TSCA Occupational Conditions of Use and Exposure Scenario Workshop

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U.S. EPA 1200 PA Ave. NW, Washington D.C. 20004

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Quantifying *safe** Conditions of Use

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*Conditions of Use (CoU) describe the operational conditions (OCs) and Risk Management Measures (RMMs) that are appropriate to maintain exposure at a safe level
NOTE Safe ≈ adequality controlled

VS

15 USC § 2602(4): the circumstances, as determined by the Administrator, under which a chemical substance is intended, known, or reasonably foreseen to be manufactured, processed, distributed in commerce, used, or disposed of

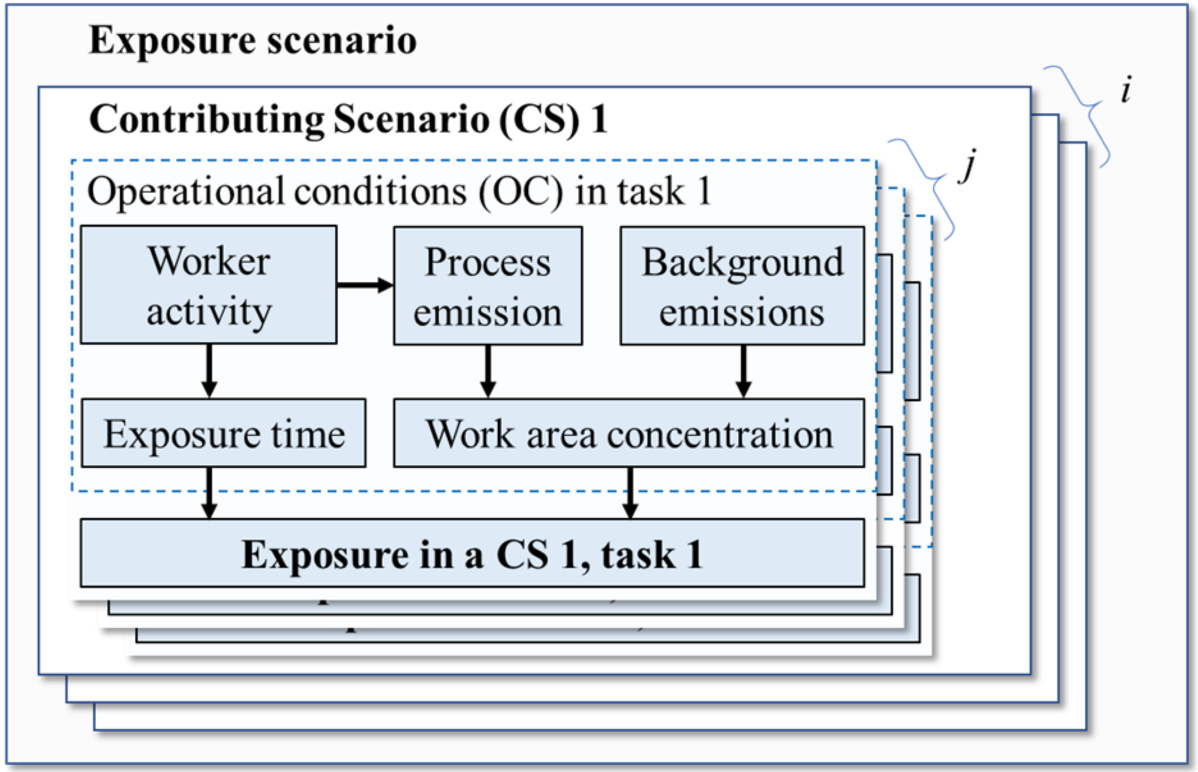
ASINA (GA 862444), SABYDOMA (GA 862296), SABYNA (GA 862419), SBD4Nano (GA 862195) and Repoxyble (GA 101091891) have received funding from the European Union's Horizon research and innovation programme.

Conditions of Use (CoU)

- CoU describe the operational conditions (OCs*) and Risk Management Measures (RMMs) that are appropriate to maintain exposure at a safe level.
- Setting CoU requires the risk assessment of all relevant Contributing Scenarios (CSs) in an exposure scenario.
- A new CS has to be created whenever an OC is changed.

***Operational conditions ≈ Exposure determinants:**

- **Process emissions** (flow rate, energy level, emission controls, etc.)
- **Environmental conditions** (dilution and removal of emissions, background concentration, etc.)
- **Personal behaviours** (proximity to the source, exposure time in different areas, working practices, experience, etc.)

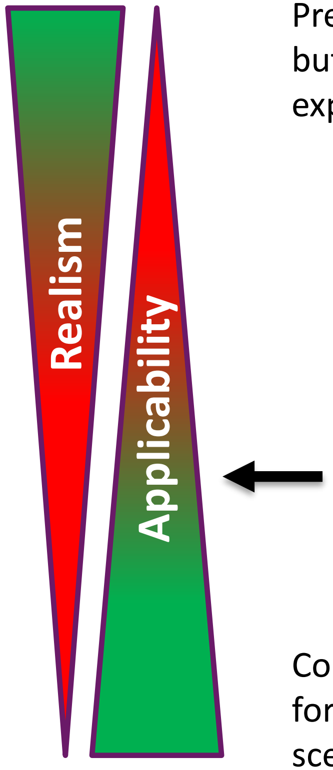


A simplified concept of an occupational exposure scenario consisting of *i* CSs with *j* OCs. Arrows shows exposure determinants relations affecting on the personal exposure level. Adopted from Koivisto et al. (2021a).

Setting generic CoUs

CoU objective is to find broadly applicable conditions where the exposure is classified as adequately controlled (risk characterization ratio; RCR < 0.1)

Low RCR



High RCR

Precise exposure estimates but limited for specific exposure scenarios

Optimize applicability
Find limit for adequately controlled exposure (RCR < 0.1) → Efficient risk communication

Conservative exposure estimates for broadly applicable exposure scenarios

When exposure is adequately controlled?

- **The predicted exposure risk is considered highly-controlled when a 95th percentile (P95) of the exposure distribution is below 10% of the occupational exposure limit value (Torres et al 2014; Hewett et al. 2006)**

How about allocation factors?

- **Limits for integrated exposure (occupational and public exposure)?**
- **Process specific limit, i.e. how much one process machine can increase the exposure (e.g. P95 < 0.01 × OEL)?**

"This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 862444".

Innovative CoU assessment

Current approach

- Risk assessment is mainly based on personal exposure measurements
  → Scenario based RA
- Subjective assessment

Proposed approach

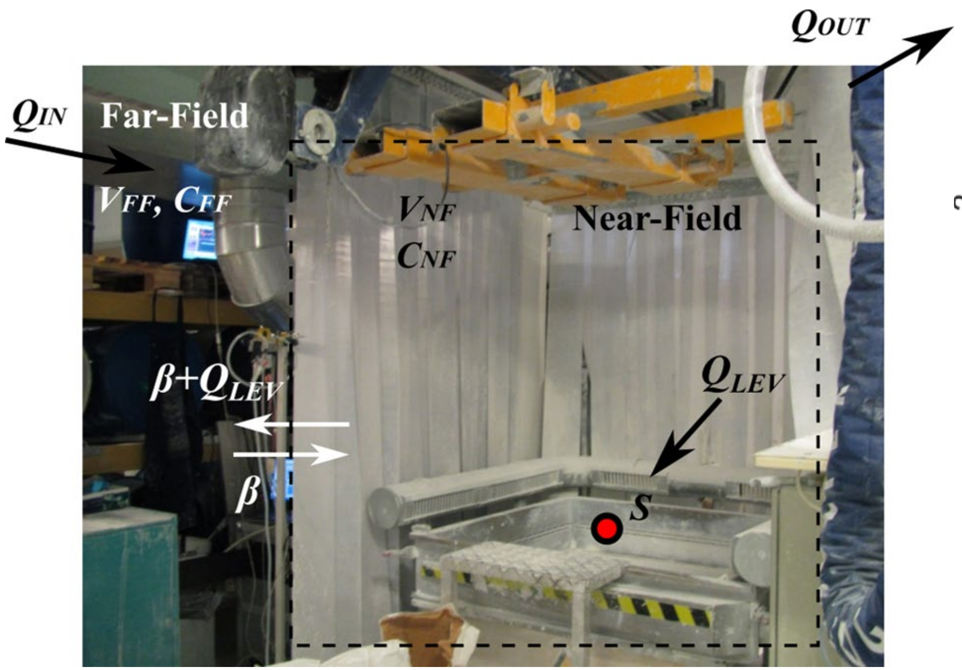
Apply probabilistic exposure model to (Koivisto et al. 2021):

- Quantify process emissions and predict their risk at any scenario → Generic approach
- *Quantify* relevant exposure determinants
  → Efficient safety communication

New

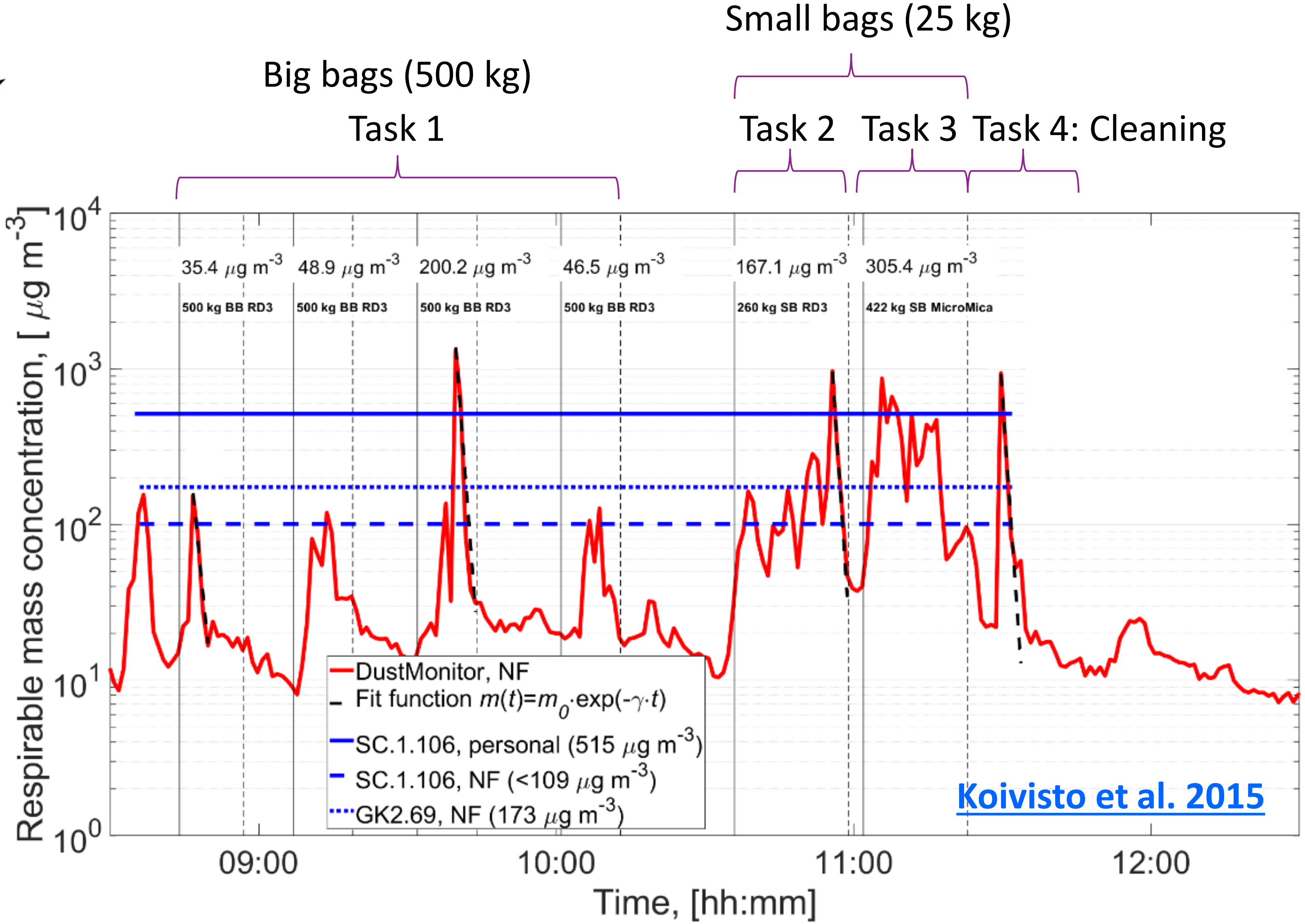
Example: Pouring pigments and fillers in a paint factory (Koivisto et al. 2015; Fonseca et al. (2021).

Example: Pouring processes and concentrations



8-h TWA occupational exposure limit values (OELVs):

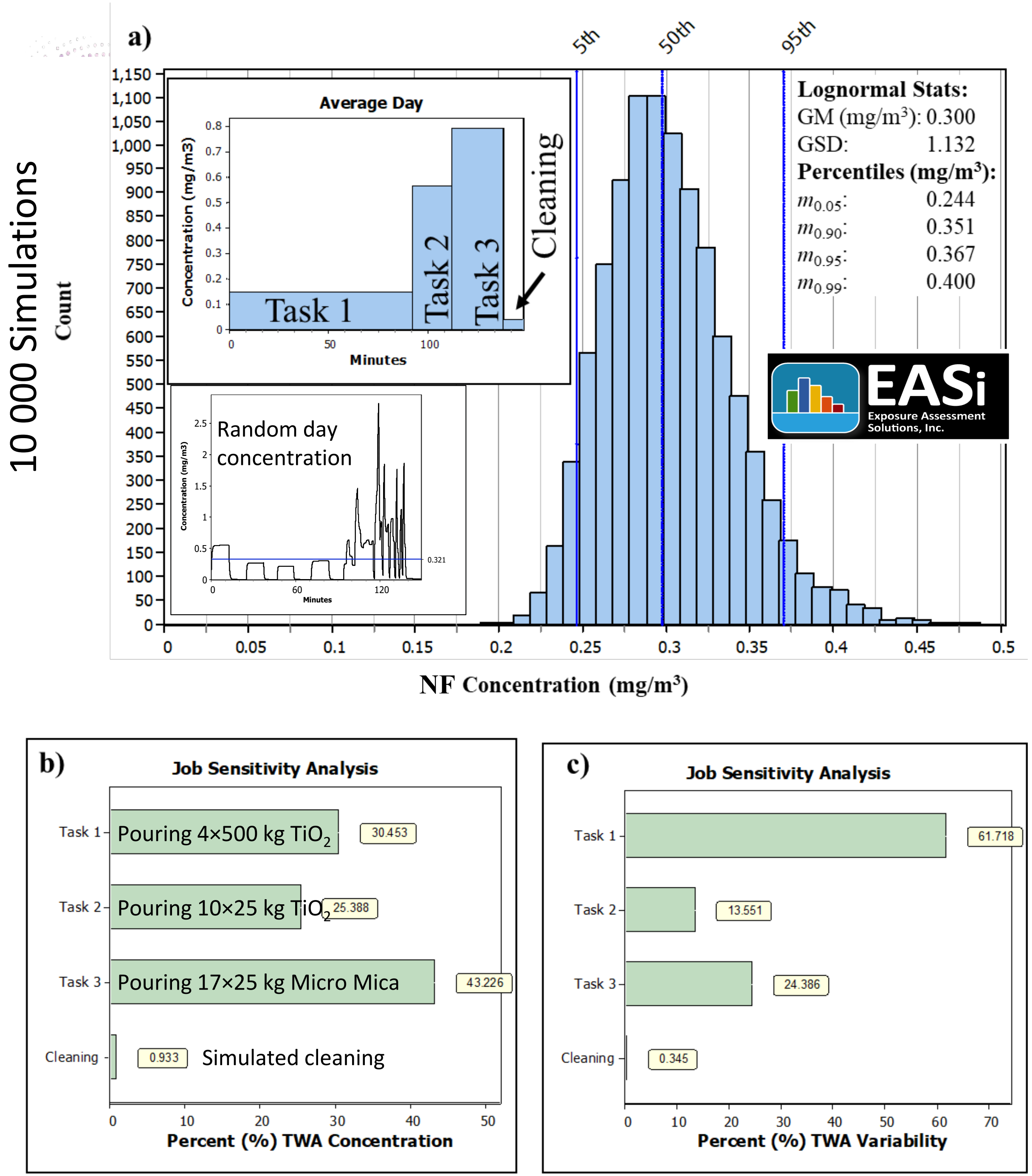
- TiO_2: 10 mg/m^3
- Micro Mica (inorganic dust): 5 mg/m^3



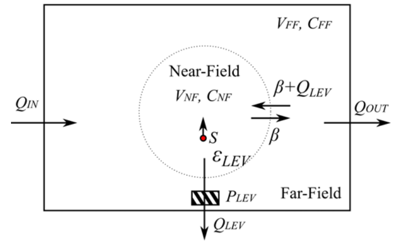
Koivisto et al. 2015

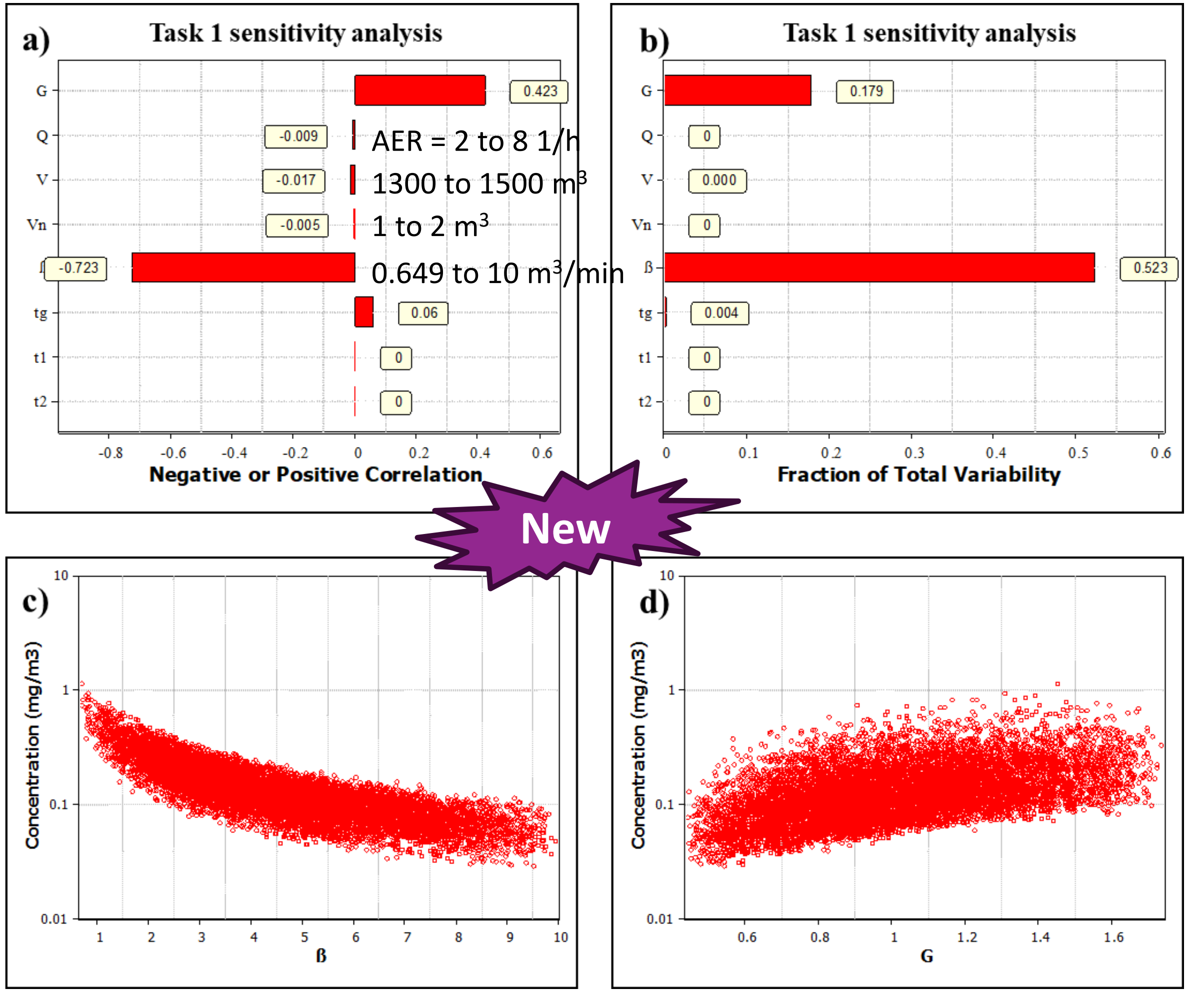
Probabilistic exposure modeling

(Koivisto et al. 2021)



Time Weighted Average (TWA): In this shift 150 minutes





Effect of exposure determinants to NF concentration level (Koivisto et al. 2021a)

Near-Field (NF) concentration levels as geometric mean (GM), 95th percentile and normalized with observed scenario GM concentration. **The exposure time is *ca.* 150 min.**

No. / scenario	NF GM, [mg/m³]	95th percentile, [mg/m³]	GM normalized with scenario no. 1
1. Observed scenario	0.30	0.37	1.00
2. G range increased by ×2	0.51	0.64	1.71
3. β decreased by ×2	0.55	0.67	1.83
4. AER reduced by ×5 to 0.4 to 1.6 1/h	0.32	0.37	1.05
5. A small room (V_{room} = 100 m³)	0.43	0.53	1.42
6. A large room (V_{room} = 10,000 m³)	0.29	0.36	0.97
7. NF including LEV at 9.6 m³/min	0.08	0.39	0.28
8. Worst-case: G increased, β decreased, AER decreased and small room (V_{room} = 100 m³)	1.57	1.92	5.23

Relevant exposure determinants (red):

- Emission rate (*G*)
- Air mixing between NF and FF (β)
- NF local exhaust ventilation (Q_{LEV})

Less relevant exposure determinants (blue):

- Room volume (V_{room})
- General ventilation air exchange rate (*AER*)

RWC-NF 95th percentile concentration level (without NF LEV) is 1.92 mg/m³ (in 150 min)

- 8-h TWA RWC-NF 95th percentile is 0.59 mg/m³ (0.13 × OEL) → **Apply NF LEV**
- If two baches are manufactured the exposure is 0.25 × OEL → **Apply NF LEV**

TARGET USERS

- **Occupational safety managers**:
  - Mandatory by OSH and ECHA legislation
- **Process equipment manufacturers**:
  - Process safety data sheets makes possible to comply with EN689 (reduced safety management costs → Improved sales)
- **Material manufacturers**:
  - Material safety data sheets
  - Chemical safety reports
- **Product manufacturers** (optional):
  - Quantify CoU for consumer products

"This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 862444".

Conclusions

- A method to quantify relevant exposure determinants and CoU:
    - Probabilistic exposure assessment & sensistivity analysis
    - Simplifies safety communication: Focus only on *relevant* exposure determinants

- Examples of applicability:
    - Paint factory pigment formulation (Koivisto et al. 2021)
    - Industrial nanocoating process (Koivisto et al. 2022)

- **CONS:** Emissions (rates/factors) needs to be known (basic requirement for any predictive exposure assessment)

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Extra slides

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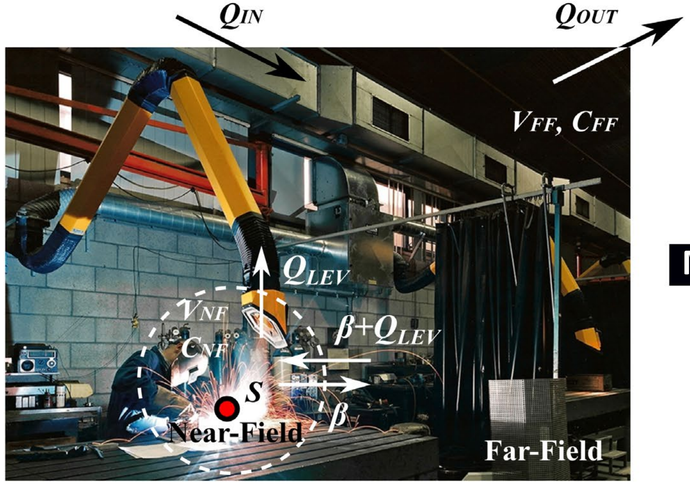
ASINA

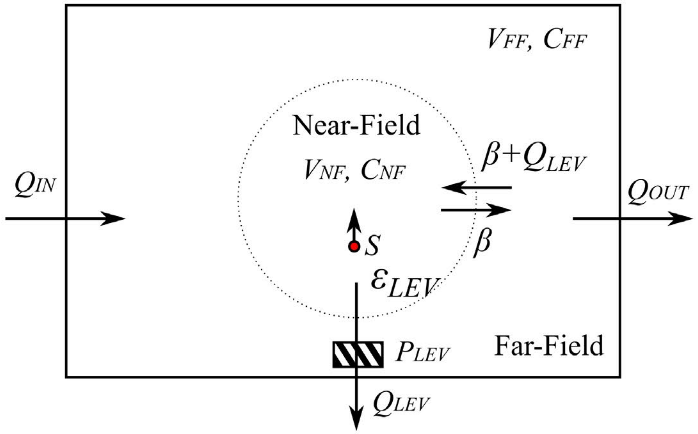
Near-Field/Far-Field (NF/FF) model

Workplace



Model

Simplified physical concept



Exposure determinant	Symbol, [units]
Emission rate from process	S, [µg s^{-1}]
Far-Field volume	V_{FF}, [m^3]
Near-Field volume	V_{NF}, [m^3]
Air mixing between NF and FF	β, [m^3 s^{-1}]
Incoming ventilation	Q_{IN}, [m^3 s^{-1}]
Outgoing ventilation	Q_{OUT}, [m^3 s^{-1}]
Local exhaust ventilation	Q_{LEV}, [m^3 s^{-1}]
Local control efficiency	ε_{LEV}, [-]

Mathematical representation (*e.g.* Ganser and Hewett, 2017):

$$V_{FF}\frac{dC_{FF}}{dt} = \beta \cdot C_{NF} - (\beta + Q_{LEV} + Q_{FF})C_{FF}$$

$$V_{NF}\frac{dC_{NF}}{dt} = (1 - \varepsilon_{LEV}) \cdot S + (\beta + Q_{LEV})C_{FF} - (\beta + Q_{LEV})C_{NF}$$

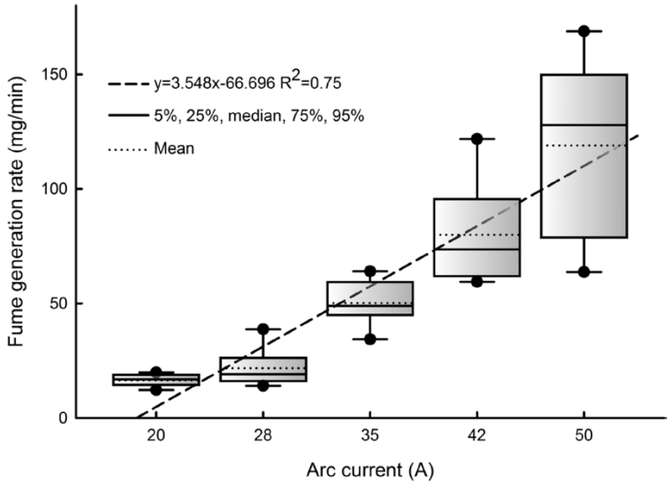
Assumptions:

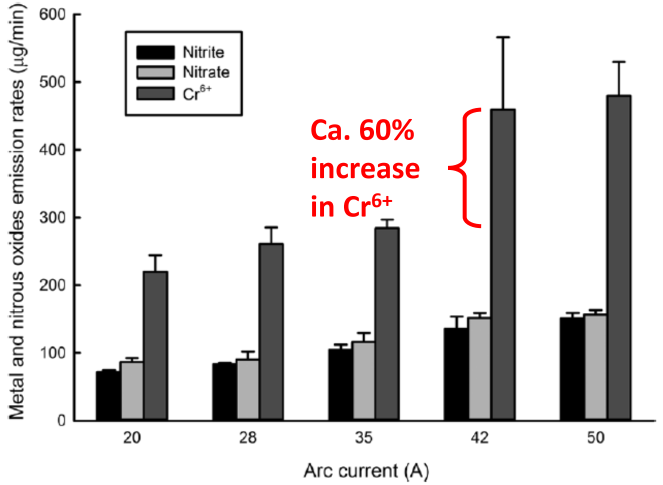
- All mass entering the model volume is created at a source inside the NF volume or from incoming ventilation air.
- Particles are fully mixed at all times in the NF and FF.
- There is limited air exchange between NF and FF volumes.
- There are no other particle losses than the FF and NF ventilation.

Some examples of exposure determinant libraries

Plasma cutting (Wang et al. 2017)

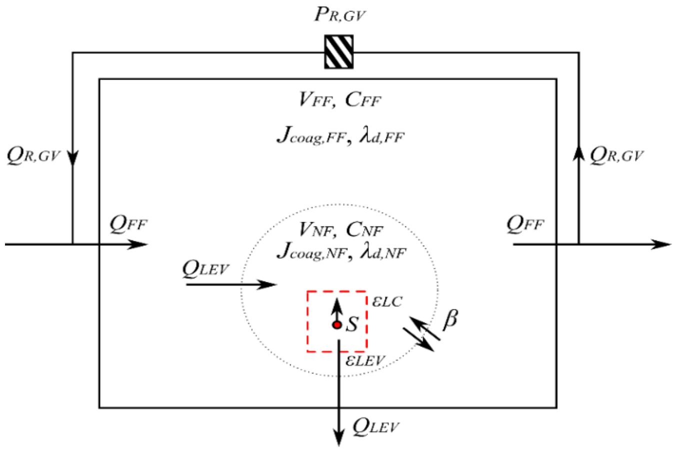
- **Emission/release libraries:**
  - Welding and allied processes (HSL, 2000)
  - Volatile organic compounds (Abadie and Blondeau, 2011)
  - Nano-enabled articles and products (Koivisto et al., 2017)
  - Microbial VOC emissions (Lemfack et al., 2018)
  - 3D printer emissions (Byrley et al., 2020)
- **Emission control efficacy library** (Fransmann et al., 2008; Goede et al., 2018)
- **Air mixing between NF and FF** (see Table 3 in Koivisto et al., 2019)



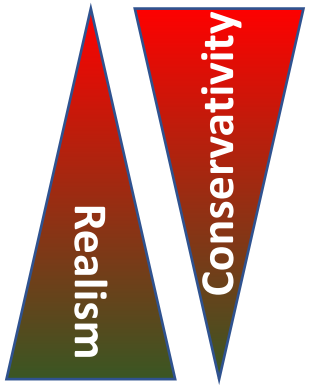


Summary of mass-balance models

- Widely used and well accepted
- Can be very dynamic but preserves transparency
- Available knowledge (parameterization) defines the model complexity
- Less knowledge more precautionary
- NF/FF model precision is good, similar results when single box model, when applied accordingly



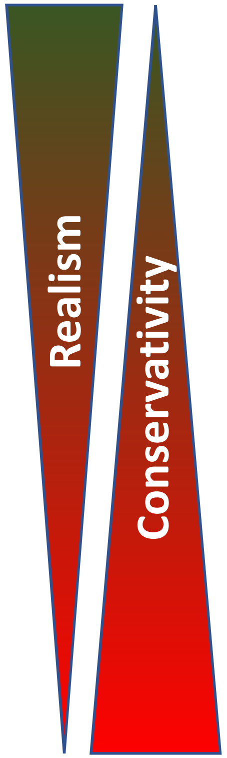
Example of parameterization in Tiered approach: WC = worst case, DP = Default parameterization, Mo = modelled and Me = measured,.



Free parameters	Variables									
	S, [X s^{-1}]	V_{FF}, [m^3]	V_{NF}, [m^3]	β, [m^{3}s^{-1}]	Q_{FF}, [m^{3}s^{-1}]	ε_{LC}, [-]	ε_{LEV}, [-]	Q_{LEV}, [m^{3}s^{-1}]	$\varepsilon_{R,GV}$, [-]	$Q_{R,GV}$, [m^{3}s^{-1}]
1	WC	20	8	20	0	0	0	0	0	0
2	WC/Mo	20	8	20	WC	0	0	0	0	0
1 to 8	WC/Mo	WC/DP	WC/DP	WC/DP	WC/DP	WC/DP	WC/DP	WC/DP	0	0
4 to 8	Mo/Me	DP	DP	DP	DP	Me	Me	Me	DP	DP
4 to 8	Mo/Me	DP/Me	DP/Me	DP/Me	DP/Me	Me	Me	Me	DP/Me	DP/Me

Penny Nymark, Martine Bakker , Susan Dekkers et al., (2020) Toward Rigorous Materials Production: New Approach Methodologies Have Extensive Potential to Improve Current Safety Assessment Practices. Small 16, 1904749. https://doi.org/10.1002/smll.201904749

Model parametrization



The most relevant exposure determinants are typically: 1. emission source, 2. emission control efficacy, 3. air mixing near the source and 4. worker location and exposure durations.

Tiered parametrization:

- *In-situ* observations (measured emission rates, air mixing,…)
- Extrapolation and read-across from similar conditions: A 25th or 75th (5th or 95th) percentile of probability density function depending which one favours higher exposure level (Bremmer et al., 2006).
- Theoretical predictions, such as for emission source:
  - Volatiles: Henry's Law or Raoult's Law (Abattan et al. 2021)
  - Powders: Material dustiness (Ribalta et al. 2021)
- RWC conditions: e.g. worker is near the source 6-h during a work shift.
- Worst case conditions: e.g. worker all the time near the source, all material losses in process becomes inhalable.

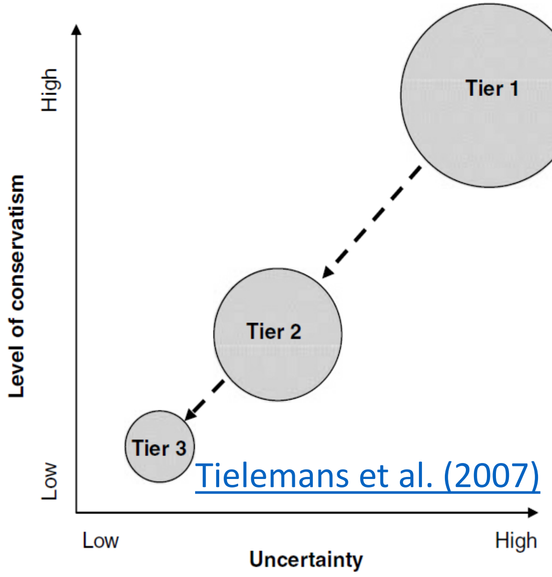
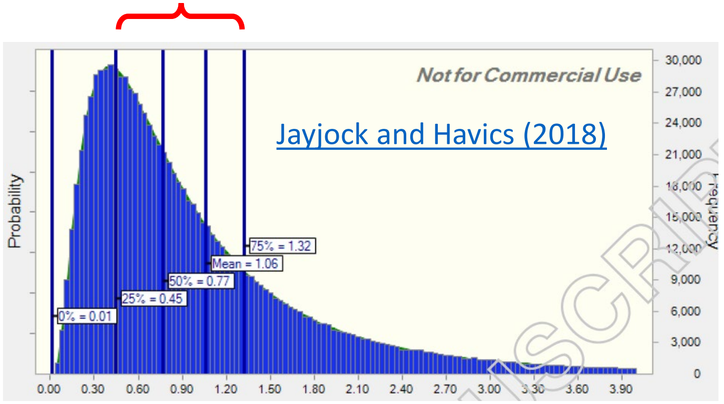


Figure 1. Tiered exposure assessment approach in relation to uncertainty and level of conservatism.

AER estimate: Mean 1.06 [0.45 (25%); 1.32 (75%)]

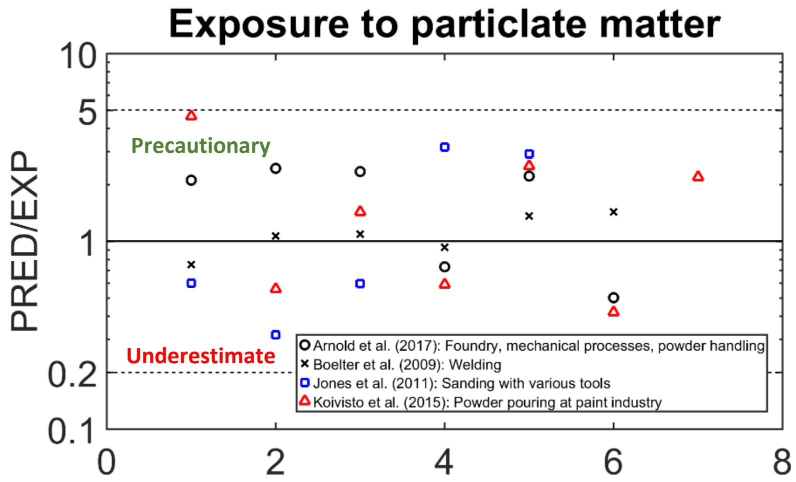


Example of assessing default value for households air exchange ratio

Performance of the well-parametrized NF/FF model

Definition: Performance is the ratio of predicted exposure and measured exposure (<1 underestimate; >1 overestimate).

- Typical performance of NF/FF model is:
  - **0.3–3.7 times for solvent vapours** (Abattan et al., 2021).
  - **0.5 to 5 for powders** when source is estimated with powder dustiness (Ribalta et al., 2021)
  - **0.3 to 5 for different processes** emitting particulate matter (e.g. Iron foundry, Dry wall finishing, weighing and transferring, Mixing and cleaning, Welding, Sanding, powder pouring, laser-generated particles).
- Good evidence that NF/FF model is useful tool for predicting worker exposure at reasonable precision
- Better understanding is needed to understand when model can fail i.e. when the model concept or parametrization is not reflecting the exposure situation (Abattan et al., 2021).



NF/FF model performance for different industrial processes (See Table 1 in Koivisto et al., 2019)

Data collection for exposure assessment

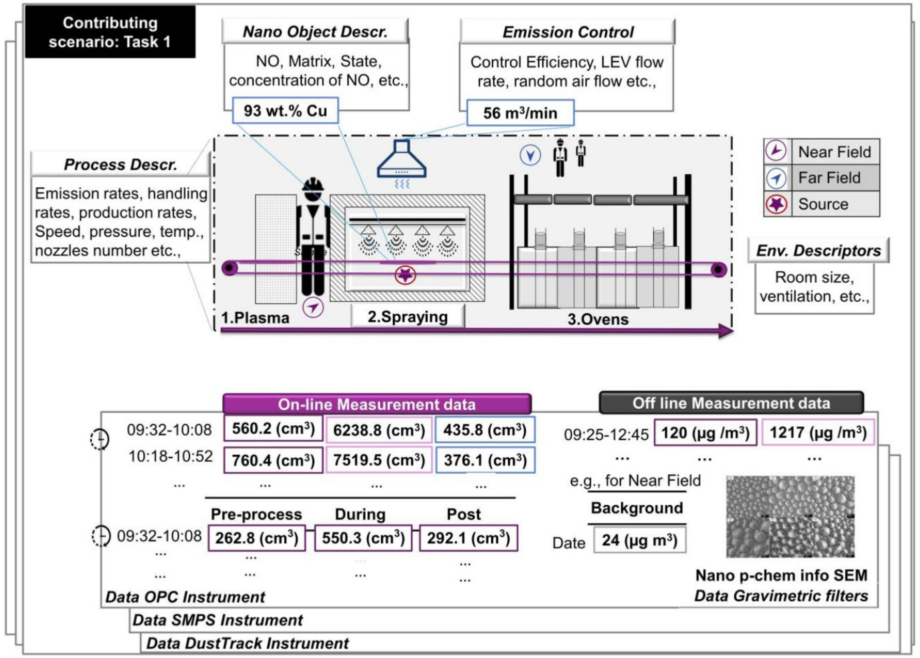
nanomaterials MDPI

Article

Data Shepherding in Nanotechnology. The Exposure Field Campaign Template

Irini Furxhi [1,2,*], Antti Joonas Koivisto [3,4,5], Finbarr Murphy [1,2], Sara Trabucco [6], Benedetta Del Secco [6] and Athanasios Arvanitis [7]

Provides the fundamental principles for occupational exposure data collection in scientifically Findable, Accessible, Interoperable and Reusable format (FAIR principles)



Tools for rapid chemical safety assessment (Koivisto et al. 2019)

Example of using novel safety concepts (occupational exposure)

1. Process emission

Fume and Cr^{VI} generation rates during gas (95% Ar/5% CO_2) metal arc welding of stainless steel (Keane et al. 2009).

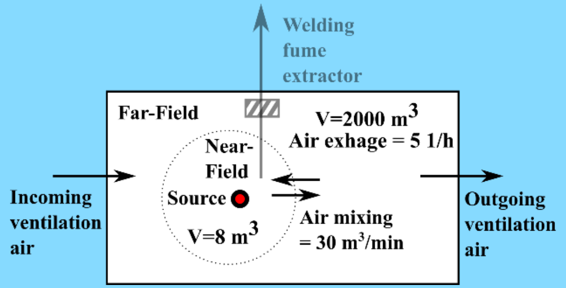
BLUE MAX® MIG 308 LSi

Component	Emission rate (µg/min)	Emission index (µg/kg wire*)
Total fume	1700	28400
Cr^{VI}	**4.4**	**73.4**

*Wire feed rate v = 760 cm/min; $\dot{m}$ = 60 g/min

2. Default Exposure scenario

Assumption: Typical welding hall with or without fume extractor. Short term 15-min welding (0.9 kg) and continuous 8-h welding (28.8 kg)



3. Operator mean exposure (Cr^{VI} in µg/m³)

C_{NF} (8-h)	C_{NF} (15-min)	$TLV_{8\text{-}h}$*	$TLV_{15\text{-}min}$*
0.17	0.022	0.2	0.5

*US. ACGIH Cr^{VI} treshold limit value

4. Relative risk

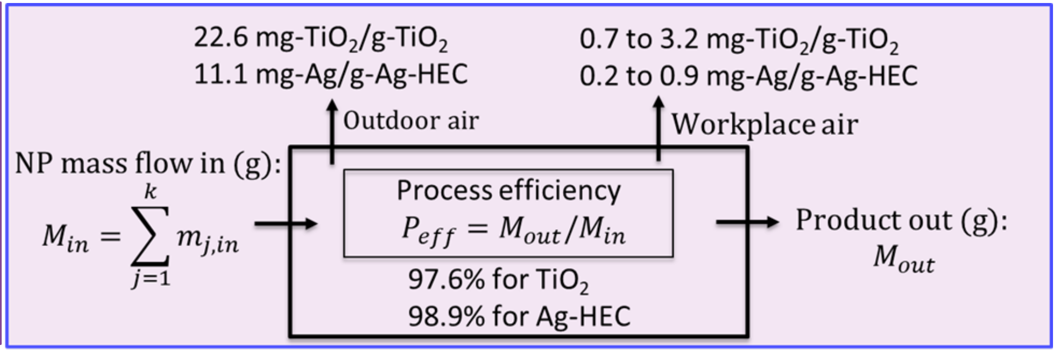
Scenario	$RR_{8\text{-}h}$	$RR_{15\text{-}min}$
RR(Cr^{VI})	0.85	0.04
RR(Cr^{VI}) LEV*	0.02	0.001

*Capturing efficiency 90%; Q_{LEV} = 100 m³/min

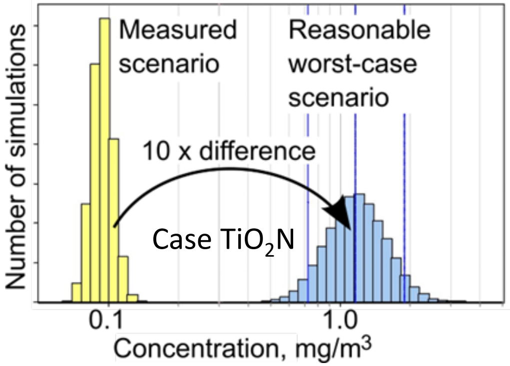
5. Safety decision: Long term welding requires respirator or an emission control. Total fume emissions is *ca.* 30 mg/kg of wire. **Operator exposure can be estimated as $C = E_{SF} \times M_{wire}$**, where E_{SF} exposure scaling factor is $5.1\times10^{-3}\ \frac{\mu g}{m^3 \cdot kg}$ and M_{wire} is use of wire in kg during 8-h (V_{NF} = 8 m³ and $Q_{air\ mixing}$ = 30 m³/min and infinitive dilution in far-field.

Example: CoU for Nanocoating process (Koivisto et al. 2022)

Del Secco et al. 2022



Reasonable worst-case conditions compared to measurement conditions
2 × smaller room
2 × smaller ventilation
2 × smaller air mixing
2 × mixing volume
Highest emitting process parameters
14 × longer process time
26 × higher consumable use



Extrapolation of NF concentrations from measured scenario to RWC scenario with 6-h of spraying per work shift

Setting CoUs for continuous process

- Recommended limit values (NIOSH: TiO_2 300 μg m^{-3}, Ag 0.9 μg m^{-3}) → Recommended CoUs
- TiO_2 TWA exposure under RWC 171 TiO_2-μg/m^3 (0.6 × REL_{TiO2}) → Under RWC conditions a control reducing exposure by a factor of 6 is needed OR perform personal measurements to verify EN689 compliance OR wear RPE

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Exposure model regulatory compliance

- Raul and Dwyer (2003) used to assess whether expert witnesses' scientific testimony is methodologically valid is the Daubert standard (Daubert v. Merrell Dow Pharmaceuticals, Inc., 509 U.S. 579, 1993)

Daubert criteria	Compliance
Is applicable and has been tested	The models have been validated and tested only at 'operational analysis' level
Has been subjected to peer review and is generally accepted	Calibration database is not subjected to peer review and this is the first study evaluating the theoretical background in detail. It is the scientific community's responsibility to evaluate findings in this study and decide if the models constructs are acceptable for regulatory chemical safety decision making
The rate of error is known and acceptable, i.e. 'Does the chosen model, with its simplifying assumptions, adequately simulate conditions to give reasonable estimates and useful insights?' (Jayjock *et al.*, 2011)	The rate of error has been shown very high. The models have shown high uncertainty why their applicability in a chemical safety decision making should be revised
The existence and maintenance of standards and controls concerning the operation	The models fulfills this condition
Is generally accepted in the relevant scientific community	This should be revised by including the findings from this study and the calibration data bases

The Dutch Social Economic Council (Rijksoverheid) lists following criteria:

1. Twenty comparisons per application domain.
2. Evaluation is done separately for solids, liquids, and/or gases/fumes.
3. The Spearman correlation in comparison is at least 0.6.
4. The tool estimates a reasonable worst-case which represents the upper-end side of possible exposure values.
5. Measurements do not exceed the model estimates for more than 10% of the total comparisons.

NF/FF model complies the criteria by Daubert and the Dutch Social Economic Council (Jayjock et al. 2011)
ECHA regulatory exposure models Stoffenmanager, ART, MEASE, ECETOC TRA regulatory compliance have not been assessed (Koivisto et al. 2022, see also review comments at Zenodo)

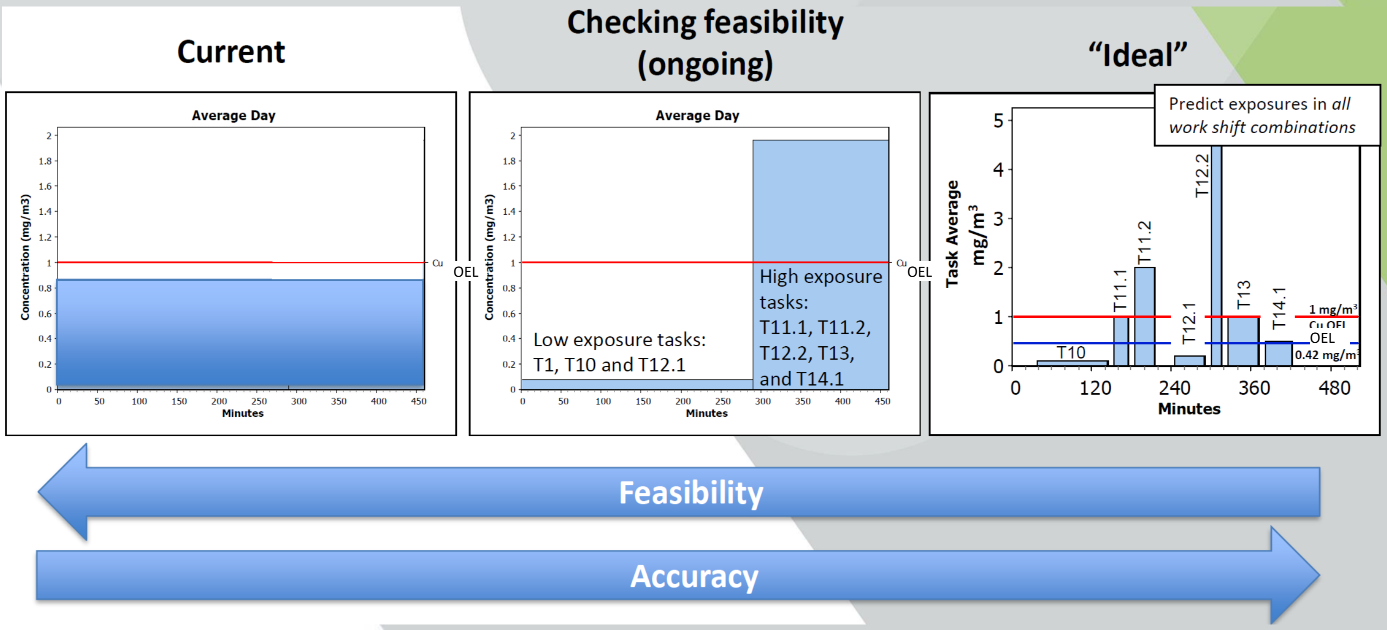
Exposure data collection for setting CoU

Data collection for setting Conditions of Use (CoU):

- Worker performs many tasks with varying durations and it is challenging to combine similar exposure groups (SEGs)
- Exposure assessment:
  - Quantitative (measurements) is limited
  - Qualitative is available (e.g. PPE specification)
  - Task specific exposure assessment was not considered feasible
  - Exposure categorization to low/high exposure scenarios is considered

Exposure taxonomy

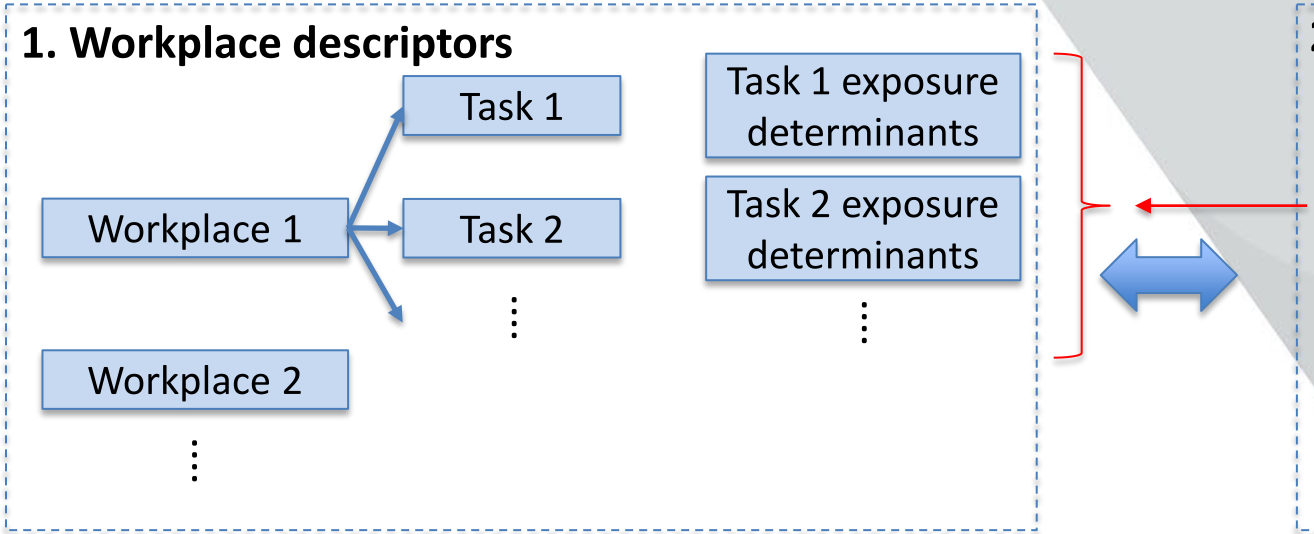
Taxonomy can vary between companies, national level, or down-stream use → Harmonization needed



Data collection questionnaire

Exposure grouping requires information about exposure determinants:

- Dividing a data collection to 1) workplace descriptors and 2) measurements → Simplifies contextual data collection!



2. Exposure

Measurement	Exposure, [mg/m³]
Workplace 1: • T1 140 min • T2 100 min • T3 60 min	0.01
	0.02
	0.03
Workplace 1: • T1 150 min • T2 150 min	0.001
	0.002
	0.003
⋮	⋮

Requirements:

- Registration of workplace exposure determinants
- Measurer register performed tasks during sample collection