Data Generation for Emission Rates

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Need for high quality generation rates

- Model performance is heavily influenced by our ability to generate high quality emission rates
  - Need for reasonably accurate estimates, rather than significantly overestimating them promotes efficient and effective use of resources to those control exposures and risks that most need mitigating
  - Use of tiered approach that starts with screening level models and applies higher tier models as necessary to refine exposure estimates
- Requires a non-trivial investment of resources
  - That will lead to accurate emission rates and exposure estimates
  - For a wide-range of exposure scenarios and conditions of use
  - Delivering a high return on investment

Demonstrating feasibility and impact

While there are no conventions or standards (yet) for generating emission rates, there are numerous examples that demonstrate the feasibility and impact of high-quality generation rates.

In this presentation, we will focus on three as illustrative case studies.

1. All purpose cleaner – aqueous chemical mixture
2. Medical device manufacturing – metal powder
3. Fiber settling study

Case Study 1

- All-purpose floor cleaner – mopping exposure scenario
- Chamber and Field Study
  - Chamber environment supports development of emission rates under tightly controlled conditions that simulate specific scenarios/conditions of use
- Field Study
  - Real world environment provides confidence in accuracy of emission rate
  - Also demonstrated portability of emission rate

Study Objectives (Arnold et al. 2020)

This study was motivated by the need to refine a highly overestimating screening level assessment. Modeling evaporation from aqueous mixture required the development of an emission rate

Objectives:

1. Develop a reasonably accurate emission rate for acetic acid evaporating from an all-purpose cleaner aqueous mixture
2. Evaluate the accuracy of the emission rate in a real-world environment by comparing measured and modeled exposures

Emission Rate Development - Chamber Study

ESTIMATING A TIME -VARYING GENERATION RATE

$$G_1(t) = M_0 k e^{-kt} \tag{1}$$

$$G_2(t) = G_1(t) + M_0\, k e^{-k*(t\_2-t\_1)} \tag{2}$$

$$G_n(t) = M_0 k e^{-kt}\left[\frac{1-e^{-kn}}{1-e^{k}}\right] \tag{3}$$

where
$G_1(t)$ is the generation rate at time t (mg/min)
M_0 is the mass applied at t = 0 (mg)
k is the unknown evaporation rate (min^{-1})
t is the time over which the first spill occurs, 0 < t < 1

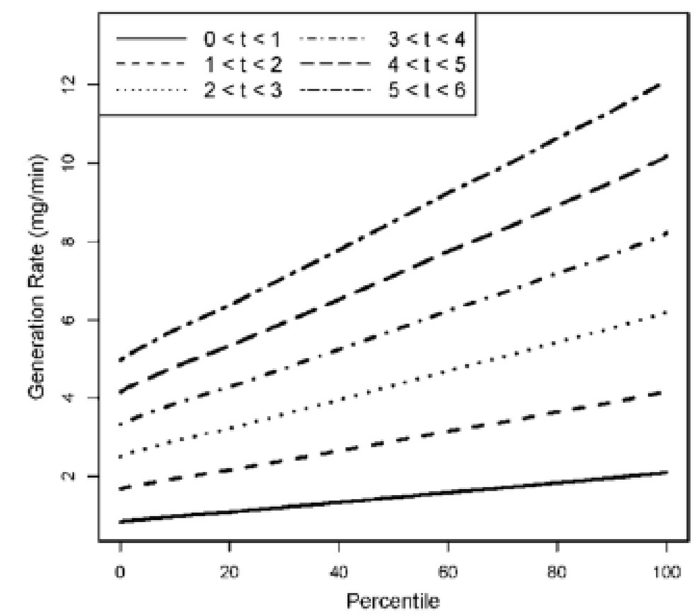


Fig. 3 Cumulative plot of time-varying generation rates. After solving for the evaporation rate, *k*, accounting for differences associated with measurement averaging time, a range of values for *k* was generated. By incorporating this range of values of *k*, a distribution of time-varying generation rates was generated for each "small spill" over a 6 min period

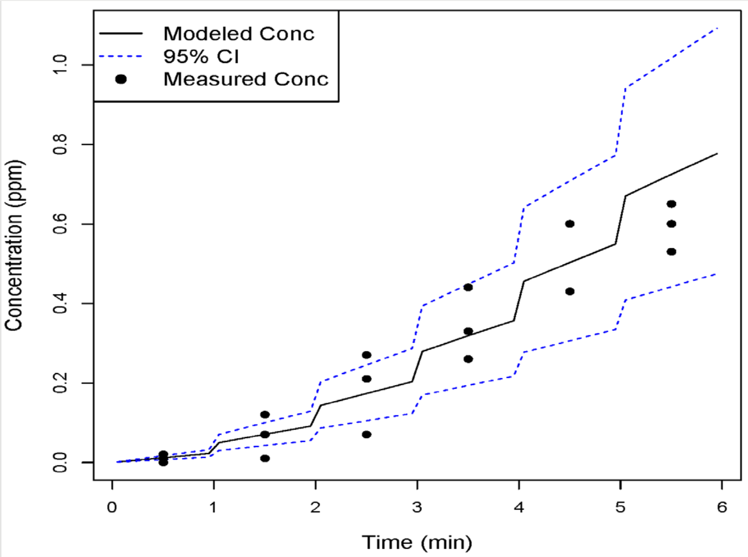
Arnold, S., Ramachandran, G., Kaup, H., & Servadio, J. (2020). Estimating the time-varying generation rate of acetic acid from an all-purpose floor cleaner. Journal of exposure science & environmental epidemiology, 30(2), 374-382. https://doi.org/10.1038/s41370-019-0142-5

Field Evaluation of Emission Rate using the Well Mixed Room (WMR) model

TIME WEIGHTED AVERAGE (TWA) MEASURED AND MODELED ACETIC ACID CONCENTRATIONS

	Time Weighted Average Concentration (ppm)	
	Measured	WMR
Room 1	0.413 (0.334)	0.305 (0.272)
Room 2	0.281 (0.229)	0.301 (0.267)
Room 3	0.864 (0.822)	0.777 (0.681)

Showing mean and (SD) concentrations averaged over six minutes (n=3).
WMR: Well Mixed Room model.



Measured and Modeled (WMR model) Acetic Acid Concentrations in Room 2

- Using the time-varying emission rate, the WMR model accurately predicted exposures to acetic acid
- The refined exposure estimates were three orders of magnitude lower than the screening level estimate.

Case Study 2

- Weighing and Mixing Cobalt Lithium Powders
- Field Study
  - Tasks that create airborne particulate
  - Emission rates of powders and aerosols are difficult to predict, and typically need to be determined using field/laboratory measurements
  - This is feasible in real-world environments with direct reading instruments
    - Often combined with integrated measurement methods when speciation is needed

Study Objectives (Arnold et al. 2017)

This study was motivated by the need to evaluate the performance of two commonly used models, the well mixed room (WMR) and near field far field (NF FF) models.

Objectives:

1. Characterize exposure determinants and exposure to Lithium Cobalt in a manufacturing clean room
2. Model exposures using the WMR and NF FF models
3. Evaluate agreement between measured and modeled estimates

Emission Rate Development – Field Study

- Weighing and mixing Lithium Cobalt in clean room
- Estimating the emission rate using source sampling: $G = CQ_{NF}$
  - Using direct reading instruments to measure C
  - Applying Monte Carlo approach to model exposures using the WMR and Near Field Far Field (NF FF) models

Comparing $C_{measured}$ and $C_{modeled}$ Exposures

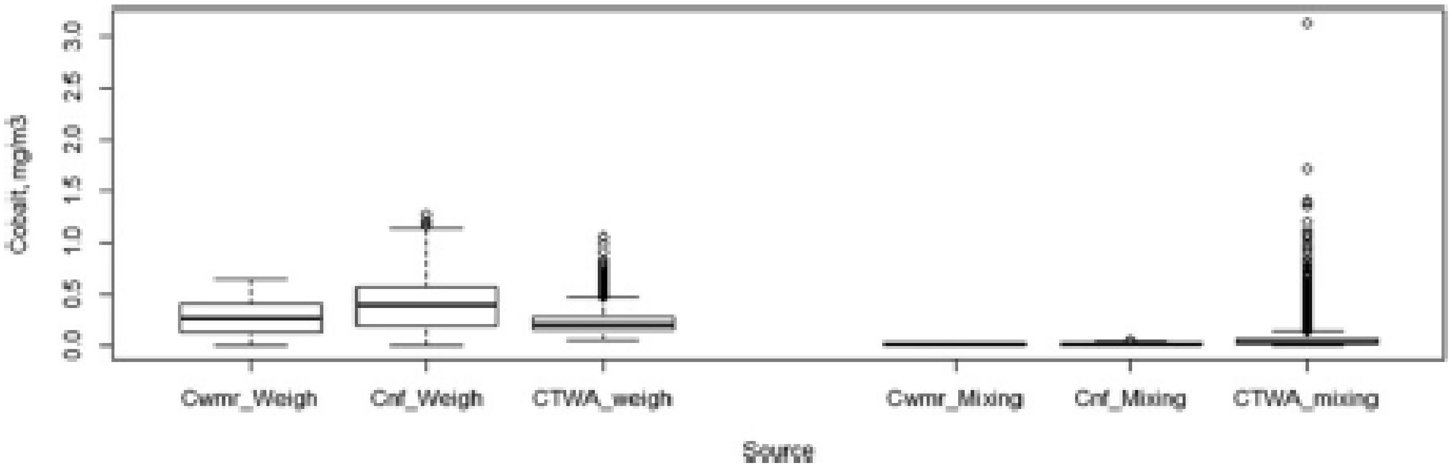


Figure 1. Comparison of modeled and measured Cobalt (mg/m^3) for weighing and mixing tasks. Cwmr_Weigh is the weighing task exposure estimate based on WMR model. Cnf_Weigh is the NF weighing task exposure estimate based on the NF FF model and CTWA_weigh is the TWA Cobalt exposure calculated from personal exposure measurements, n = 6. Cwmr_Mixing is the mixing task exposure estimate based on WMR model. Cnf_Mixing is the NF mixing task exposure estimate based on the NF FF model and CTWA_mixing is the TWA Cobalt exposure calculated from personal exposure measurements, n = 6.

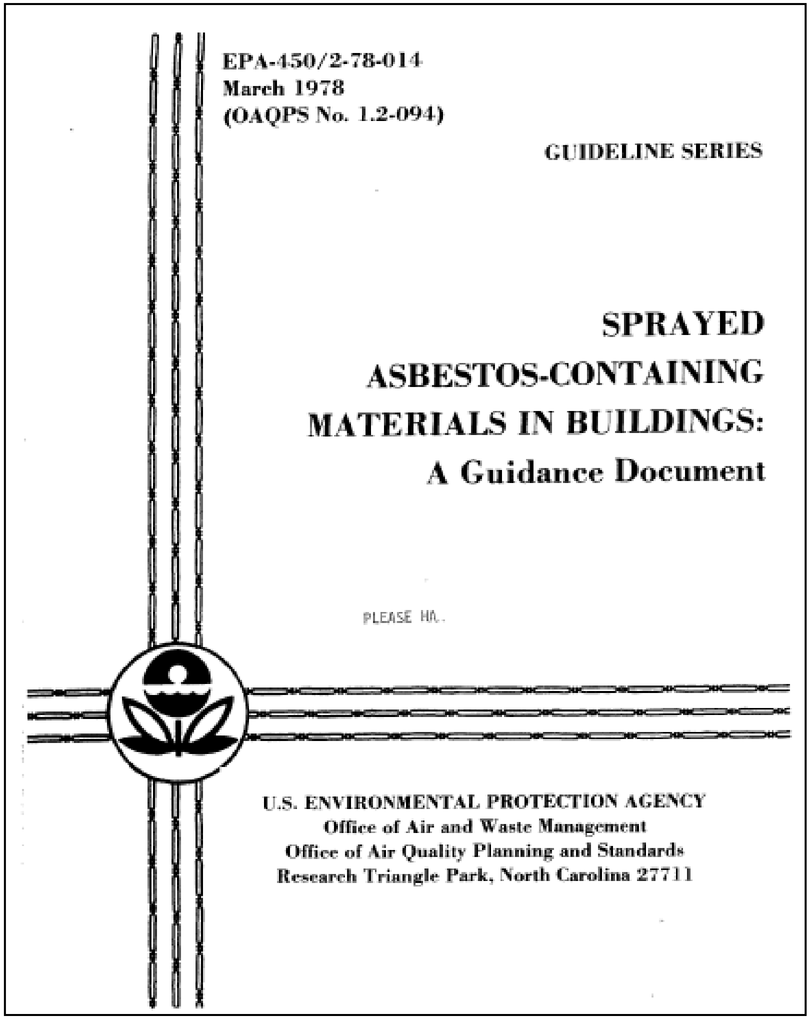
Susan F. Arnold, Yuan Shao & Gurumurthy Ramachandran (2017) Evaluation of the well mixed room and near-field far-field models in occupational settings, Journal of Occupational and Environmental Hygiene, 14:9, 694-702 https://doi.org/10.1080/15459624.2017.1321843

Case Study 3

- Evaluating Fiber Settling
- Chamber Study

Fiber Settling: Historical Modeling Estimates

- U.S. EPA (1978):
  - Fibers of 5 µm in length with a 5:1 aspect ratio would require 4 hours to settle out of still air from a height of 9 feet.
  - Fibers 2 µm and 1 µm in length would require 20 and 80 hours, respectively, to settle.



EPA-450/2-78-014
March 1978
(OAQPS No. 1.2-094)

GUIDELINE SERIES

SPRAYED ASBESTOS-CONTAINING MATERIALS IN BUILDINGS: A Guidance Document

PLEASE HA

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Waste Management
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina 27711

Study Objectives (Sahmel et al. 2015)

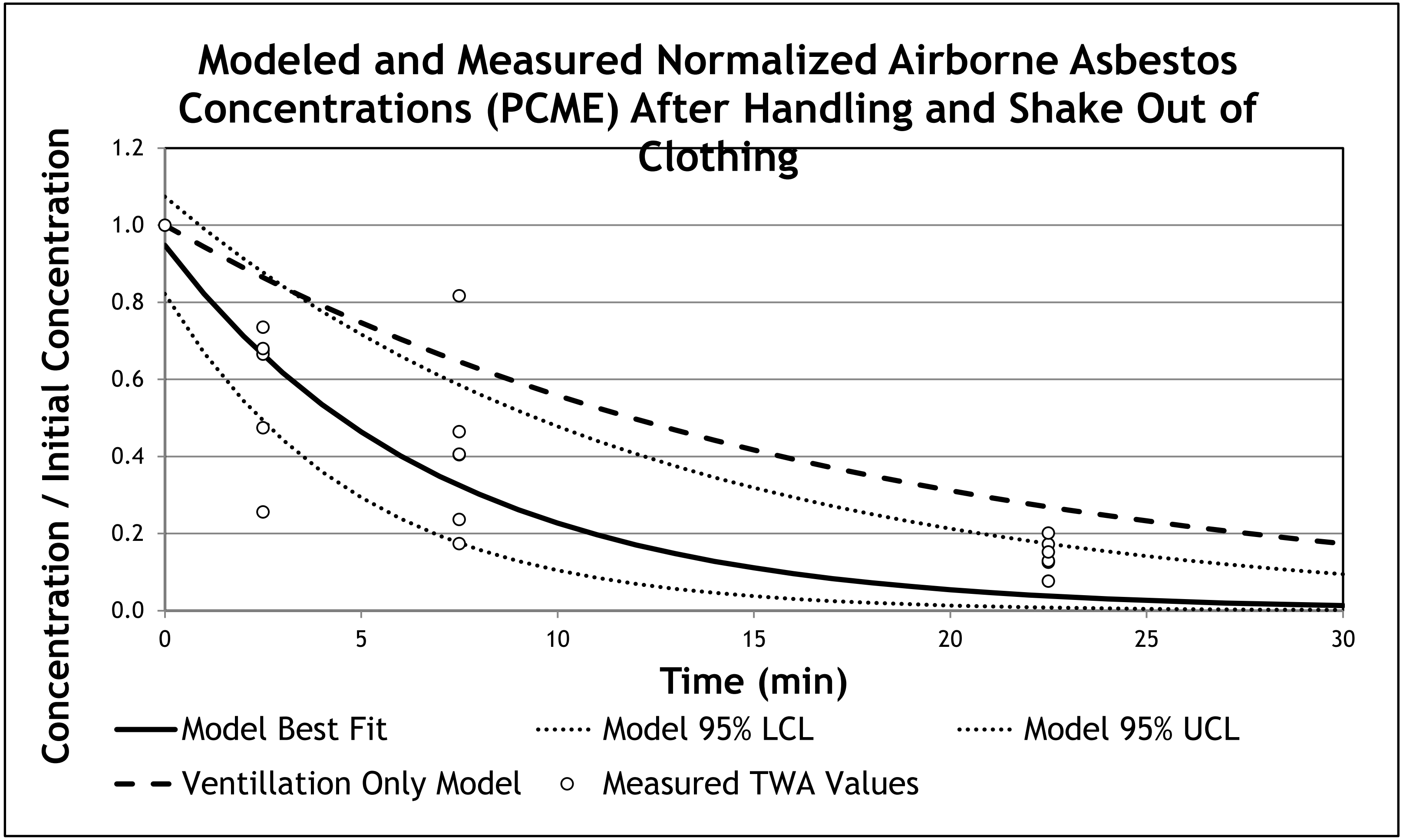
- Measure the rate of removal from air of chrysotile fibers in the PCME size range over 6 replicate tests

  and

- Compare this rate to calculated estimates based on historical models:
  - gravitational settling
  - dilution ventilation

Sahmel, J., H.J. Avens, P.K. Scott, K. Unice, A. Burns, C.A. Barlow, A.K. Madl, J. Henshaw, and D.J. Paustenbach. 2015. Measured removal rates of chrysotile asbestos fibers from air and comparison with theoretical estimates based on gravitational settling and dilution ventilation. Inhal Tox. 27(14):787-801.

Fiber Settling Using Measurements: All Events Combined



Comparison of PCME Fiber Settling Rates (Time to 99% Removal)

Approach to Estimating Removal	Est. Minutes to 99% PCM Fiber Settling
Best fit based on measured data	32 (22 – 57)
Ventilation only (3.5 ACH)	79
Measured data assuming zero ventilation	55
Theoretical: Gravitational settling	420 – 9,600
Theoretical: Gravitational settling and ventilation	60 – 79

Recommendations

- Call for a particle emission library
  - with statistical estimates for average and reasonable worst case emissions (e.g. for different sanding processes)
  - E.g. PANDORA (Pandora (univ-lr.fr)) (includes particle emissions)
- Follow a tiered approach
- Starting with fewer inputs (model parameters) at the screening level and refining with additional inputs as necessary
  - This will make interpretation easier to understand and will be more applicable over a broad range of operating conditions
- Establish or sponsor a lab-field evaluation research program to systematically assess the applicability of lab-generated emission rates for predicting real-world airborne contaminant/exposure levels across a wide range of emission types and operating conditions

Conclusions

- Model input values are portable, meaning that they can be used to estimate exposures under different conditions, different locations, different temporal periods – but more research is needed to determine how well we can characterize sources under different circumstances
- Tiered approaches allow for efficient use of resources, producing refined exposure estimates where necessary, to ensure reasonably accurate and representative exposure and risk estimates
- Selecting and applying models, given real world complexities requires non-trivial but worthwhile investment in training and practice – guidance on selecting and applying models are needed

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