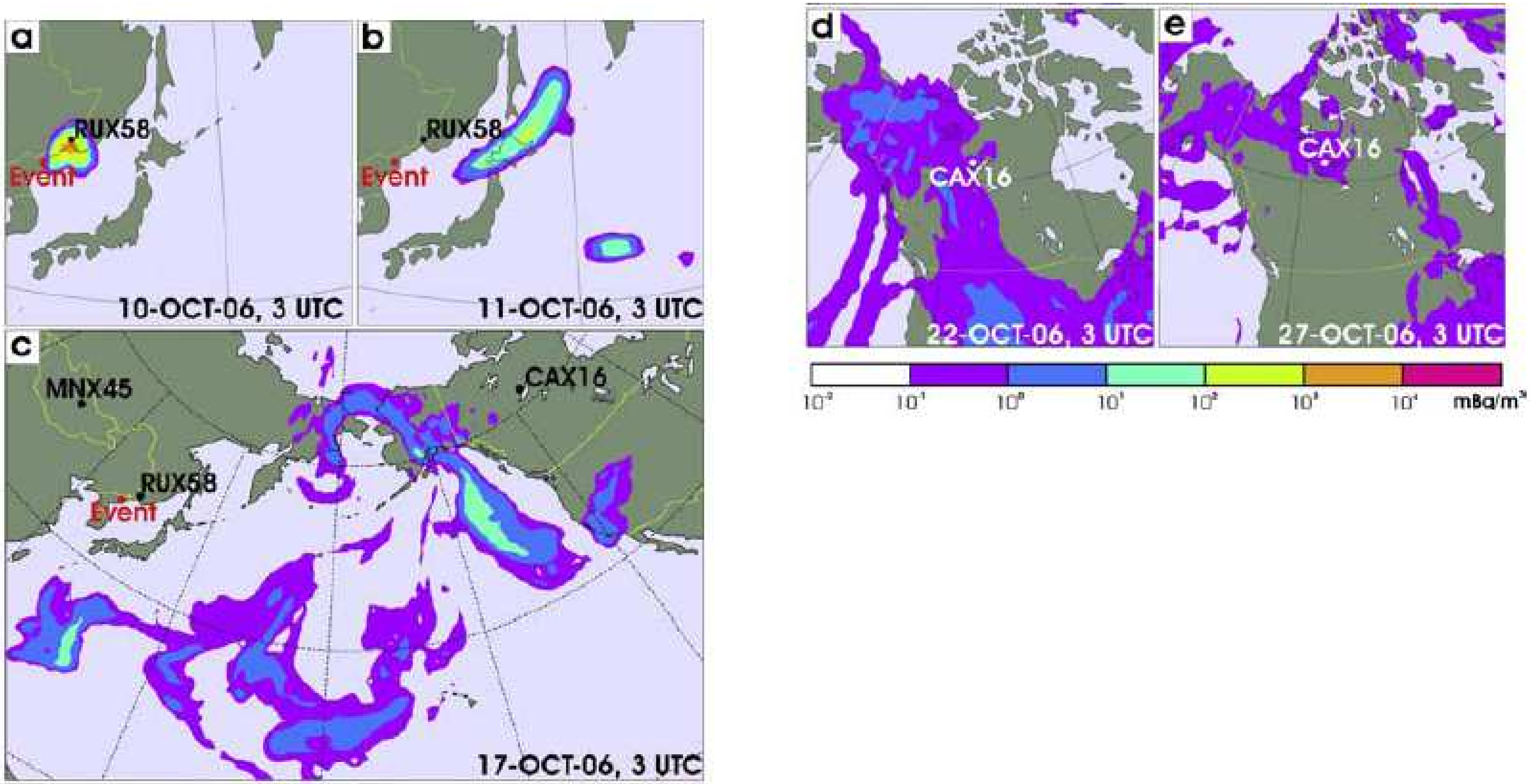
PS Primary Seismic · AS Auxiliary Seismic · I Infrasound · H Hydroacoustic · R Radionuclide · R+ Radionuclide w/ Noble Gas · L Radionuclide Lab

The boundaries and presentation of material on this map does not imply the expression of any opinion on the part of the Provisional Technical Secretariat concerning the legal status of any country, territory, city or area or its authorities, or concerning the delimitation of its frontiers or boundaries.

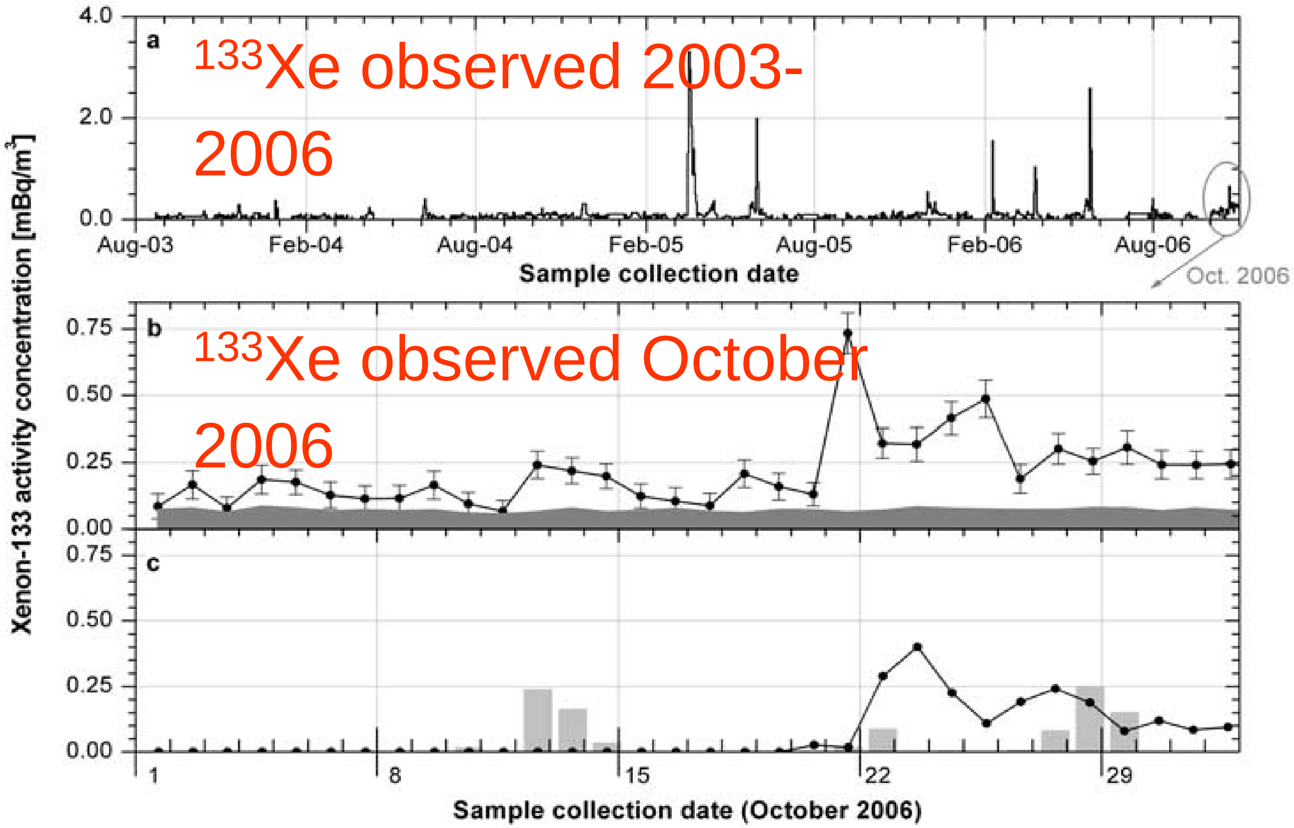
WWW.CTBTO.ORG

DPKR 2006

Calculations showed that radionuclides released **immediately** after the test would spread across Pacific towards the south and east, eventually reaching North America

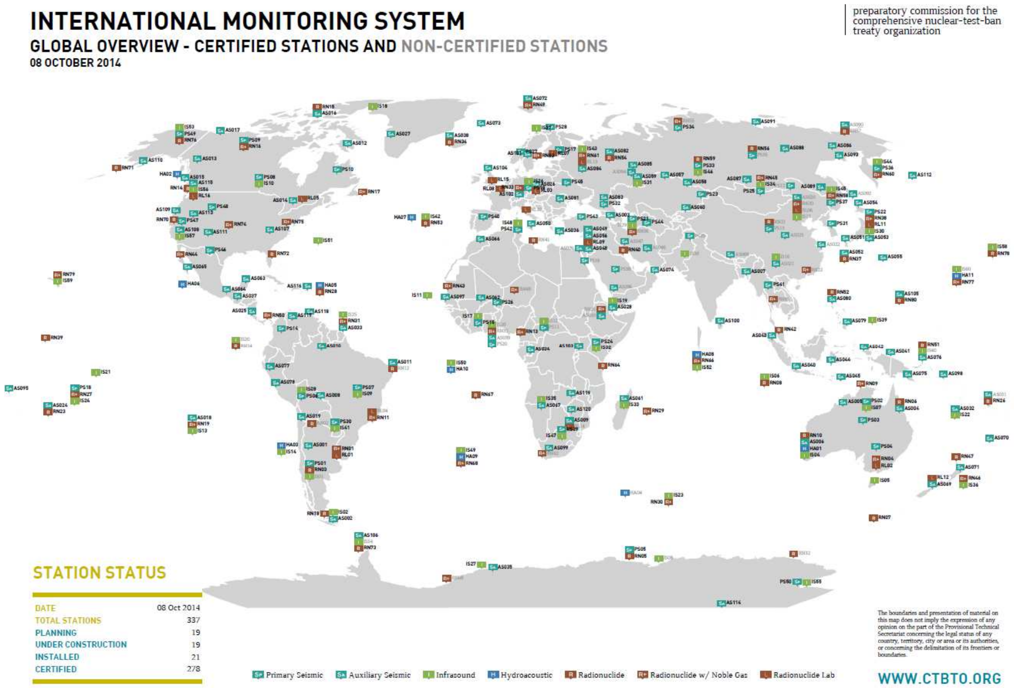


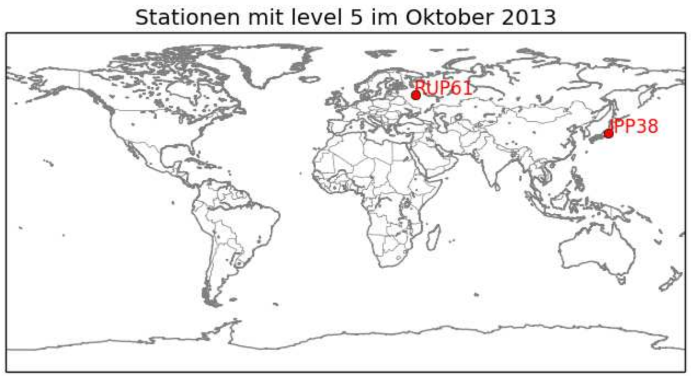
The FLEXPART simulation shows that ^{133}Xe detected in Yellowknife between 22 and 27 October 2006 may have originated from the DPRK event location



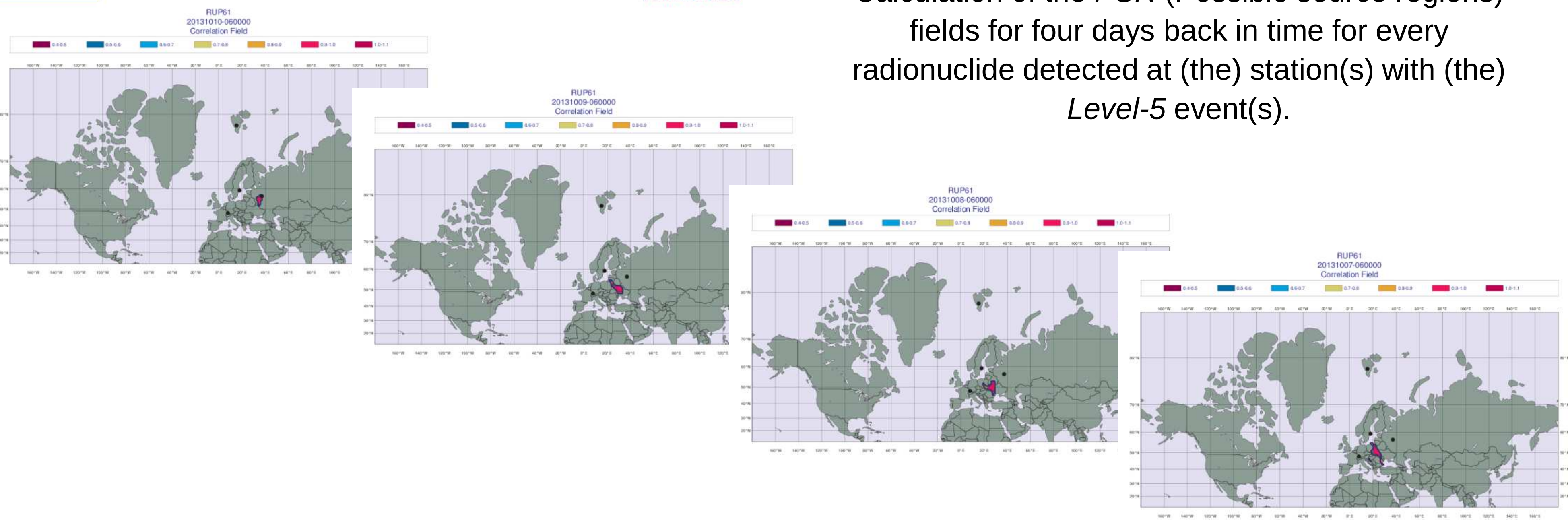
^{133}Xe predicted October 2006 (instantaneous release at REB location (boxes: Chalk River influence)

ZAMG – NDC



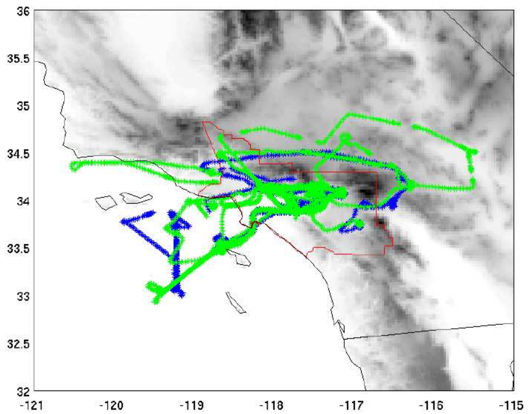


Calculation of the *PSR* (Possible source regions) fields for four days back in time for every radionuclide detected at (the) station(s) with (the) *Level-5* event(s).



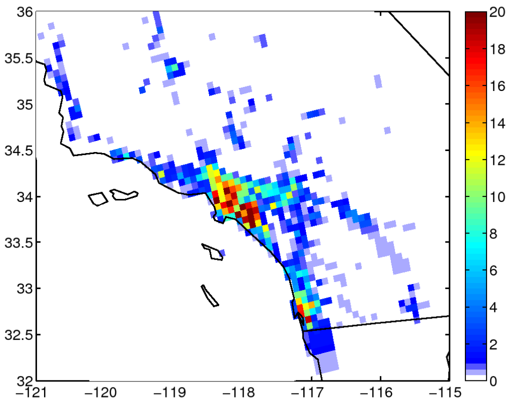
Emission inventories via inversion

Example of backtracking airplane measurements to obtain the model sensitivities for an inversion of surface fluxes of CO, NOx and CO2 (Brioude et al. 2013) courtesy of Jerome Brioude

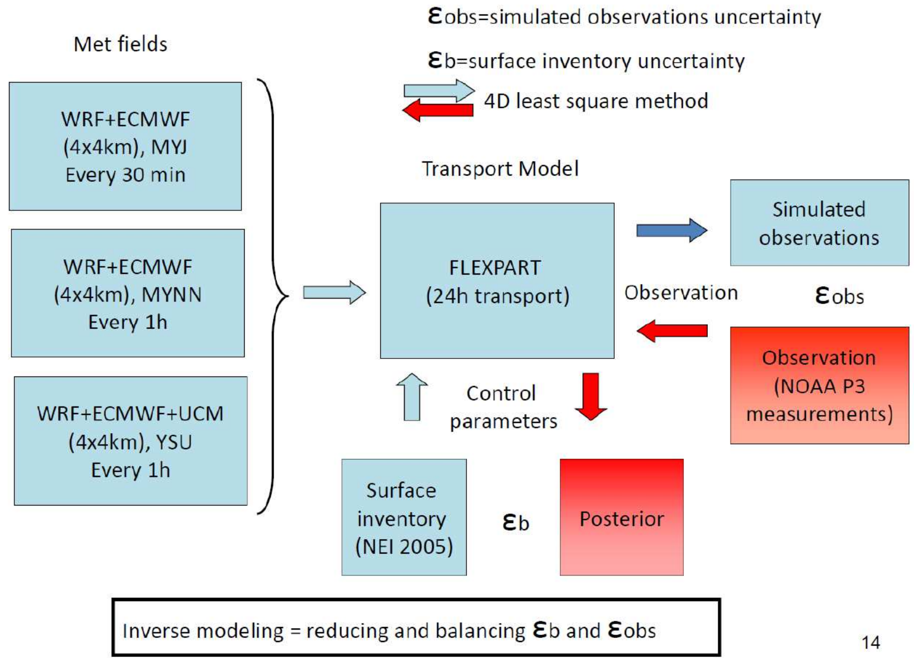


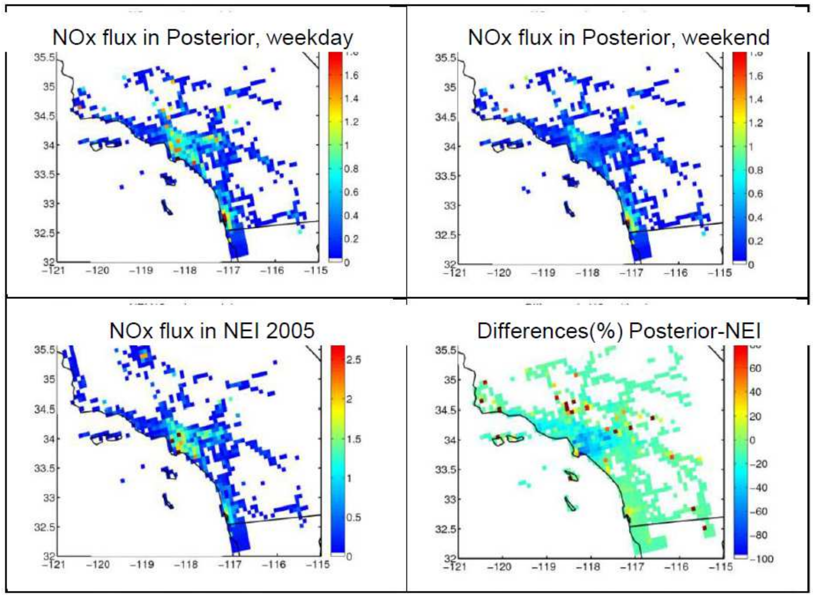
6 flights during CALNEX 2010 used to evaluate LA basin anthropogenic emissions

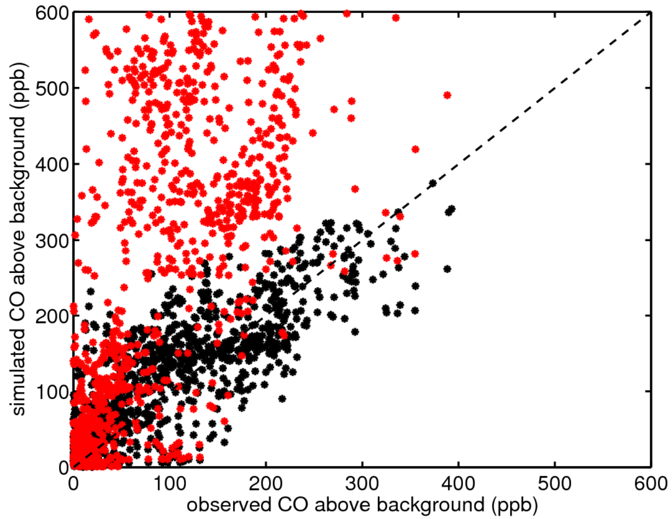
3 flights during weekdays, 3 flights during weekends



flux in NEI 2005







- Using NEI

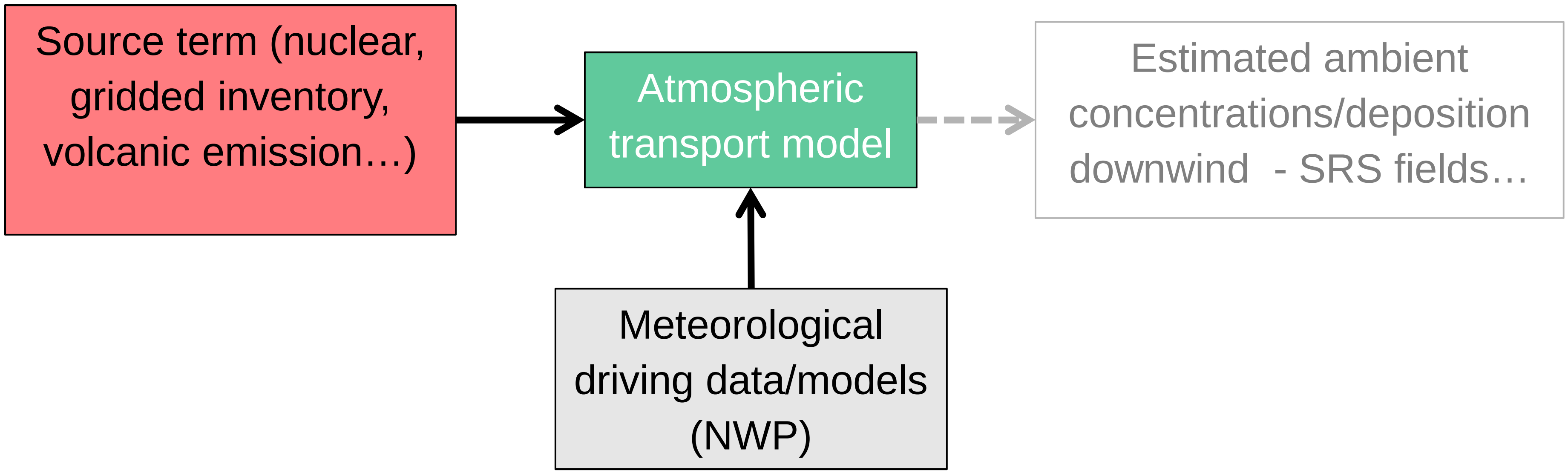
- Using Posterior

Remarks

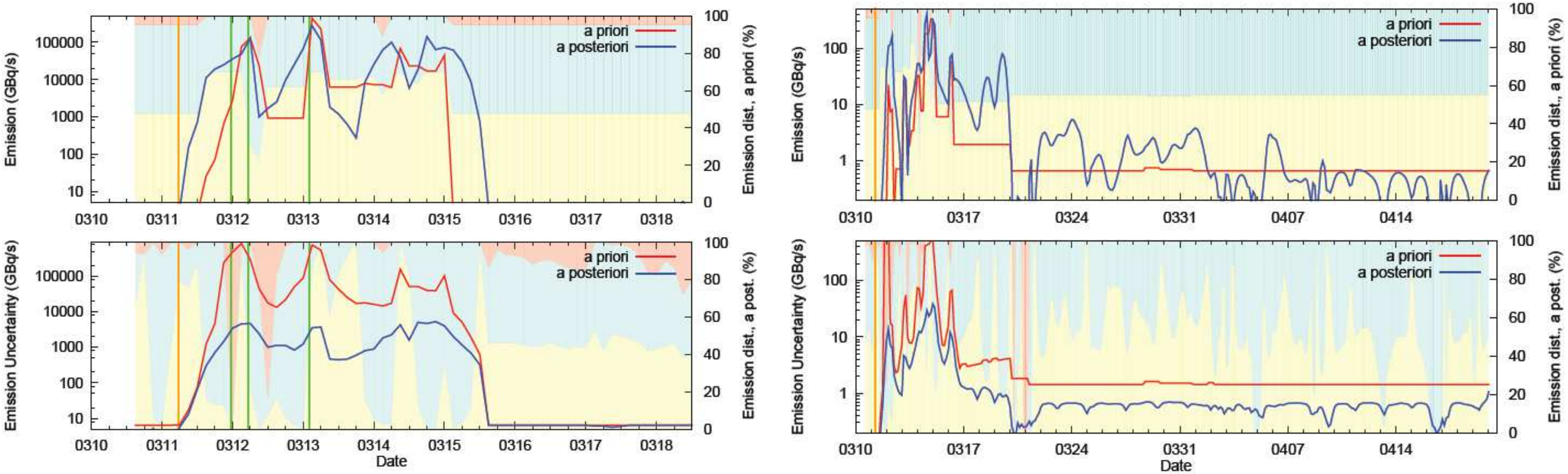
- Backtracking is very useful and computationally very efficient (consider doing fwd runs from all the potential source locations, strengths and times to understand ONE single measurement at one time!). Usually constrains in the information are needed to narrow down possibilities, for example point emission, time of emission, a priori estimate of the emission, data fusion with independent data sources (i.e., seismic, infrasound…)

Model uncertainties

- Let’s have a look at some of the uncertainties involved in the modelling procedure:



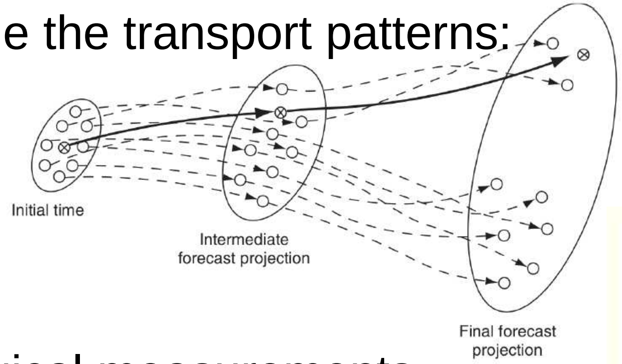
- Source term:
  - Nuclear accident: known location, uncertain emission time, strength, release shape and radionuclide mixture.



  - Volcanic emissions: known location, known (under some circumstances) emission time, uncertain emission height, strength, time evolution, ash particle size distribution (volcano dependent).
  - Anthropogenic emission inventories (bottom-up, top down) relying on relatively sparse measurements (errors on the observations), on state members information, …

Model uncertainties

- Meteorological driving data (analysis or forecasts) – errors in wind fields are the most important since they largely define the transport patterns:
  - Forecast errors
  - For analyses:
    - Inaccuracy of meteorological measurements
    - limited data coverage in some regions of the globe
    - analysis schemes
  - Precipitation errors due to parameterizations involved, often lack of analysis of precipitation and also due to the often sub-grid variability of the precipitation



Wilks (2006)

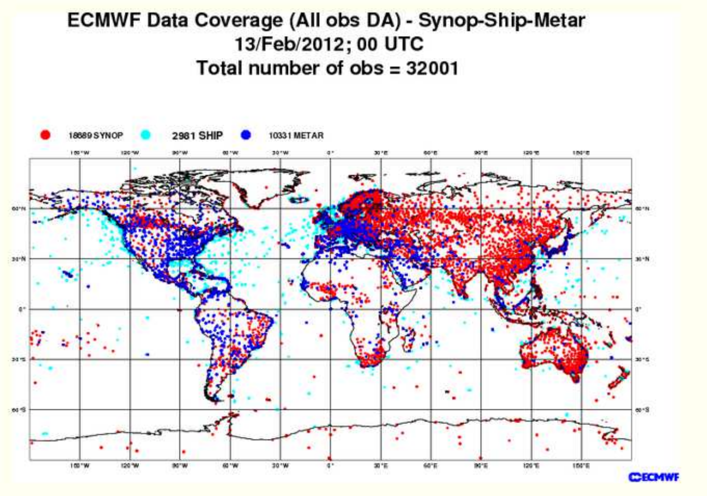


Figure 11: Data coverage of observations used for soil initial conditions on 13 February 2012.

http://old.ecmwf.int/products/changes/ifs_cycle_38r1/soil_reanalysis_impact.html

Model uncertainties

- Dispersion models:
  - Parameterization errors:
    - **Vertical** and horizontal turbulent mixing. Parameterisations are based on analytical relationships often derived in idealised conditions (for example: relatively flat and homogeneous terrain)
    - Dry / **Wet** deposition. Specially convection, which is subgrid in the horizontal and grid-scale in the vertical and which strongly affects the distribution of particles (for LPDM) in vertical but also horizontal due to the updraft-downdrafts systems
  - Numerical errors:
    - Eulerian models – discretization of the equations and specially important the advection schemes (numerical diffusion and phase errors), narrow plumes purely represented
    - Puff models – very stretched puffs in non-homogeneous conditions
    - Lagrangian particle dispersion models – errors associated to particle number, low statistics and discretisation
    - Interpolation errors – all models require interpolation of the fields to either the computational grid/integration time step or the output grid/integration-output time step.

Model uncertainties

- How to asses and quantify these uncertainties?
  - Model intercomparisons
    - **Who is rigth?**
  - Controlled experiments (CAPTEX, ETEX, …):
    - Limited meteorological situations
    - Limited species (tracers, non deposition…)
    - Data often collected only at surface stations (limited vertical information)
  - Tracers of opportunity (Fukushima, Algeciras, Chernobyl, ANSTO, Eyja, …):
    - Limited knowledge of the source term and therefore an additional important source of uncertainty unknown
  - Error propagation /error incorporation along all the processes – not straight forward since each independent uncertainty is already difficult to identify and quantify and because ATM alone have already quite important algorithms.

It is good to identify/understand (pdf?) the main sources of uncertainty, characteristics of the errors and focus on them

Model intercomparisons

Model intercomparisons are very useful (depending on set-up: same source? Same driving data? …) BUT the question of “who is right?” will always appear unless good and independent observational data is available

- Call for model intercomparison after the Fukushima Dai-ichi modelling studies:

Atmospheric removal times of the aerosol-bound radionuclides ^{137}Cs and ^{131}I during the months after the Fukushima Dai-ichi nuclear power plant accident – a constraint for air quality and climate models

N. I. Kristiansen, A. Stohl, and G. Wotawa

Review Status

This discussion paper has been under review for the journal Atmospheric Chemistry and Physics (ACP). Please refer to the corresponding final paper in ACP.

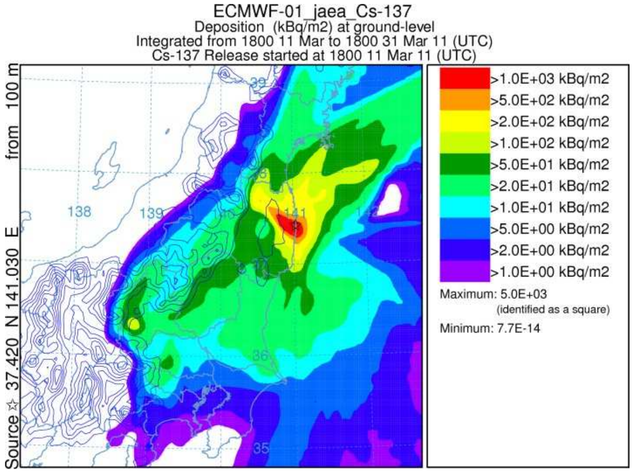
Interactive Discussion **Status: Clos**

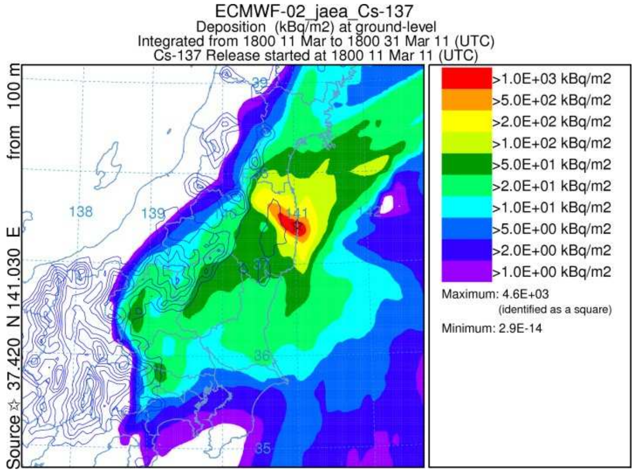
AC: Author Comment | **RC**: Referee Comment | **SC**: Short Comment | **EC**: Editor Comment

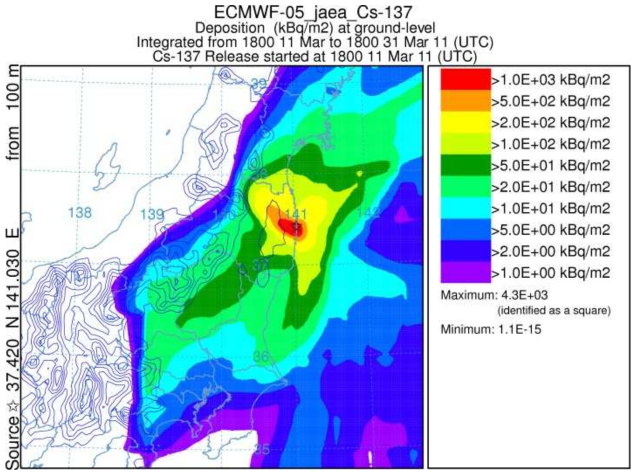
- Printer-friendly Version - Supplement

SC C2516: 'Encouragement for modelers: Follow-up study on comparisons of modeled and observed aerosol lifetimes', Nina Iren Kristiansen, 14 May 2012

- ZAMG Fukushima TT work (see G. Wotawa‘s presentation) – variation of resolution of input data with the same JAEA source term:

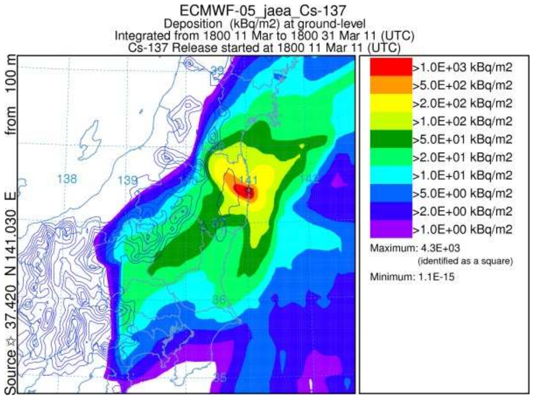


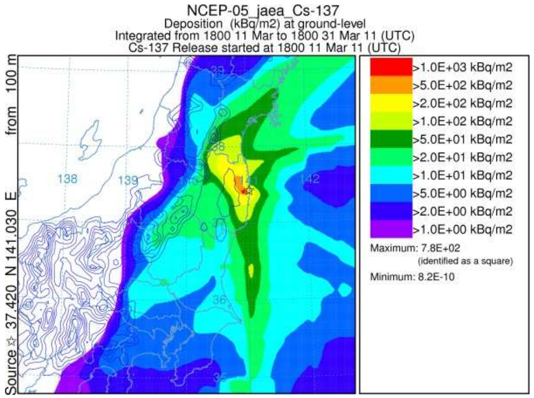




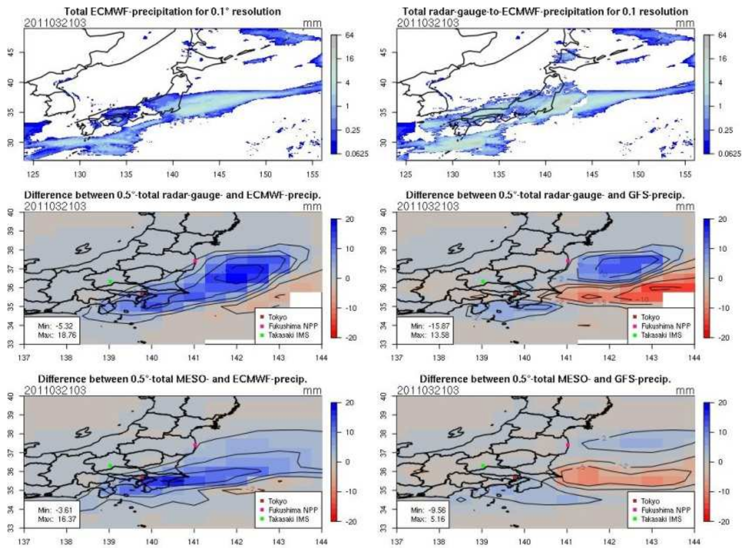
Model intercomparisons

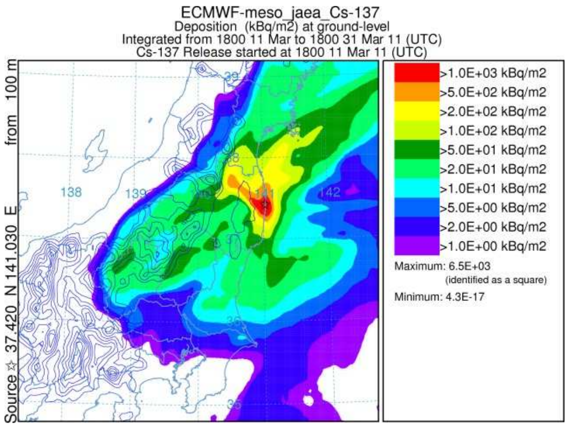
- ZAMG Fukushima TT work (see G. Wotawa‘s presentation) – variation of type of input data (ECMWF – NCEP) with the same JAEA source term

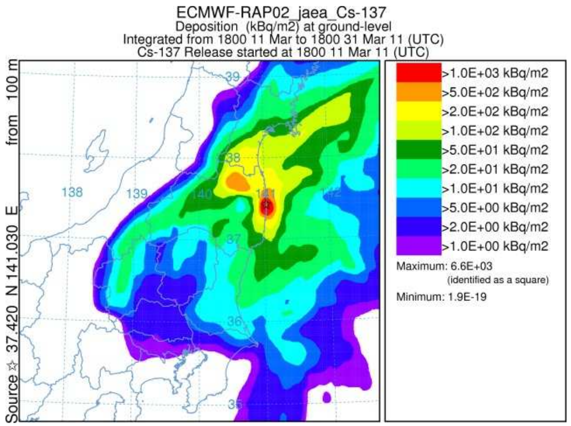




- ZAMG Fukushima TT work (see G. Wotawa‘s presentation) – influence of mesoscale precipitation information – only 0.2 deg resolution shown (NWP, mesoscale models, radar rain gauge information)

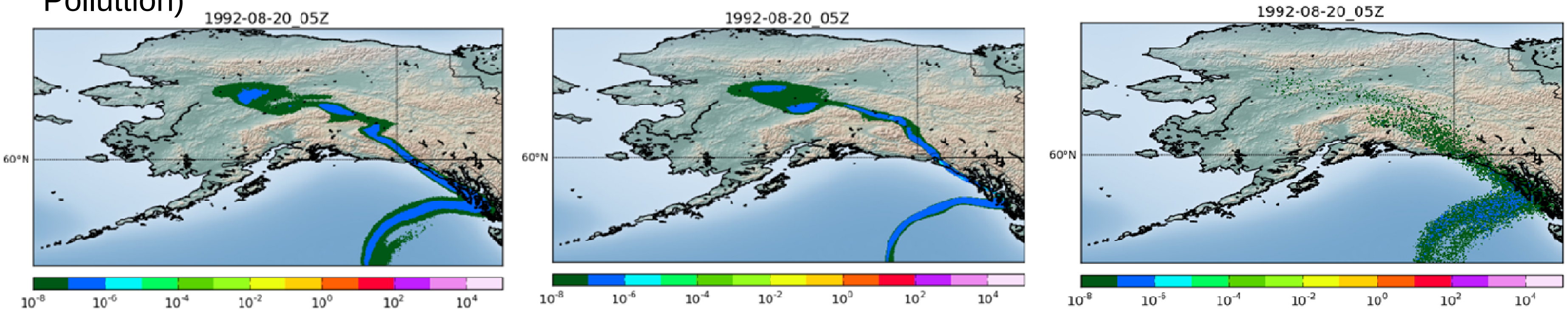




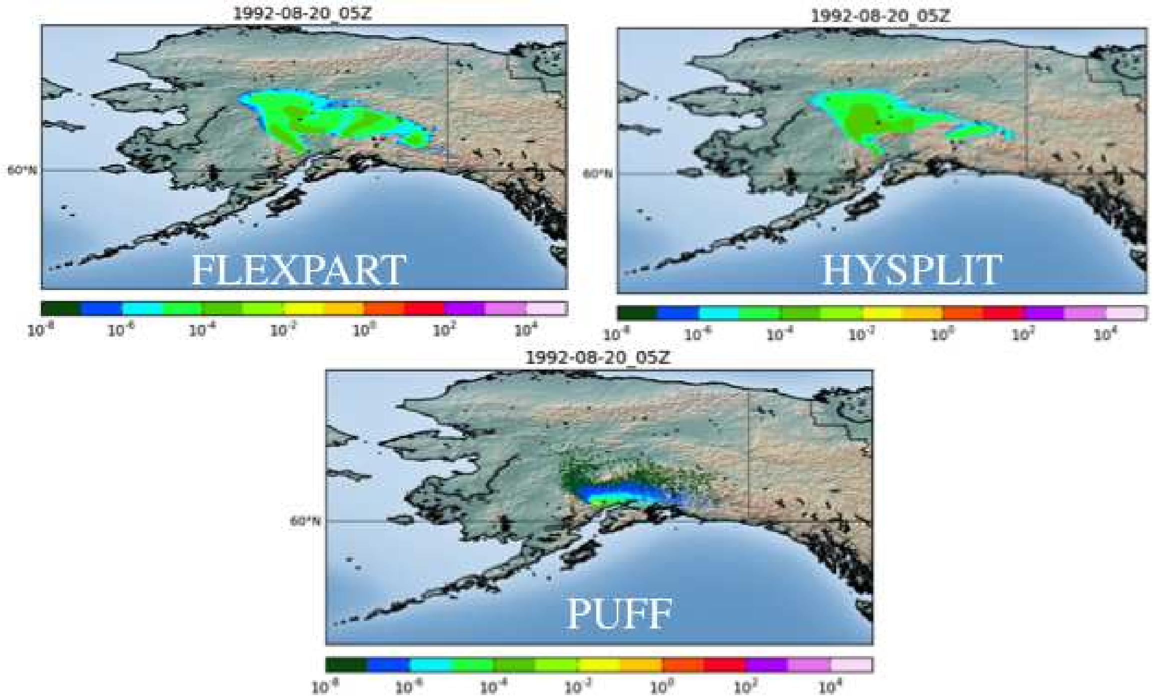


Model intercomparisons

- Volcanic ash transport model intercomparisons – VATMIS (led by D. Morton, UAF, Borealscicomp.com). **Unified model intercomparison for volcanic ash transport modelling** *by Don Morton, Dèlia Arnold Dèlia Arnold, Peter Webley, Gerhard Wotawa, Barbara Stunder* (soon published in International Journal of Air Polluttion)



SO_2 total column concentration (kg m^{-3}). FLEXPART, HYSPLIT and PUFF



Some thoughts on evaluation/verification

- Atmospheric transport studies often rely on observational data (e.g. inverse modelling studies). Verification can only be properly made with independent observational data.
- Point to grid comparisons (goodness according to co-location and strength) may become problematic for small grid cells.
- Verification with controlled experiments can only be made with the scales and species characteristics the experiments were thought for.
- Some natural traces may be as well useful for model evaluation. Traditionally, radon has been used as tracer for a wide range of scales (careful with radon flux variations though)
- How to choose the metrics? There is not real rule of thumb. A combined rank can be an option and the scientist may define what to weight or penalize more.