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

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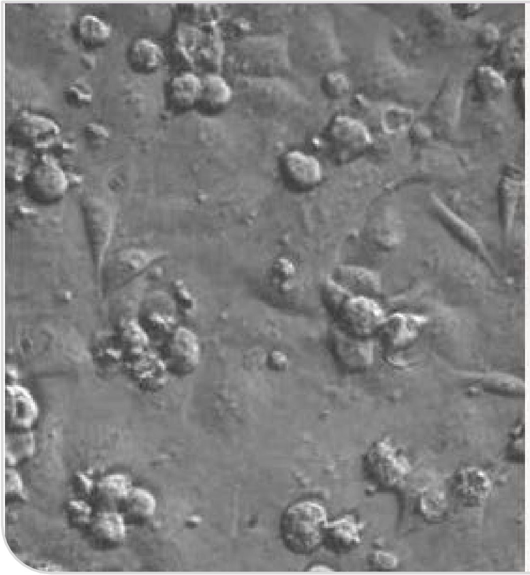
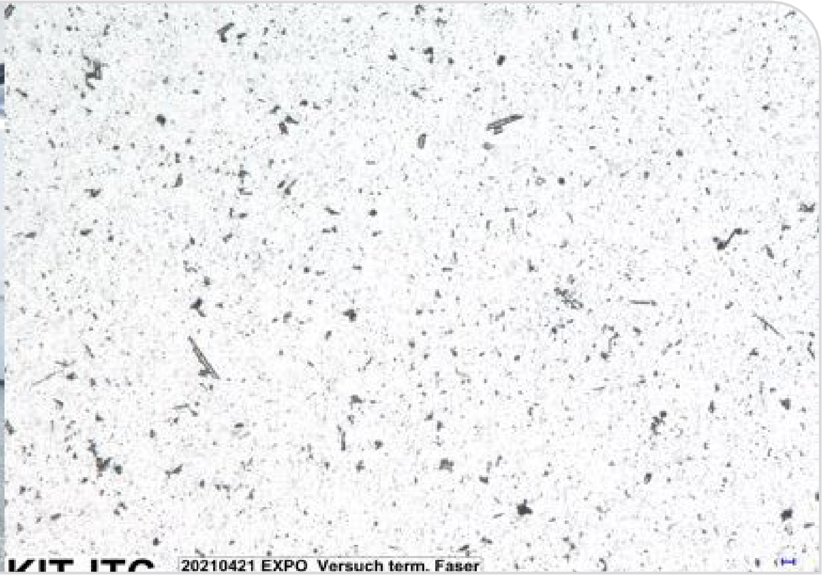
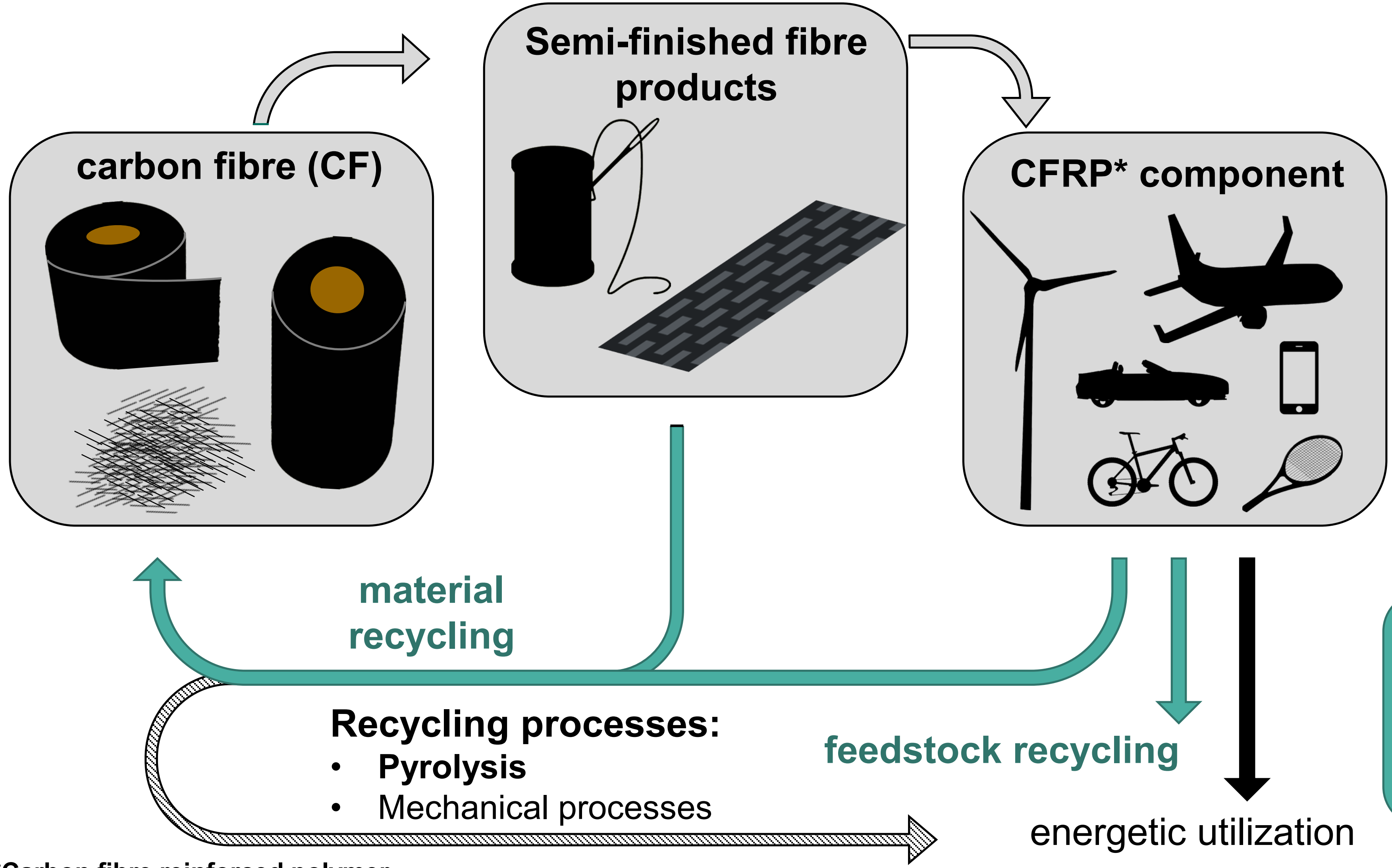


Life cycle of carbon fibres



Processing of CF/CFRP
including

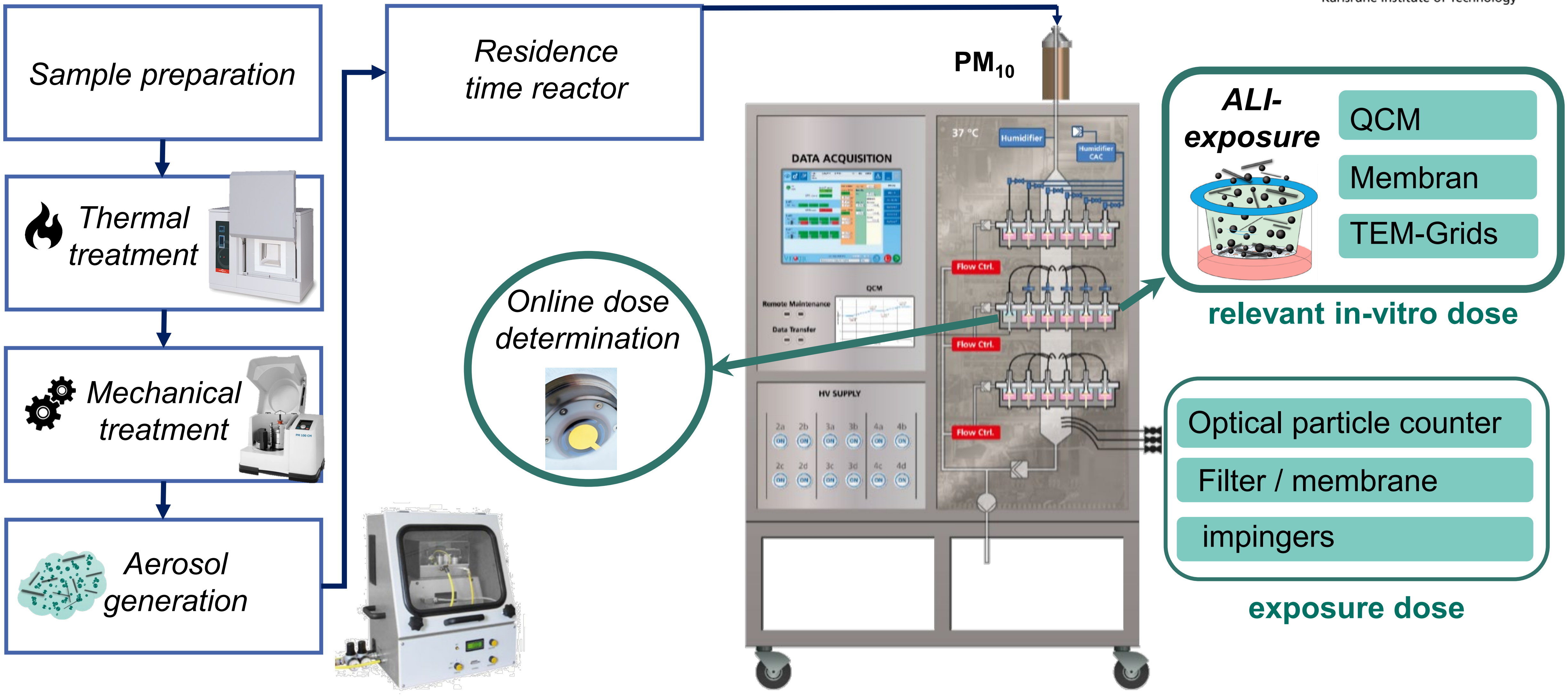
- Mechanical processes like
  - Cutting
  - Sawing
  - Grinding
  - …
- Thermal processes like
  - Energetic disassembly
  - Pyrolysis
  - …

➔ **Change of properties possible**
➔ **Release of fibres and fibre fragments possible**

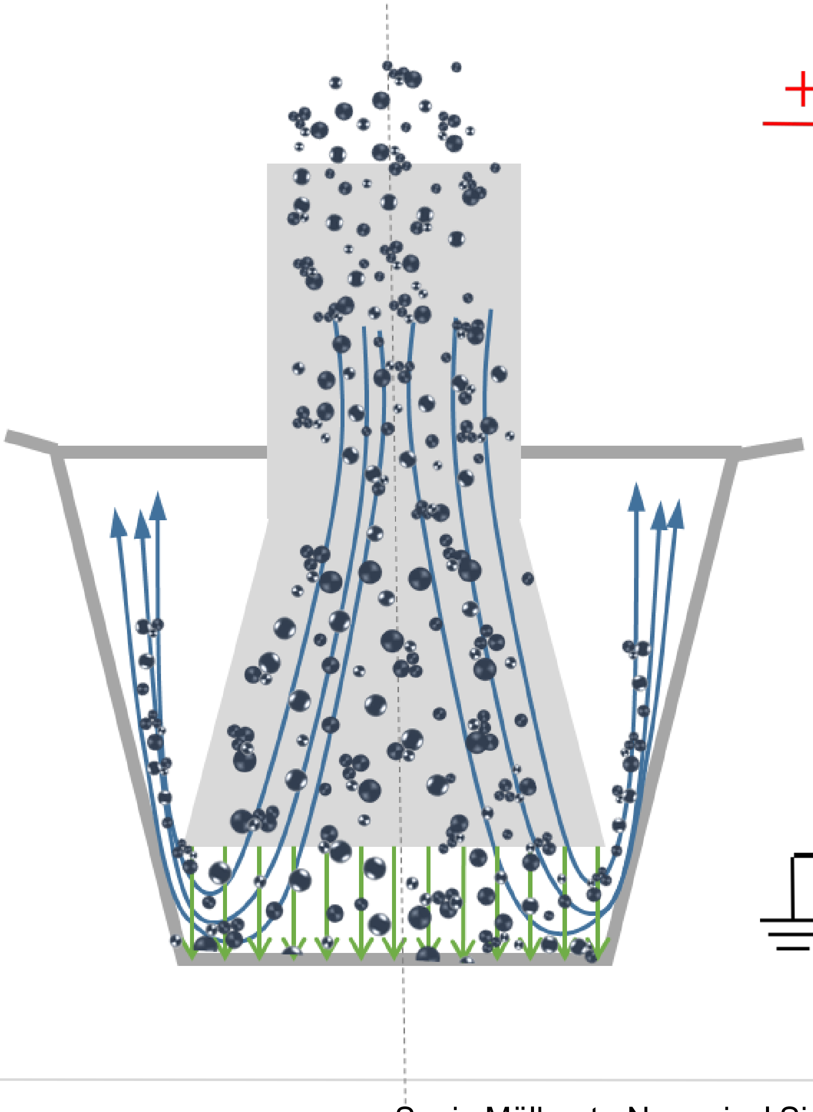
Courtesy: Manuela Wexler

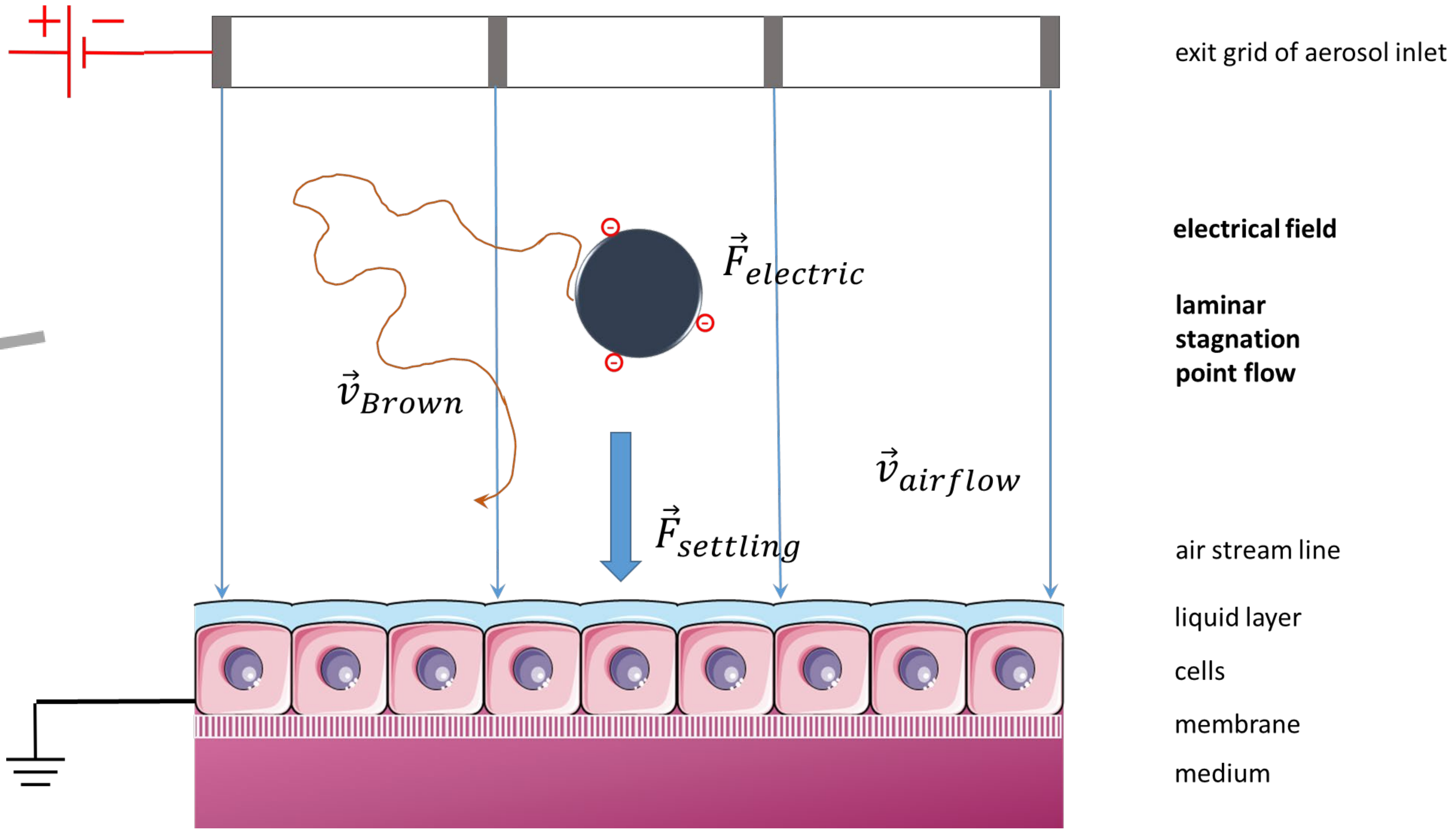
***Carbon fibre reinforced polymer**

CF aerosols for toxicological testing



Forces acting on airborne particles





Inhalable fibres („WHO fibres“)

Definition of
World Health Organisation (WHO)

- **L > 5 µm**
- **D < 3 µm**
- **L:D > 3:1**

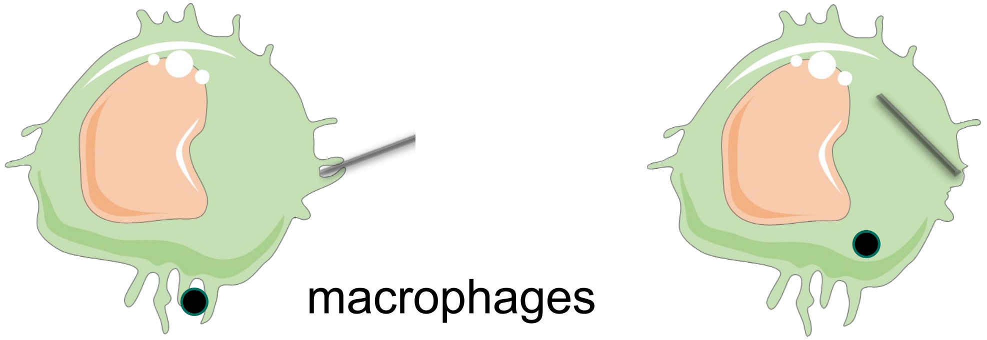
Properties increasing the risk

- **biopersistancy**
- **rigidity**

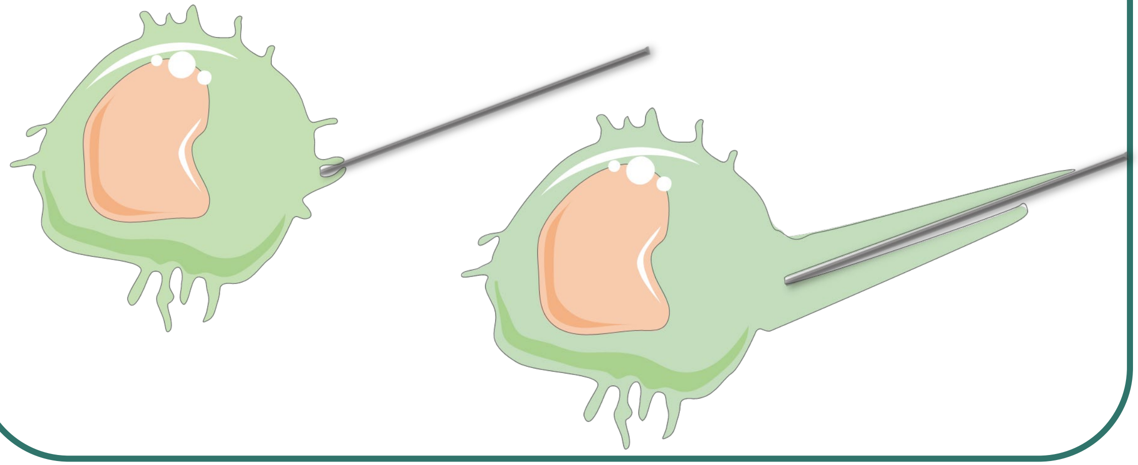
Typical disease patterns

- **Asbestosis (lung fibrosis)**
- **Lung cancer**
- **Mesotheliomas**

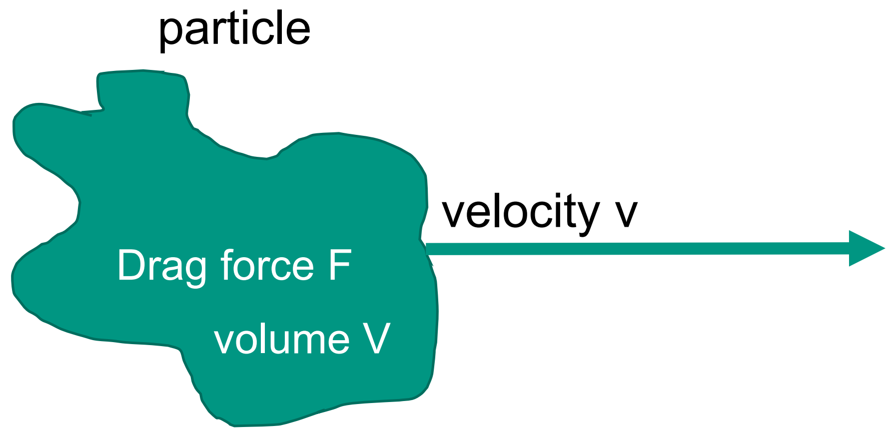
Phagocytosis of particles or short fibres



Frustrated phagocytosis of critical fibres

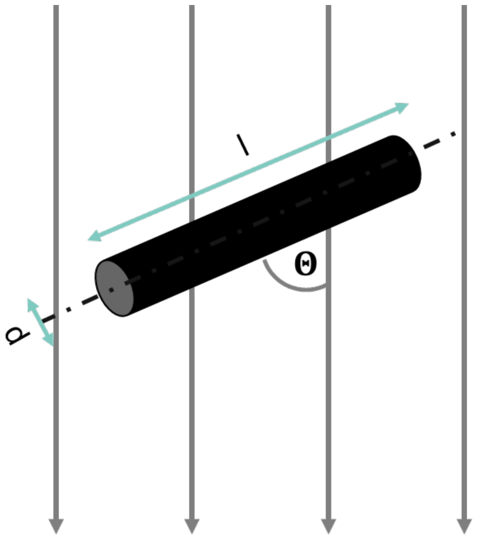


Stokes behaviour of non-spherical particles



dynamic shape factor:
describes the force ratio of the irregularly shaped particle to the spherical particle

$$F = 6\,\pi\,\mu\,R\,v_s\,\chi$$



Dynamic shape factor $$\chi = \frac{F}{F_S}$$

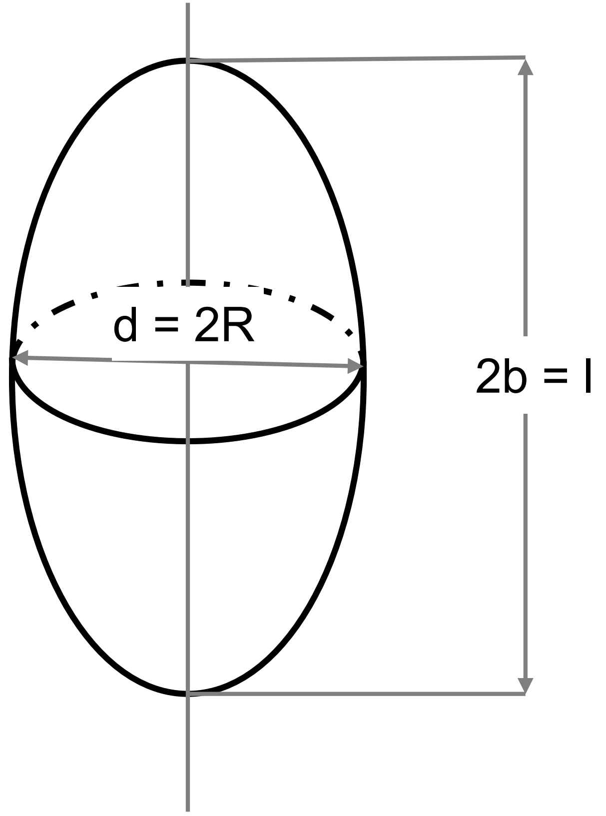
Χ depends on

- the geometry
- the orientation of the particle in the flow field

Determination of the shape factor Χ with the stretched ellipsoid of revolution approach

$$F = 6\,\pi\,\mu\,R\,v_s\,\chi$$

$$aspect\ ratio\ \beta = \frac{length\ l}{diameter\ d}$$



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

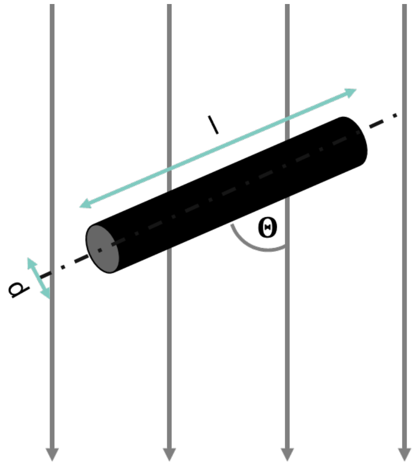
$$\chi^{\parallel} = {}^{4}/_{3}\,(\beta^2 - 1)/\left\{\frac{2\beta^2 - 1}{\sqrt{\beta^2 - 1}} \cdot ln\left[\beta + \sqrt{\beta^2 - 1}\right] - \beta\right\}$$

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

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

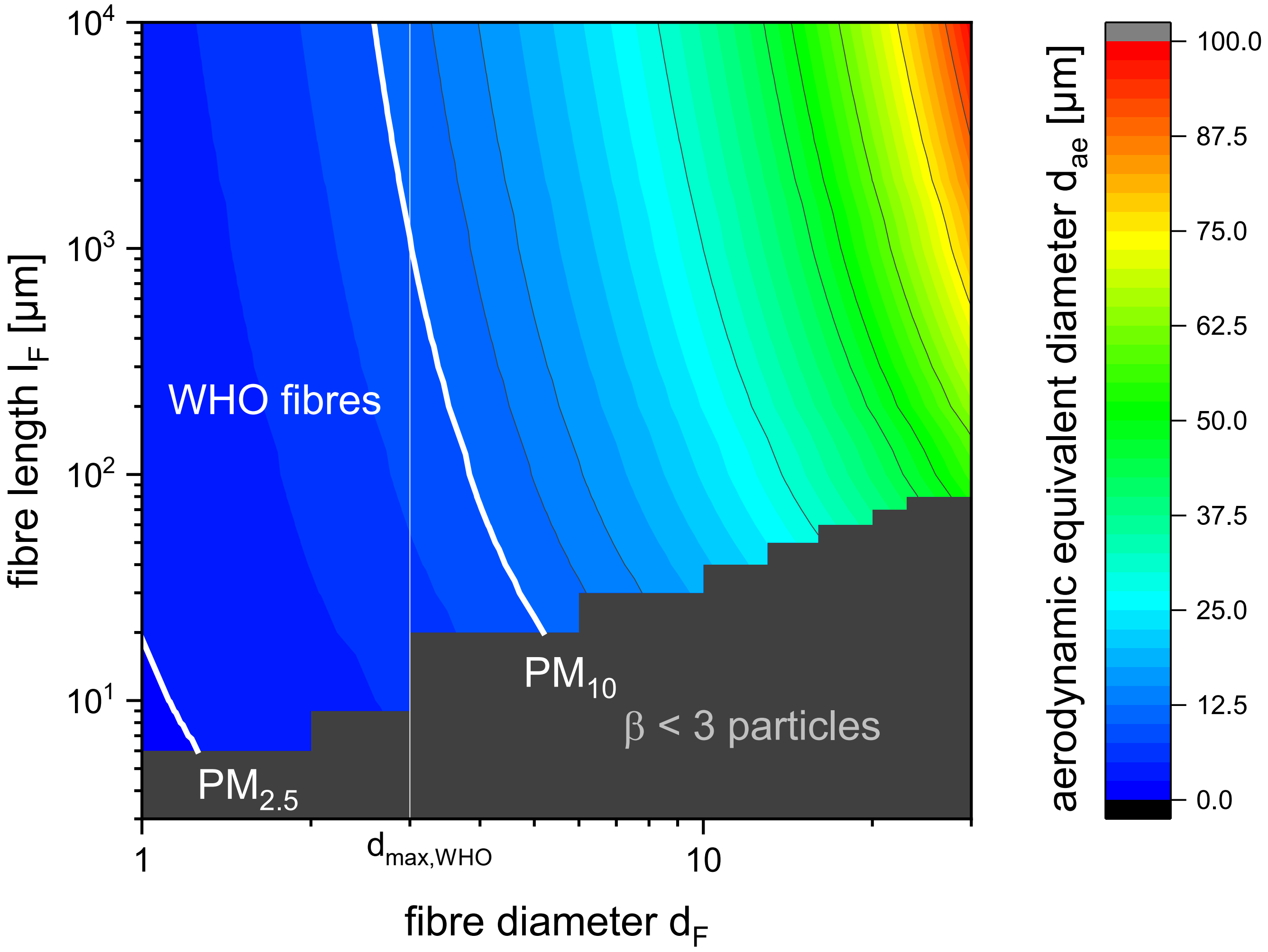
Liu, B.Y.H., Pui, D.Y.H., Wang, X.Q., and Lewis, C.W. (1983). Sampling of Carbon Fiber Aerosols. Aerosol Science and Technology, 2, pp. 499–511.
Fuchs (1964) The Mechanics of Aerosols

The aerodynamic equivalent diameter d_{ae}



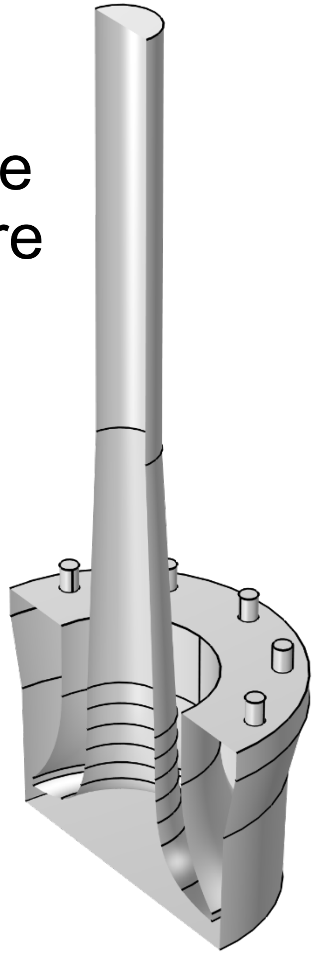
$$\beta = \frac{l_F}{d_F}$$

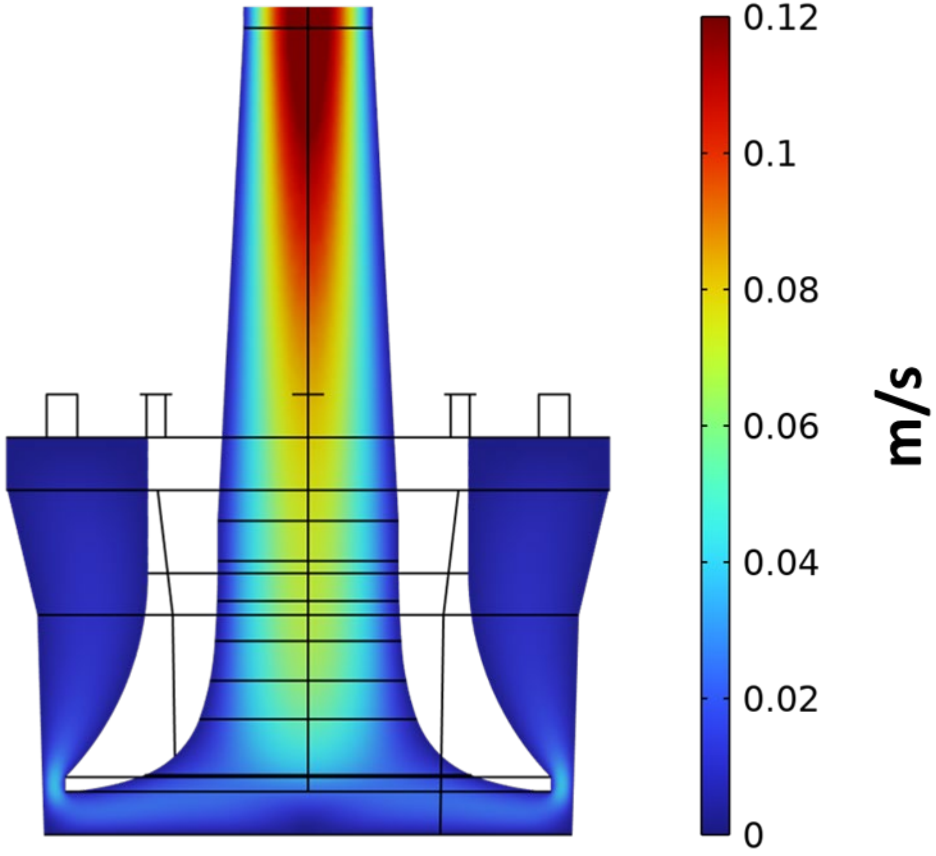
$$d_{ae} = d\sqrt{\frac{\delta_P\,\beta}{\delta_0\,\chi}}$$



Numerical simulation of deposition efficiency

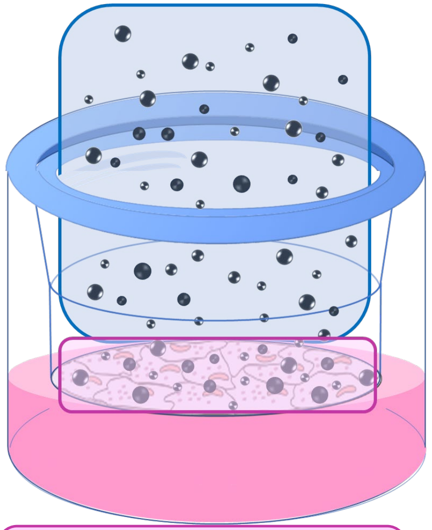
- Two steps:
  1. Steady-state flow for gas phase flow rate, temperature, pressure = constant
  2. Time-dependant particle trajectories
- Forces affecting particles:
  - Drag force
  - Electrostatic field with different potentials
  - Brownian motion





Dose determinations

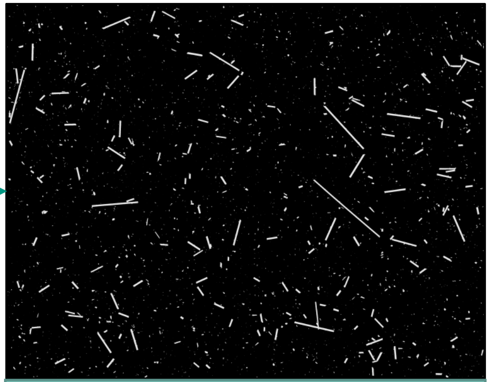
Dose type	Measurement	Analyse
Exposure dose	Nuclepore membran in filter sampling	Scanning electron microscopy
		Digital microscopy
	Quartz filter in filter sampling	Gravimetric analysis
Surface dose / RID	Membrane of insert	Digital microscopy
		Scanning electron microscopy
	QCM-Sensor	QCM signal



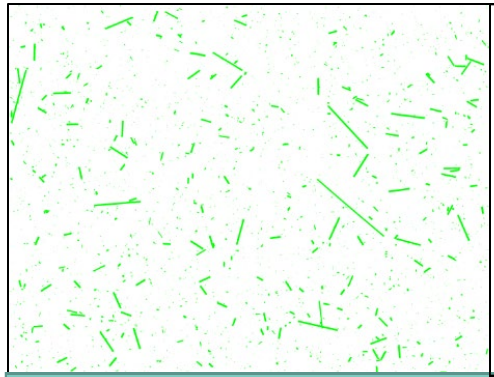
Characterisation of CF and CF fragments

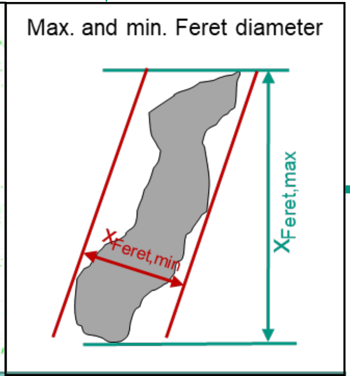
Image analysis of micrographs

micrograph



Binary image





Counting and measurement of objects

Excel macro — Categorisation of objects and evaluation of data

Rejection of agglomerates

Criterium for agglomerates:

- $d_{Objekt} > d_{Rohfaser}$

Classification of objects
- Fibres
- WHO fibres
- particles

Criterium for fibres:

- Length/Diameter $\frac{L_F}{d_F} \geq 3$

Criteria for WHO fibres:

- Fibre diameter $d_F \leq 3\ \mu m$
- Fibre length $L_F \geq 5\ \mu m$
- Length/Diameter $\frac{L_F}{d_F} \geq 3$

Criterium for particles:

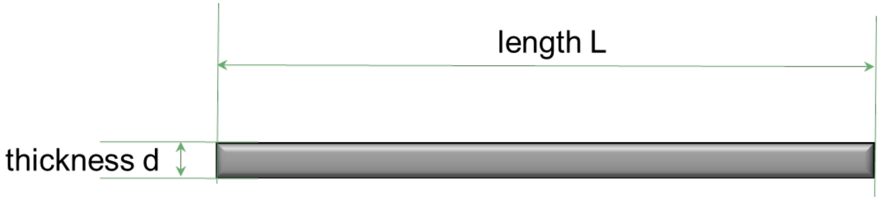
Length/Diameter $\frac{L_F}{d_F} < 3$

Statistical evaluation

Source: Jonathan Mahl

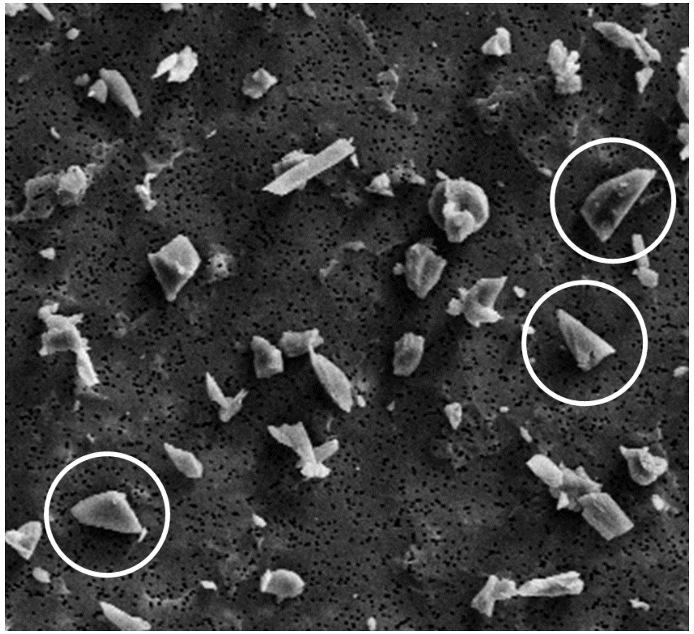
Object analysis

The Rectangular model

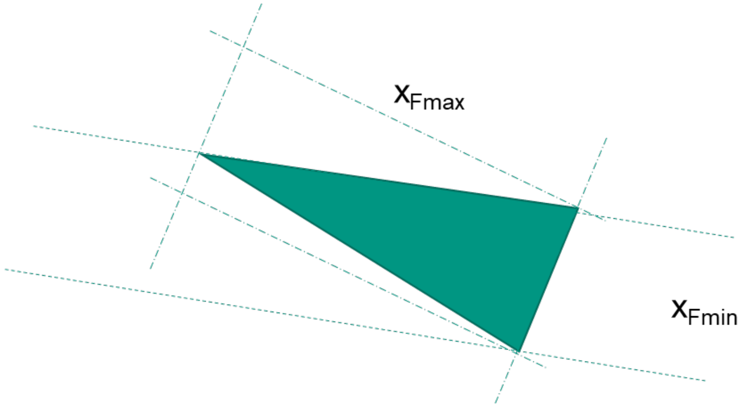


circumference $U = 2D + 2L$ $\qquad$ $area\ A = L \cdot D$

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



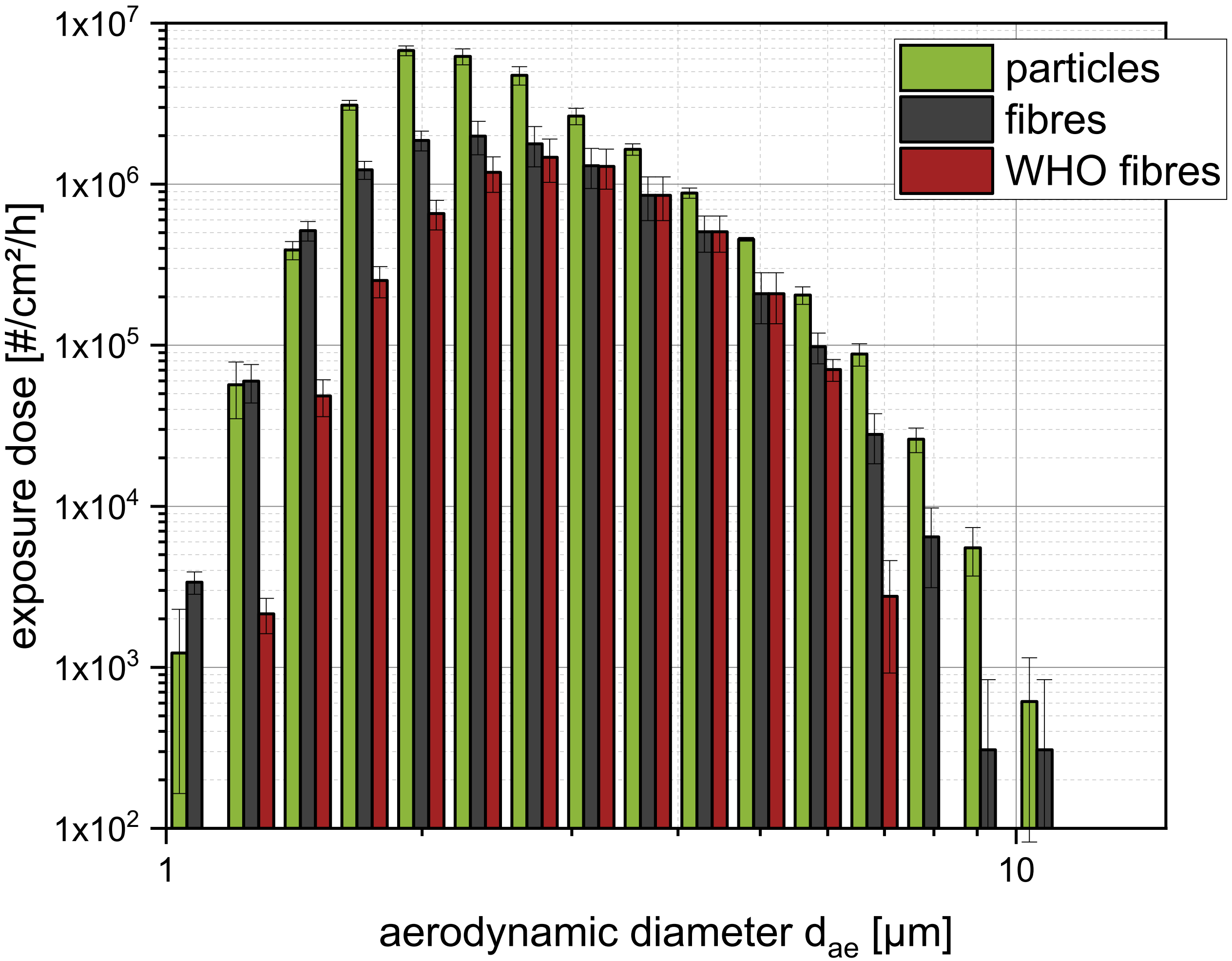
The Feret diagram



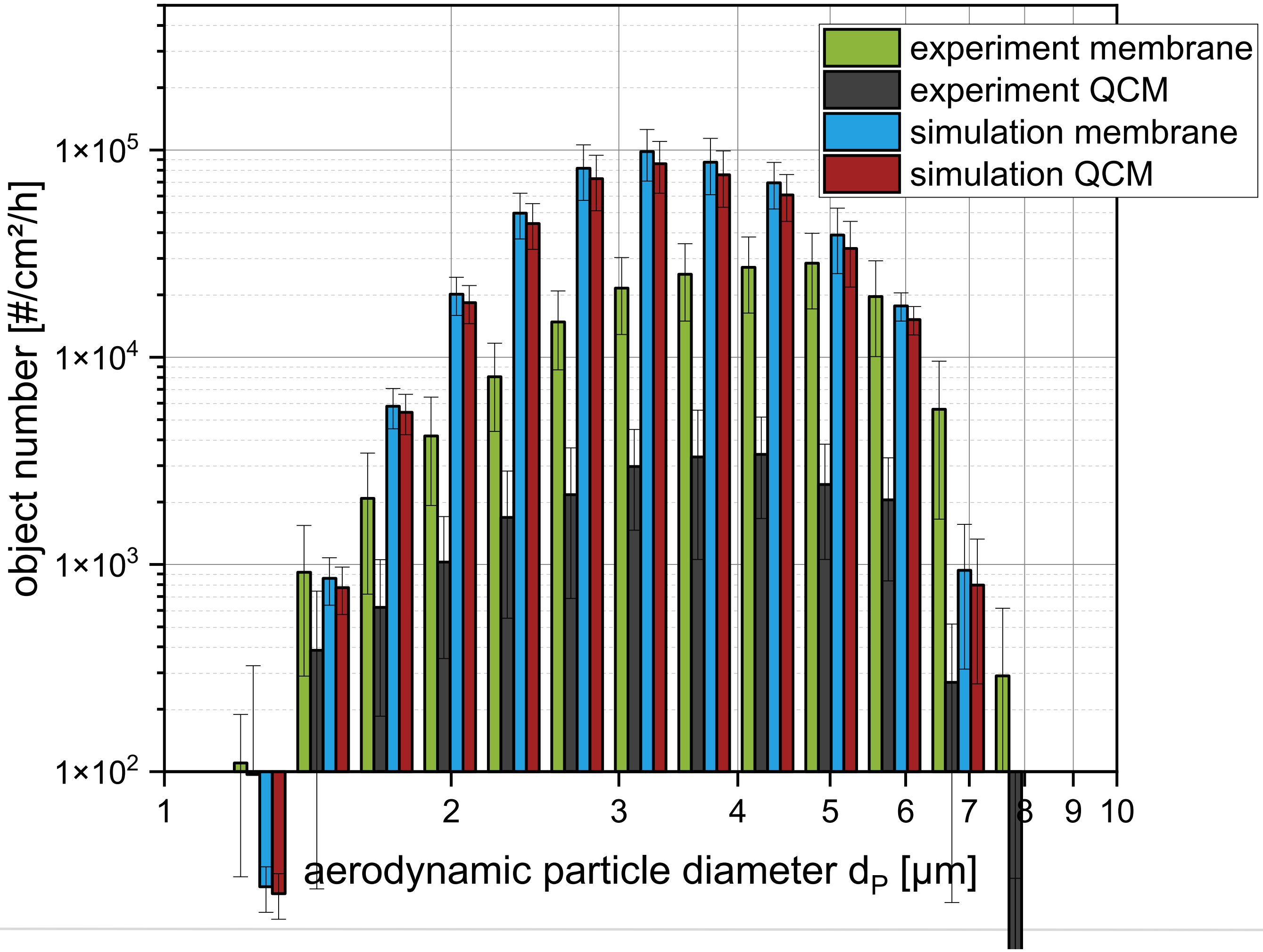
→ fragments with an approximate triangular shape are interpreted too broadly.

→ **Rectangular model**

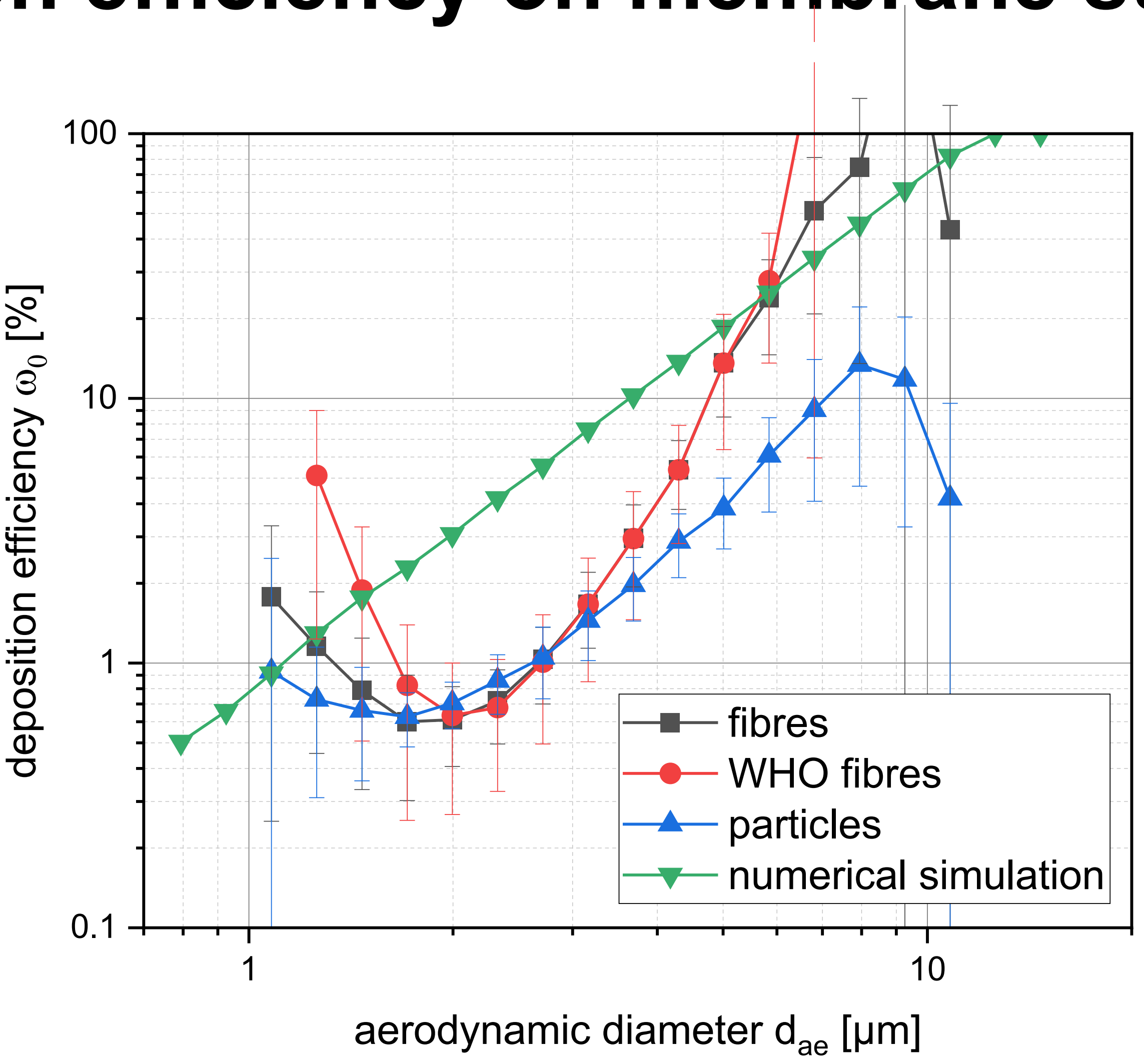
The Exposure Dose



Deposited WHO fibre doses



Deposition efficiency on membrane surface



Summary

- Various dosimetry methods established for fibres
- Comparison simulation - measurements
  - At the edges of the measurements, the standard deviation becomes larger and thus the deviation from the simulation.
  - Comparison with the membrane dose is very good.
  - The application of the aerodynamic diameter to particles with a high aspect ratio is well suited.

Thank you!

My colleagues

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