Theoretical Background and Application of Occupational Exposure Models

Mass balance modelling approach

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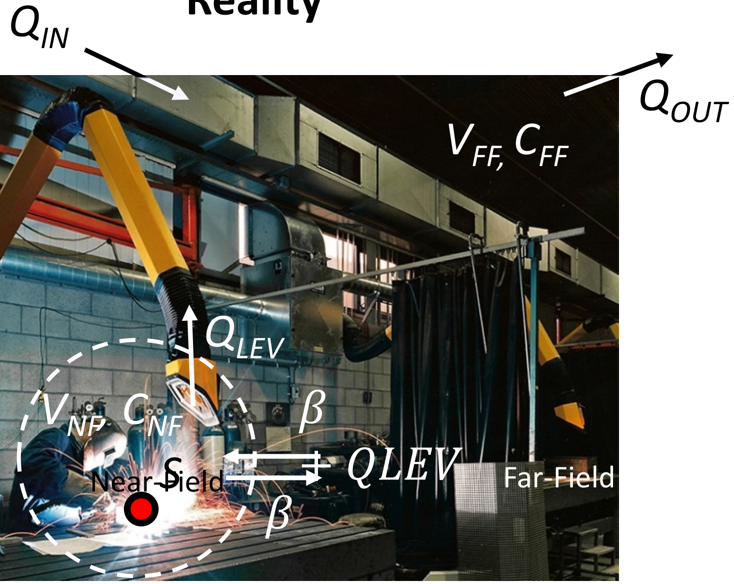
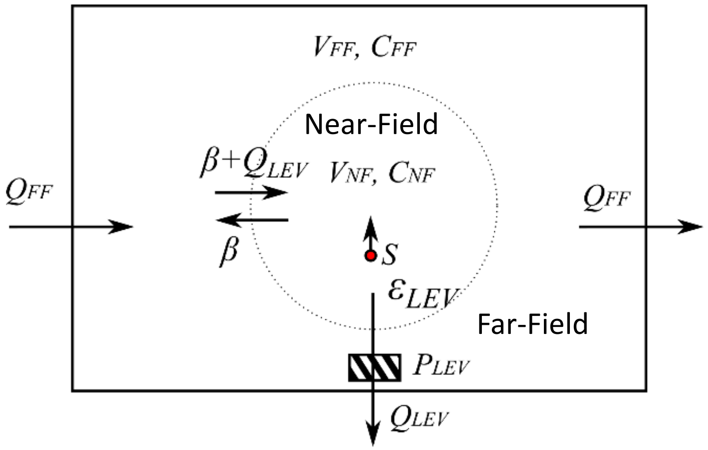
Reality



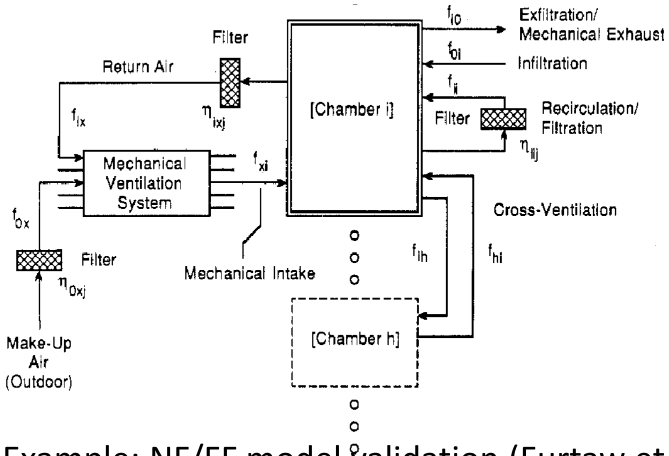
Simplification

Mathematical model and parametrization



Mass-balance models

Example: General form of indoor mass balance model (William Nazaroff, 1989)



Example: NF/FF model validation (Furtaw et al., 1996)

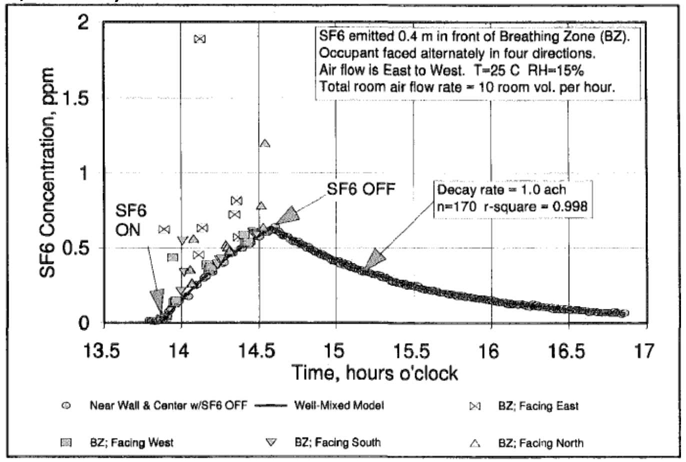


Figure 7. Experiment No. 2. Concentrations in breathing zone (0.4 meters from source) exceed well-mixed model predications.

Applied long time in exposure sciences: E.g. NF/FF model (Hemeon, 1955) and multi-compartment model (Nazaroff, 1989)

Validated and tested*: Langstroth and Gillespie (1947), Corner and Pendlebury (1951), Nazaroff (1989), Furtaw et al. (1996), Nicas (1996;2016), Zhang et al. (2009), …

Regulatory applicability evaluated (Jayjock et al., 2011, EPA???)

Models are widely available: E.g. PANDORA, MOEEBIUS, CONTAM, IH-MOD 2.0 , TEAS, GuideNano, and ConsExpo

Broadly developed, such as:

- *Bayesian approach* (e.g. Zhang et al. 2009)
- *Physical and chemical processes*: e.g. deposition, coagulation, condensation, evaporation, and chemical transformations (e.g. Seinfeld & Pandis, 2016)
- *Parameter measurements*: Emission libraries (VOC ~9000, mVOC ~2000), emission control efficacy libraries (>400), air mixing (~100) and ventilation (Q) (see review from Koivisto et al. 2019)
- *Default values* (e.g. Bremmer et al., 2006 and Oltmanns et al., 2015)

Can be combined with other models: E.g.

- Ambient air pollution (Hussein et al. 2015),
- Surface contamination (Schneider et al. 1999), and
- Physiologically based toxicokinetic models (Webster et al. 2016)

Applicable for both consumer and occupational exposure assessment

*Validation = Testing that the model theory (within boundaries) agree with observations (within tolerances) and computational algorithms are correct.

Parameterization

Easy to understand:

- Parameters are physical quantities (measurables)
- No conversions (“as observed”)
- Variation and uncertainties can be quantified

Parameters relative effects are easy to estimate (e.g. particle removal rate via deposition vs. ventilation):

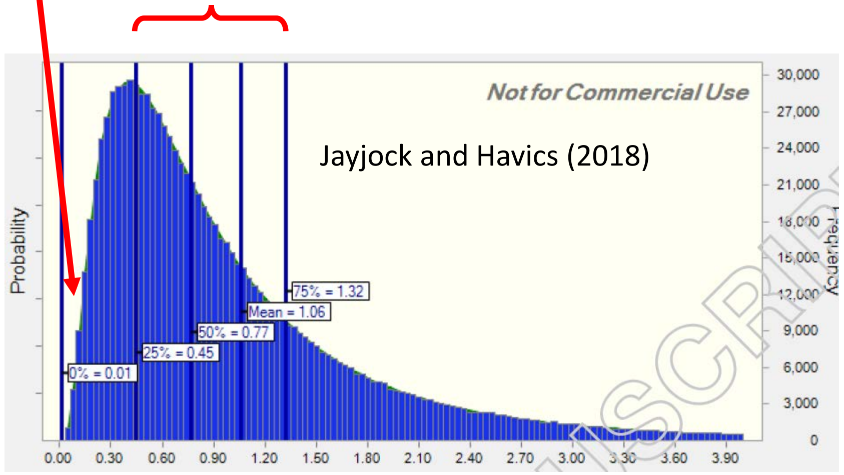
- Can be used to justify complex models simplification!

Can be extended for unique processes, such as e.g.:

- Air flows across open/closed doors (McGarth et al. 2014)
- Air cleaner particle removal rates (Mølgaard et al. 2015)
- Photoactive surfaces (Shayegan et al. 2018)
- Recirculation air filtration efficiencies from manufacturers

Conservative estimate for AER: Lowest 5% percentile

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



Example of assessing default value for households air exchange ratio

Conservativity

- Defined by parameterization and model construct
- Follows "truly" tiered approach: Reducing model complexity increases conservativity (e.g. 1-parameter model very simple but highly conservative)
- Conservativity is well-justified (i.e., can be quantified) and is not only based on model variation or uncertainty
  - Conservativity can be assigned parameter basis, such as e.g. source is measured but use conditions are not specified → conservative single box model
- Common default values can be set at international level to ensure harmonization and conservativity

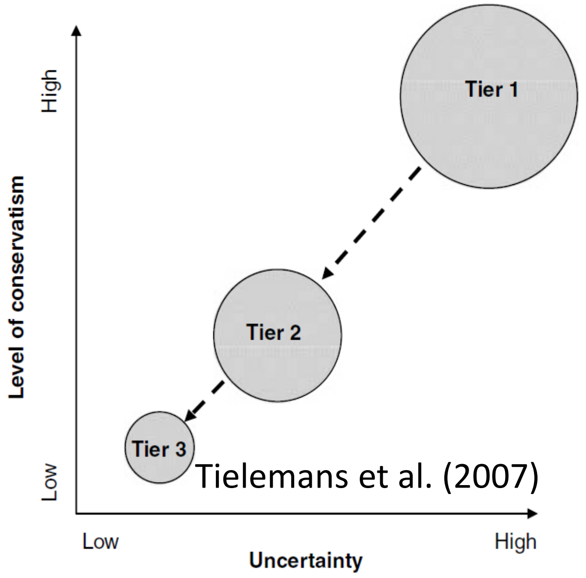
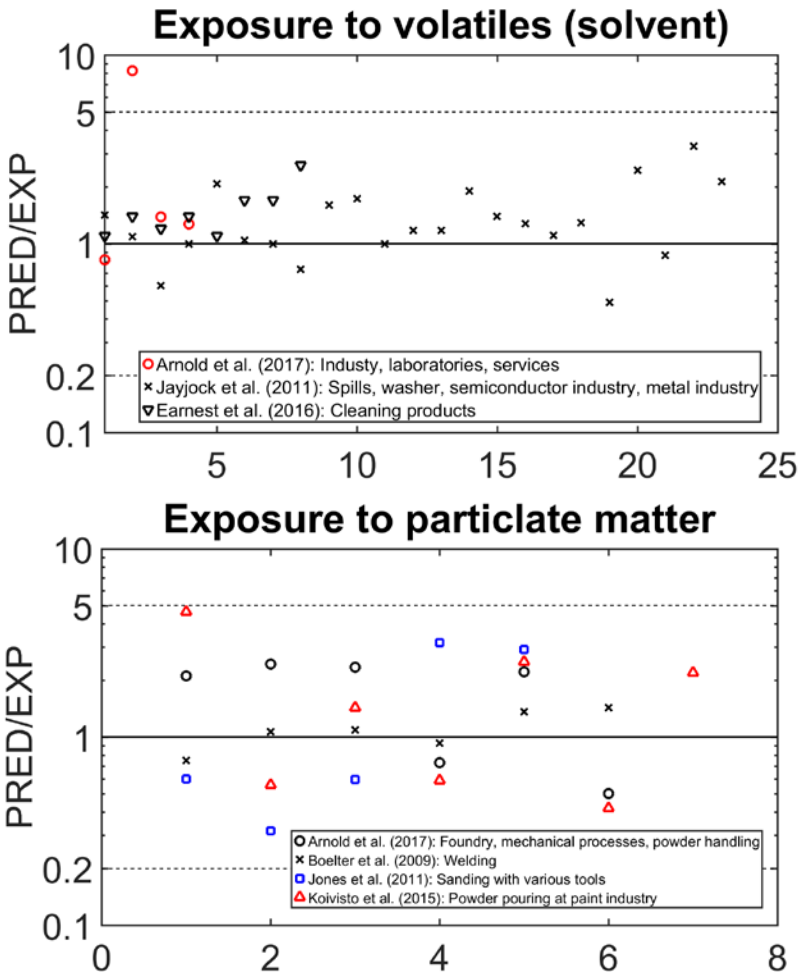


Figure 1. Tiered exposure assessment approach in relation to uncertainty and level of conservatism.

Predictability (model testing/validation/…)

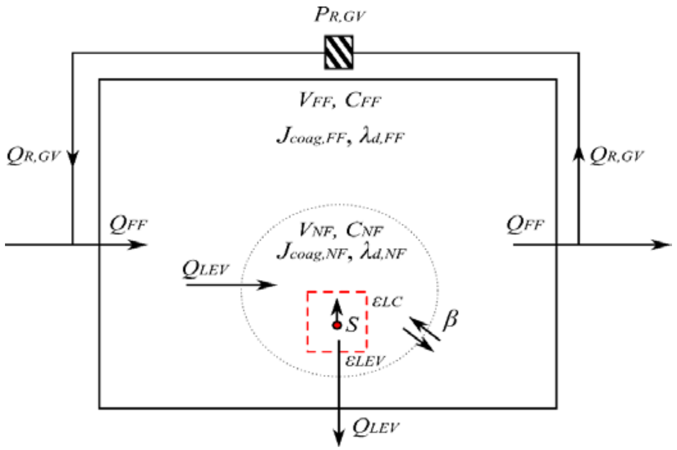


Ratio of predicted (PRED) and measured exposure (EXP) assigned for various occupational exposure scenarios.

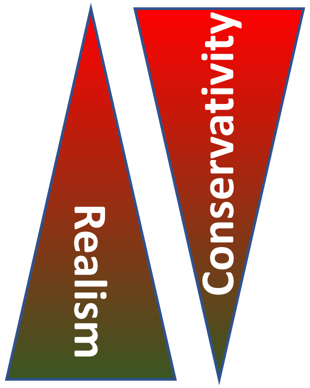
- The NF/FF model predictability usually within the range of 0.5- to 2-fold (Jayjock et al. 2011; the Figure), Arnold et al., 2016
- Single box model results similar when applied accordingly (fully mixed)
- StM and the ART calibration databases can be used:
  - For model applicability testing
  - To assign similar exposure groups
  - To identify relevant exposure determinants
  - To quantify the exposure determinants (e.g. source, handling energy factor)

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

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Key points

- Use for exposure analysis is well established
- Model parameterization, such as conservativity, is well-justified and transparent
- Model limitations, variation and uncertainty evaluation is well established and transparent
- Model developmental opportunities are unlimited
- Exposure data with contextual information is needed to understand appropriate model parametrization and limitations