TECHNISCHE UNIVERSITÄT DRESDEN

**Faculty of Mechanical Engineering** Institute of Process Engineering and Environmental Technology

# Propagation Modeling based on airborne particle release data of nanostructured materials for exposure estimation and prediction

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# Motivation

## TUD release studies on nanostructured materials

- ❑ powder handling (🗐 Göhler & Stintz 2015)
- ❑ spray can/gun application of liquid coatings (🗐 Göhler & Stintz 2014)
- ❑ weak abrasion of solid composites (🗐 Vorbau et al. 2009)
- ❑ sanding of solid composites; also aged ones (🗐 Göhler et al. 2010, 2013)
- ⇨ release data: particle size distributions & fractional particle release numbers

## risk assessment requires data on exposure !

- ❑ release (≠) exposure
- ❑ release = state of dispersion (particle size and concentration) at source
- ❑ exposure = state of dispersion at entrance to subject of protection
- ❑ exposure = f(release, transport & transformation)
- ⇨ exposure data: release data in combination with propagation modeling

# Modeling details

## Computational tools and simplifications

### propagation modeling (FEM)

- ❑ computational fluid dynamics (ParallelNS, e.g. 🗐 Knopp et al. 2005)
- ❑ thermal building simulation (TRNSYS-TUD)
- ⇨ module combination in parallel virtual machine (e.g. 🗐 Gritzki et al. 2003)

### main appointed simplifications regarding release

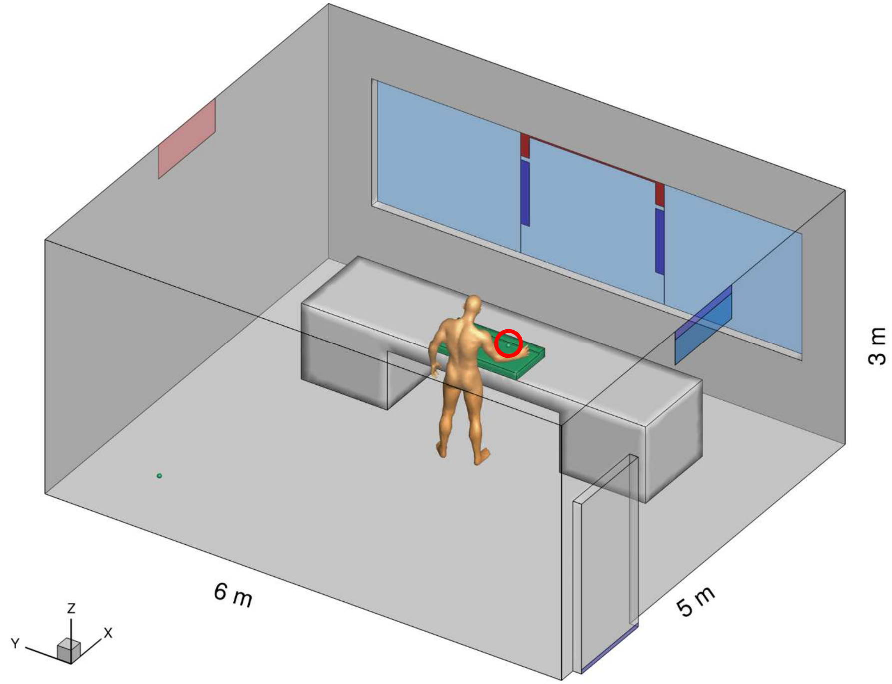
- ❑ release processes do not interact with the environment
- ⇨ no flow displacement (i.e. interference-free particle supply)
- ⇨ no directional momentum
- ⇨ …
- ❑ gas-like behavior of released airborne particles
- ⇨ no particle-particle interaction (e.g. reagglomeration)
- ⇨ no particle-wall interactions (e.g. particle losses)
- ⇨ …

# Modeling details

## Selected specifications

### model room (e.g. workshop)

- room envelope
  - ⇨ 5 m x 6 m x 3 m = 90 m³
  - ⇨ triple-part window ($\vartheta_{outdoor} \stackrel{def}{=} 5$ °C)
  - ⇨ floor heating ($\vartheta_{room} \stackrel{def}{=} 20$°C)
- room interior
  - ⇨ workbench
  - ⇨ person (1.8 m, $\vartheta_{clothes} \stackrel{def}{=} 26$°C)




### 3 ventilation scenarios (blue = inlet air; red = exit air)

- natural ventilation by door slit infiltration (NVD) $0.5\ h^{-1}$
- natural ventilation by pivot-hung window (NVW) $1.5\ h^{-1}$
- "improved" technical ventilation system (TVS) $8.0\ h^{-1}$

# Modeling details

## Selected specifications

### 3 release scenarios

- wiping (WIP)
  - ⇨ procedure: dry wiping of a coated item with a surface area of 0.5 m² for 10 s
  - ⇨ conditions: Vorbau et al. 2009 (UV-ZnO)
    area specific particle release number < 10 µm = $5.0 \cdot 10^{05}$ #/m²
    very low release -> particle size distribution (PSD) could not measured
- sanding (SAN)
  - ⇨ procedure: sanding of a coated item with a surface area of 0.5 m² for 60 s
  - ⇨ conditions: Göhler & Stintz 2010, 2013, 2014 (UV*-ZnO)
    area specific particle release number < 10 µm = $1.0 \cdot 10^{11}$ #/m²
    lognormal PSD ($x_{50,0}$ = 240 nm; GSD = 1.4); density "1000" kg/m³
- spraying (SPR)
  - ⇨ procedure: standard spray can application for 60 s
  - ⇨ conditions: Göhler & Stintz 2014 (PU-ZnO)
    particle release rate x < 10 µm = $7.5 \cdot 10^{09}$ #/s
    lognormal PSD ($x_{50,0}$ = 120 nm; GSD = 2.0); density 1000 kg/m³

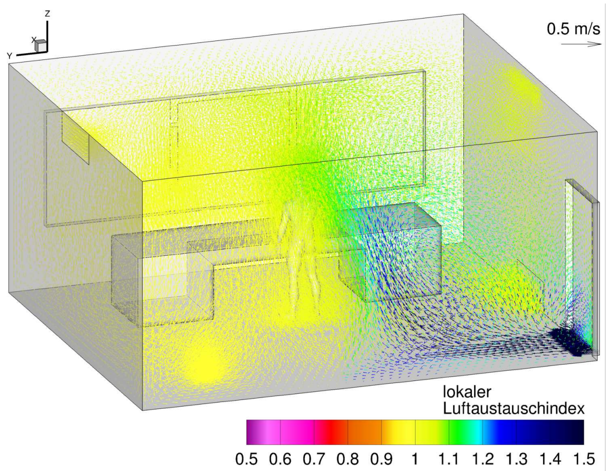
# Results - Ventilation scenarios, steady state

## Velocity field and local air exchange quality

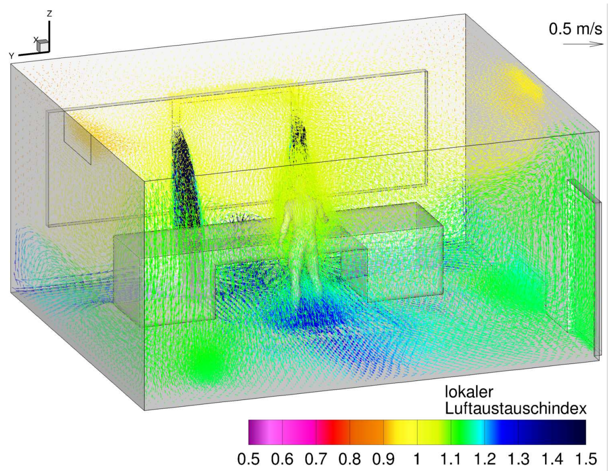
**steady state conditions reached after 30 min**

- ⇨ purple/orange regions: local air exchange is less than mean air exchange rate
- ⇨ yellow regions: local air exchange corresponds to mean air exchange rate
- ⇨ green/blue regions: local air exchange is better than mean air exchange rate

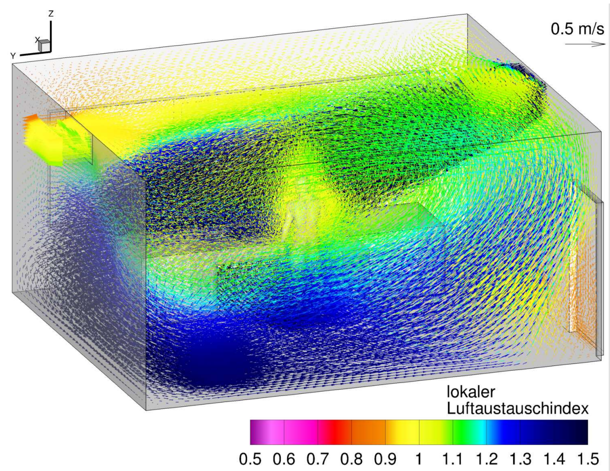
**NVD (0.5 $h^{-1}$)**




**NVW (1.5 $h^{-1}$)**




**TVS V3 (8.0 $h^{-1}$)**

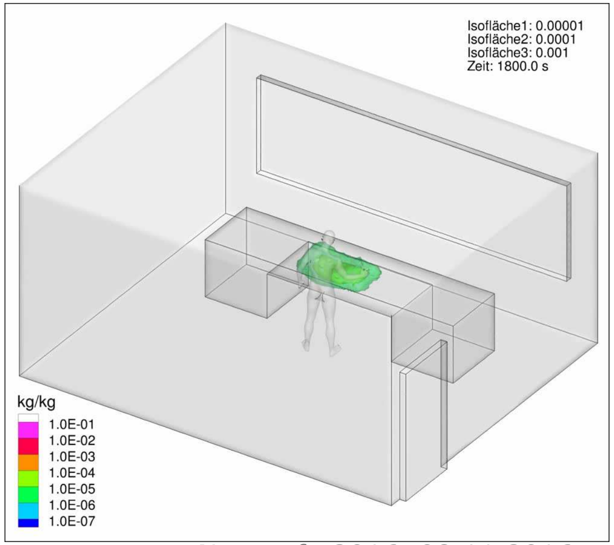


# Results - Exposure Scenarios

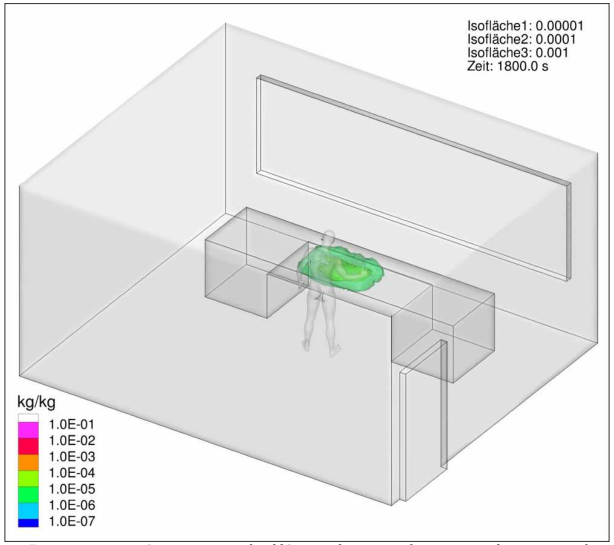
## Aerosol propagation: Wiping

- 3 iso-surfaces of relative gas exchange (~ particle concentration)
- release process (duration 10 s) starts at 1800 s, videos run until 1900 s
- tenfold playback speed

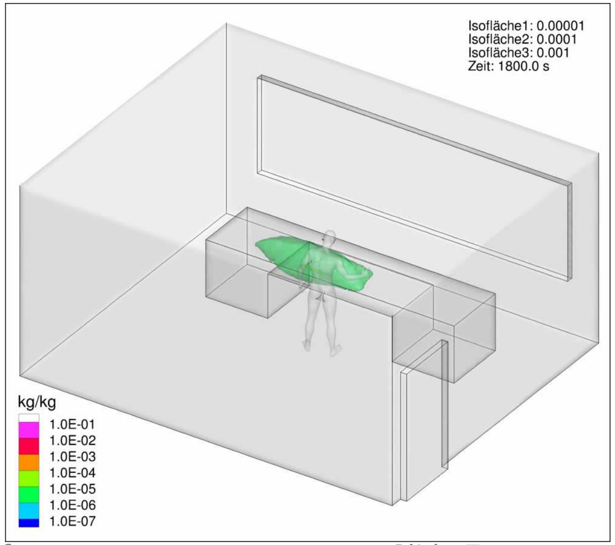
**NVD (0.5 $h^{-1}$)**




**NVW (1.5 $h^{-1}$)**




**TVS V3 (8.0 $h^{-1}$)**

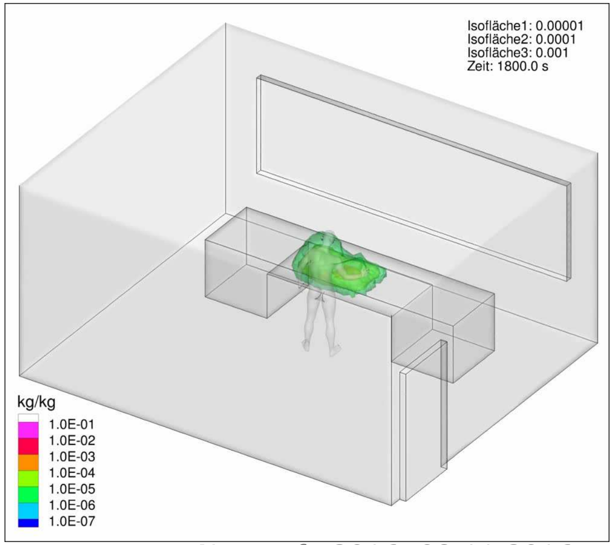


# Results - Exposure Scenarios

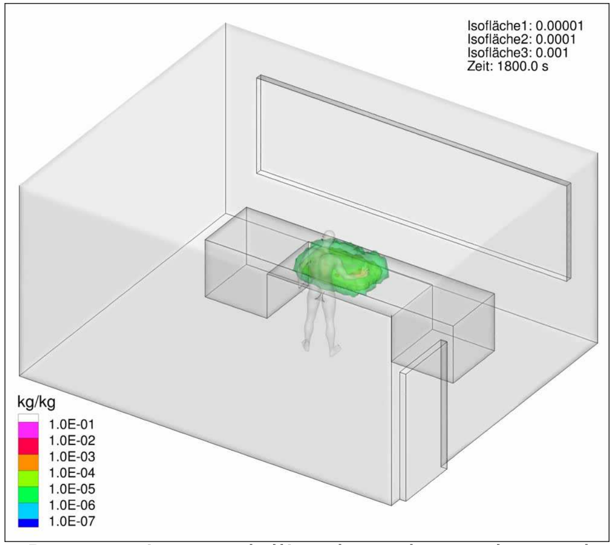
## Aerosol propagation: Sanding

- 3 iso-surfaces of relative gas exchange (~ particle concentration)
- release process (duration 60 s) starts at 1800 s, videos run until 1900 s
- tenfold playback speed

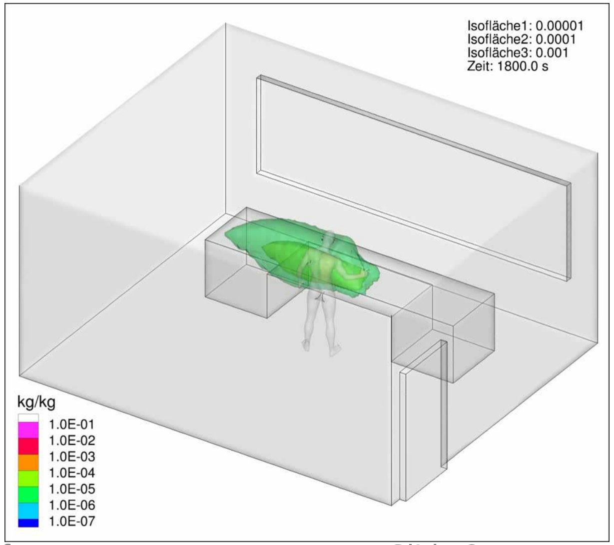
**NVD (0.5 h$^{-1}$)**




**NVW (1.5 h$^{-1}$)**




**TVS V3 (8.0 h$^{-1}$)**

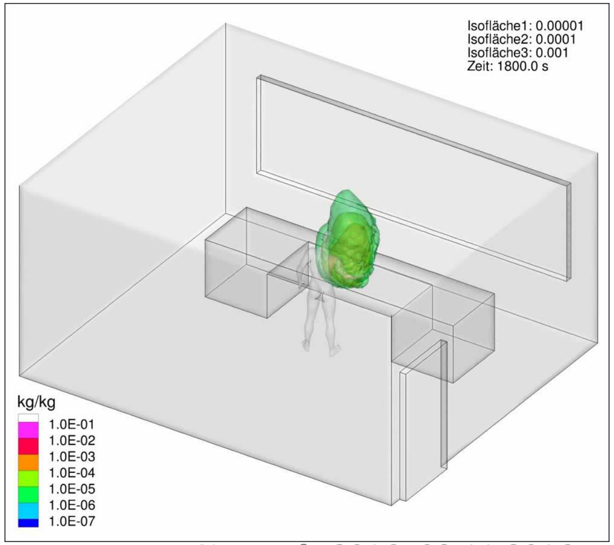


# Results - Exposure Scenarios

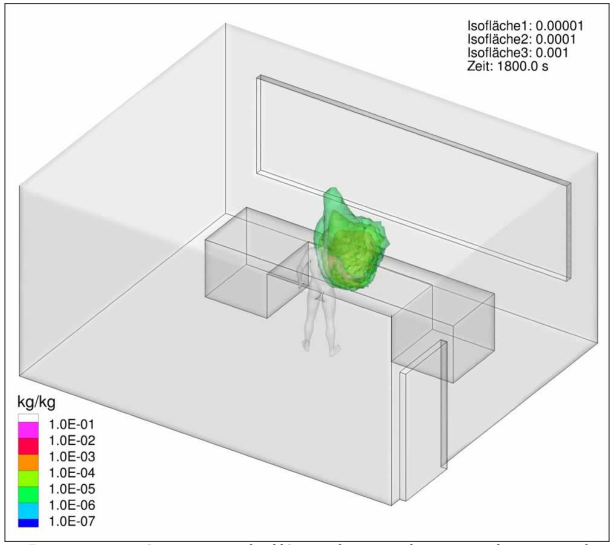
## Aerosol propagation: Spraying

- 3 iso-surfaces of relative gas exchange (~ particle concentration)
- release process (duration 60 s) starts at 1800 s, videos run until 1900 s
- tenfold playback speed

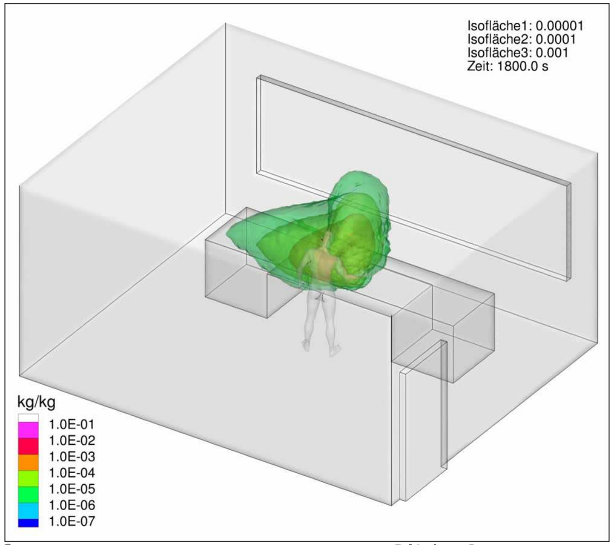
**NVD (0.5 $h^{-1}$)**




**NVW (1.5 $h^{-1}$)**




**TVS V3 (8.0 $h^{-1}$)**



# Results - Exposure Scenarios (spraying)

## from exposure via inhalation to deposition

**exposure**

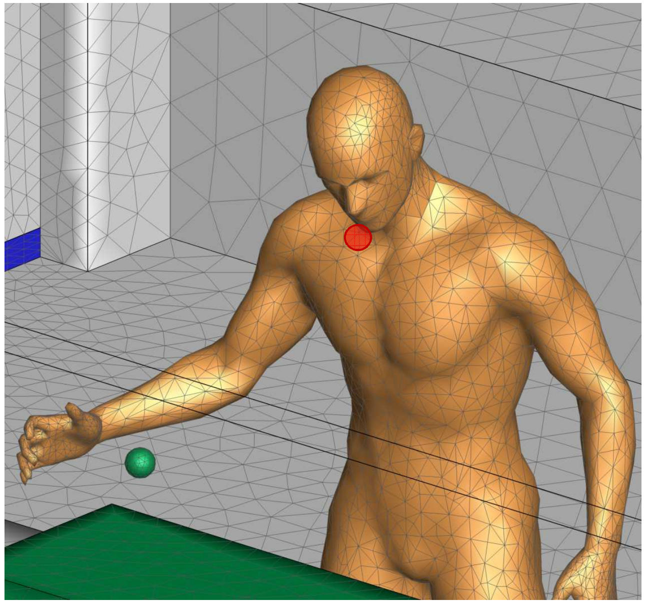
- ❑ sensor at person in breathing zone
- ⇨ particle number concentration over time
- ⇨ particle mass concentration over time

**inhalation**

- ❑ gender averaged breathing rate 383cm³/s
- ⇨ cumulative number of inhaled particles
- ⇨ cumulative mass of inhaled particles

**deposition in human airways**

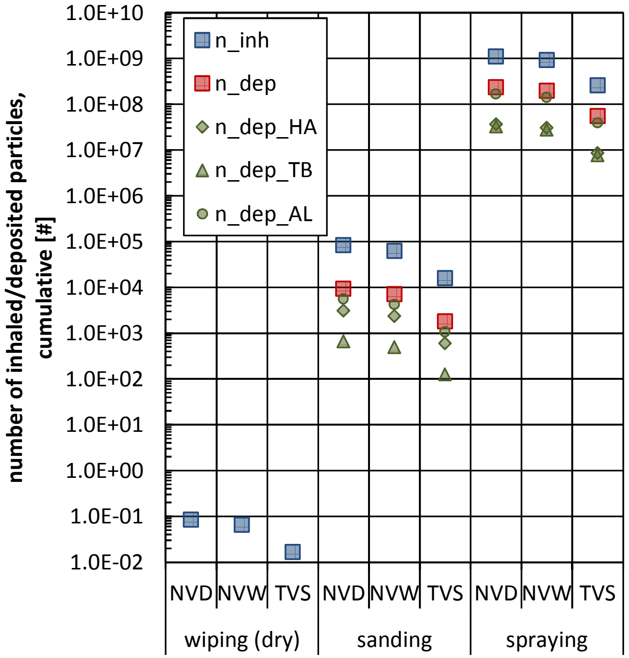
- ❑ modified IRCP 66 Modell (Hinds 1999); gender/activity averaged
- ⇨ deposition fraction based on PSDs
- ⇨ combination with inhalation

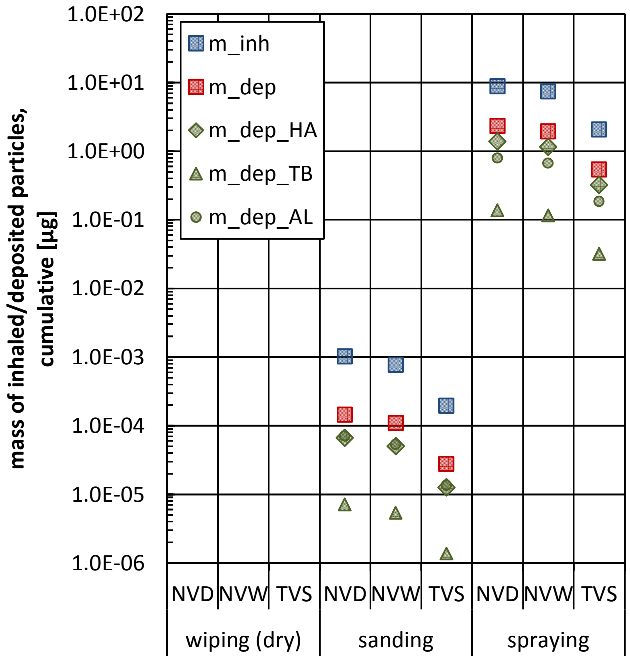


# Results - Inhalation & Deposition

## number/mass of inhaled/deposited particles

- negligible exposure levels by wiping, highest exposure levels by spraying
- $n_{released}/n_{inhaled}$ depends on exposure scenario and varied from 4E2 … 3E8




**$n_{released}/n_{inhaled}$**

| | NVD | NVW | TVS |
|---|---|---|---|
| **SPR** | 4E2 | 5E2 | 2E3 |
| **SAN** | 3E5 | 4E5 | 2E6 |
| **WIP** | 6E7 | 8E7 | 3E8 |

**Values are provided in the annex!**

# Summary and conclusions

## propagation modeling

- ❑ 3 ventilation scenarios x 3 release scenarios = 9 exposure scenarios
- ❑ artificial observation of air condition in breathing zone for exposure
- ❑ calculation of cumulative number/mass of inhaled/deposited particles
- ⇨ Attention! PSD-conversion from „number-world" into „volume/mass-world" and vice versa can lead to huge errors, especially by operating lognormal PSD fits (e.g. 🗐 Babick & Ullmann, 2016)

## general conclusions

- ❑ condition of ventilation defines fundamentally the level of exposure
- ❑ convective flows due to personal heat can cause particle availability in BZ
- ❑ highest exposure levels arise immediate during material processing
- ⇨ measured release/emission data are more resistant than exposure ones, because they are less affected from conditions of the surrounding scenario

# Thank you for your attention !

**Acknowledgement**
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# Cumulative inhalation/deposition values

| release scenario | ventil. scenario | n_inh | n_dep | n_dep_HA | n_dep_TB | n_dep_AL | m_inh | m_dep | m_dep_HA | m_dep_TB | m_dep_AL |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | **SPR** | **[no.-%]** | **21.52** | 3.37 | 3.04 | 15.12 | **[wt.-%]** | **26.21** | 15.67 | 1.56 | 8.98 |
| | **SAN** | **[no.-%]** | **11.30** | 3.80 | 0.80 | 6.70 | **[wt-%]** | **14.10** | 6.50 | 0.70 | 6.90 |
| **[-]** | **[-]** | **[#]** | **[#]** | **[#]** | **[#]** | **[#]** | **[µg]** | **[µg]** | **[µg]** | **[µg]** | **[µg]** |
| **wiping (dry)** | **NVD** | 8.49E-02 | | | | | | | | | |
| | **NVW** | 6.51E-02 | | | | | | | | | |
| | **TVS** | 1.64E-02 | | | | | | | | | |
| **sanding** | **NVD** | 8.30E+04 | 9.37E+03 | 3.15E+03 | 6.64E+02 | 5.56E+03 | 1.02E-03 | 1.44E-04 | 6.63E-05 | 7.14E-06 | 7.03E-05 |
| | **NVW** | 6.27E+04 | 7.09E+03 | 2.38E+03 | 5.02E+02 | 4.20E+03 | 7.71E-04 | 1.09E-04 | 5.01E-05 | 5.39E-06 | 5.32E-05 |
| | **TVS** | 1.59E+04 | 1.79E+03 | 6.03E+02 | 1.27E+02 | 1.06E+03 | 1.95E-04 | 2.75E-05 | 1.27E-05 | 1.36E-06 | 1.34E-05 |
| **spraying** | **NVD** | 1.10E+09 | 2.36E+08 | 3.69E+07 | 3.33E+07 | 1.66E+08 | 8.79 | 2.30 | 1.38 | 0.14 | 0.79 |
| | **NVW** | 9.20E+08 | 1.98E+08 | 3.10E+07 | 2.79E+07 | 1.39E+08 | 7.38 | 1.93 | 1.16 | 0.12 | 0.66 |
| | **TVS** | 2.55E+08 | 5.49E+07 | 8.59E+06 | 7.75E+06 | 3.86E+07 | 2.05 | 0.54 | 0.32 | 0.03 | 0.18 |