

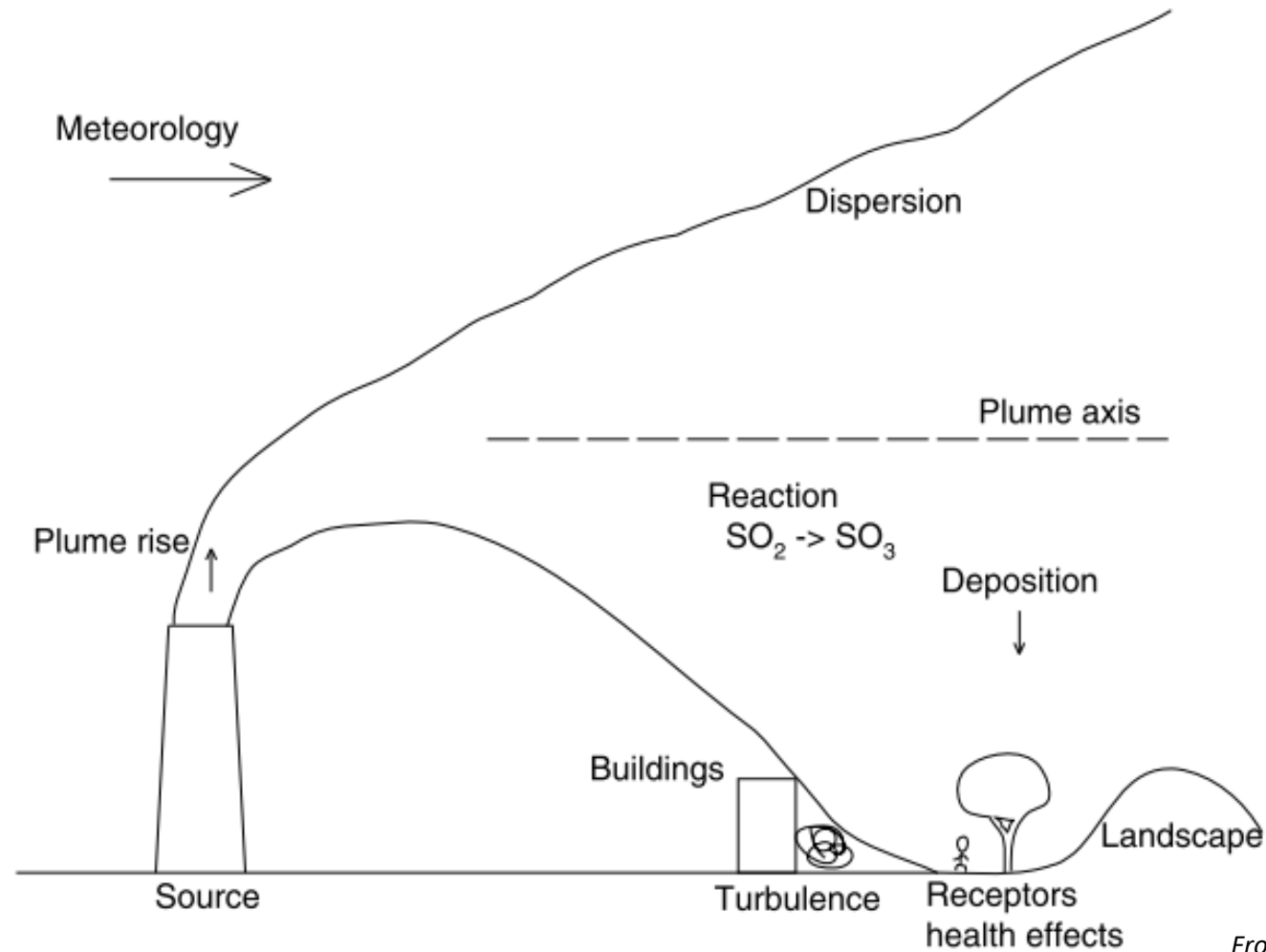
Atmospheric Modelling With FLEXPART

A Lagrangian particle dispersion model

Workshop 2026 (University of Vienna)

A short introduction from
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Atmospheric Transport Model



Events of an air pollution problem.

From: Air dispersion modelling -2013- Visscher

Atmospheric Transport Model

AtmosphericTransportModel or AtmosphericDispersionModel

What:

Atmospheric Transport Modelling: using mathematical theory to **understand**, or **predict** the way atmospheric components behave/get transported in the atmosphere.

Why:

Modelling can be used to **run scenarios**, to **test theories** and **understand environmental impact** under different emission rates, weather and development scenarios.

How:?

Atmospheric Transport Model

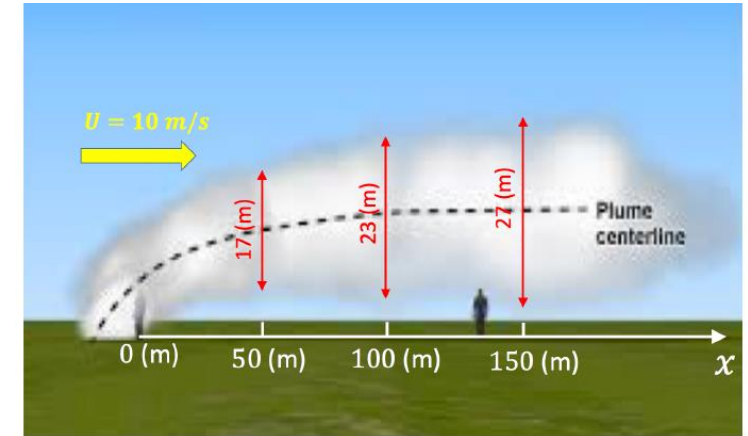
Atmospheric Transport Model or Atmospheric Dispersion Model

The advection-diffusion equation is the equation of continuity for the pollutant concentration C

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = - \frac{\partial}{\partial x} \overline{u'C'} - \frac{\partial}{\partial y} \overline{v'C'} - \frac{\partial}{\partial z} \overline{w'C'} + S_o + S_i$$

- Advection (mean wind)
 - +
 - Diffusion (mixing by unresolved turbulent wind eddies)
- } Dispersion
- Emission (sources)
 - Removal (sinks)

Those includes effects of clouds and precipitation (wet scavenging), radioactive decay, and deposition on the ground due to the various capturing properties of the surface (dry deposition).



Two transport model approaches

Two basic reference frames: **Lagrangian** and **Eulerian** that present complementary information

Lagrangian perspective follows an “air parcel” around.

It is the situation of a sensor which monitors the fluid following its movement.

Eulerian perspective, we observe changes of fluid properties at a fixed location, as the parcels pass by.

This is what happens with ground stations for example.

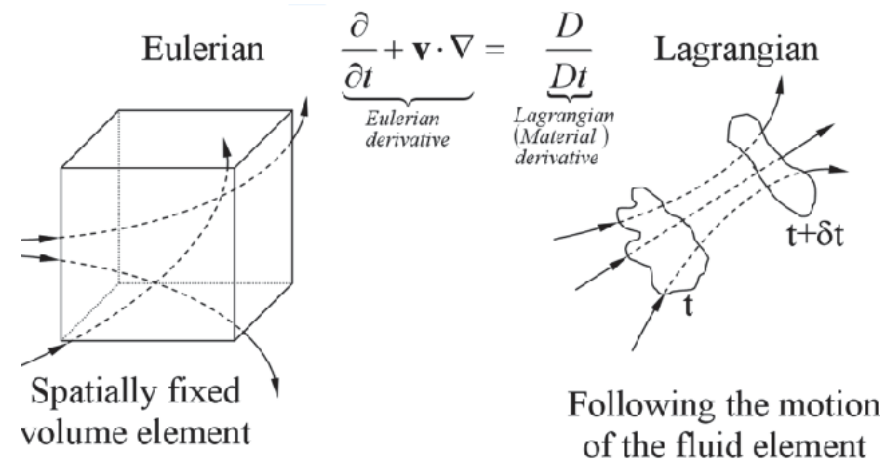


Image from Shadloo et al. 2016

Lagrangian vs. Eulerian

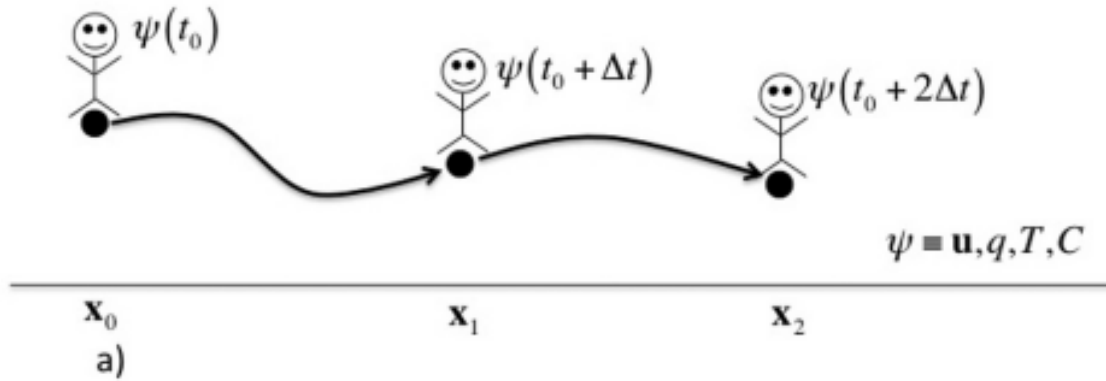
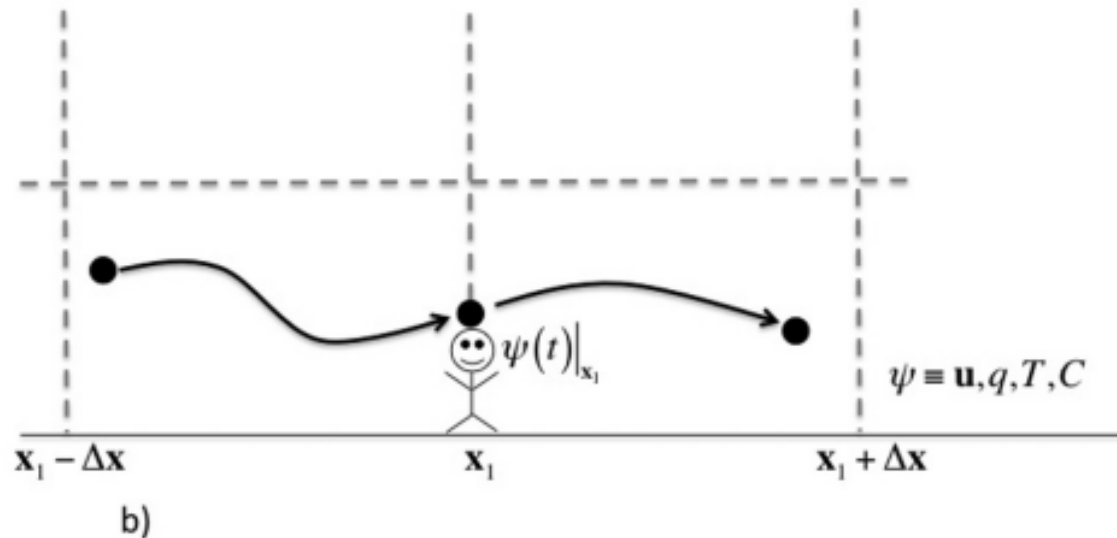


Image from: Lin et al. 2012: Lagrangian modelling of the atmosphere



Ψ is a state variable
 S is the generic source

$$\frac{D\Psi}{Dt} = S,$$

Trajectory: $D\mathbf{x}/Dt = \mathbf{u}$

$$\mathbf{x}(t_0 + \Delta t) = \mathbf{x}(t_0) + \mathbf{u}(t_0) \cdot \Delta t + \dots,$$

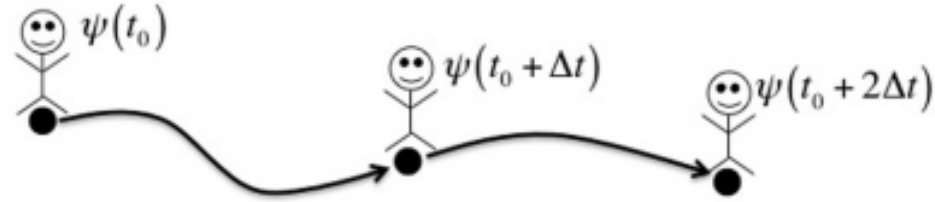
First order, «zero acceleration» solution

$$\frac{\partial \Psi}{\partial t} + \mathbf{u} \cdot \nabla \Psi = S,$$

Why Lagrangian?

PROS:

- Point by point informations along trajectories
- Closer to a „real“ atmosphere (so it can follow mixing, transport barriers, turbulent eddies and convection)
- Numerical stability due to the linearity of Lagrangian advection and lack of numerical diffusion: it preserves distributions where sharp gradients exist in the atmosphere, e.g., the polar vortex (better parameterization of mixing processes)
- conservation of energy, mass, and momentum while Eulerian advection schemes may not conserve mass for example!



Why Lagrangian?

CONS:

- Computational cost! (they do not solve the atmosphere's equations of motions, as they ingest it directly as input BUT they solve the turbulent velocity fluctuations!). **BUT**, they can be parallelized.
- The position of the particles in output may not be in a regular grid! Needs additional procedure of parcel insertion or merging, parcel counting within regular grid cells, kernel density estimators, or parcels representing dynamic volume.

$$C_{T_s} = \frac{1}{V} \sum_{i=1}^N (m_i f_i) ,$$

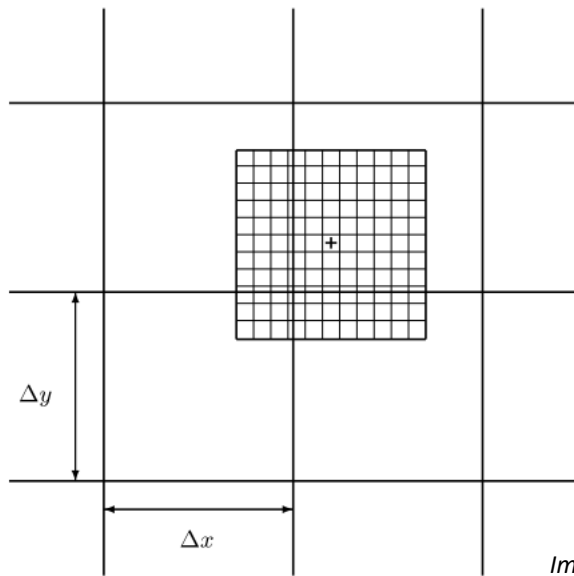


Image from: Stohl et al. 2005, Technical note

Fig. 1. Illustration of the uniform kernel used to calculate gridded concentration and deposition fields. The particle position is marked by “+”

V being the grid cell volume

m_i particle mass

N the total number of particles

f_i the fraction of the mass of particle per grid cell.

This mass fraction is calculated by a uniform kernel with bandwidths (Δx , Δy), where Δx and Δy are the grid distances on the longitude-latitude output grid.

Why Lagrangian?

CONS:

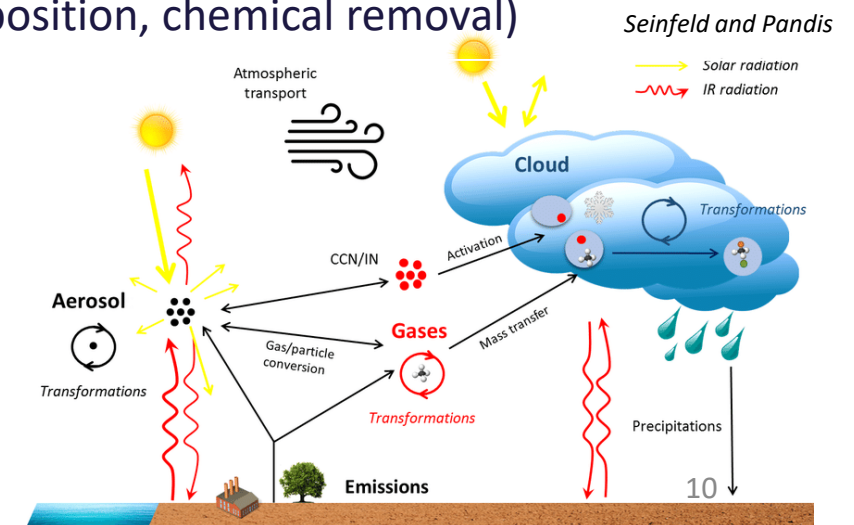
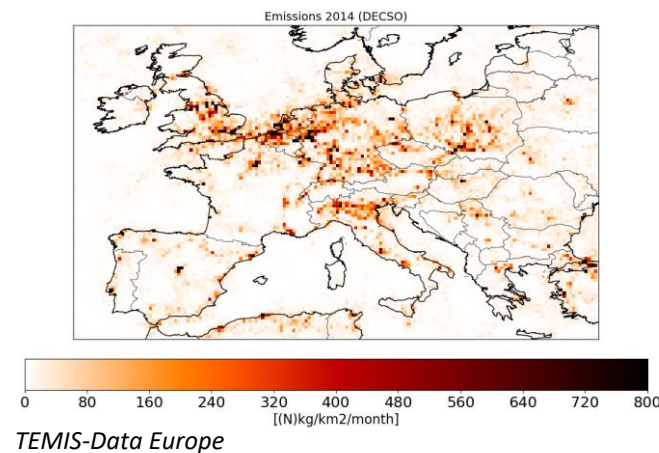
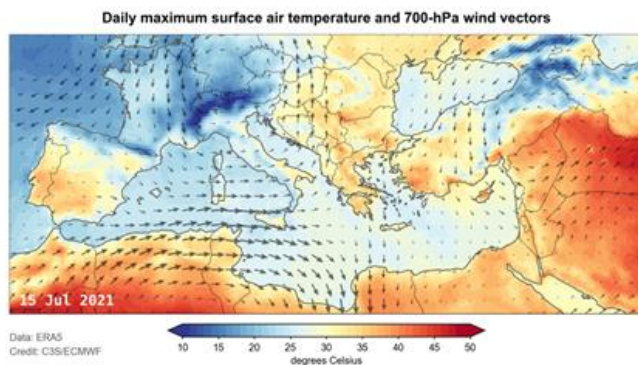
- Computational cost! (they do not solve the atmosphere's equations of motions, as they ingest it directly as input BUT they solve the turbulent velocity fluctuations!). **BUT**, they can be parallelized.
- The position of the particles in output may not be in a regular grid! Needs additional procedure of parcel insertion or merging, parcel counting within regular grid cells, kernel density estimators, or parcels representing dynamic volume.
- Inconsistencies with the feeding Eulerian model (for the meteorological variables). The two models can be inconsistent with one another, especially if variables are omitted in the output or interpolated from internal model coordinates to common pressure levels. This can be solved, though!

Uncertainties sources

- 'All models are wrong but some are useful' (George Box)

The ATM rely on a series of information that can introduce errors and inaccuracies

1. The meteorological input data
2. The emission data or any additional input/ancillary data (e.g. land-use, precursors concentrations, orography)
3. The parametrization/description of certain processes (e.g. turbulence, deposition, chemical removal)

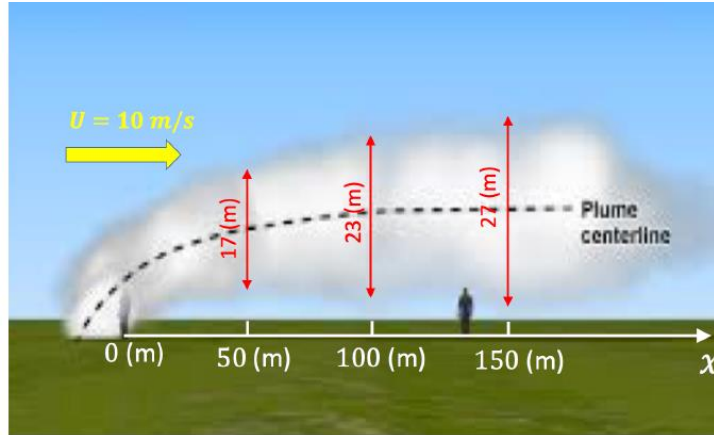


Lagrangian

Lagrangian: They include all models in which plumes can be broken down into segments, puffs or particles.

Advection:

Modelled from the mean wind field.



Diffusion:

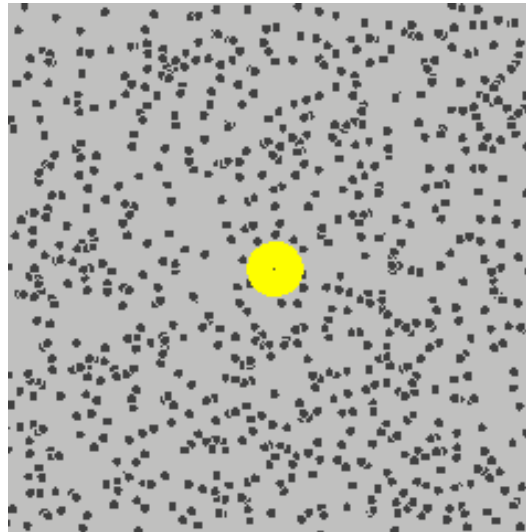
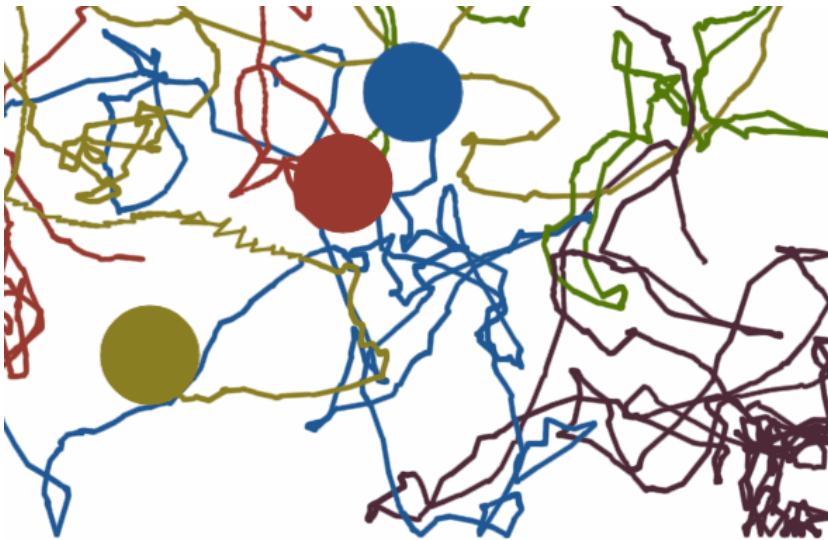
- *low number of elements* (puffs or plume segments): diffusion is usually simulated by a **Gaussian model applied to each plume elements**. The standard deviation is calculated taking into account the atmospheric mixing layer structure.
- *very large number of particles*: diffusion is modelled by adding a "**semi-random**" component **to the large scale wind**. The probability density function for the random component, which simulates the atmospheric turbulence, is also dependent on the state of the atmospheric mixing layer.

Diffusion/Turbulence

Turbulence: Random motion of the particles as they travel in a turbulent flow.

The basic theory is the Brownian motion, in particular the Langevin equation.

In Brownian motion, a particle of colloidal size (1 nm – 100 nm, called a Brownian particle) undergoes random collisions in succession ($\sim 10^{21}$ collisions per second) with the molecules of the surrounding fluid.



RandoWalk.gif and Brownian motion large.gif from Wikimedia Commons

The Brownian particle experiences a **viscous resistance in the fluid**, which damps its velocity.

The time scale (τ_B) at which the particle ceases to “remember” its initial velocity due to this viscous resistance is very small (one-hundredth of a μs) and it's called **relaxation or dissipation time**

If $t \gg \tau_B$: we only see random jumps of velocity after every time interval.

If $t \leq \tau_B$: Langevin equation. Deterministic part (overall viscous resistance) + Random part (collision)

The Langevin equation

- Turbulent diffusion, like molecular diffusion (Brownian motion), can be described as a **Markov process**: the particles forget their current velocity state after **the Lagrangian time scale**.
- This is written as the Langevin equation (Thomson, 1987)

$$w(t + \Delta t) = aw(t) + b\sigma_w\zeta \qquad a = \exp(-\Delta t/T_L); \quad b = (1 - a^2)^{1/2}$$

ζ : random number drawn from a Gaussian distribution with zero mean and unit standard deviation.

σ_w : standard deviation of the vertical turbulence velocity.

- Given a state of the turbulent vertical velocity of a particle at time t , a future state at time $t + \Delta t$ can be determined using the **autocorrelation coefficient a** . T_L is the Lagrangian time scale for the vertical velocity

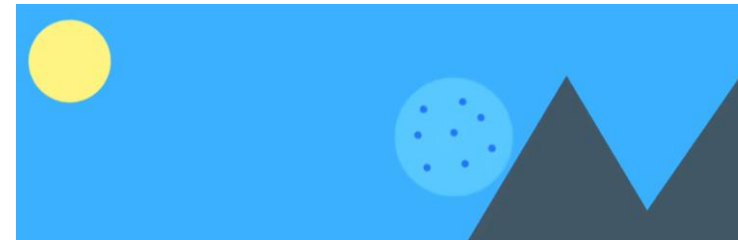
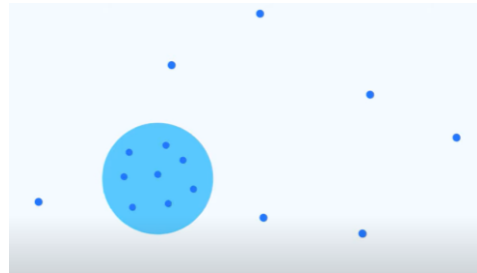
Both T_L and σ_w can be calculated diagnostically based on certain boundary layer characteristics (Hanna, 1982) or can be related to the turbulent kinetic energy (Fay et al., 1995).

Lagrangian

What Is an Air Parcel?

It is a “ chunk ” of the atmosphere, a blob!

- **Large enough** to encompass enough molecules to be able to represent certain properties (temperature in the sense of kinetic energy for example, or a pollutant concentration)
- **Small enough** such that the parcel can be thought of as occupying an infinitesimal location in space that represents a single value of density, temperature, humidity, and pollutant concentration. Same conditions anywhere inside! And it's a sealed box



From youtube: what is an air parcel anyway?

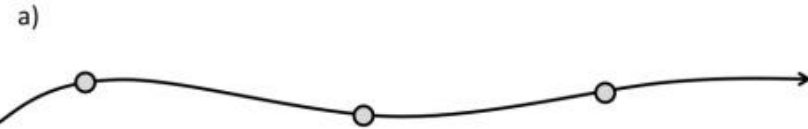
The **boundaries** of an air parcel **are not well defined** and an hypothetical surface wrapping the parcels **constantly deforms** due to molecular and turbulent diffusion!

Parcels may lose their identities so we use many parcels in aggregate: as a **box or a puff**.
Or we use numerous parcels to be handled more explicitly: as an **ensemble of particles**.

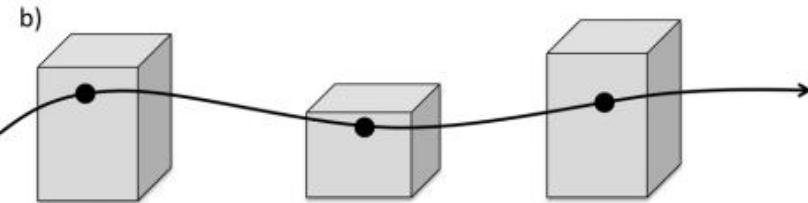
Lagrangian Approaches

Reynolds decomposition of $\mathbf{u}$

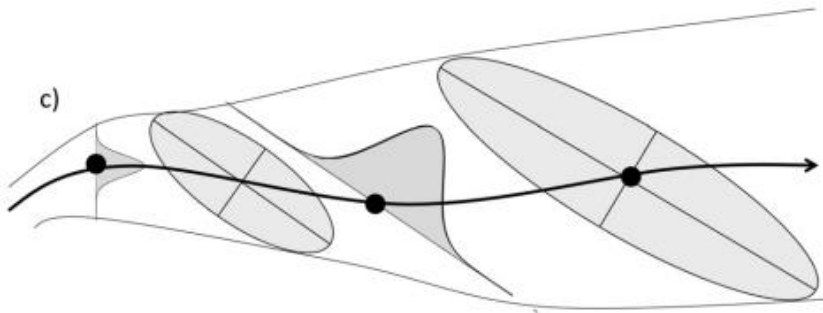
$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'.$$



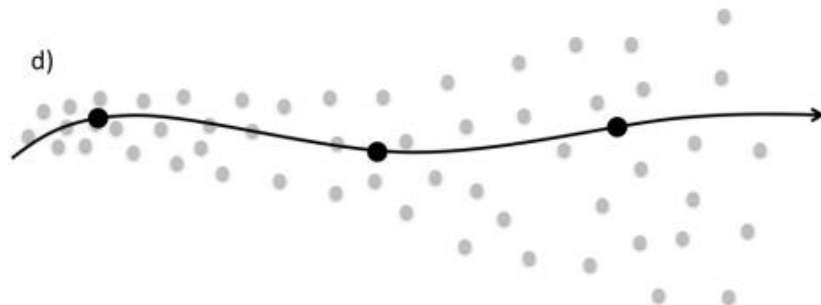
Mean trajectories (no diffusion)



Lagrangian box model, it aggregates parcels. Volumes describe the extent of mixing. The boxes do not interact and they can be distorted. Ex. CiTTYCAT



Puff models: account for turbulent dispersion by Gaussian distributions in all three dimensions (puff expansion). Distortion causes peaks tilting and plume area changes. Ex. CALPUFF



Lagrangian particle dispersion models (LPDMs), represent air parcels as particles of equal mass that are transported with random velocities generated by a Markov process. Stochastic effects of turbulence are captured because of the large number of particles. Computationally expensive. Ex. FLEXPART. It solves $\mathbf{u}'$!!!!

Lagrangian, some comments

It is not possible to follow an infinitesimal air parcel path with infinite accuracy. **A real parcel of finite size** may become **distorted** so strongly in a divergent flow that it is **torn apart** by inhomogeneities of the wind field, by turbulent and convective motions and by precipitation processes.

The combined action of these factors is the reason for the fact that in general a **single trajectory is not sufficient for a description of the path of an air parcel** and the mass center of gravity of the air parcel does not exactly follow the path of the computed trajectory!

Hence, a computed trajectory is representative for the path of an air parcel only for a limited period.

Lagrangian Backward and Forward!

$$\frac{d\mathbf{X}}{dt} = \dot{\mathbf{X}}[\mathbf{X}(t)]$$

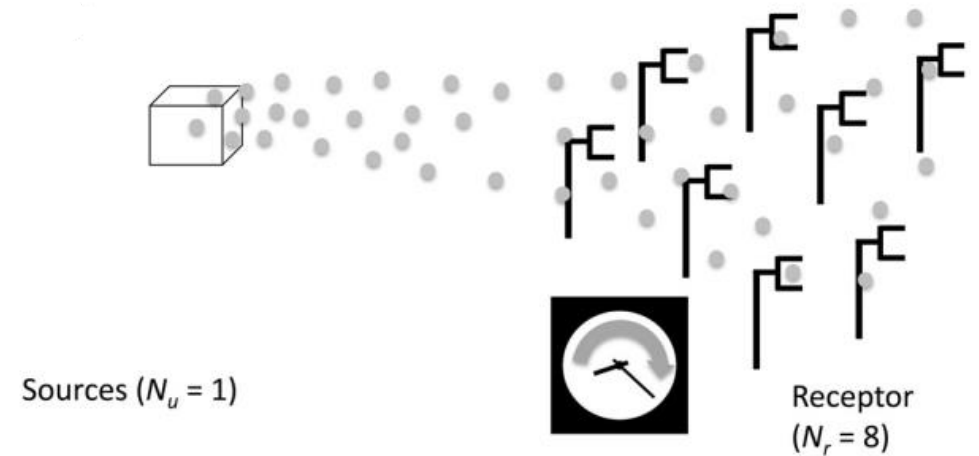
Trajectory equation

$$\mathbf{X}(t) = \mathbf{X}(\mathbf{X}_0, t)$$

Forward solution

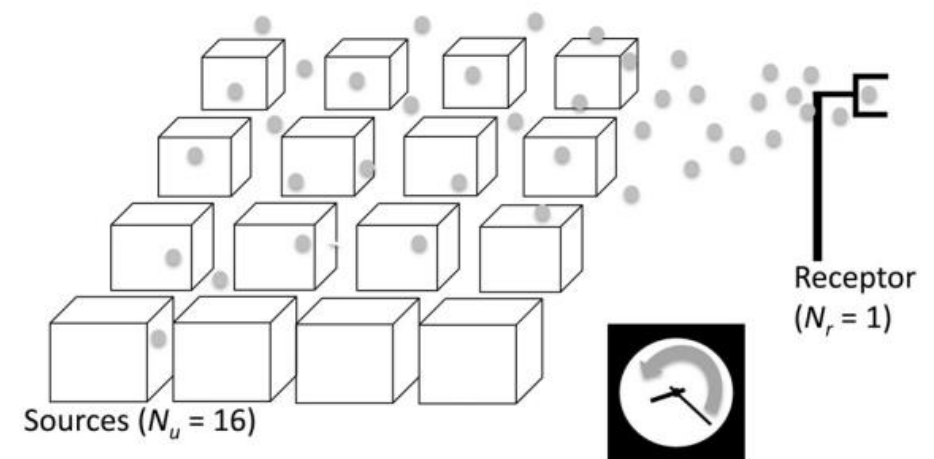
$$\mathbf{X}_0(t = t_0) = \mathbf{X}_0(\mathbf{X}, t)$$

Backward solution



Forward

Andreas Hiboll lectures 2019, «Different kinds of atmospheric models»

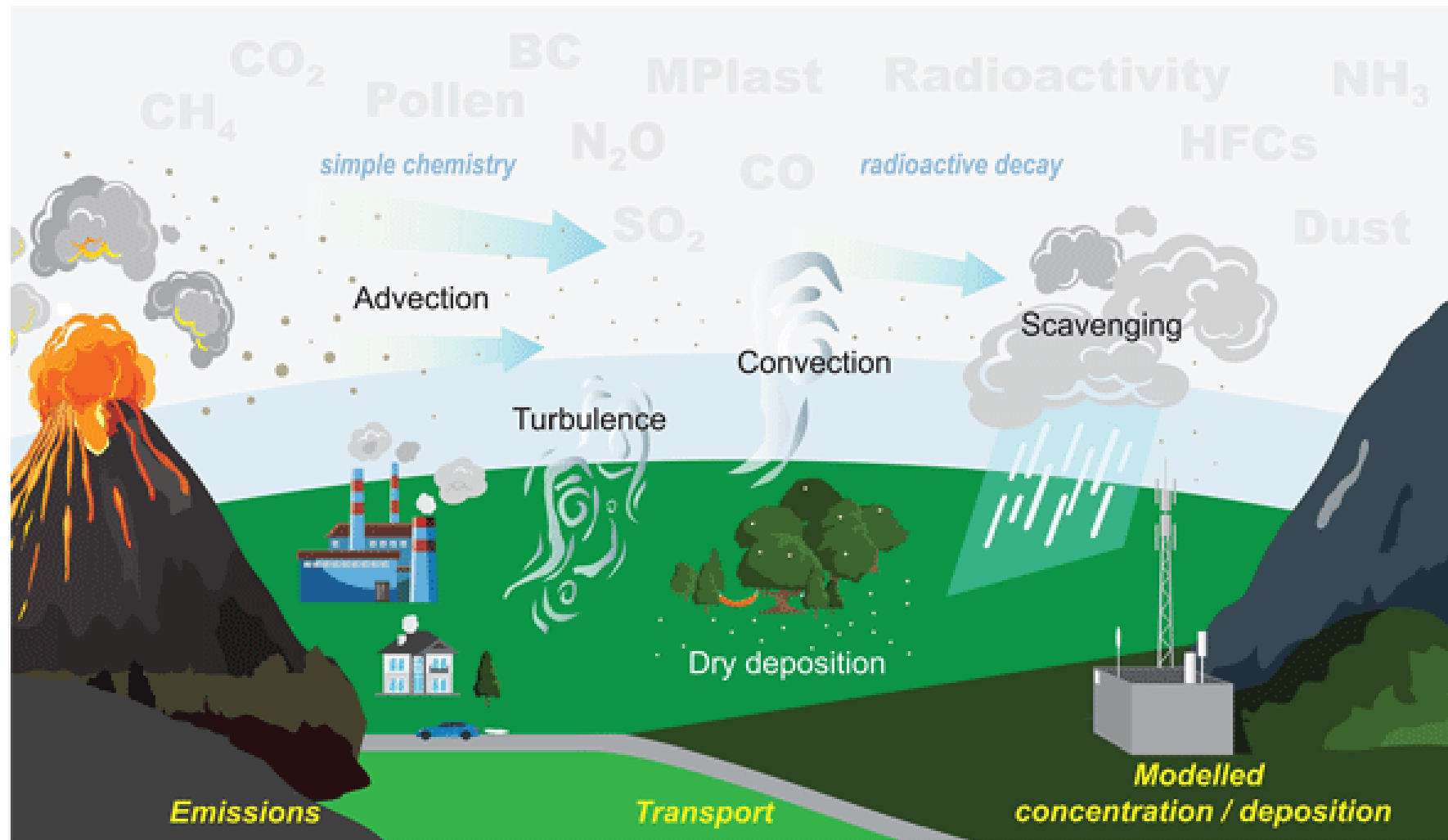


Backward

Backward or Forward?

- What are the upwind influences on the location of interest (receptor)? **Backw**
- Where are the source regions of tracers? **Backw**
- Where do tracers get transported? **Forw**
- How much is the concentration of a passive tracer at downwind locations affected by a unit emission from the source? **Forw**
- What is the downwind impact of air originating from a location of interest (source)? **Forw**
- How strong is the sensitivity of the receptor to a particular upwind source region? **Backw**
- Where does the air come from? **Backw**

FLEXPART v11



FLEXPART

You will find most of the description of the model and its evolution in:

- Bakels et al. 2024 (Flexpart v11)
- [Pisso et al. 2019](#) (Flexpart v10.4)
- [Stohl et al. 2005](#) (Flexpart v6.2)
- [Stohl et al. 1998](#)

An example: FLEXPART backward

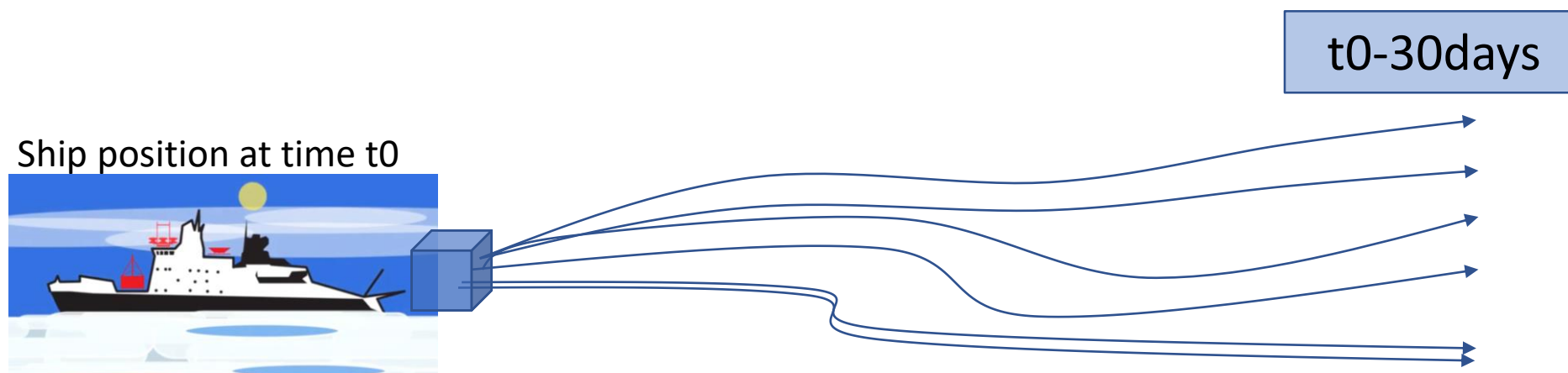
- Release points

Ship position at time t_0



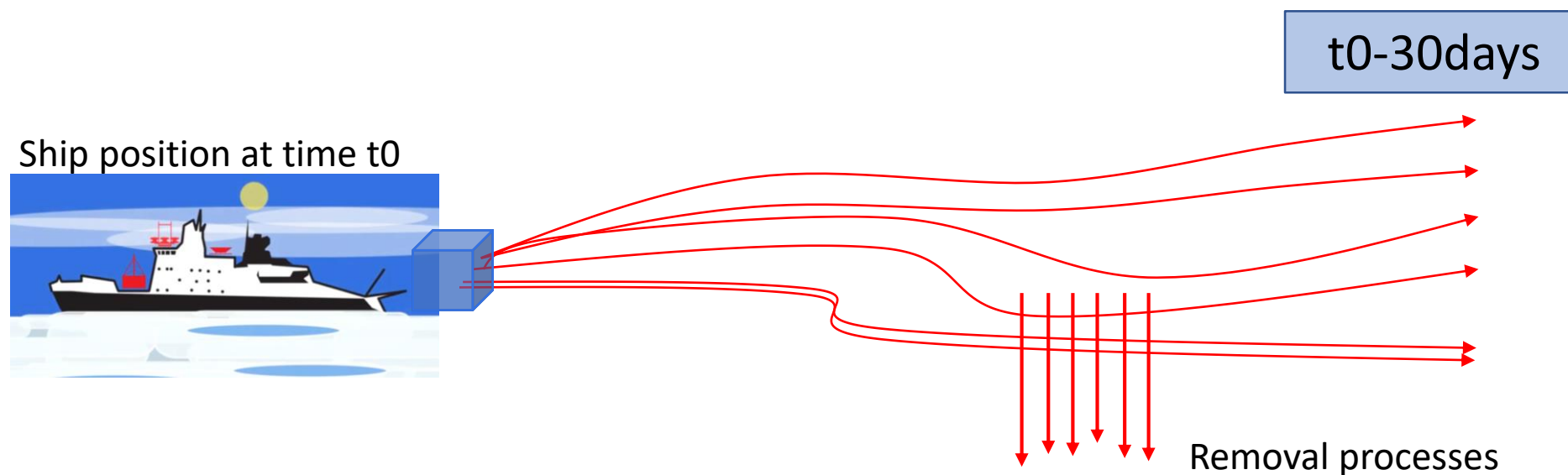
An example: FLEXPART backward

- Release points
- Length of simulations and number of trajectories



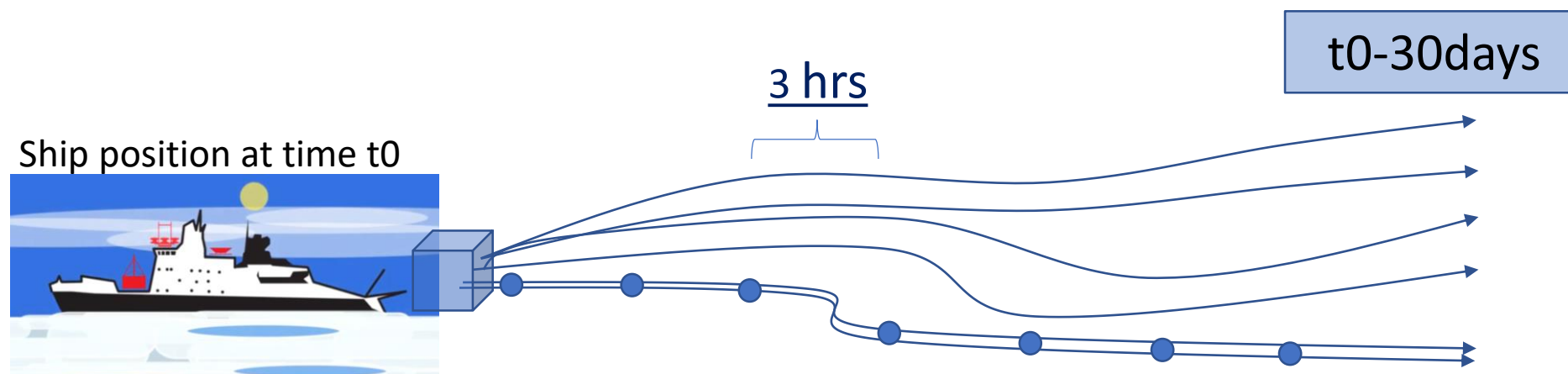
An example: FLEXPART backward

- Release points
 - Length of simulations and number of trajectories
 - Species



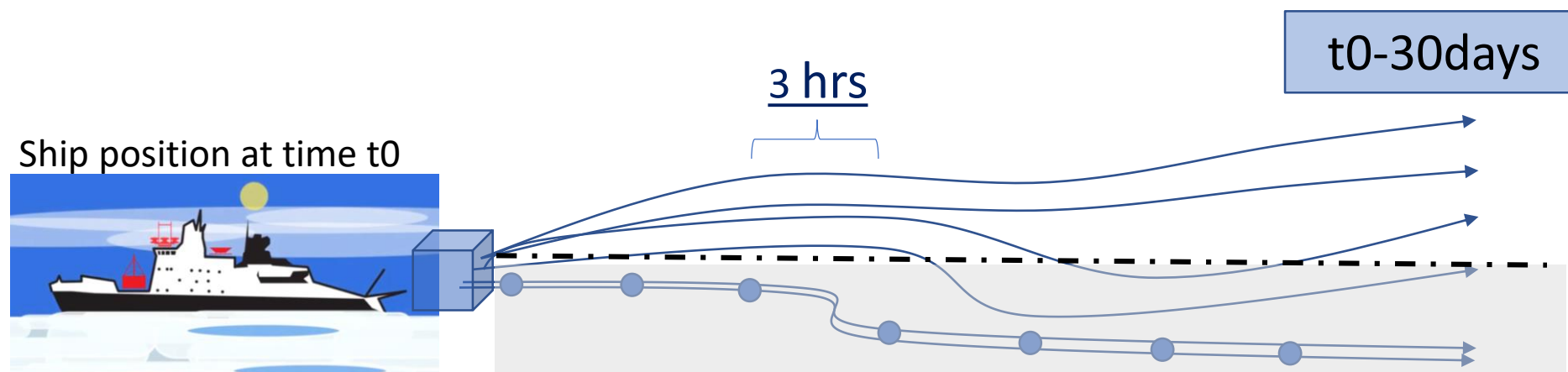
An example: FLEXPART backward

- Release points
 - Length of simulations and number of trajectories
 - Species
 - Resolution



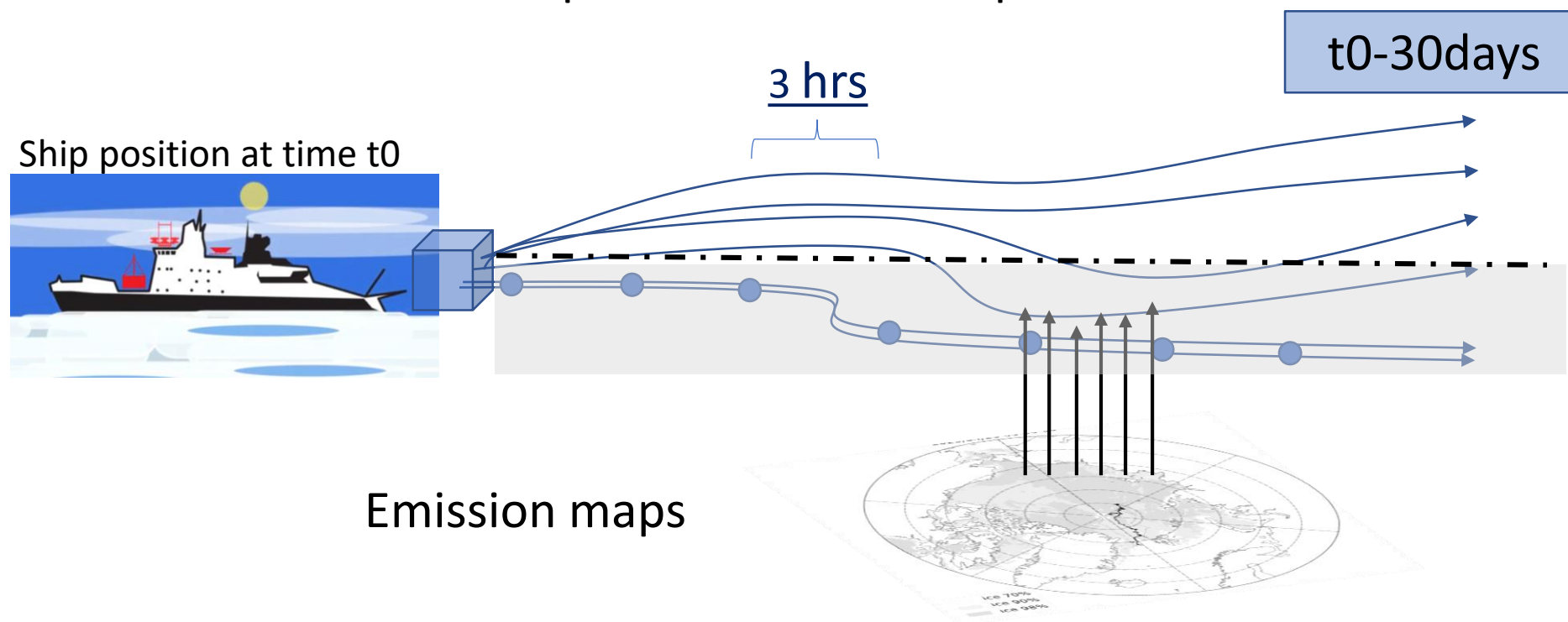
An example: FLEXPART backward

- Release points
 - Length of simulations and number of trajectories
 - Species
 - Resolution
 - Layer of interaction



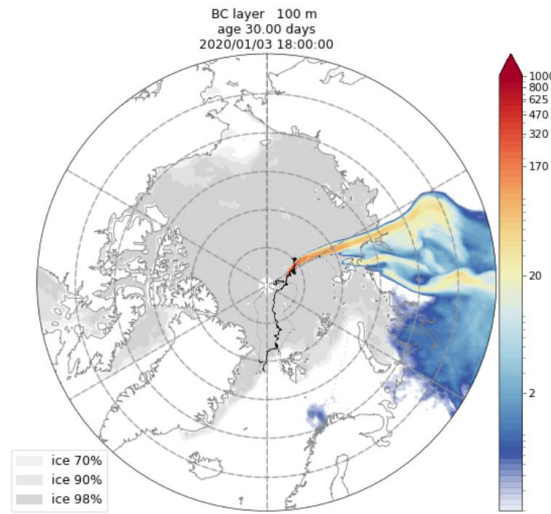
An example: FLEXPART backward

- Release points
 - Length of simulations and number of trajectories
 - Species
 - Resolution
 - Layer of interaction
- Maps of sources to couple with



Coupling of trajectories with emissions / maps

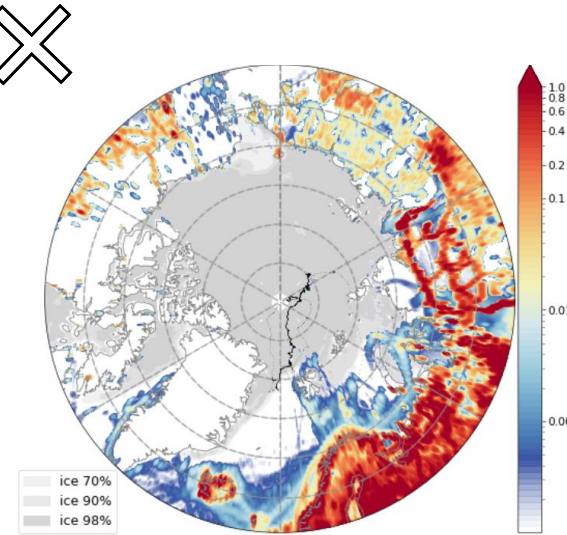
Emission Sensitivity FLEXPART
(proportional to residence time of the particles, loss processes included)



It indicates regions contributing to the air masses composition at the point of release

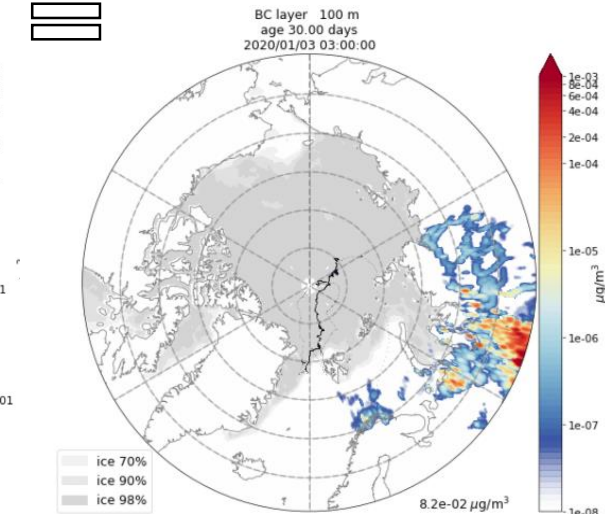
[s]

Emission fluxes from **INVENTORIES**



[ug/m2/s]

Source Contribution
in [ug/m3]



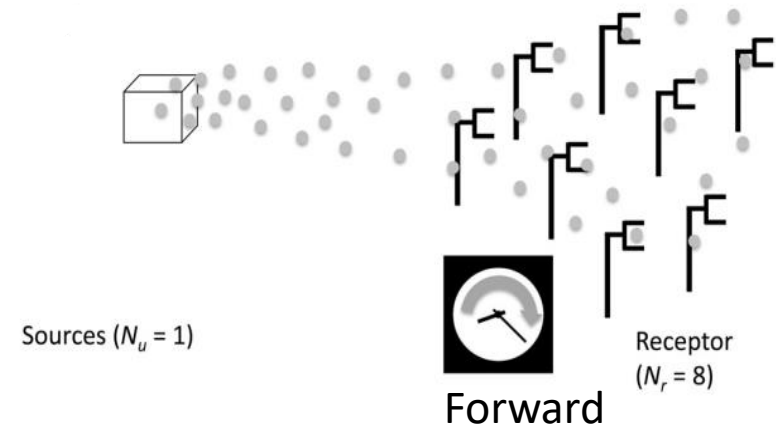
$$\sum (s) \times (ug/m^2/s)/m = ug/m^3$$

Backward vs. Forward

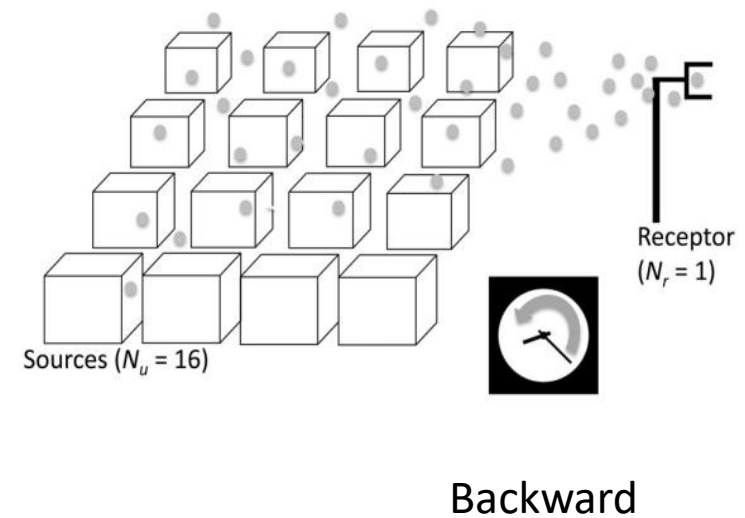
Direction	ind_source	ind_receptor	input unit	output unit
Forward	1	1	kg	ng m^{-3}
Forward	1	2	kg	ppt by mass
Forward	2	1	1	ng m^{-3}
Forward	2	2	1	ppt by mass
Backward	1	1	1	s
Backward	1	2	1	$\text{s m}^3 \text{kg}^{-1}$
Backward	2	1	1	s kg m^{-3}
Backward	2	2	1	s

1 refers to mass units

2 to mass mixing ratio units



Andreas Hiboll lectures 2019, «Different kinds of atmospheric models»



Backward vs. Forward

Direction	ind_source	ind_receptor	input unit	output unit
Forward	1	1	kg	ng m^{-3}
Forward	1	2	kg	ppt by mass
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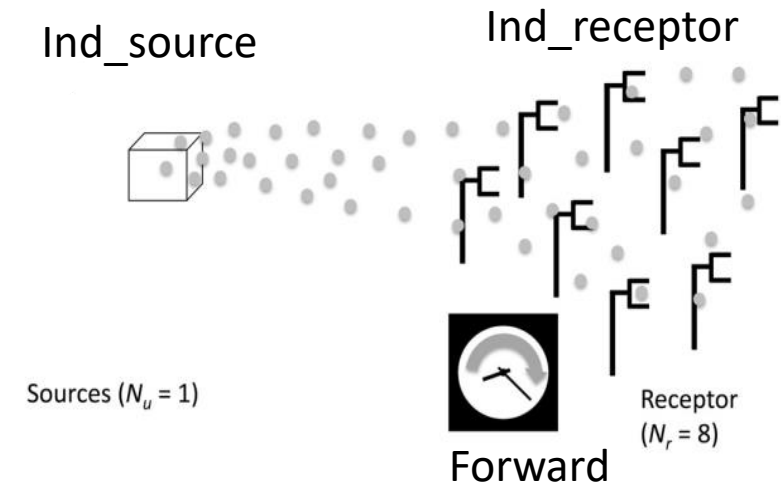
2 to mass mixing ratio units

You start with mass – you end with mass concentration

You start with mass – you convert in mass mixing ratio

You start with a mass mixing ratio – you convert in concentration

You start with a mass mixing ratio – you end with a mass mixing ratio



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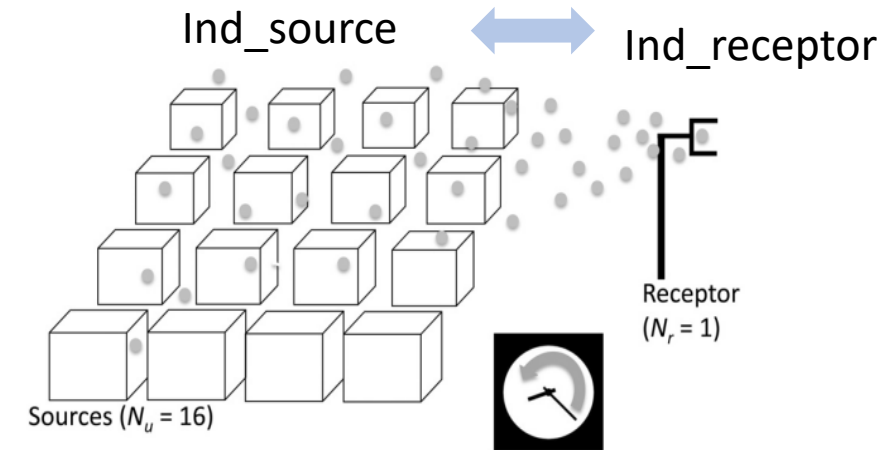
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Forward	2	2	1	ppt by mass
Backward	1	1	1	s
Backward	1	2	1	$\text{s m}^3 \text{kg}^{-1}$
Backward	2	1	1	s kg m^{-3}
Backward	2	2	1	s

You will use an
emissive field!

$$x \quad \text{kg m}^{-3} \text{s}^{-1}$$

Or $x \quad g \text{ kg}^{-1} \text{s}^{-1}$



Backward

1 refers to mass units

2 to mass mixing ratio units

You start with mass – you end with residence time (to get back a mass)

You start with mass – you convert (to get back a mixing ratio)

You start with a mass mixing ratio – you convert (to get a concentration)

You start with a mass mixing ratio – you end with a residence time (to get back a mass mixing ratio)

Backward vs. Forward

Backward	1	1	1	s
Backward	1	2	1	$\text{s m}^3 \text{kg}^{-1}$
Backward	2	1	1	s kg m^{-3}
Backward	2	2	1	s

You will use an
emissive field!

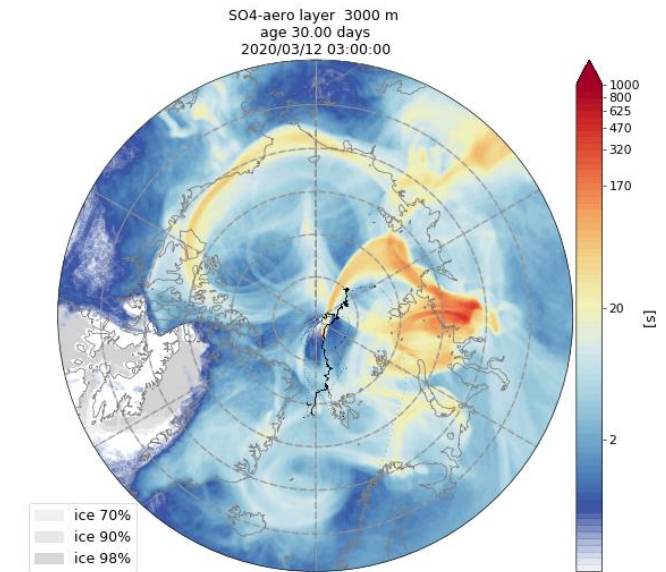
$$\times \text{ kg m}^{-3} \text{ s}^{-1}$$

$$\text{Or } \times \text{ g kg}^{-1} \text{ s}^{-1}$$

1 refers to mass units

2 to mass mixing ratio units

- The residence time is also referred to as “emission sensitivity (ES)” as it express how „sensitive“ you are to the possible emission fluxes.
- It is also referred to as “source-receptor relationship”



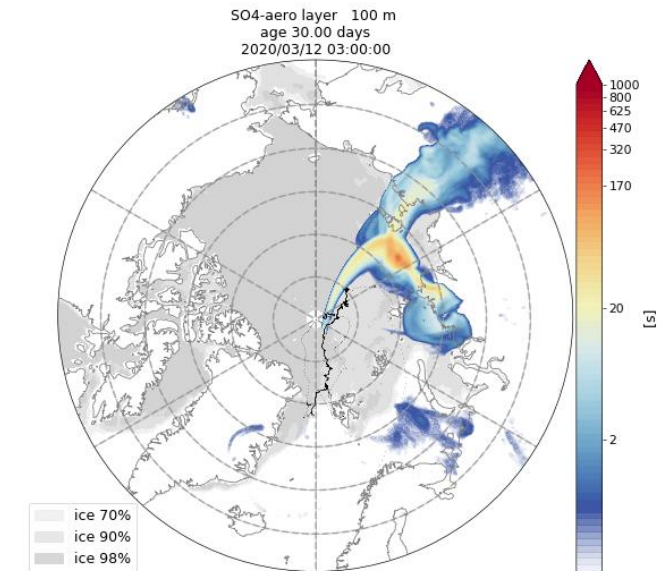
Backward vs. Forward

Backward	1	1	1	s
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Backward	2	2	1	s

You will use an
emissive field!

$$\times \text{ kg m}^{-3} \text{ s}^{-1}$$

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1 refers to mass units
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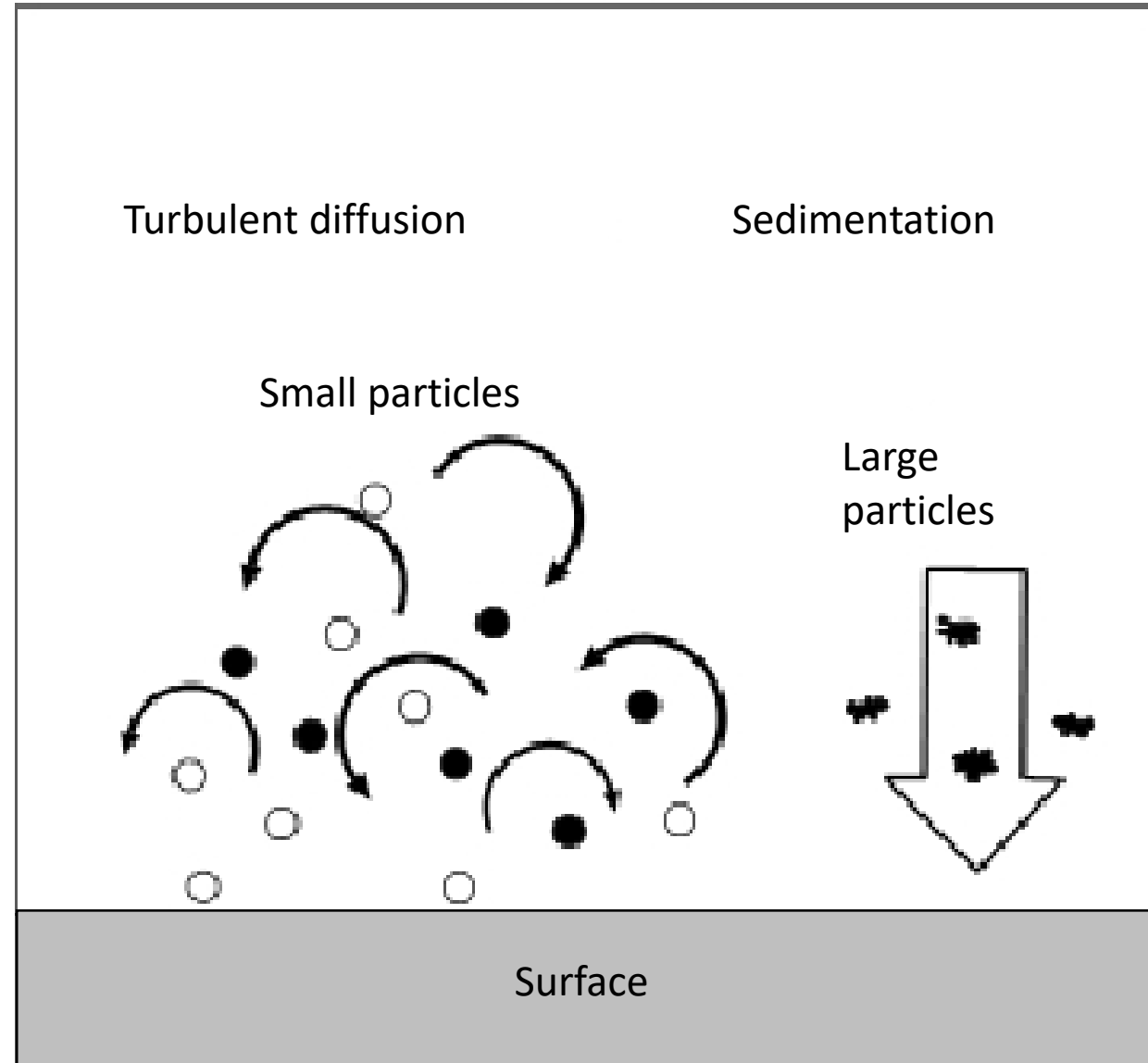
- The residence time is also referred to as “emission sensitivity (ES)” as it express how „sensitive“ you are to the possible emission fluxes.
- It is also referred to as “source-receptor relationship”
- If you consider **only** the layer closer to the ground it is then also called “footprint emission sensitivity” as it is related to the surface fluxes

The removal mechanisms

FLEXPART can also compute some of the removal mechanisms that can affect the concentration of an atmospheric species. Among the most important:

- WET and DRY deposition of both **gas and aerosols** -> **let's briefly look into that**
- Radioactive decay (or anything with an half-life)
- Chemical reactions with the hydroxyl radical (OH)

Aerosol dry deposition



We will see it
better tomorrow!

Adapted from
Leelőssy et al. 2014

Gas dry deposition

Dry deposition is the transport of gases and particles from the atmosphere onto surfaces (usually Earth's surface) in the absence of precipitation.

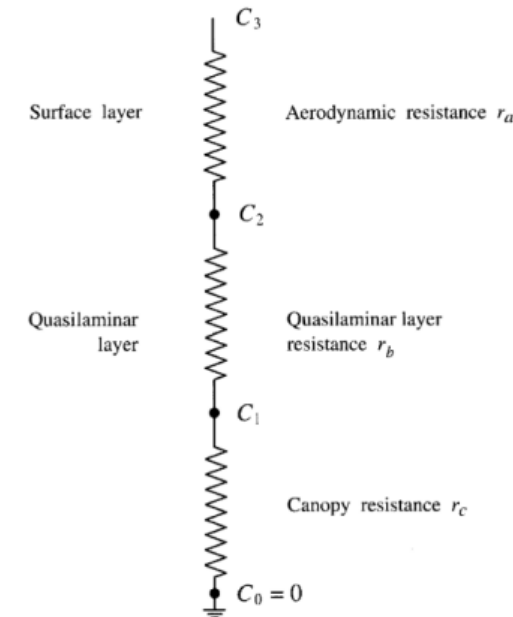
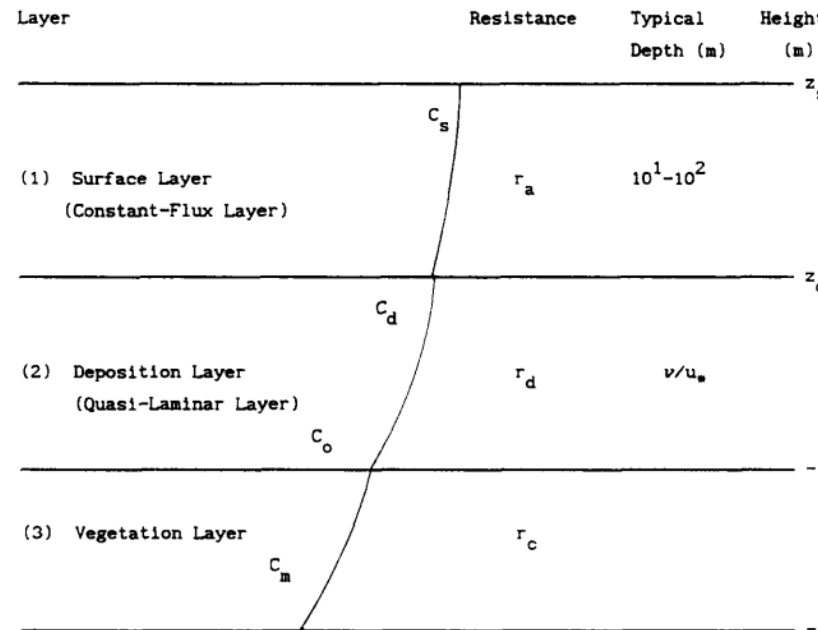


FIGURE 19.1 Resistance model for dry deposition.

Seinfeld and Pandis, 2nd edition

r_a depends (inversely) on the turbulence intensity

r_b depends (inversely) on the diffusivity of the gas

r_c depends (inversely) on the reactivity and solubility of the gas

The deposition velocity of a gas is calculated with the *resistance method* (Wesely and Hicks, 1977) in subroutine `getvdep.f` according to

$$|v_d(z)| = [r_a(z) + r_b + r_c]^{-1}, \quad (42)$$

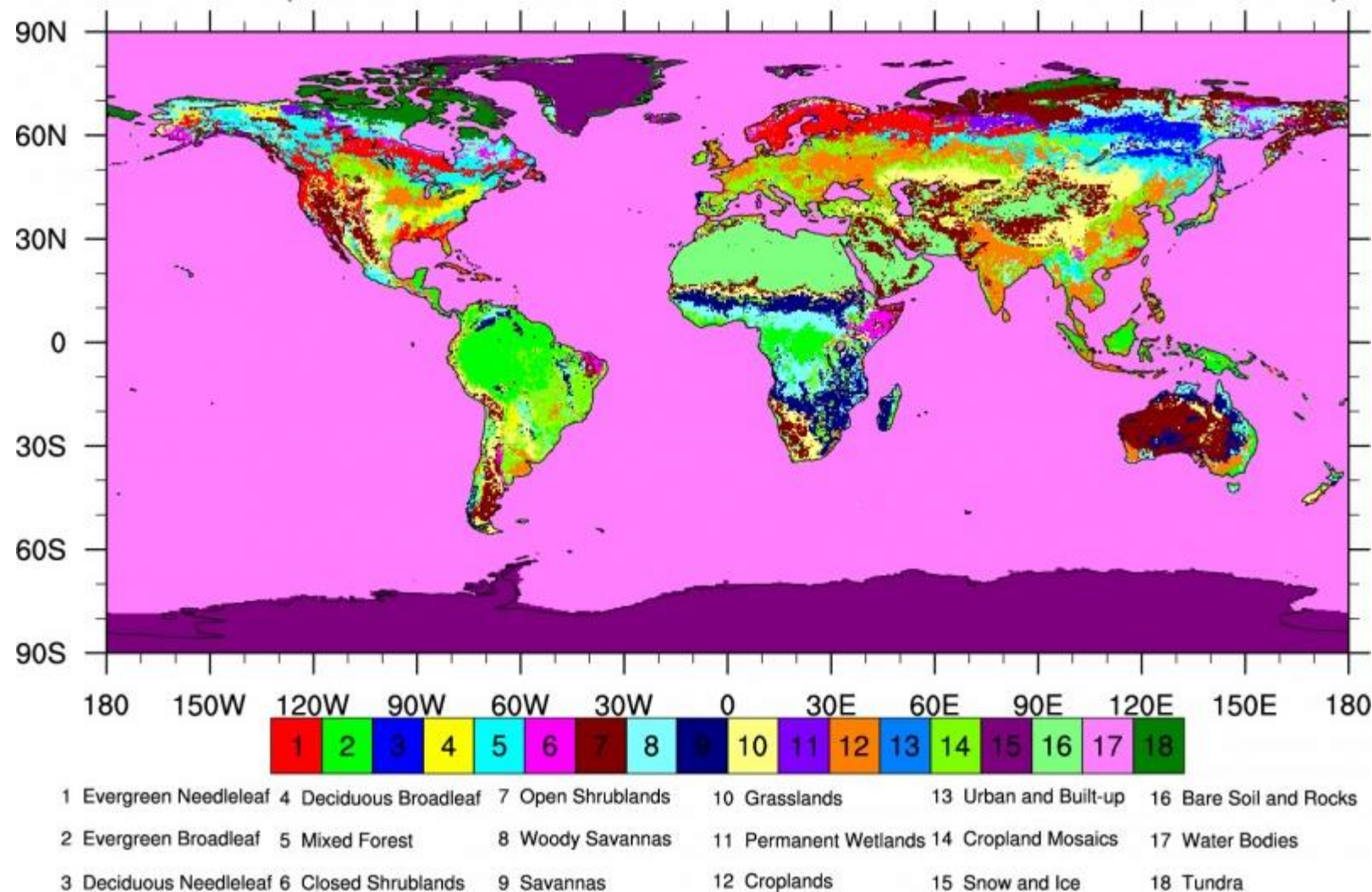
Gas Dry deposition



...but also on the surface conditions!
Leaves (small) vs dry surfaces (large)

IGBP_int1.dat

The IGBP-DIS 1-Km Land-Cover Data Set DISCover:



Contains the 3 most dominant land classes per bin , with their percentage

IGBP: International Geosphere Biosphere Program

Which are the surface types?

13 landuse categories are related roughness length

landuse	comment	z0
1	Urban land	0.7
2	Agricultural land	0.1
3	Range land	0.1
4	Deciduous forest	1.
5	Coniferous forest	1.
6	Mixed forest including wetland	0.7
7	water, both salt and fresh	0.001
8	barren land mostly desert	0.01
9	nonforested wetland	0.1
10	mixed agricultural and range land	0.1
11	rocky open areas with low grow shrubs	0.05
12	snow and ice	0.001
13	rainforest	1.

What are the aerodynamic properties of those surfaces?

INPUT RESISTANCES (s/m) FOR THE COMPUTATION OF SURFACE RESISTANCES TO
DRY DEPOSITION

AFTER WESELY, 1989

1 to 11: Landuse types after Wesely; 12 .. snow, 13 .. rainforest

Values are tabulated for 5 seasonal categories:

- 1 Midsummer with lush vegetation
- 2 Autumn with unharvested cropland
- 3 Late autumn after frost, no snow
- 4 Winter, snow on ground and subfreezing
- 5 Transitional spring with partially green short annuals

	1	2	3	4	5	6	7	8	9	10	11	12	13
ri	9999.	60.	120.	70.	130.	100.	9999.	9999.	80.	100.	150.	9999.	200.
rlu	9999.	2000.	2000.	2000.	2000.	2000.	9999.	9999.	2500.	2000.	4000.	9999.	1000.
rac	100.	200.	100.	2000.	2000.	2000.	0.	0.	300.	150.	200.	0.	2000.
rgss	400.	150.	350.	500.	500.	100.	0.	1000.	0.	220.	400.	100.	200.
rgso	300.	150.	200.	200.	200.	300.	2000.	400.	1000.	180.	200.	10000.	200.
rcls	9999.	2000.	2000.	2000.	2000.	2000.	9999.	9999.	2500.	2000.	4000.	9999.	9 999.
rclo	9999.	1000.	1000.	1000.	1000.	1000.	9999.	9999.	1000.	1000.	1000.	9999.	9999

This is just the example for the
Midsummer with lush vegetation

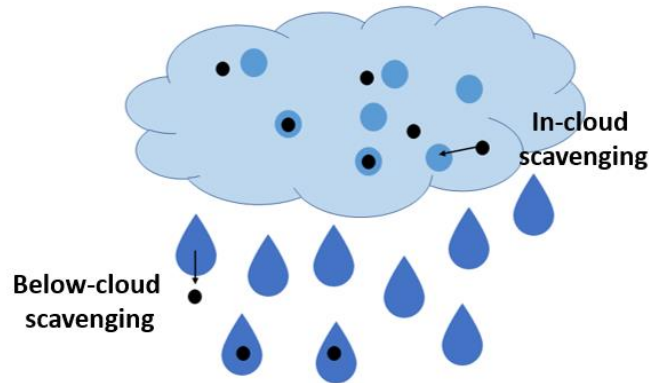
How efficiently they take up
deposition?

! rcl [s/m] Lower canopy resistance (+s=SO₂, +o=O₃)
 ! rgs [s/m] Ground resistance (+s=SO₂, +o=O₃)
 ! rlu [s/m] Leaf cuticular resistance
 ! rac [s/m] Transfer resistance (depending on canopy height)
 ! ri [s/m] Stomatal resistance

Wet deposition of gas and aerosols

1

Where and which type of scavenging



- No clouds
- Above the top of the clouds
- Precipitation rate $< 0.01 \text{ mm h}^{-1}$

-> no scavenging occurs

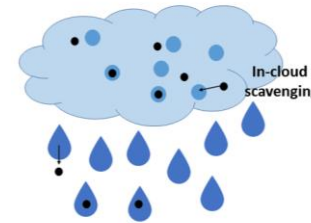
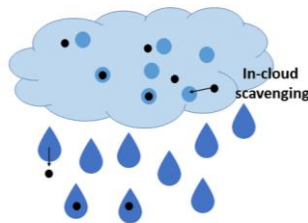
2

Scavenging coefficient computation
 $\Lambda \text{ (s}^{-1}\text{)}$

Below cloud

In cloud

Vs.



3

Estimate of mass loss

$$m(t + \Delta t) = m(t) \exp(-\Lambda \Delta t)$$

We can also use them in backward!

Useful for wet and dry or bulk deposition data

In COMMAND:

IND_SOURCE= 1, ! Unit to be used at the source; [1]mass 2]mass mixing ratio

IND_RECEPTOR= 1, ! Unit to be used at the receptor; [0]no receptor [1]mass 2]mass mixing ratio 3]wet depo. 4]dry depo.

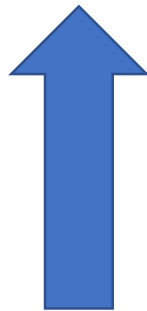
They need to be run separately.
Same instrument point?
Two simulations 😊 one wet, one dry



An example of a Wet&Dry collector

How to handle the variables of the problem within FLEXPART!

AVAILABLE options output pathnames



How to handle the variables of the problem within FLEXPART!

Characterizing the main content of the simulation:

COMMAND

- Timing (resolution and boundaries) and direction,
- Turbulence yes/no,
- Type of units,
- Output style and content,
- Auxiliary inputs

Resolution of the output grid:

OUTGRID

Do you want to interpolate the output in specific locations?

RECEPTORS

How the lagrangian plume will be released:

RELEASE

- species
- timing
- 3-D location/extent
- emitted mass
- number of particles

Which variables do you want along all trajectory points?:

PARTOPTIONS

Which are the features of the species you want to simulate
SPECIES -> this is a directory! In it, every time, you define your own species with its characteristics and you give it an identifier e.g. SPECIES_025

How to handle the variables of the problem within FLEXPART!

```
&SPECIES_PARAMS  
PSPECIES="AIRTRACER",    ! Tracer name  
PWEIGHTMOLAR=29.0,      ! molweight /
```

If we suppose that we have no removal mechanism (AIRTRACER)

Which are the features of the species you want to simulate
SPECIES -> this is a directory! In it, every time, you define your own species with its characteristics and you give it an identifier e.g. SPECIES_025

How to handle the variables of the problem within FLEXPART!

If we have a simple gas, e.g. CO

```
&SPECIES_PARAMS
PSPECIES="CO",           ! Tracer name
PWETA_GAS=8.62E-5,       ! Below-cloud scavenging (gases) - A (weta_gas) [Calculated accord to Asman (1995)]
PWETB_GAS=0.62,          ! Below-cloud scavenging (gases) - B (wetb_gas) [Asman (1995)]
PRELDIFF=1.3,            ! Dry deposition (gases) - D [Calculated accord to Asman (1995)]
PHENRY=9.7E-04,          ! Dry deposition (gases) - Henrys const. [henrys-law.org]
PF0=0.0,                 ! Dry deposition (gases) - f0 (reactivity) [Clifton et al. (2020)]
PWEIGHTMOLAR=28.0,       ! molweight
/
```

Which are the features of the species you want to simulate
SPECIES -> this is a directory! In it, every time, you define your own species with its characteristics and you give it an identifier e.g. SPECIES_025

How to handle the variables of the problem within FLEXPART!

```
&SPECIES_PARAMS
PSPECIES="AEROSOL",      ! Tracer name
PCRAIN_AERO=1.0,         ! Below-cloud scavenging (particles) - Crain (crain_aero) [arbitrary value]
PCSNOW_AERO=1.0,         ! Below-cloud scavenging (particles) - Csnow (csnow_aero) [arbitrary value]
PCCN_AERO=0.9,           ! In-cloud scavenging (particles) - CCNeff (ccn_aero) [arbitrary value]
PIN_AERO=0.1,            ! In-cloud scavenging (particles) - INeff (in_aero) [arbitrary value]
PDENSITY=1.4E3,          ! Dry deposition (particles) - rho [arbitrary value]
PDIA=2.5E-07,            ! Dry deposition (particles) - dquer [arbitrary value]
PDSIGMA=1.25,            ! Dry deposition (particles) - dsig [arbitrary value]
PSHAPE=1,                ! 0 for sphere, 1 any shape (defined by axes PLA,PIA,PSA), 2-cylinder, 3-cube, 4-tetrahedron, 5-octahedron,
6-ellipsoid
PASPECTRATIO=50.0        ! Aspect ratio of cylinders: works for PSHAPE=2 only
PLA=1.8E-06,             ! Longest axis in meters (Bagheri & Bonadonna 2016): only for PSHAPE=1
PIA=0.6E-06,             ! Intermediate axis in meters: only for PSHAPE=1
PSA=0.6E-06,            ! Smallest axis in meters: only for PSHAPE=1
PORIENT=0,              ! 0 for random orientation of particles, 1 for horizontal, 2 for an average between random and horizontal
/
```

If we suppose that we have a simple aerosol (AEROSOL TRACER)

Which are the features of the species you want to simulate
SPECIES -> this is a directory! In it, every time, you define your own species with its characteristics and you give it an identifier e.g. SPECIES_025

```

*
*      Input file for the Lagrangian particle dispersion model FLEXPART
*      Please select your options
*
*****

```

```

&COMMAND
LDIRECT=      -1, ! Simulation direction in time      ; 1 (forward) or -1 (backward)
IBDATE=       20170925, ! Start date of the simulation ; YYYYMMDD: YYYY=year, MM=month, DD=day
IBTIME=       000000, ! Start time of the simulation  ; HHMISS: HH=hours, MI=min, SS=sec; UTC
IEDATE=       20170928, ! End date of the simulation  ; same format as IBDATE
IETIME=       000000, ! End time of the simulation   ; same format as IBTIME
LOUTSTEP=     3600, ! Interval of model output; average concentrations calculated every LOUTSTEP (s)
LOUTAVER=     3600, ! Interval of output averaging (s)
LOUTSAMPLE=   600, ! Interval of output sampling (s), higher stat. accuracy with shorter intervals
LOUTRESTART=  86400, ! Interval of writing restart files (s)
LSYNCTIME=    600, ! All processes are synchronized to this time interval (s)
CTL=          -5.0000000, ! CTL>1, ABL time step = (Lagrangian timescale (TL))/CTL, uses LSYNCTIME if CTL<0
IFINE=        10, ! Reduction for time step in vertical transport, used only if CTL>1
IOUT=         9, ! Output type: [1]mass 2]pptv 3]1&2 4]plume 5]1&4, +8 for NetCDF output
IPOUT=        0, ! Particle position output: 0]no 1]every output 2]only at end 3]time averaged
LSUBGRID=     0, ! Increase of ABL heights due to sub-grid scale orographic variations;[0]off 1]on
LCONVECTION=  1, ! Switch for convection parameterization;0]off [1]on
LTURBULENCE=  1, ! Switch for turbulence parameterisation;0]off [1]on
LAGESPECTRA=  0, ! Switch for calculation of age spectra (needs AGECLASSES);[0]off 1]on
IPIN=         0, ! Warm start from particle dump (needs previous partposit_end file); [0]no 1]yes
IOUTPUTFOREACHRELEASE= 1, ! Separate output fields for each location in the RELEASE file; [0]no 1]yes
IFLUX=        0, ! Output of mass fluxes through output grid box boundaries
MDOMAINFILL=  0, ! Switch for domain-filling, if limited-area particles generated at boundary
IND_SOURCE=   1, ! Unit to be used at the source; [1]mass 2]mass mixing ratio
IND_RECEPTOR= 1, ! Unit to be used at the receptor; [1]mass 2]mass mixing ratio 3]wet depo. 4]dry depo.
MQUASILAG=    0, ! Quasi-Lagrangian mode to track individual numbered particles
NESTED_OUTPUT= 0, ! Output also for a nested domain
LINIT_COND=   0, ! Output sensitivity to initial conditions (bkw mode only) [0]off 1]conc 2]mmr
SFC_ONLY=     0, ! Output only for the lowest model layer, used w/ LINIT_COND=1 or 2
CBLFLAG=      0, ! Skewed, not Gaussian turbulence in the convective ABL, need large CTL and IFINE
NXSHIFT=      0, ! Shift of the global meteorological data. Default 359 for ECMWF and 0 for GFS if not given
OHFIELDS_PATH= "../../flexin/", ! Default path for OH file
/

```



COMMAND

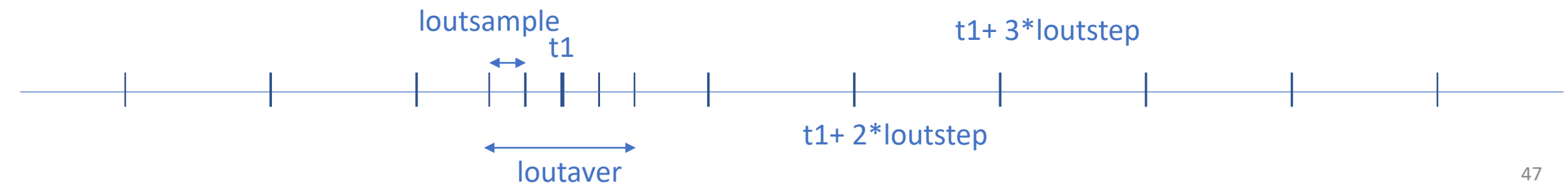
```

*
*      Input file for the Lagrangian particle dispersion model FLEXPART
*      Please select your options
*
*****
&COMMAND
LDIRECT=      -1, ! Simulation direction in time   ; 1 (forward) or -1 (backward)
IBDATE=       20170925, ! Start date of the simulation ; YYYYMMDD: YYYY=year, MM=month, DD=day
IBTIME=       000000, ! Start time of the simulation ; HHMISS: HH=hours, MI=min, SS=sec; UTC
IEDATE=       20170928, ! End date of the simulation   ; same format as IBDATE
IETIME=       000000, ! End time of the simulation     ; same format as IBTIME
LOUTSTEP=     3600, ! Interval of model output; average concentrations calculated every LOUTSTEP (s)
LOUTAVER=     3600, ! Interval of output averaging (s)
LOUTSAMPLE=   600, ! Interval of output sampling (s), higher stat. accuracy with shorter intervals
LOUTRESTART=  86400, ! Interval of writing restart files (s)
LSYNCTIME=    600, ! All processes are synchronized to this time interval (s)
CTL=         -5.000000, ! CTL>1, ABL time step = (Lagrangian timescale (TL))/CTL, uses LSYNCTIME if CTL<0
IFINE=        10, ! Reduction for time step in vertical transport, used only if CTL>1

```

← COMMAND

$$\Delta t_i = \frac{1}{c_{tl}} \min \left(\tau_{L_w}, \frac{h}{2w}, \frac{0.5}{\partial \sigma_w / \partial z} \right)$$



```

*****
!
!      Input file for the Lagrangian particle dispersion model FLEXPART
!      Please specify your output grid
!
! OUTLON0 = GEOGRAPHICAL LONGITUDE OF LOWER LEFT CORNER OF OUTPUT GRID
! OUTLAT0 = GEOGRAPHICAL LATITUDE OF LOWER LEFT CORNER OF OUTPUT GRID
! NUMXGRID = NUMBER OF GRID POINTS IN X DIRECTION (= No. of cells + 1)
! NUMYGRID = NUMBER OF GRID POINTS IN Y DIRECTION (= No. of cells + 1)
! DXOUT    = GRID DISTANCE IN X DIRECTION
! DYOUT    = GRID DISTANCE IN Y DIRECTION
! OUTHEIGHTS = HEIGHT OF LEVELS (UPPER BOUNDARY)
*****
&OUTGRID
OUTLON0= 10.00,
OUTLAT0= 20.00,
NUMXGRID= 80,
NUMYGRID= 120,
DXOUT= 0.50,
DYOUT= 0.50,
OUTHEIGHTS= 100.0, 500.0, 1000.0 , 50000.0,
/

*****
!
!      Input file for the Lagrangian particle dispersion model FLEXPART
!      Please select your options
!
*****
&RELEASES_CTRL
NSPEC = 1, ! Total number of species
SPECNUM_REL= 24, ! Species numbers in directory SPECIES
/
&RELEASE ! For each release
IDATE1 = 20170928, ! Release start date, YYYYMMDD: YYYY=year, MM=month, DD=day
ITIME1 = 000000, ! Release start time in UTC HHMISS: HH hours, MI=minutes, SS=seconds
IDATE2 = 20170928, ! Release end date, same as IDATE1
ITIME2 = 000000, ! Release end time, same as ITIME1
LON1 = 35.000, ! Left longitude of release box -180 < LON1 < 180
LON2 = 35.000, ! Right longitude of release box, same as LON1
LAT1 = 40.000, ! Lower latitude of release box, -90 < LAT1 < 90
LAT2 = 40.000, ! Upper latitude of release box same format as LAT1
Z1 = 0.000, ! Lower height of release box meters/hPa above reference level
Z2 = 1000.000, ! Upper height of release box meters/hPa above reference level
ZKIND = 2, ! Reference level 1=above ground, 2=above sea level, 3 for pressure in hPa
MASS = 5.09256513E18, ! Total mass emitted, only relevant for fwd simulations
PARTS = 100000, ! Total number of particles to be released
COMMENT = "RELEASE 1", ! Comment, written in the outputfile
/

```

RELEASE



OUTGRID

