

Examples of applications: microplastic as a special aerosol

Silvia Bucci

Silvia.bucci@unitus.it



Life in PLASTIC

Cheap, versatile, **light**, resistant, waterproof, hygienic
Crucial for food security (e.g. packaging, see FAO)

- We use it in large quantities and we produce it in large quantities (Million tons per year)
- It's very hard to get rid of!
- It carries toxic contaminants
- It is **easily spread around the globe**

Advised Ted Talk:

Leyla Acaroglu: Paper beats plastic? How to rethink environmental folklore

...and PLASTIC Life



The Lifecycle of Plastics

What does it happen in this timeframe?



Plastic bag
20 years



Coffee cup
30 years



Plastic straw
200 years



6-pack plastic rings
400 years



Plastic water bottle
450 years



Coffee pod
500 years



Plastic cup
450 years



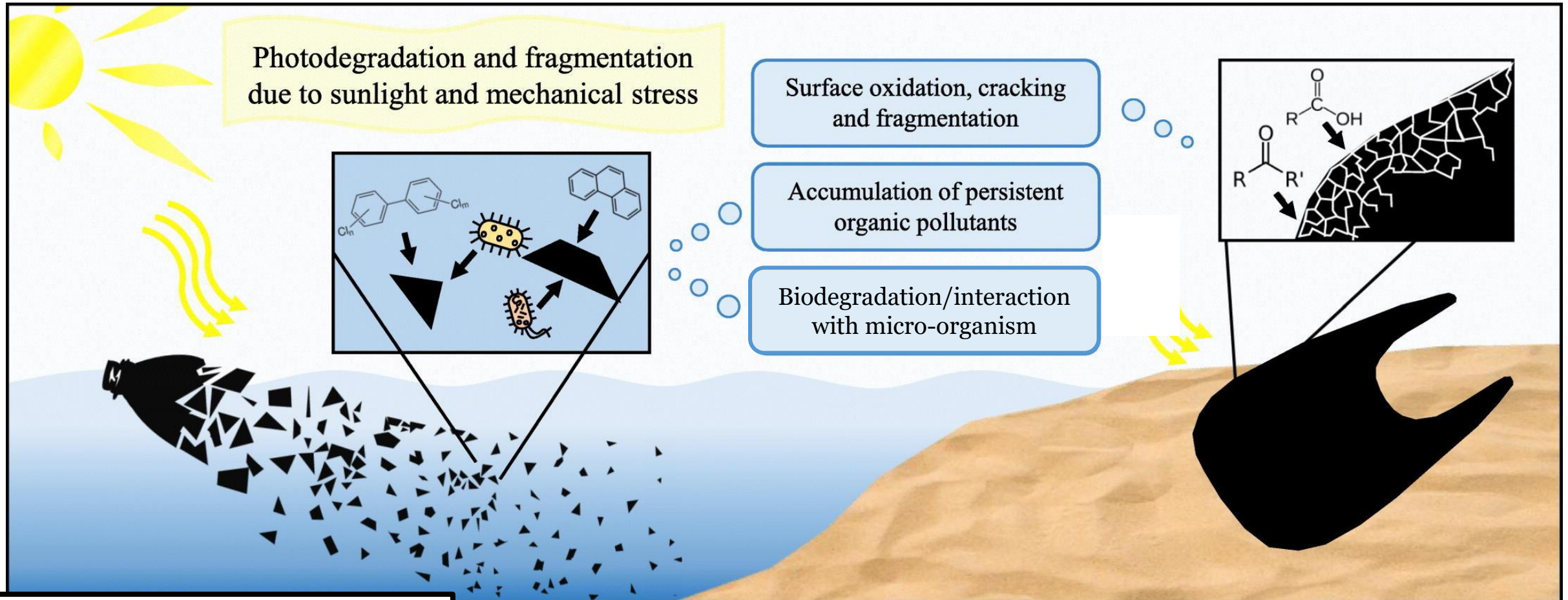
Disposable diaper
500 years



Plastic toothbrush
500 years

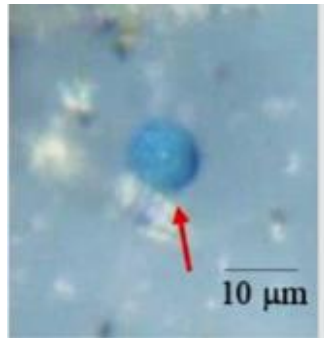
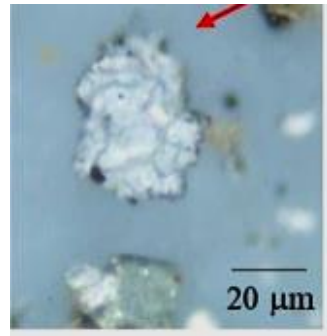
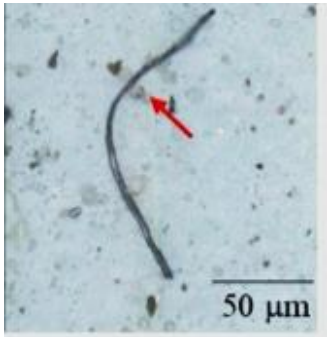
...and PLASTIC Life

It degrades and fragments!



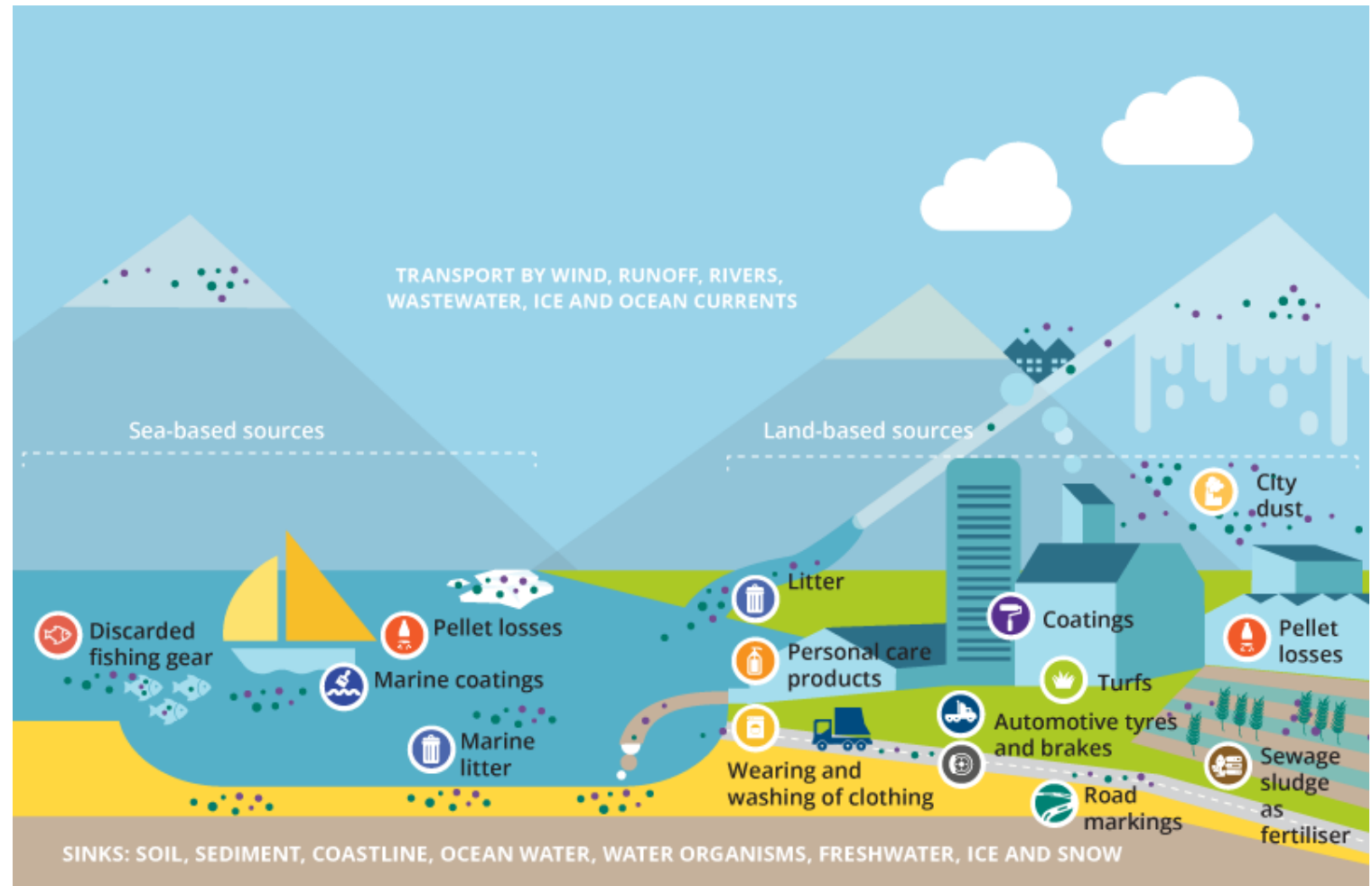
Microplastics: a “special” atmospheric pollutant

Large variety of sizes, chemical compositions & shapes



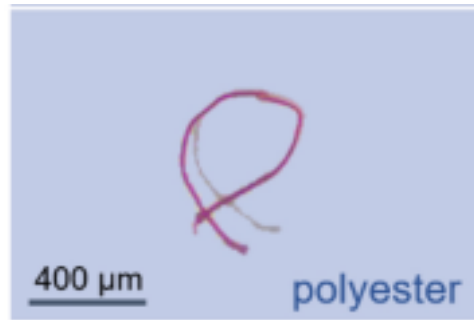
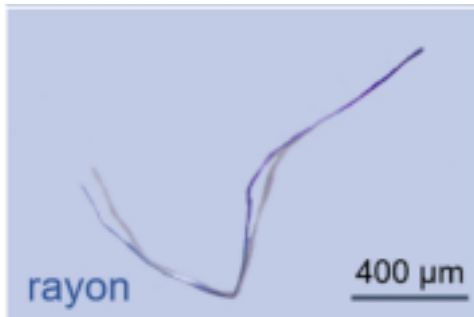
(Xie et al. 2022)

Complexity of sources



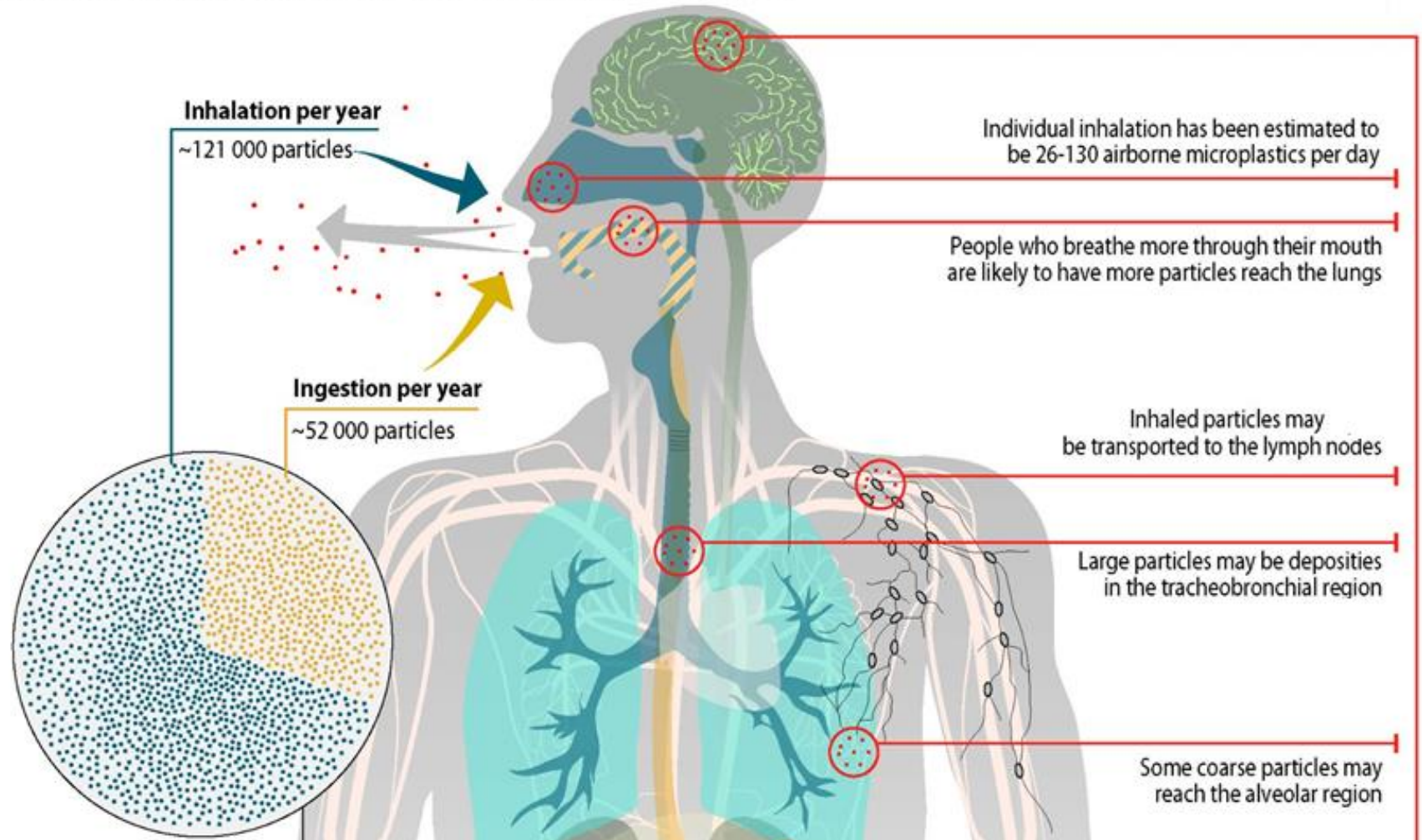
We breathe it

Microfibers found in the lungs!
(as long as mm!!!)



Chen et al., 2022

Human exposure to microplastic and nanoplastic particles

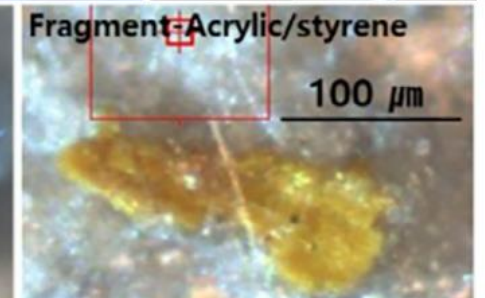
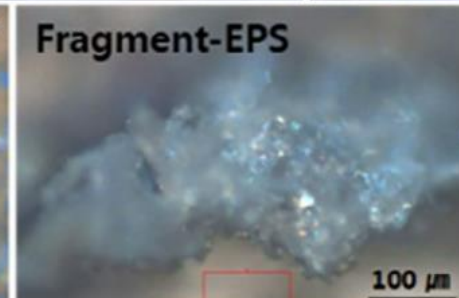
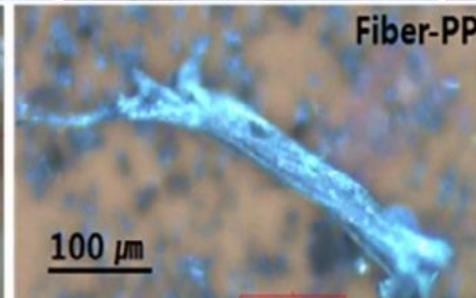
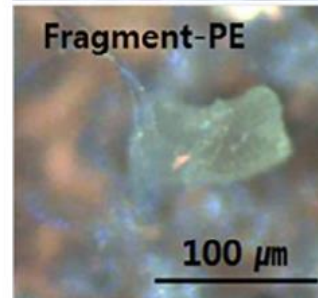
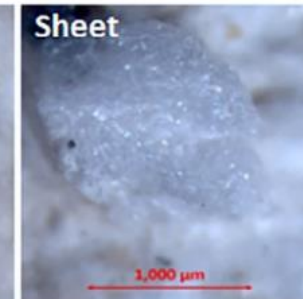
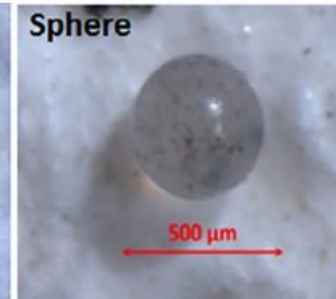
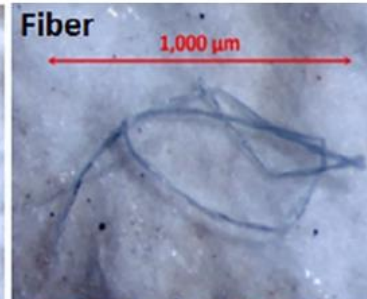
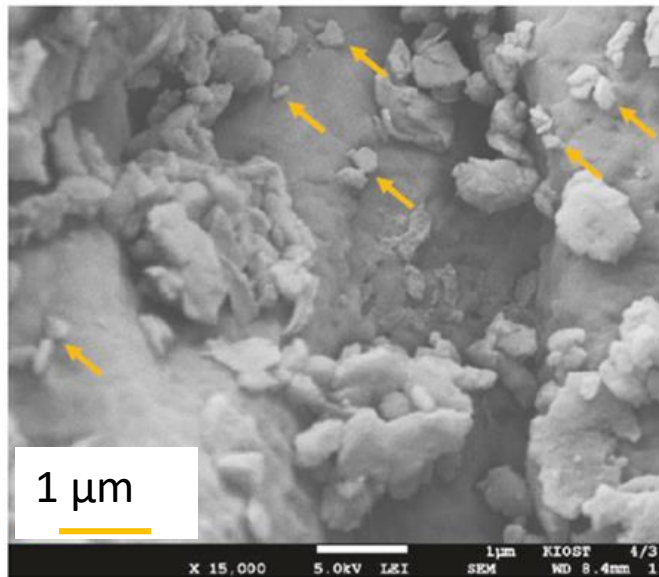


We get it in all sizes and shapes!

Particle category	Diameter range
	(mm = millimetres)
Nanoplastics	< 0.0001 mm (0.1µm)
Small microplastics	0.0001 – 1 mm
Large microplastics	1 – 4.75 mm
Mesoplastics	4.76 – 200 mm
Macroplastics	>200 mm

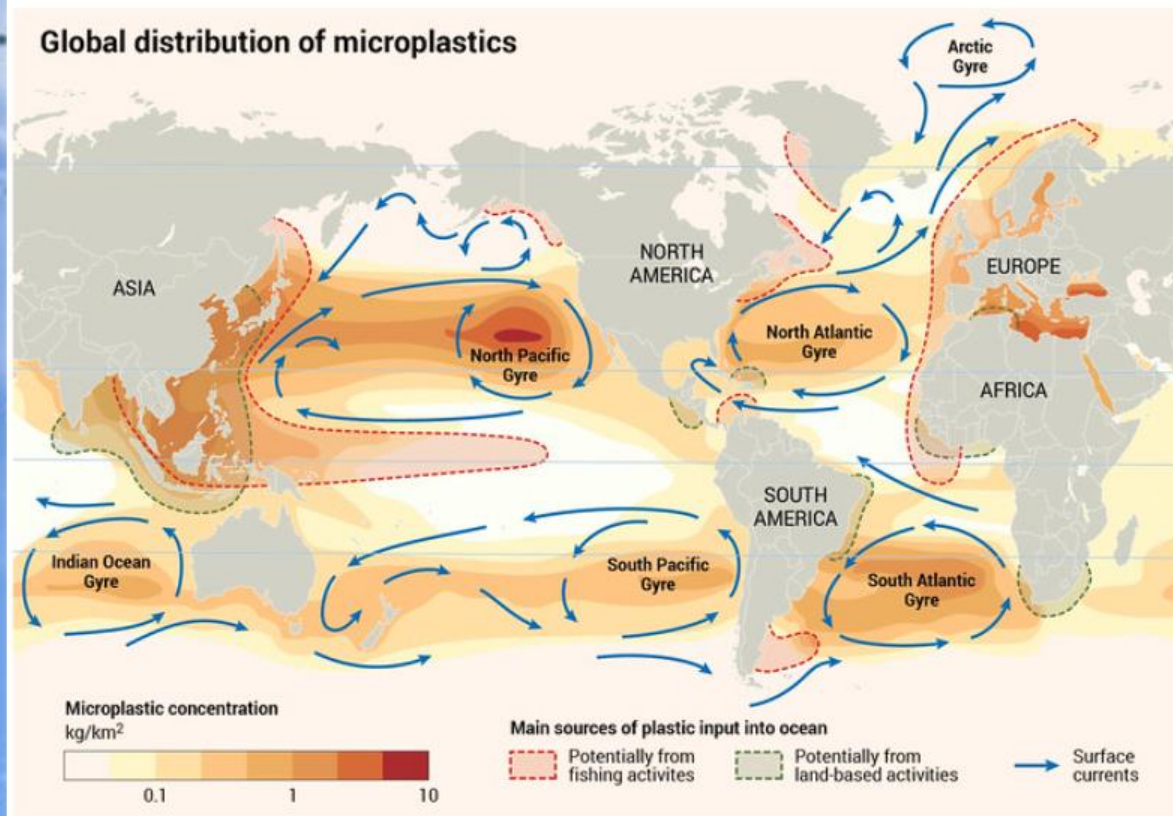
Those factors affects the **transport properties** of the microplastic in the different environmental sectors

Shim et al.,
2018

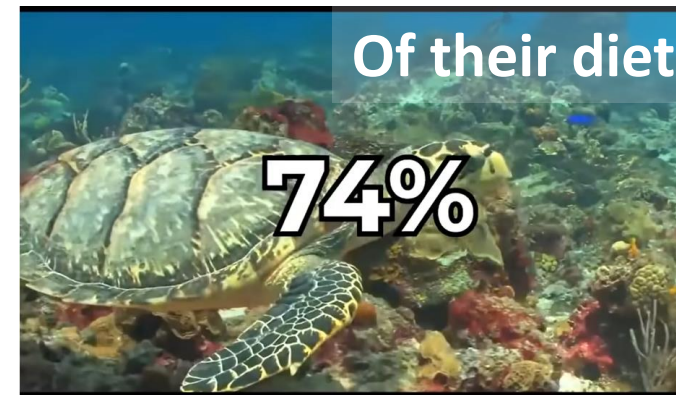


We get it everywhere

Floating on the surface of the ocean



Sebille et al., 2015

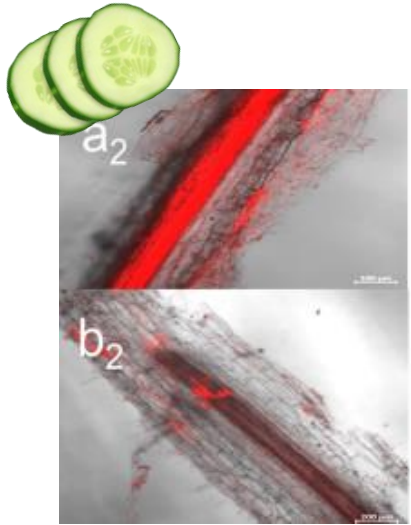


<https://theoceancleanup.com/trash-island/>

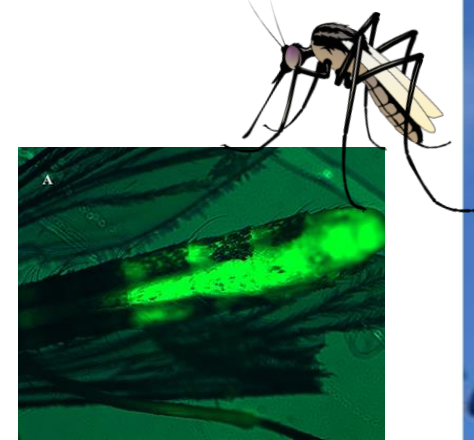
We get it everywhere

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In marine and terrestrial living organisms, plants, animals, our organs



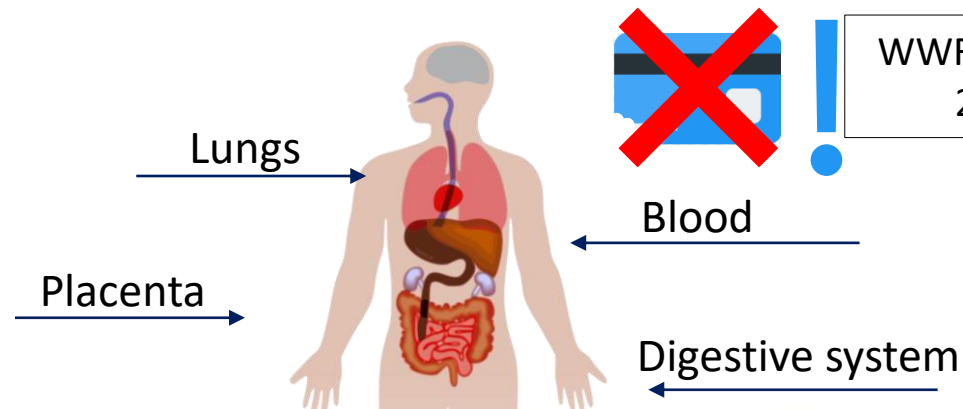
Li et al. 2021



Al-Jaibachi et al. 2018



Cole et al. 2013



WWF analysis
2019

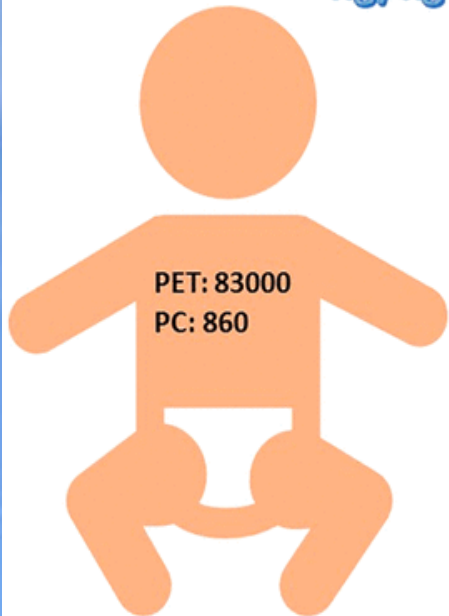


e.g. Fournier 2021, Ragusa et al. 2021, Leslie et al. 2021, Amato-Lourenço et al. 2021

We get it everywhere

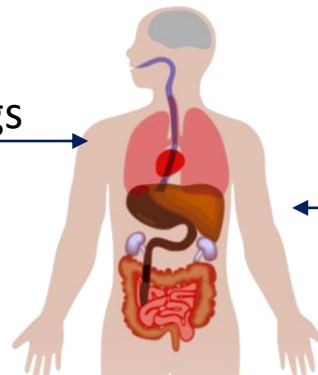
MICROPLASTICS EXPOSURE

ng/kg-bw/day



Placenta

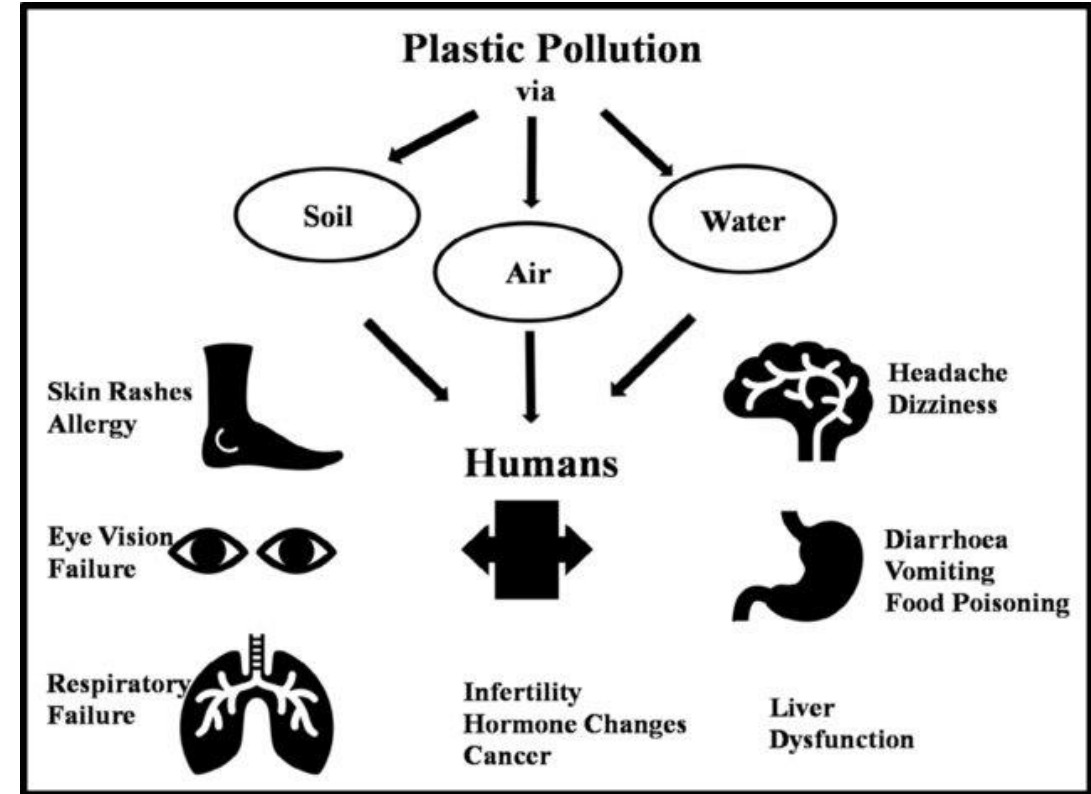
Lungs



WWF analysis
2019

Blood

Digestive system

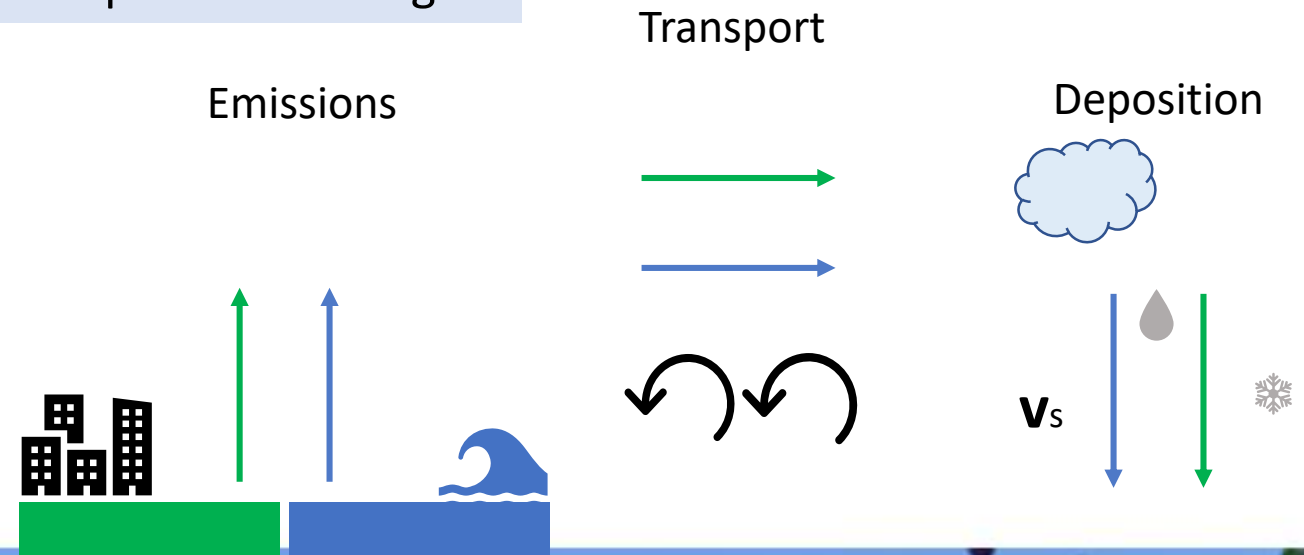


Limitations and challenges in modelling

- Very few emission inventories
- Transport processes are complex: shape, density, hygroscopicity, removal, reactions.
- Off-the-shelf aerosol models are not adequate

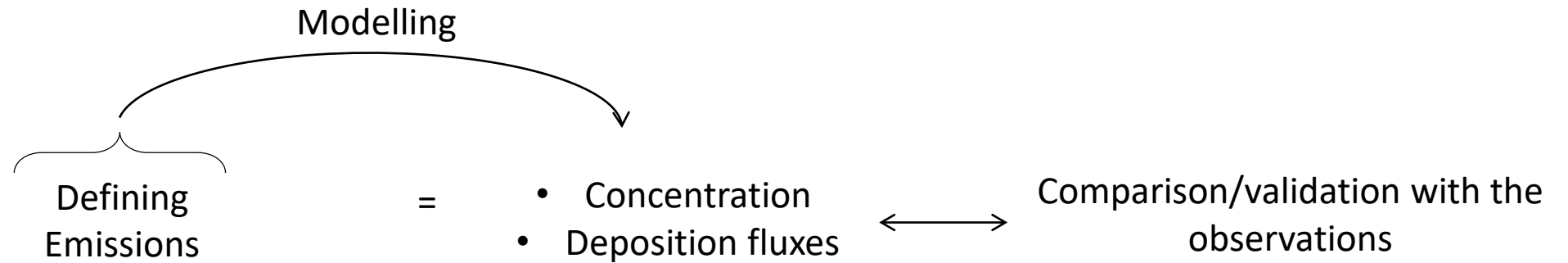
- Need proper source estimates
- Need dedicated particle models

Microplastic challenges:



Emission inventories

The approach:



First steps undertaken:



Oceanic source

~1 kton/year, (**Bucci** et al, 2024)



Arid regions source

~0.1 kton /year, (Evangelou et al 2024)



Road traffic source

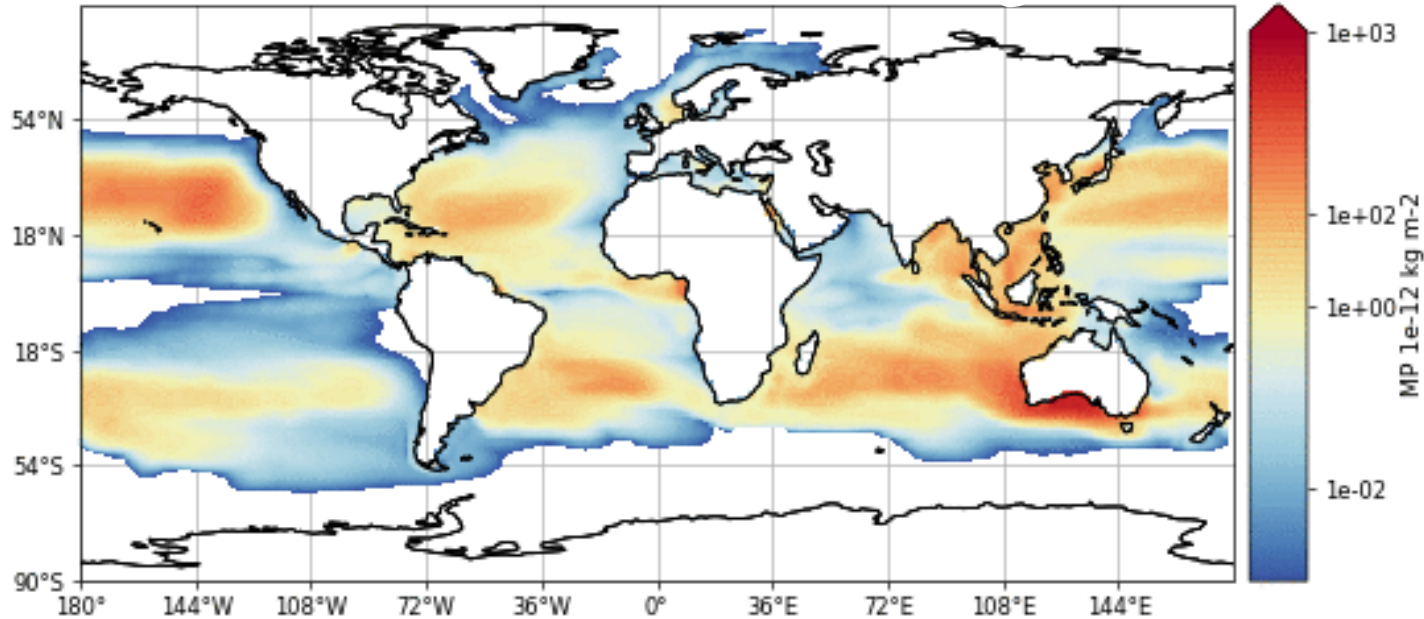
~4000 kton /year, (Tatsii et al, 2025)



An example

Ocean: From emissions to dispersion and deposition

MP emissions tot 2014-01-01 00:00



Flexpart trajectories simulations:

- 50 million trajectories in total
- Every 6 hours
- Travelling forward for 2 months

3D Simulations for a whole year



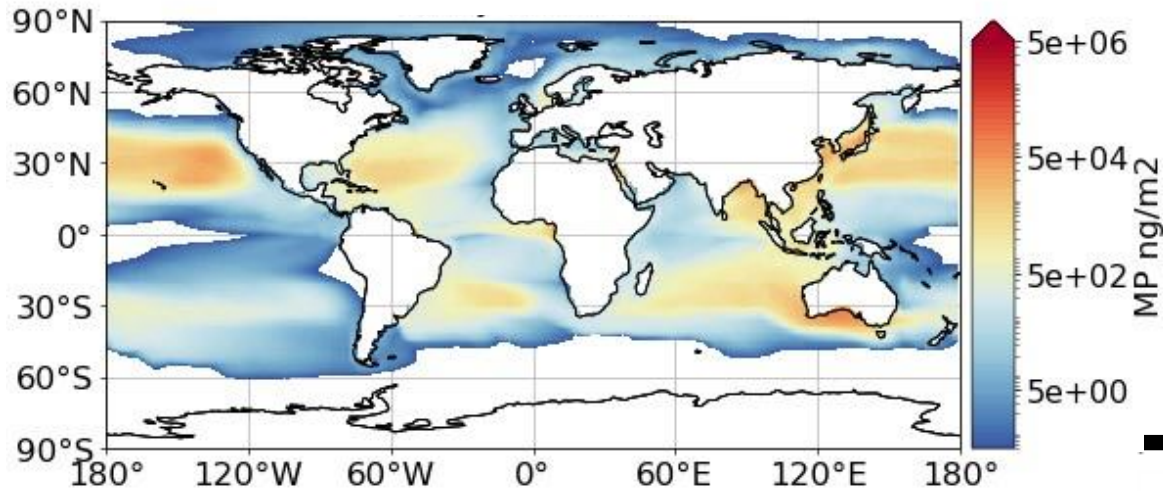
One simulation for each size range
($D_p=1, 5, 10, 25, 50 \mu\text{m}$)



Bucci et al. 2024

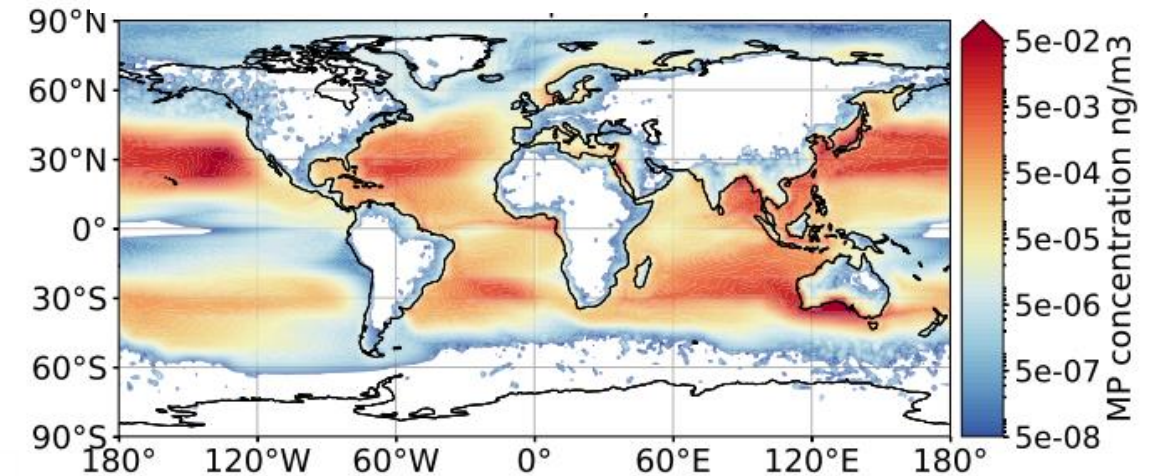
Global dispersion of MP 50 μm

MP emissions (yearly)



Atmospheric
transport

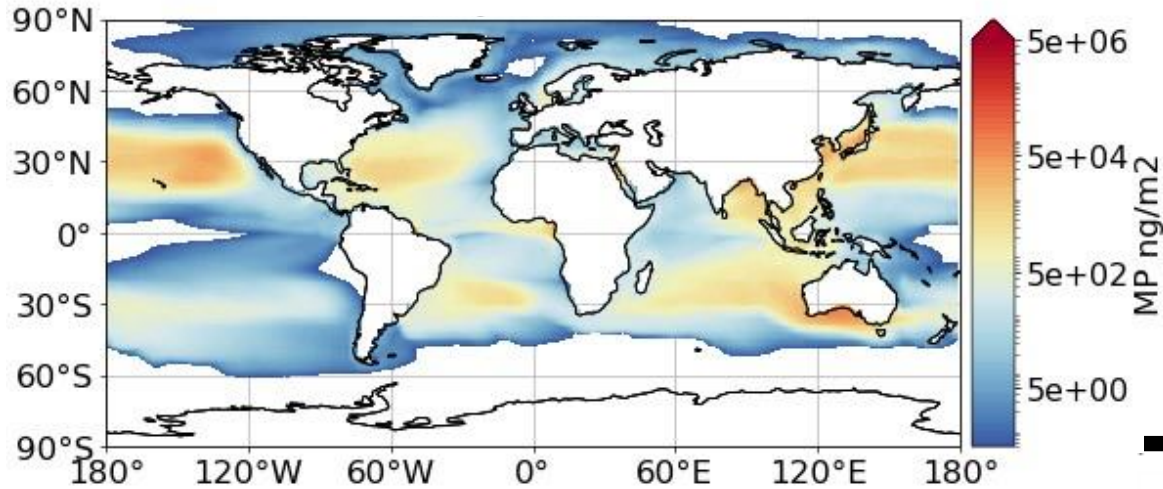
MP concentration (Big particles)



- MP distributed **close to the sources**, it hardly reaches the inland but rather the **coast**.

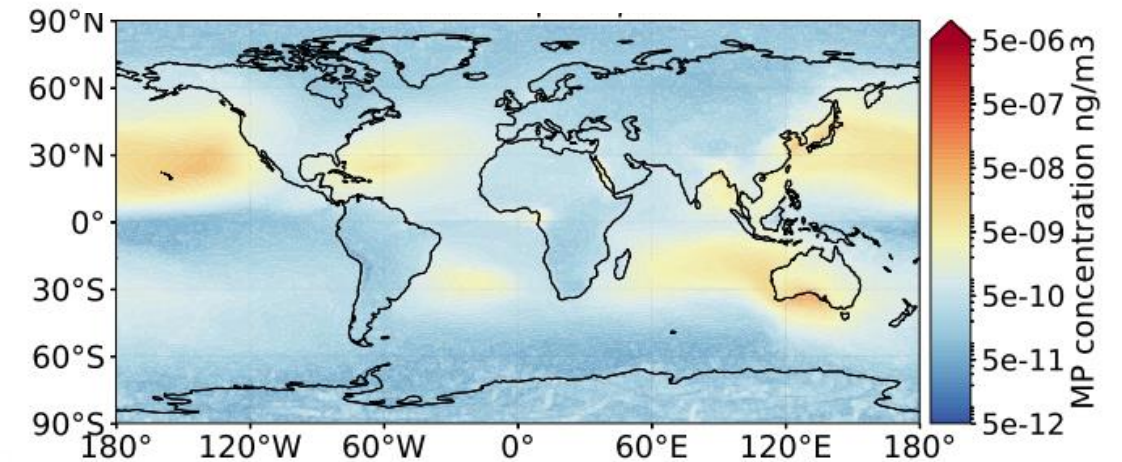
Global dispersion of MP 1 μm

MP emissions (yearly)



Atmospheric
transport

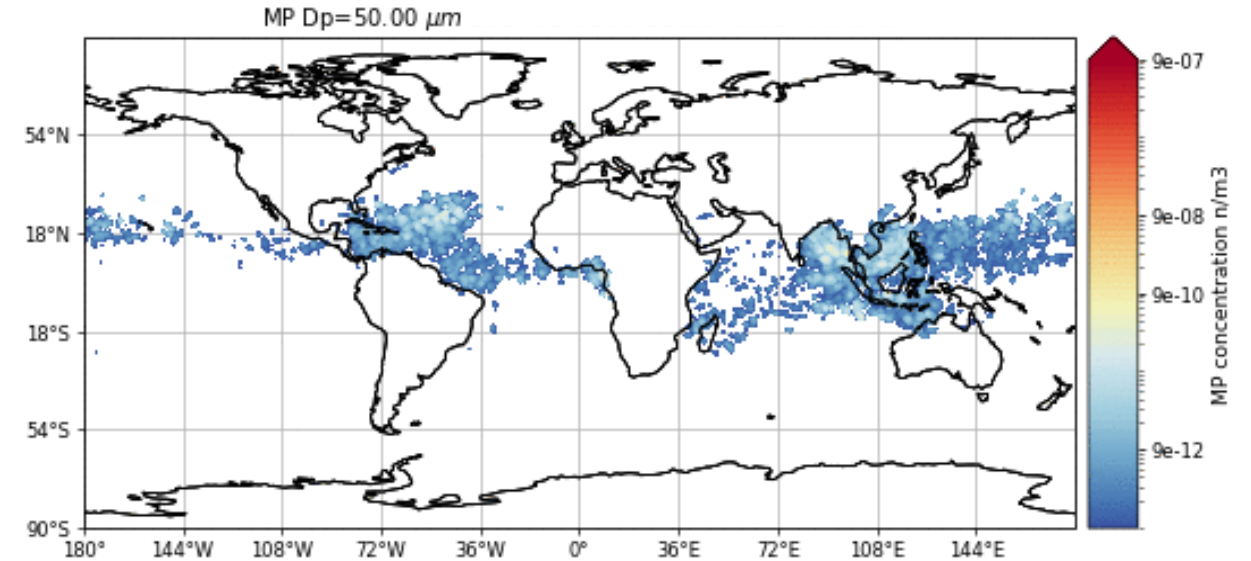
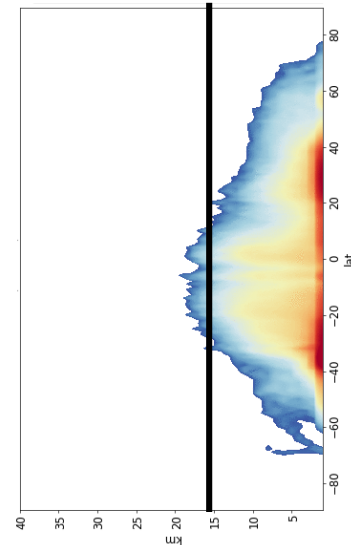
MP concentration (Small particles)



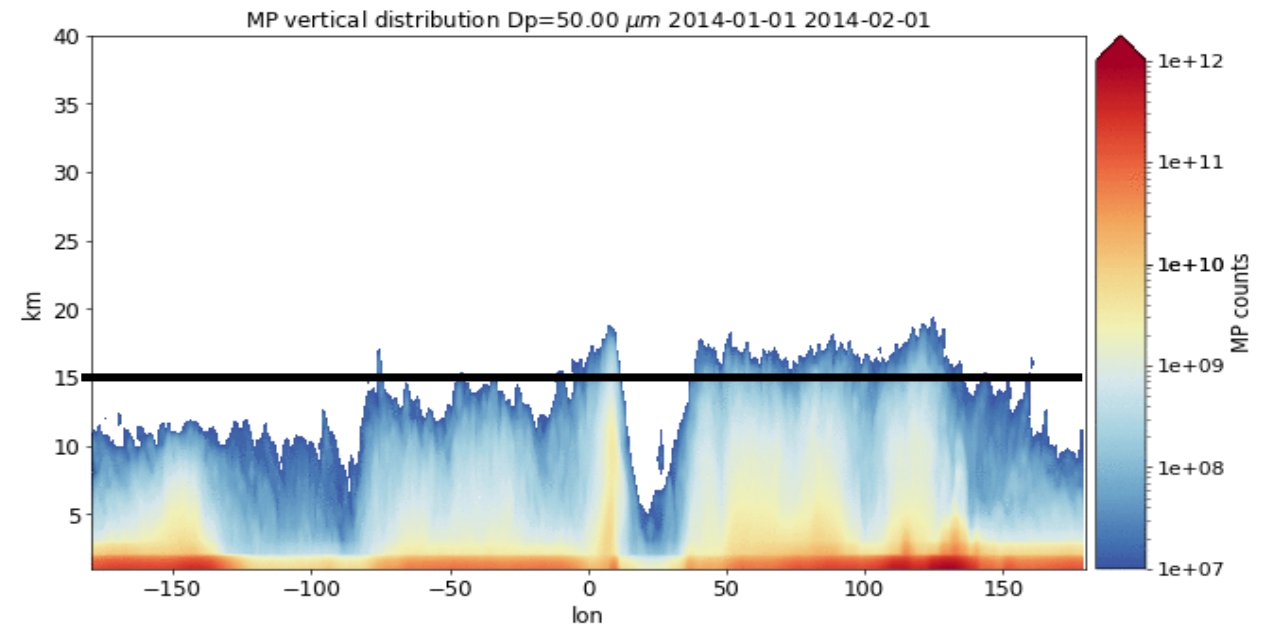
- Widespread distribution for smaller particles!

Vertical distribution: big particles

$D_p = 50 \text{ } \mu\text{m}$

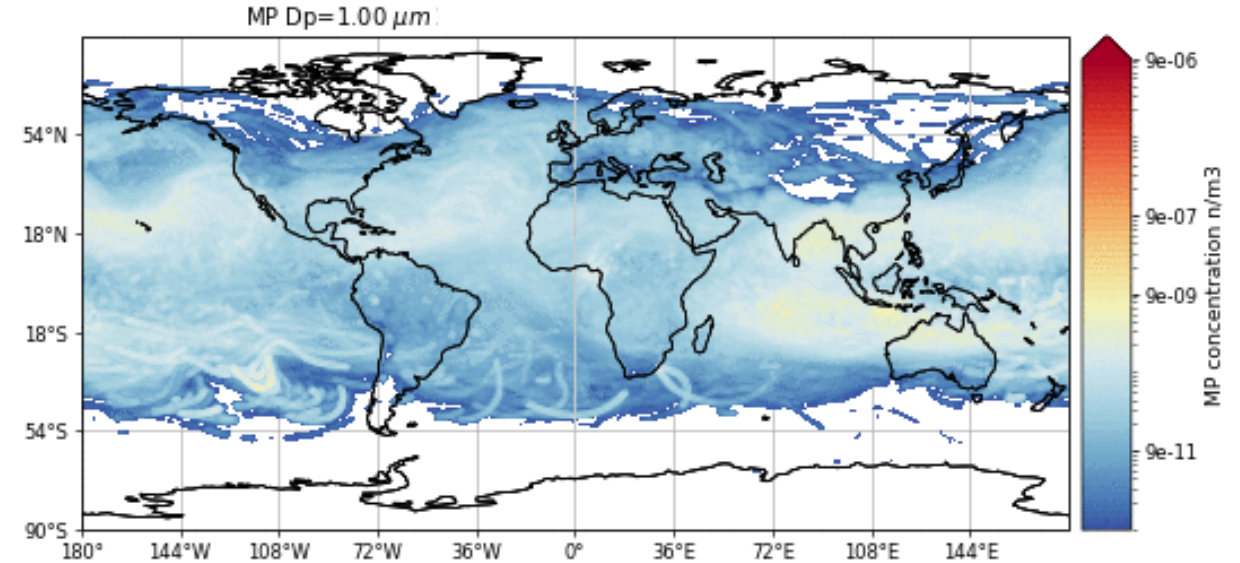
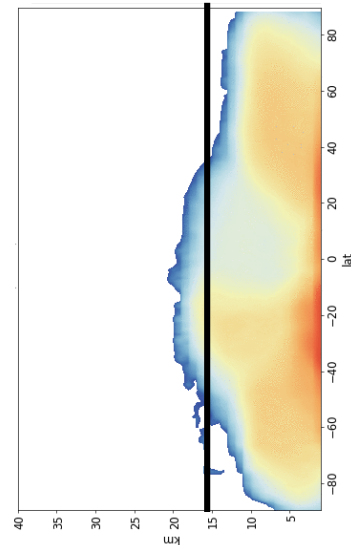


Injections of MP of relatively big dimensions (up to the $\sim 50 \text{ } \mu\text{m}$) in the free troposphere!

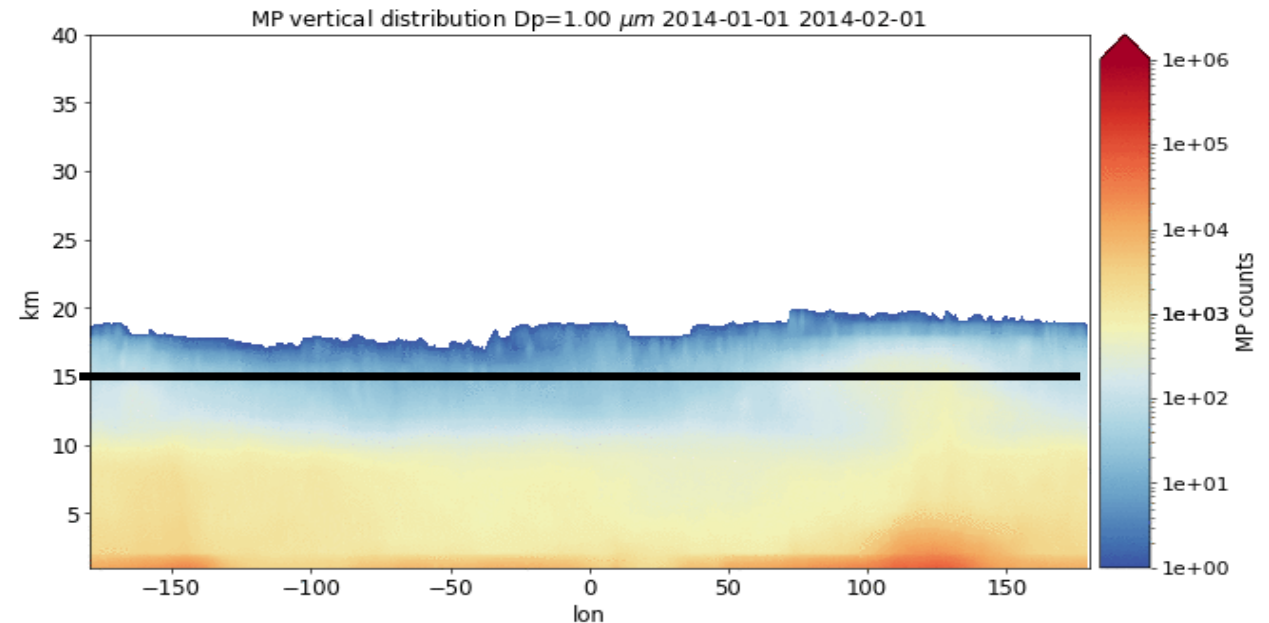


Vertical distribution: small particles

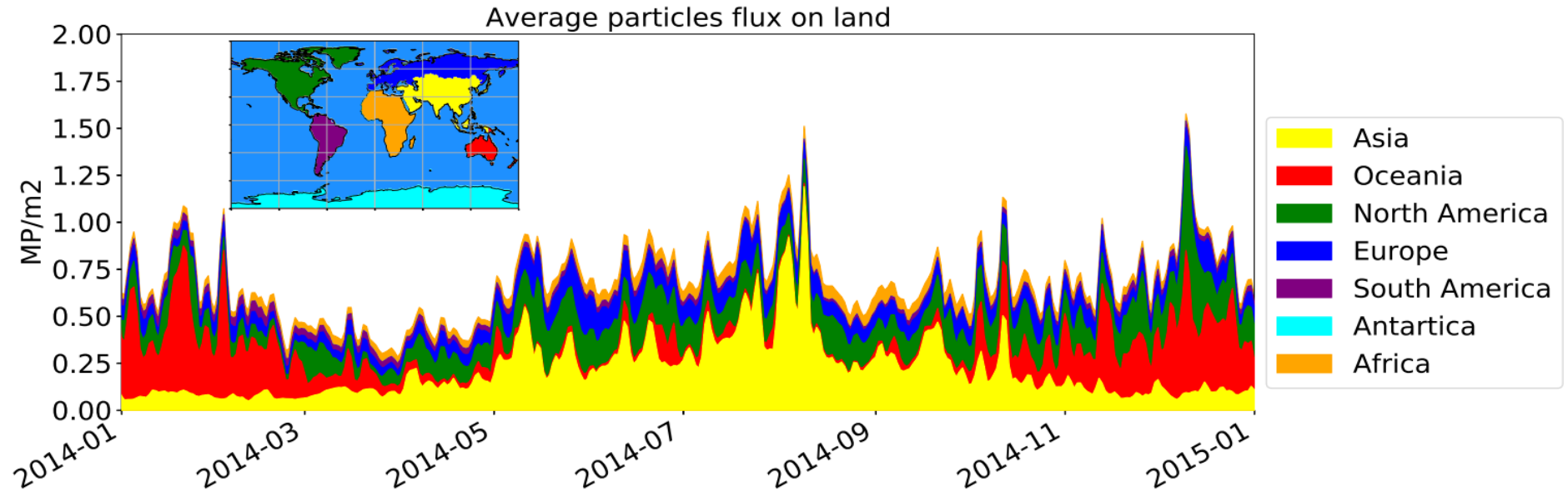
$D_p = 1 \mu\text{m}$



Injections of MP of relatively big dimensions (up to the $\sim 50 \mu\text{m}$) in the free troposphere!



Deposition fluxes



Larger deposition fluxes in

ASIA

OCEANIA

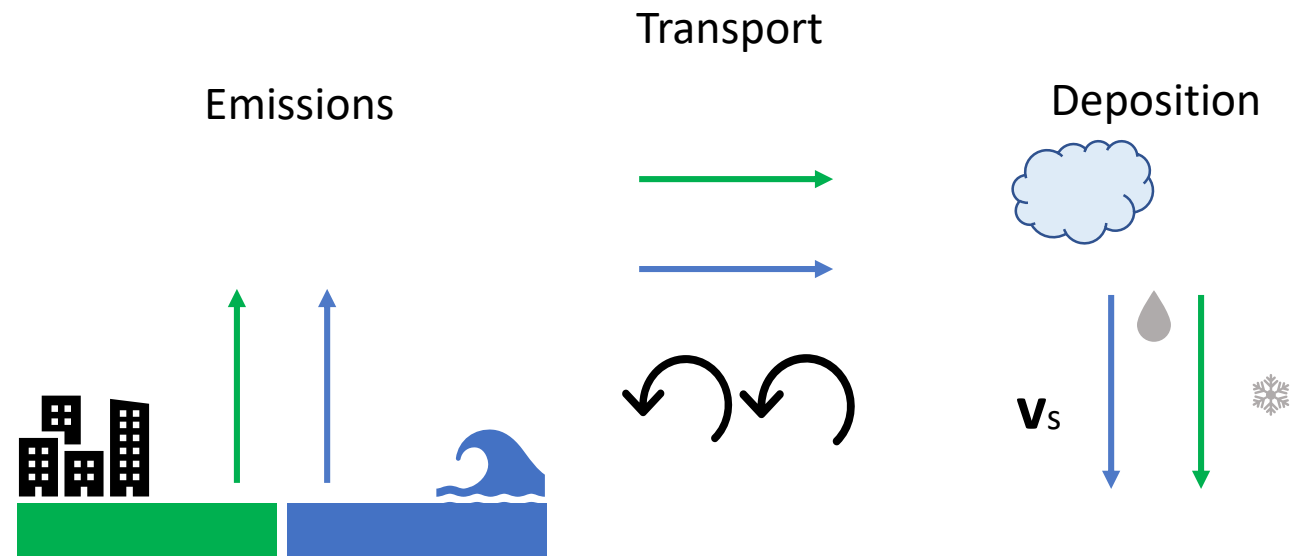


The model needs to be adjusted to account for the **aerodynamic behaviour of microplastic**.

E.g. shape effect on settling velocity (Tatsii et al. 2024)

Microplastic challenges:

Let's understand first how we compute the dry deposition of aerosols

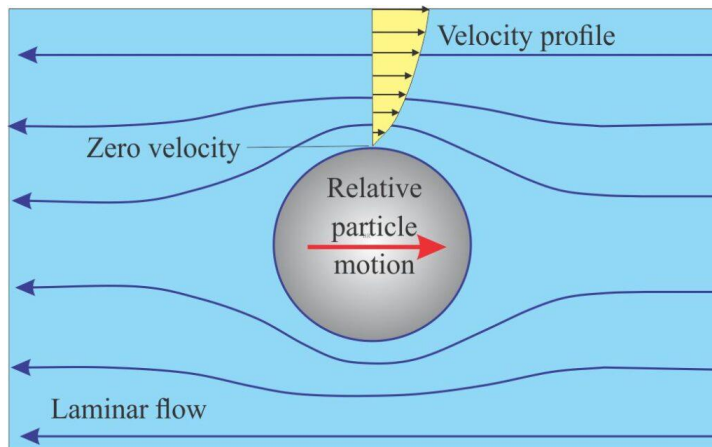


The settling velocity: we start with Stokes Law

Stokes Law

Stokes assumed particles were spherical

Stokes analysis requires laminar flow with **Reynolds Numbers** < 1 (this avoids the problem of turbulence).



Stokes Law expresses the fluid drag $\mathbf{F_d}$ as:

$$\mathbf{F_d} = 6\pi\mu\mathbf{vR} \text{ where}$$

μ is viscosity, $\mathbf{v}$ is mean velocity, and $\mathbf{R}$ is particle radius

Hence...Stokes' law and a constant viscosity estimate are used to start an iterative loop

The settling velocity: the initial computation

Settling velocity (w_s) occurs at the point where the buoyancy force equals the drag force.

$0 = \text{Drag force} - \text{buoyancy force}.$

The buoyancy weight is written as:

$$\frac{4}{3}\pi(D/2)^3\gamma \quad \text{where } \gamma \text{ is } \gamma = (\rho_p - \rho_a)g$$

ρ is the density of the particle and air respectively.

Therefore, the equality is written as:

$$\frac{1}{6}\pi D^3 \gamma = 3\pi\mu V D$$

such that the settling velocity w_s for $Re < 1$ is:

$$w_s = \frac{1}{18} (\rho_p - \rho_a)g D^2 / \mu$$

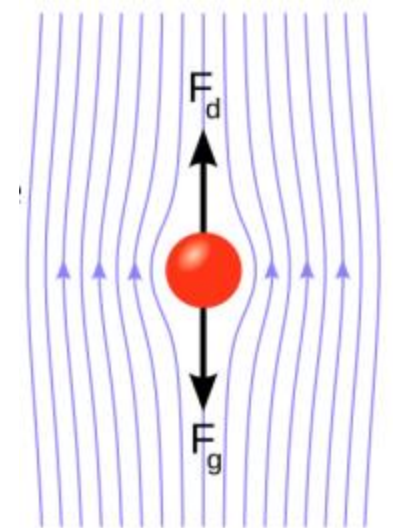
This is our initial settling velocity!

$$\nu = \frac{\mu}{\rho_{\text{air}}}$$

$$Re = \frac{d_{\text{eq}}|v_s|}{\nu}$$

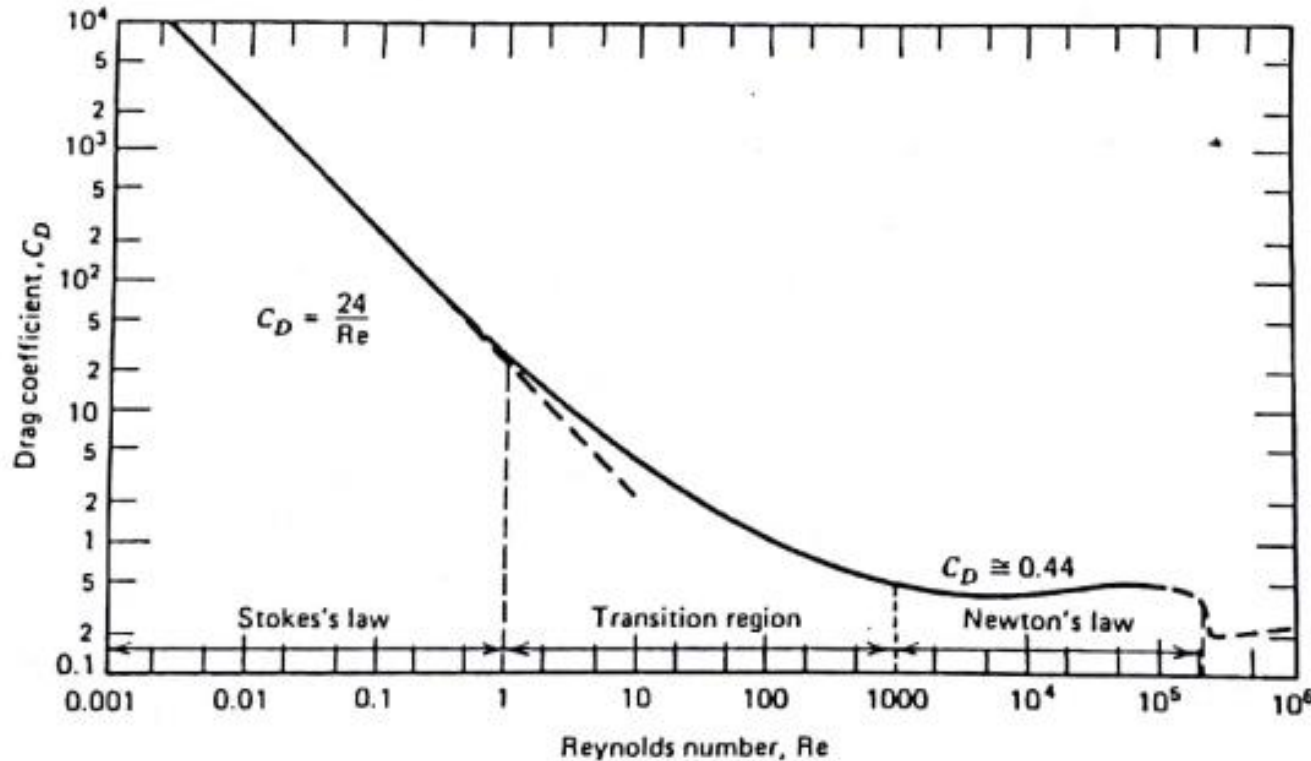
And this is our initial Re !

$$\text{Drag force } F_d = 6\pi\mu\nu R = 3\pi\mu\nu D$$



$$\text{Buoyancy force } F_b = -F_g = \rho V g$$

Settling velocity: we determine the drag coefficient



A well-known relation is given by Bird et al. (1960):

$$C_d = \frac{24}{Re} \quad (Re < 0.1, \text{ Stokes regime});$$

$$C_d = \frac{18.5}{Re^{3/5}} \quad (Re < 500, \text{ intermediate regime});$$

$$C_d = 0.44 \quad (Re > 500, \text{ turbulent regime})$$

After the first initialization with the Stokes Law we need to take into account all the following processes.
We introduce the Drag Coefficient C_D

Beware that what I am showing here is a simplification, FLEXPART v11 has a more complex C_d computation now
See Bakels et al. 2024

Settling velocity: we determine the drag coefficient

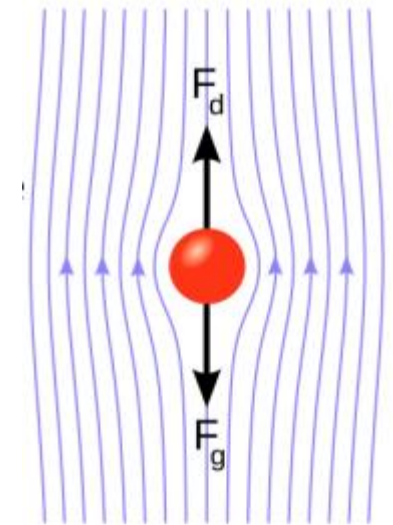
If Re is not < 1 , as for larger particles, inertial forces become important, increasing the drag. Numerical iterative solutions are needed, as the drag depends on the Reynolds number!

do $i=1,20$! do a few iterations

```
if (reynolds.lt.1.917) then
  c_d=24./reynolds
else if (reynolds.lt.500.) then
  c_d=18.5/(reynolds**0.6)
else
  c_d=0.44
endif
```

```
settling=-1.* &
  sqrt(4*ga*dquer(nsp)/1.e6*density(nsp)*cunningham(nsp)/ &
  (3.*c_d*airdens))
```

The iteration is stopped when converging



Terminal settling velocity

$$V_{TS} = [(4 d \rho_p g) / (3 C_D \rho_g)]^{1/2}$$

Settling velocity: we determine the drag coefficient

If Re is not < 1 , as for larger particles, inertial forces become important, increasing the drag. Numerical iterative solutions are needed, as the drag depends on the Reynolds number.

do i=1,20 ! do a few iterations

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 c_d=24./reynolds

else if (reynolds.lt.500.) then

 c_d=18.5/(reynolds**0.6)

else

 c_d=0.44

endif

Just to clarify what we use for what...

settling=-1.* &

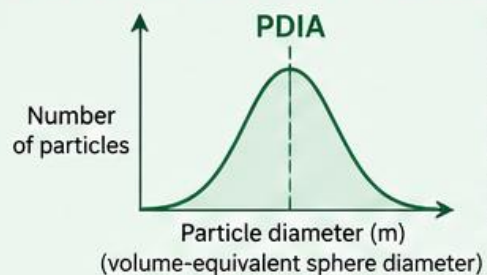
 sqrt(4*ga*dquer(nsp)/1.e6*density(nsp)*cunningham(nsp)/ &
 (3.*c_d*airdens))

The iteration is stopped when converging

reynolds=dquer(nsp)/1.e6*abs(settling)/vis_kin

How aerosol shapes are handled in FLEXPART

PDIA and PDSIGMA – size distribution

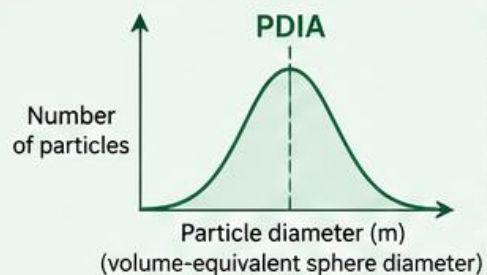


PDIA = geometric mean diameter (m)

PDSIGMA = geometric standard deviation (spread of the size distribution)

How aerosol shapes are handled in FLEXPART

PDIA and PDSIGMA – size distribution

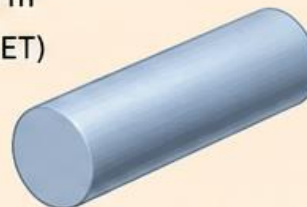


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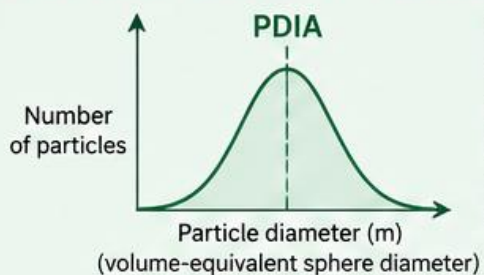
PDENSITY – particle material density

$\rho_p = 1.4 \times 10^3 \text{ kg m}^{-3}$
(e.g. polyester/PET)



How aerosol shapes are handled in FLEXPART

PDIA and PDSIGMA – size distribution

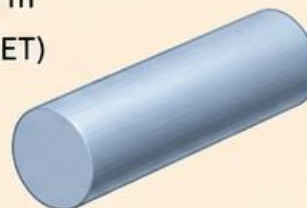


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PCRAIN_AERO, PCSNOW_AERO, PCCN_AERO, PIN_AERO – wet scavenging



Parameters controlling below-cloud and in-cloud scavenging. Values are uncertain for microplastics and are often kept fixed in sensitivity studies.

How aerosol shapes are handled in FLEXPART

PSHAPE – particle shape



0 = sphere
(PDIA)



1 = general ellipsoid
(PLA, PIA, PSA)



2 = cylinder (fibre)
(PDIA, PASPECTRATIO)



3 = cube



4 = tetrahedron



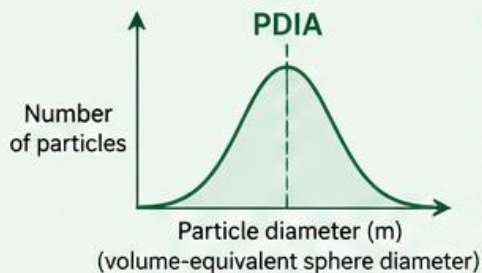
5 = octahedron



6 = ellipsoid

Among all shapes,
let's take the «cylinder»
as an example

PDIA and PDSIGMA – size distribution

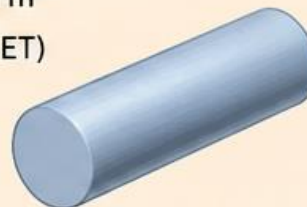


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How aerosol shapes are handled in FLEXPART

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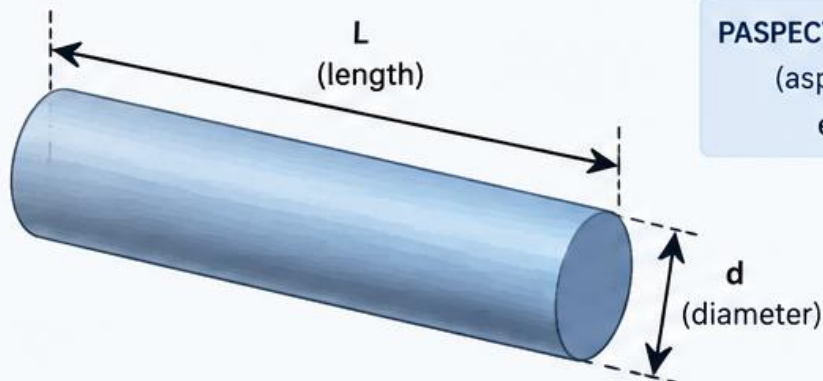
5 = octahedron



6 = ellipsoid

Cylinder (PSHAPE = 2)

Defined by an equivalent-volume diameter (PDIA) and an aspect ratio (PASPECTRATIO)

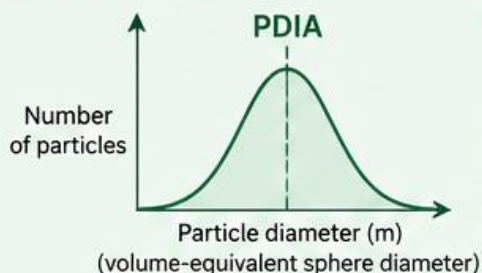


$$\text{PASPECTRATIO} = L / d$$

(aspect ratio)
e.g. 10

How does PDIA relate to the cylinder dimensions?

PDIA and PDSIGMA – size distribution



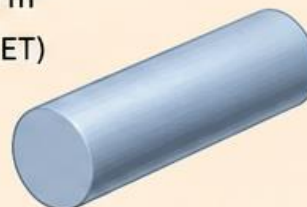
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(e.g. polyester/PET)



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How aerosol shapes are handled in FLEXPART

PSHAPE – particle shape



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(PDIA, PASPECTRATIO)



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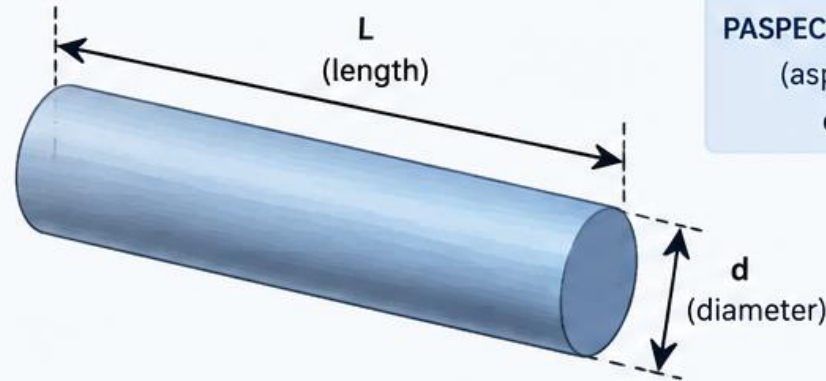
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Cylinder (PSHAPE = 2)

Defined by an equivalent-volume diameter (PDIA) and an aspect ratio (PASPECTRATIO)



$PASPECTRATIO = L / d$
(aspect ratio)
e.g. 10

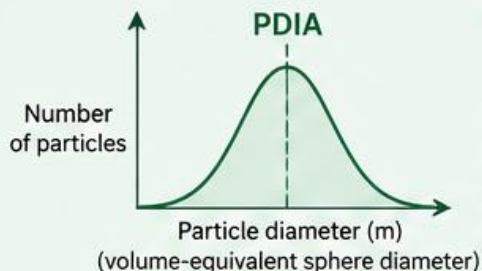
How does PDIA relate to the cylinder dimensions?

PDIA is the diameter of a sphere with the same volume as the cylinder.

For a cylinder with diameter d and length L :

$$V_{cyl} = \pi \left(\frac{d}{2} \right)^2 L = \frac{\pi d^2 L}{4}$$

PDIA and PDSIGMA – size distribution

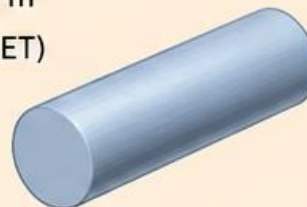


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$\rho_p = 1.4 \times 10^3 \text{ kg m}^{-3}$
(e.g. polyester/PET)



PCRAIN_AERO, PCSNOW_AERO, PCCN_AERO, PIN_AERO – wet scavenging



Parameters controlling below-cloud and in-cloud scavenging. Values are uncertain for microplastics and are often kept fixed in sensitivity studies.

How aerosol shapes are handled in FLEXPART

PSHAPE – particle shape



0 = sphere
(PDIA)



1 = general ellipsoid
(PLA, PIA, PSA)



2 = cylinder (fibre)
(PDIA, PASPECTRATIO)



3 = cube



4 = tetrahedron



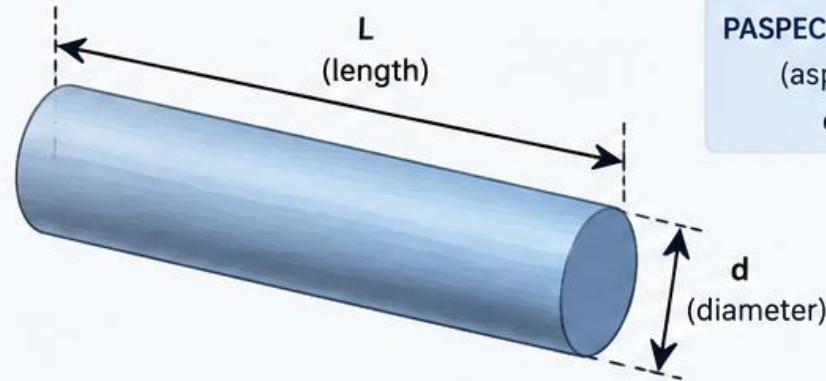
5 = octahedron



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Cylinder (PSHAPE = 2)

Defined by an equivalent-volume diameter (PDIA) and an aspect ratio (PASPECTRATIO)



$PASPECTRATIO = L / d$
(aspect ratio)
e.g. 10

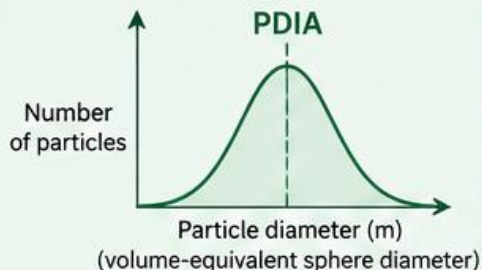
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PDIA and PDSIGMA – size distribution

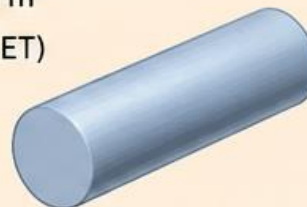


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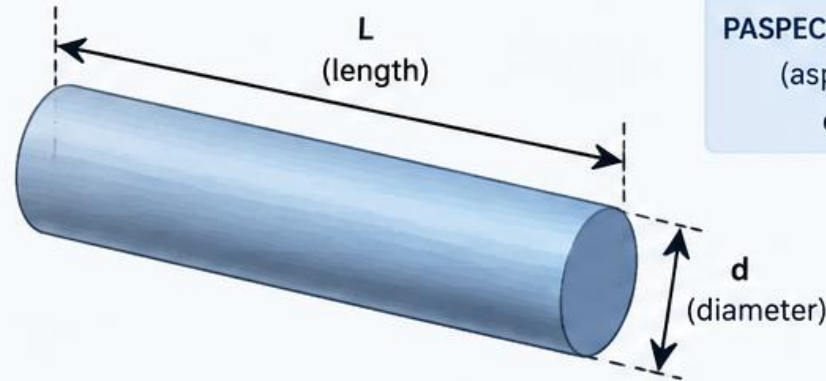
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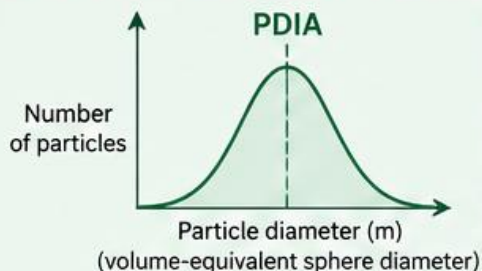
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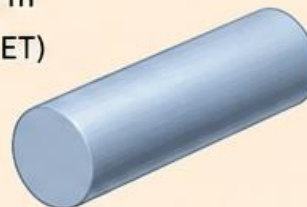


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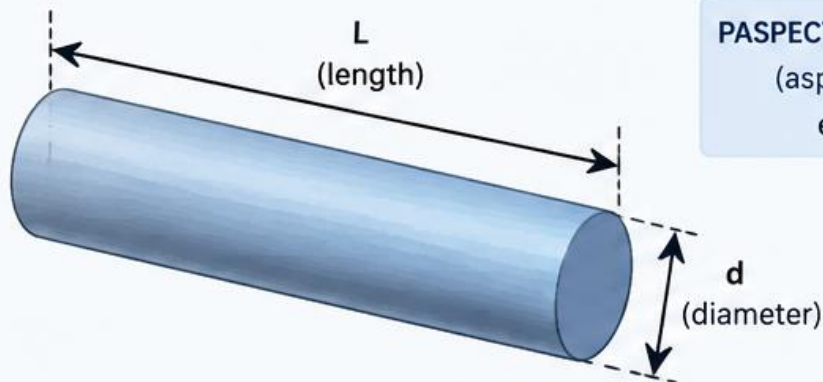
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$PASPECTRATIO = L / d$
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e.g. 10

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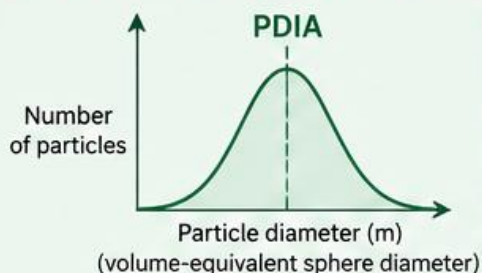
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For a cylinder with diameter d and length L :

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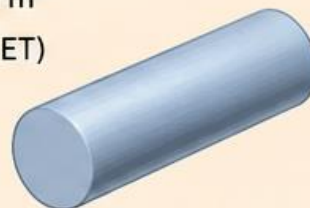


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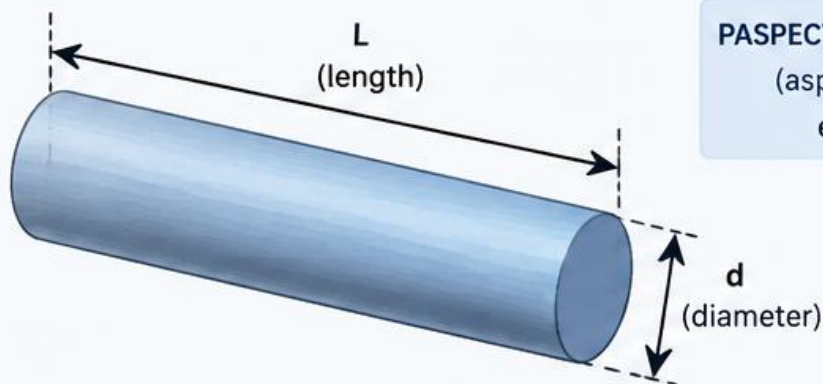
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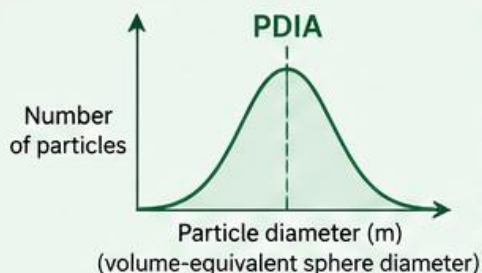
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PORIENT – particle orientation

0 = horizontal
Particles oriented horizontally



PDIA and PDSIGMA – size distribution

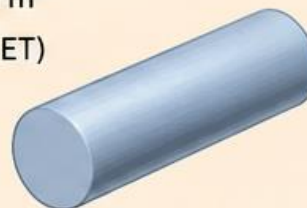


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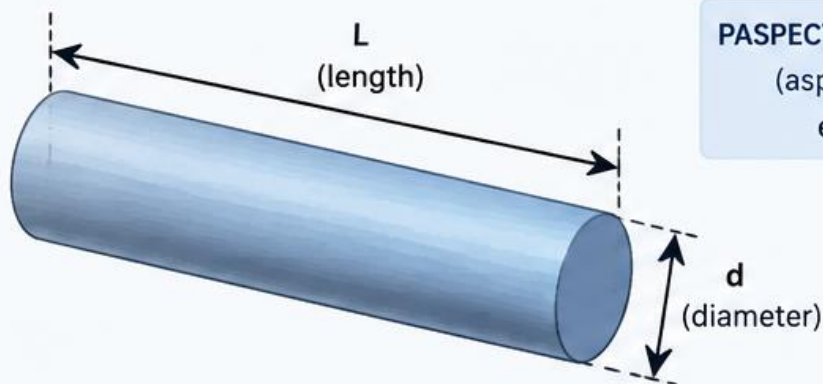
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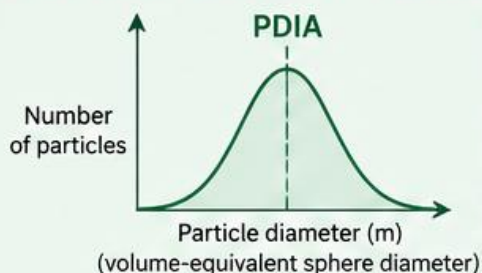
0 = horizontal
Particles oriented horizontally



1 = random
Random orientation of particles



PDIA and PDSIGMA – size distribution

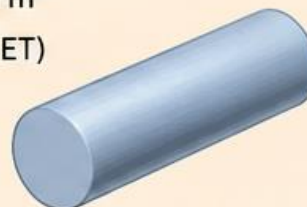


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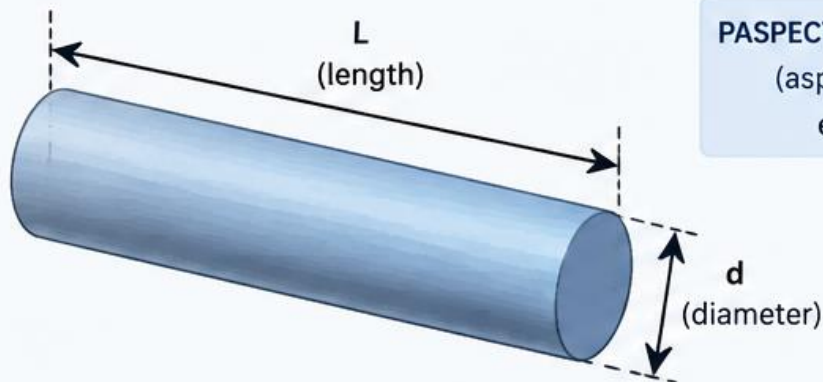
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Particles oriented horizontally



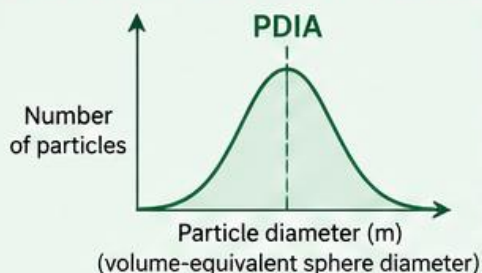
1 = random
Random orientation of particles



2 = averaged
Average between random and horizontal



PDIA and PDSIGMA – size distribution

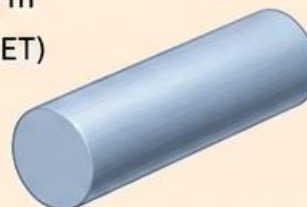


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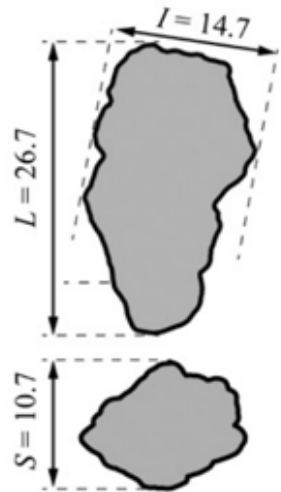
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Corrected drag coefficient: Tatsii et al. 2024

Equations to predict gravitational settling

Bagheri and Bonadonna 2016 shape-correction scheme



$$f = S/I$$

$$e = I/L$$

$$F_N = f^2 e$$

$$F_S = f e^{1.3}$$

The scheme is semi-empirical, based on experiments with irregular volcanic ash particles, cylinders, cubes, disks and ellipsoids.

We need to know three dimensions of a particle: longest (L), intermediate (I) and smallest (S) axes.

$$\alpha = 0.45 + 10/(\exp(2.5 \log \rho') + 30)$$

$$\beta = 1 - 37/(\exp(3 \log \rho') + 100)$$

$$\rho' = \frac{\rho_f}{\rho_p}$$

$$w_t = \sqrt{\frac{4gd_{eq}\rho_p C_{cun}}{3C_d \rho_f}}$$

$$C_d = \frac{24k_S}{Re} (1 + 0.125(Re \cdot k_N/k_S)^{2/3}) + \frac{0.46k_N}{1 + 5330/(Re \cdot k_N/k_S)}$$

$$k_{S,rand} = (F_S^{1/3} + F_S^{-1/3})/2$$

$$k_{N,rand} = 10^{\alpha[-\log(F_N)]^\beta}$$

The scheme considers two types of orientation: random and horizontal (max-drag).

w_t - settling velocity

C_d - drag coefficient

d_{eq} - volume equivalent diameter

g - gravitational acceleration

ρ_p - density of particle

ρ_f - density of fluid

C_{cun} - Cunningham slip correction factor

k_N - Stokes' drag correction

k_S - Newton's drag correction

α, β - empirical expressions

Re - Reynolds number

F_S - Stokes' form factor

F_N - Newton's form factor

4

Slide provided by
Dr. Daria Tatsii

Break time!

Let's do it ourselves: simulations with shape

Which morphology remains airborne longest and why?



Let's test a 1 week long simulation from an instantaneous release for the following cases:

Case	Equivalent diameter	Orientation	What are we testing?
Sphere (020)	30 μm	—	Reference case
Fibre AR_10 (021)	30 μm	Average	Effect of elongation
Fibre AR_50 (022)	30 μm	Average	Effect of elongation
Fibre AR_50 horizontal (023)	30 μm	Horizontal	Effect of orientation
Film (033) with 1 μm thickness	30 μm	Average	Effect of flattened shape

Let's do it ourselves: simulations with shape

Which morphology remains airborne longest and why?



Let's test a 1 week long simulation from an instantaneous release for the following cases:

*Beware that, while for the cylinders the dimensions from the equivalent spherical diameter are automatically computed, for the flat film you will have to compute the three sides of the film. **We will suppose that the film will have 1 μm thickness, and that it is a square!***

Volume of the film = $PLA \times PIA \times PSA$ with $PLA = PIA$ and $PSA = 1$ micron

SPECIES definition

Let's do it ourselves: simulations with shape

Which morphology remains airborne longest and why?



Let's test a 1 week long simulation from an instantaneous release for the following cases:

Let's say that we want to simulate a synthetic material, PET, that we said had density of around 1400 kg/m³

PDENSITY=1.4E3, ! Dry deposition (particles) – rho

Let's have a size distribution with standard deviation of 1.25 around the main equivalent diameter

PDSIGMA=1.25

SPECIES definition

Let's do it ourselves: simulations with shape

Which morphology remains airborne longest and why?



Let's test a 1 week long simulation from an instantaneous release for the following cases:

Finally for the scavenging properties...let's say it is very easily scavenged below cloud, it is a good cloud nuclei but a poor ice nuclei (for microplastic it is not well understood so far, hence it is only just an hypothesis)

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]

SPECIES definition

Let's do it ourselves: simulations with shape

Which morphology remains airborne longest and why?



Let's test a 1 week long simulation from an instantaneous release for the following cases:

We make a **forward simulation**, lasting 7 days, from 2017-09-25 00:00
(hence, start and end times are between 2017-09-25 00:00 and 2017-10-01 00:00)
Output time step to 1 hour

COMMAND, OUTGRID,
RELEASE definition

Gridded output between 20-65 E and 30-55 N with 0.5 space resolution, and from ground to 2500 m, with 100 m vertical resolution

Release at **35 E and 40 N**, between **0-1000m** , with **5000 particles, 1 kg of mass (MASS=1)**

Let's do it ourselves: simulations with shape

Which morphology remains airborne longest and why?



Let's test a 1 week long simulation from an instantaneous release for the following cases:

We also want to have some turbulence here:
CTL = 5, IFINE =10, LTURBULENCE=1

COMMAND, OUTGRID,
RELEASE definition

And we take into account convection too:
LCONVECTION=1

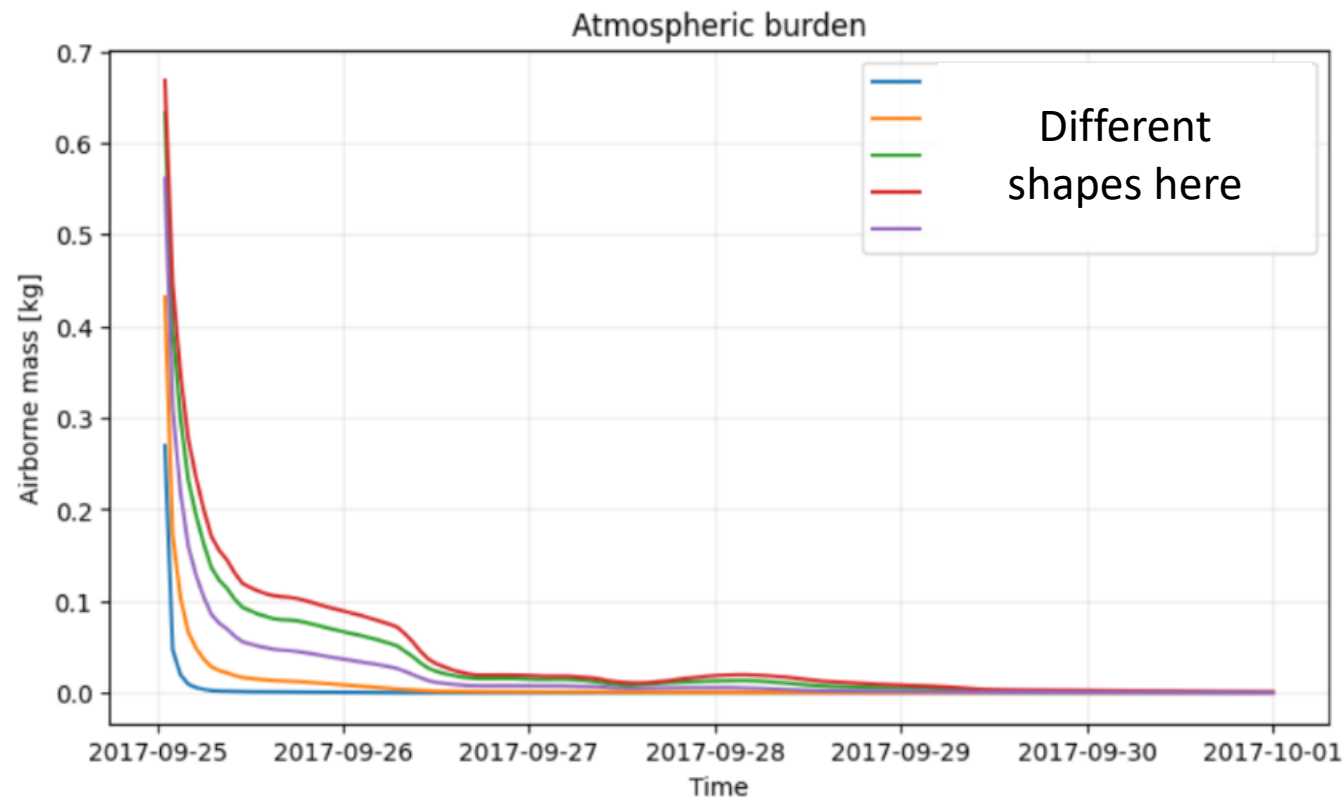
We released in mass and we want the concentration in mass too. Deposition as well, in forward mode. Hence...

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.

First question: total burden with time

Which morphology remains airborne longest and why?



To get the total burden in time in kg

Tot mass(t) =

$$\Sigma[\text{mass}(\text{ng}/\text{m}^3/\text{time}) * \text{area}(\text{m}^2) * \text{dz}(\text{m})] * 1\text{e-}12$$

For the deposition fluxes it will be

Flux mass dd(t) =

$$\Sigma[\text{mass}(\text{ng}/\text{m}^2/\text{time}) * \text{area}(\text{m}^2)] * 1\text{e-}12$$

Flux mass wd(t) =

$$\Sigma[\text{mass}(\text{ng}/\text{m}^2/\text{time}) * \text{area}(\text{m}^2)] * 1\text{e-}12$$

POINTS 3 and 4 of the notebook

POINT 5 is optional,
simply mapping the fields

Let's do it ourselves: simulations with shape

Which morphology remains airborne longest and why?

We want to get a table like this one, representing the total aerosol burden at the last time step.

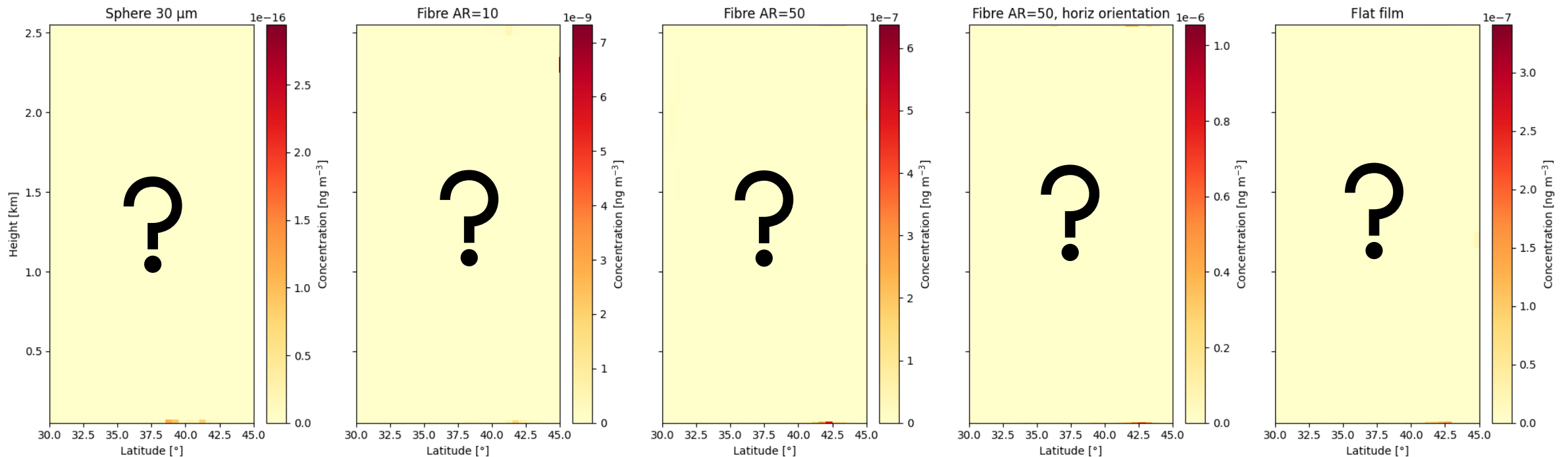
	Airborne [kg]	Dry deposited [kg]	Wet deposited [kg]	Airborne + deposited [kg]
Case				
Sphere 30 μm				
Fibre AR=10 ave.				
Fibre AR=50 ave.				
Fibre AR=50, <i>horizontal</i>				
Flat film, ave.				

POINT 6 of the notebook

Let's do it ourselves: simulations with shape

Does the shape also affect the vertical distribution?

We can check the latitude–height cross section of atmospheric concentration,
For ex. averaged over all longitudes, at the last 5 time steps



POINT 7 of the notebook

Some reflections



1. Which morphology appeared to remain airborne longest? Was your prediction correct?
2. Does changing **orientation** have an effect comparable to changing aspect ratio?
3. How does the **flat film** compare with the fibres and sphere, despite equal equivalent volume and density?
4. Why can wet deposition differ even though wet-scavenging parameters are identical?
5. If you look at the table produced in table 6, you'll notice that the total sum of airborne+deposited is <1 . Can you guess why?