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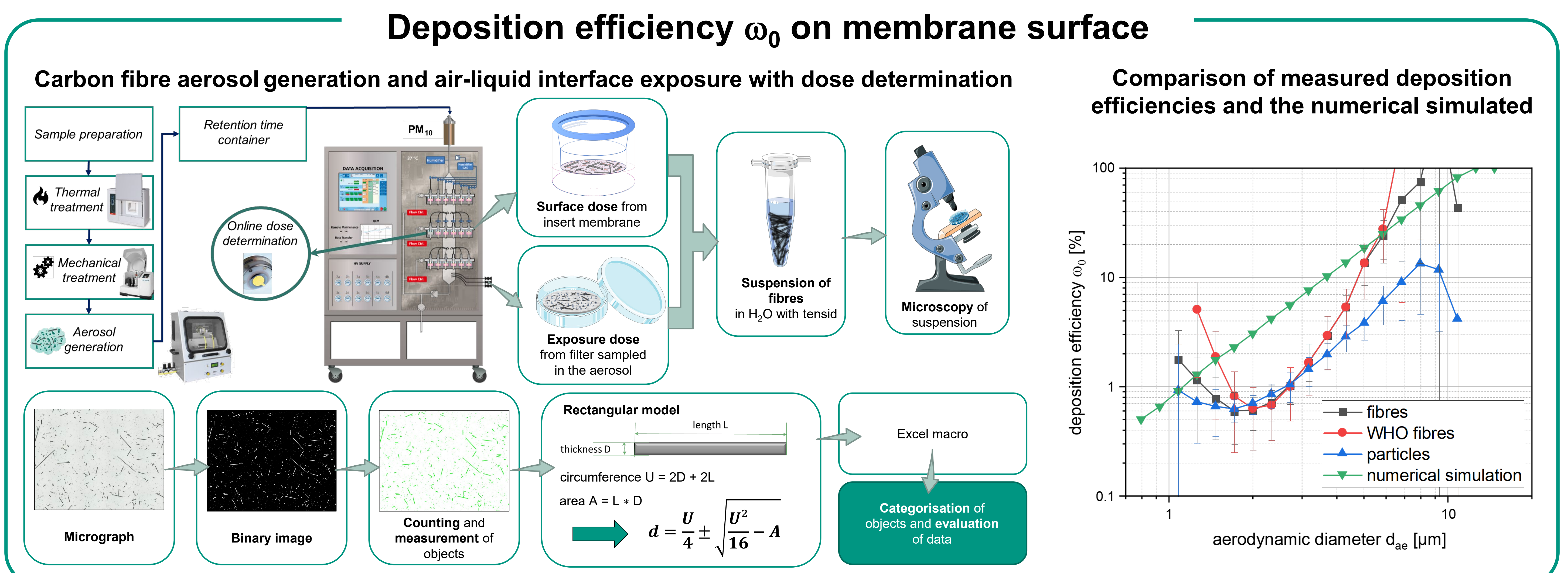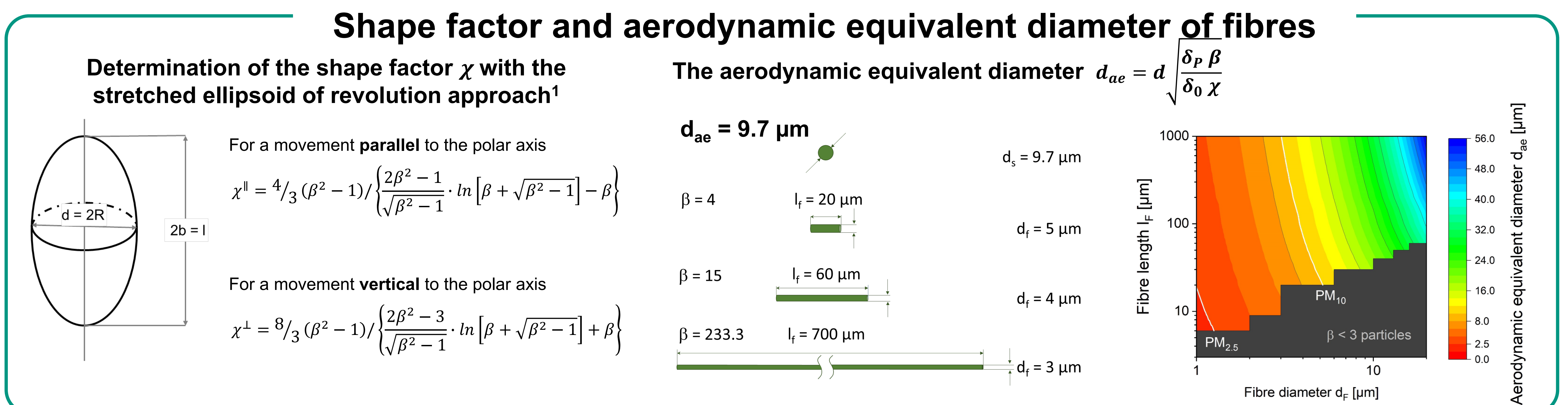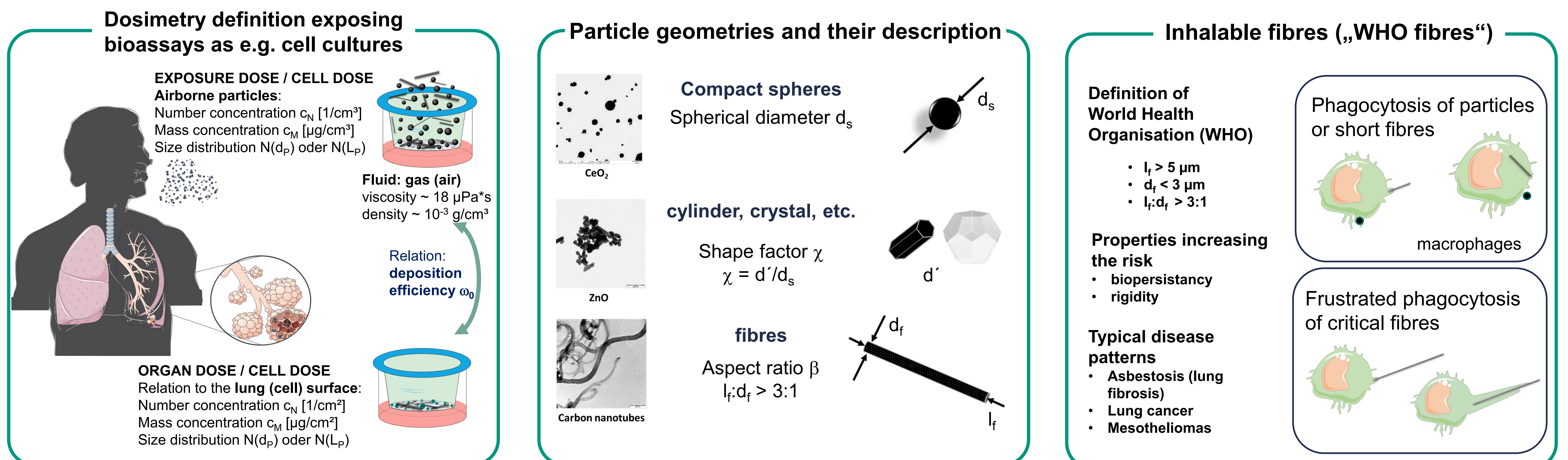**ITC** — Institute for Technical Chemistry

Numerical Simulation of Fibre Dose in an Air-Liquid-Interface Exposure System

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Dosimetry definition exposing bioassays as e.g. cell cultures

EXPOSURE DOSE / CELL DOSE
Airborne particles:
Number concentration c_N [1/cm³]
Mass concentration c_M [µg/cm³]
Size distribution $N(d_P)$ oder $N(L_P)$

Fluid: gas (air)
viscosity ~ 18 µPa*s
density ~ 10^{-3} g/cm³

Relation:
deposition efficiency ω_0

ORGAN DOSE / CELL DOSE
Relation to the **lung (cell) surface:**
Number concentration c_N [1/cm²]
Mass concentration c_M [µg/cm²]
Size distribution $N(d_P)$ oder $N(L_P)$

Particle geometries and their description

CeO₂

Compact spheres
Spherical diameter d_s

ZnO

cylinder, crystal, etc.
Shape factor χ
$\chi = d'/d_s$

Carbon nanotubes

fibres
Aspect ratio β
$l_f:d_f > 3:1$

Inhalable fibres („WHO fibres")

Definition of World Health Organisation (WHO)

- $l_f > 5$ µm
- $d_f < 3$ µm
- $l_f:d_f > 3:1$

Properties increasing the risk
- biopersistancy
- rigidity

Typical disease patterns
- Asbestosis (lung fibrosis)
- Lung cancer
- Mesotheliomas

Phagocytosis of particles or short fibres

macrophages

Frustrated phagocytosis of critical fibres

Shape factor and aerodynamic equivalent diameter of fibres

Determination of the shape factor χ with the stretched ellipsoid of revolution approach[1]

$d = 2R$
$2b = l$

For a movement **parallel** to the polar axis

$$\chi^{\parallel} = \frac{4}{3}(\beta^2-1)/\left\{\frac{2\beta^2-1}{\sqrt{\beta^2-1}}\cdot ln\left[\beta+\sqrt{\beta^2-1}\right]-\beta\right\}$$

For a movement **vertical** to the polar axis

$$\chi^{\perp} = \frac{8}{3}(\beta^2-1)/\left\{\frac{2\beta^2-3}{\sqrt{\beta^2-1}}\cdot ln\left[\beta+\sqrt{\beta^2-1}\right]+\beta\right\}$$

The aerodynamic equivalent diameter $d_{ae} = d\sqrt{\dfrac{\delta_P\,\beta}{\delta_0\,\chi}}$

d_{ae} = 9.7 µm

d_s = 9.7 µm
β = 4 l_f = 20 µm d_f = 5 µm
β = 15 l_f = 60 µm d_f = 4 µm
β = 233.3 l_f = 700 µm d_f = 3 µm

Fibre length l_f [µm] vs Fibre diameter d_F [µm]; Aerodynamic equivalent diameter d_{ae} [µm]; PM₁₀, PM₂.₅, $\beta < 3$ particles

Deposition efficiency ω_0 on membrane surface

Carbon fibre aerosol generation and air-liquid interface exposure with dose determination

Sample preparation → Thermal treatment → Mechanical treatment → Aerosol generation

Retention time container   PM₁₀

DATA ACQUISITION — Online dose determination

Surface dose from insert membrane

Exposure dose from filter sampled in the aerosol

Suspension of fibres in H₂O with tensid

Microscopy of suspension

Micrograph

Binary image

Counting and measurement of objects

Rectangular model
length L
thickness D

circumference U = 2D + 2L
area A = L * D

$$d = \frac{U}{4} \pm \sqrt{\frac{U^2}{16} - A}$$

Excel macro

Categorisation of objects and evaluation of data

Comparison of measured deposition efficiencies and the numerical simulated

deposition efficiency ω_0 [%] vs aerodynamic diameter d_{ae} [µm]
- fibres
- WHO fibres
- particles
- numerical simulation

References

1 Fuchs, N.A. (1964). The Mechanics of Aerosols. Pergamon Pr.: Oxford.
2 Friesen, A., Fritsch-Decker, S., Mülhopt, S., ..., M., Stapf, D., Hartwig, A., and Weiss, C. (2023). International Journal of Molecular Sciences, **24**, p. 1927.

More information

Please visit Poster 807:
Numerical Simulation of Fiber Deposition Behavior in an Air-Liquid Interface Exposure System, **Sven Klein et al.**

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