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Evaluation of the well mixed room and near-field far-field models in occupational settings

Susan F. Arnold[a], Yuan Shao[a], and Gurumurthy Ramachandran[b]

[a]Division of Environmental Health Sciences, School of Public Health, University of Minnesota, Minneapolis, Minnesota; [b]Department of Environmental Health and Engineering, Bloomberg School of Public Health, Johns Hopkins University, Baltimore, Maryland

ABSTRACT

Drawing appropriate conclusions about a scenario for which the exposure is truly unacceptable drives appropriate exposure and risk management, and protects the health and safety of those individuals. To ensure the vast majority of these decisions are accurate, these decisions must be based upon proven approaches and tools. When these decisions are based solely on professional judgment guided by subjective inputs, however, they are more than likely wrong, and biased, underestimating the true exposure.

Models have been shown anecdotally to be useful in accurately predicting exposure but their use in occupational hygiene has been limited. Possible reasons are a general lack of guidance on model selection and use and scant model input data. The lack of systematic evaluation of the models is also an important factor.

This research is the second phase of work building upon the robust evaluation of the Well Mixed Room (WMR) and Near Field Far Field (NF-FF) models under controlled conditions in an exposure chamber,[5] in which good concordance between measured and modeled airborne concentrations of three solvents under a range of conditions was observed. In real world environments, the opportunity to control environmental conditions is limited and measuring the model inputs directly can be challenging; in many cases, model inputs must be estimated indirectly without measurement. These circumstances contribute to increased model input uncertainty and consequent uncertainty in the output. Field studies of model performance directly inform us about how well models predict exposures given these practical limitations, and are, therefore, an important component of model evaluation.

The evaluation included ten diverse contaminant-exposure scenarios at five workplaces involving six different contaminants. A database of parameter values and measured and modeled exposures was developed and will be useful for modeling similar scenarios in the future.

KEYWORDS
Field study; model evaluation; models; Near Field Far Field; Well Mixed Room

Introduction

Decisions regarding the acceptability of occupational exposure impacts the well-being of individuals and groups of workers. Drawing appropriate conclusions about a scenario for which the exposure is truly unacceptable drives appropriate exposure and risk management, and protects the health and safety of those individuals. When these decisions are based solely on professional judgment guided by subjective inputs, they are more than likely wrong, and biased, underestimating the true exposure.[3–5] Consequently, these exposures and risks are not adequately managed, and the health and safety and lives of people are placed at risk. Approaches and tools are needed to guide professional judgment so that the vast majority of these decisions are accurate.

Models have been anecdotally reported to be useful tools[6,7,12–20,23–25,28] yet they are undervalued and underutilized. This is likely due to several factors; previously, they had not been systematically evaluated, model input data are scarce and guidance on selecting and applying models is lacking. Further, there is little guidance on how to interpret results in any kind of formal framework, or in conjunction with other information or data, such as personal exposure measurements.

Evaluation of model performance in a chamber environment allowed for direct measurement of almost all

CONTACT Gurumurthy Ramachandran gramach5@jhu.edu Department of Environmental Health and Engineering, Bloomberg School of Public Health, Johns Hopkins University, 615 N. Wolfe Street, Baltimore, MD 21205.

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model inputs of the Well Mixed Room (WMR) and Near Field Far Field (NF FF) models with a reasonable degree of confidence.[26] Evaluation in field environments takes into account uncertainty arising from challenges in measuring the model inputs and the presence of additional environmental factors not accounted for in the model but that may influence exposures. To gain a full appreciation of how well models can help guide professional judgment towards accurate decision making, both chamber and field evaluations are necessary. Controlling the conditions in a chamber and varying them one at a time allows a range of conditions to be evaluated, and facilitates capturing the time varying concentration so that model performance can be evaluated as the concentration builds, reaches steady state, and declines. This allows us to gain a sense of the overall performance of a model and understand how the model performance is impacted by changes in conditions. However, this controlled environment also means that variability and uncertainty are minimized, so model performance results likely represent a best-case assessment. In real-world environments, the opportunity to control environmental conditions is limited and measuring the model inputs directly can be challenging; in many cases, model inputs must be estimated indirectly without measurement. These circumstances contribute to increased model input uncertainty and consequent uncertainty in the output. Field studies of model performance directly inform us about how well models predict exposures given these practical limitations, and are, therefore, an important component of model evaluation.

This research builds upon a first phase of work of robust evaluation of the Well Mixed Room (WMR) and Near Field Far Field (NF-FF) models under controlled conditions in an exposure chamber,[26] in which good concordance between measured and modeled airborne concentrations of three solvents under a range of conditions was observed. The evaluation included ten diverse contaminant-exposure scenarios at five workplaces involving six different contaminants. A database of parameter values and measured and modeled exposures was developed and will be useful for modeling similar scenarios in the future.

Methods

The WMR and NF-FF models were evaluated using information and exposure data from ten contaminant-scenarios collected in five different workplaces and for six chemical agents. Several companies volunteered their worksites for this research and scenarios were selected with input from site personnel. Model inputs were directly measured wherever possible, and estimated by simulating the tasks under controlled conditions, or based on professional judgment when measuring was not feasible. Monte Carlo sampling was used to estimate and the mean and the 95th percentile exposure from the distribution of modeled exposures. Personal time weighted average (TWA) exposure measurements were collected from individuals performing tasks with the chemical agent. The mean and 95th percentile of the distribution of the TWA exposure measurements were used as the decision metric against which modeled exposures were compared. These models are described in detail elsewhere[6–8,15,16,20,22,25–28,31,32] so will be discussed here only in the context of their application to each of the scenarios.

A detailed basic characterization of each scenario was conducted providing a general description of the scenario, number of people involved in the task or tasks, a description of the physical layout, room dimensions and details of the product(s), and agent of concern. This information was recorded using the Industrial Hygiene Exposure Scenario Tool (IHEST), a tool developed specifically for this application. It is freely available and is included in the online Supplemental Materials.

A range of methods were used to define model input values. A general explanation is provided here, with additional detail about how a specific approach was selected and applied to each scenario in the Supplemental Materials.

Generation rate

The generation rate was measured or estimated using several methods. The most commonly used method was solving for G using source sampling to measure the contaminant concentration, after knowing or estimating the other model inputs. For a WMR scenario under steady state conditions, this involves only three parameters - C, G, and Q:

$$G = C \times Q, \tag{1}$$

where

C is the concentration measured in the room

Q is the airflow rate entering and exiting the room

G is the contaminant generation rate.

Real-time instruments were used to measure the time-varying contaminant concentration, C(t), and in some cases, such as the foundry scenarios, to estimate the time weighted average airborne contaminant concentrations, C. Integrated sampling methods were also used to collect personal exposure measurements to estimate the time weighted average (TWA) contaminant concentration. The ventilation rate, Q was measured or estimated using one of several methods, described below. Knowing

C and Q, the steady state equation for the WMR was used to solve for G. In field scenarios, the contaminant concentration needs to be measured very near the source. Sometime this method is not feasible, for example when the work environment is too complex or dynamic. In such cases the generation rate can be estimated by simulating the work task under controlled conditions in a chamber. Both approaches were used in this study.

When the generation rate was due to a point source, near-source sampling was conducted by collecting concentration measurements in the NF. Measuring the total airflow provided the necessary data to solve for G. Another method for estimating G was modeling it using the "drum filling" model. This generation rate model is useful for estimating generation rates involving liquid transfer of a volatile or semi-volatile chemical. The volumetric rate at which a fluid enters or is transferred to a vessel (L) is equal to the volumetric rate at which the vapors exit the vessel. It is especially useful for estimating exposures resulting from fugitive headspace vapor emissions during sample collection and from fugitive emissions while drum filling and similar types of scenarios. The drum filling model is particularly useful to hygienists because the inputs needed to apply it typically readily obtained or estimated:

$$G = L\left(\frac{m^3}{min}\right) \times C_{headspace}\ \left(\frac{mg}{m^3}\right) \qquad (2)$$

Ventilation rate

Several approaches were employed to characterize ventilation rates. The most common approach was solving for Q by collecting concentration decay data using direct reading instruments as described in Arnold et al.[26] Briefly, by plotting the logarithm of the concentration decay over time following cessation of the contaminant emission and knowing the room volume, Q can be estimated from the slope of the line of best fit.

Q was also estimated in some cases, for example for scenarios 1 and 2, from local air velocity measurement data. Specifically, multiple velocity measurements were made at the duct or hood face to obtain an average velocity. The area of the hood or duct face was measured and Q estimated according to the equation

$$Q = \upsilon A, \qquad (4)$$

Where

υ is the average velocity measured at the duct or hoodface

A is the area of the duct or hood face, e.g. for a roundduct $A = 2\pi r^2$ where r is the duct radius.

Interzonal air flow rate

The inter-zonal air flow rate, ß was estimated from the random local air speed and NF free surface area (FSA). The free surface area is determined by the geometry of the NF which is generally characterized by the work environment and task, and sized to encompass the individual's breathing zone. A hemispherical geometry was used to describe the NF in these scenarios, reflecting tasks that were conducted on a table-top surface or in which the placement of equipment limited the NF volume. For example, in Scenario 10, Cleaning the Morehouse mixer, the slurry pot was mounted on a large platform and the technician was seated very close to or directly over the pot while cleaning it. Local air dispersion patterns and random air speed were characterized using two TSI Velocicalc thermal anemometers, model 9545 (TSI, Inc., Shoreview, MN). One anemometer was positioned to measure air speed along the x-axis relative to the source and the other positioned along the y-axis, with the instrument aligned so that the orientation dimple is facing upstream. Median air speed values were used to estimate β.

Contaminant concentrations

Time-varying contaminant concentrations were measured using direct reading instruments for seven of the ten scenarios. Acetone was measured in the mixing and cleaning and nail polish scenarios (described later) using two Dräger X-am 7000 Multi-Gas Monitors (MGM) equipped with Smart PID® sensors (Dräger Safety AG & Co. KGaA). Respirable particulate measurements were collected in the foundry (Scenario 1, described later) using a TSI DustTrak (Model 8520) aerosol monitor with a respirable inlet and a co-located Dorr-Oliver cyclone to collect samples that were analyzed in accordance with NIOSH method 7500, providing real time and time weighted average (TWA) area exposure data. Respirable dust measurements for all other scenarios involving particulates were collected using a newer model of the TSI DustTrak aerosol monitor (Model 8533), that does not require an external cyclone to collect the respirable particulate fraction and correct the DustTrak measurements. All other aspects of sample collection for respirable dusts were the same.

Personal time weighted average (TWA) exposure measurements were collected using integrated sampling according to NIOSH validated methods, with sample analysis conducted at AIHA accredited laboratories. Respirable dust and silica samples were analyzed using NIOSH method 7500. Cobalt samples were collected and analyzed using NIOSH method 7027. Acetone samples were collected and analyzed using NIOSH method 1300.

To measure phenol, samples were collected and analyzed in accordance with NIOSH method 2546. Methylene chloride personal exposure measurements were collected following NIOSH method 1005. Personal exposure data sets comprised at least six personal measurements to ensure the 95th percentiles from the distributions of the SEGs and corresponding Reference Exposure Control Categories (Reference ECCs) could be calculated with a reasonable degree of confidence.

Details explaining data collection for each scenario and the application of this information to define model input values are provided in the discussion and scenario narratives in the online Supplemental Materials.

Scenarios

Each scenario in this study represents a unique contaminant-task combination. Ten scenarios involving six contaminants were used for this evaluation. Briefly, scenarios ranged from tasks conducted during medical parts manufacturing in a clean room area to sanding drywall in a hospital under construction. Exposures to respirable dust and respirable silica (quartz), cobalt, phenol, acetone, and methylene chloride were measured and modeled. The scenarios are summarized in Table 1. A more detailed description of each scenario is presented in the online Supplementary Materials.

Parameter distributions

Variability and uncertainty associated with the measured or estimated model inputs were accounted for by characterizing the model inputs as ranges or distributions and utilizing Monte Carlo simulations to produce a distribution of modeled exposures. Model input data were visually inspected before goodness-of-fit tests (GOF), W-test for normality, and lognormality were conducted. Descriptive statistics including mean and standard deviation, and for lognormally distributed data, geometric mean (GM) and geometric standard deviation (GSD) were calculated for generation rates that were estimated from repeated measurements. For the generation rates, multiple contaminant concentration measurements were made, from which multiple generation rates were estimated so that a mean and GSD were calculated, capturing the variability in the generation rate. The probability distributions assigned to the generation rate for eight of the scenarios were characterized in this manner. As an example, for Scenario 10, Cleaning Morehouse mixer, real time contaminant concentration data were collected on four separate occasions from which four generation rates were estimated, and a GM and GSD calculated from this data set of generation rates. When estimating generation rates for scenarios involving respirable silica (quartz), since these were generally identified as a weight fraction of the respirable dust in the safety data sheet or from bulk analysis, the generation rate for quartz was estimated by calculating the product of the respirable dust generation rate multiplied by a uniform distribution for quartz, spanning the plausible range of weight percent values.

Ventilation rates were described using uniform distributions. In most cases, repeated ventilation measurements were not collected so it was not possible to identify a parametric distribution. The assumption was made that since mechanical ventilation is designed to provide consistent air delivery, minimum and maximum ventilation rates were likely within $\pm$ 20% of the observed value. Interzonal airflow rates estimated from repeated random air speed measurements were characterized by lognormal distributions based on GOF tests. In Scenario 7, collecting a liquid (methylene chloride) sample from manufacturing vessel, minimum and maximum air speed values were estimated by site personnel and thus the interzonal airflow rate was defined as a uniform distribution. Model inputs are presented in Table 2. Detailed explanations for each of the model inputs are provided in the Supplemental Materials.

For each model, 10,000 simulations were run and a 95th percentile exposure was obtained from the distribution of modeled exposure concentration estimates. $C_{measured}$ and $C_{modeled}$ pairs obtained for each scenario were compared, where $C_{measured}$ was the 95th percentile value calculated from a lognormal distribution fit to a data set of six or more personal exposure measurements.

Model evaluation criteria

Measured and modeled TWA exposure estimates were evaluated by comparing mean modeled and measured concentrations and categorically, comparing the 95th percentiles using the AIHA Exposure Assessment Exposure Control Categories (ECC) framework. This method is described in detail in Arnold et al.[26] Categorical model evaluation reveals the practical value of these models for assessing occupational exposures by identifying when the modeled exposure estimates are likely to accurately predict the ECC and consequently drive exposure and risk management consistent with those based on a robust set of personal exposure measurements. Model performance was evaluated categorically, using the Exposure Control Categories (ECC) defined in the AIHA Exposure Assessment Strategies framework.[11] Reference ECCs were identified by determining the category to which the 95th percentile of the measured exposure distribution most likely belonged (calculated from personal exposure measurements assuming a lognormal distribution). The ECC

Table 1. Summary description of field scenario tasks, agents and exposure limits included for model evaluation.

Scenario 1	Removing iron parts from sand molds in an iron foundry - Respirable Dust
Description:	Foundry molds, containing iron parts are lifted by crane pulley and placed on a vibrating platform called a shaker, where the iron part and sand are knocked onto the platform. The sand mixture is removed by the shake-out conveyor. The iron parts move to the back end of the shake-out area, where they are manually broken into individual pieces. A layout of the area and pictures are included in the Supplemental Materials.
Tasks:	The operator in the front end of shake-out moves the mold (cope and drag) to the shaker using a crane pulley. After transferring the mold onto the conveyor, the vibrating shaker removes and separates the sand mixture and casting parts from the cope and drag by shaking the mold apart. The sand gradually falls off the conveyor, where it is removed from the area by another, open conveyor system. A second operator works at a station on the back end of shake-out, breaking the molded parts into individual pieces by picking and dropping them onto table, then tosses them into a bin.
Agent and Exposure Limit:	ACGIH TLV for 8 hour TWA respirable dust = 3 mg/m^3
Scenario 2	**Removing iron parts from sand molds in an iron foundry - Respirable Silica (Quartz)**
Description:	Foundry molds, containing iron parts are lifted by crane pulley and placed on a vibrating platform called a shaker, where the iron part and sand are knocked onto the platform. The sand mixture is removed by the shake-out conveyor. The iron parts move to the back end of the shake-out area, where they are manually broken into individual pieces. A layout of the area and pictures are included in the Supplemental Materials.
Tasks:	The operator in the front end of shake-out moves the mold (cope and drag) to the shaker using a crane pulley. After transferring the mold onto the conveyor, the vibrating shaker removes and separates the sand mixture and casting parts from the cope and drag by shaking the mold apart. The sand gradually falls off the conveyor, where it is removed from the area by another, open conveyor system. A second operator works at a station on the back end of shake-out, breaking the molded parts into individual pieces by picking and dropping them onto table, then tosses them into a bin.
Agent and Exposure Limit:	ACGIH TLV 8 hour TWA for quartz = 0.025 mg/m^3 (Quartz is present at 5 – 20% respirable dust).
Scenario 3	**Dry wall finishing in a new construction environment - Respirable Dust**
Description:	Five dry wall finishers sand dry wall during construction of a new hospital suite. Drywall dust is generated. Respirable dust is comprised of, among other things, 1–2% respirable silica (quartz).
Tasks:	Drywall finishers use pole and block (hand) sanding methods to sand drywall in a large hospital suite. Multiple finishers work in the same area, sometimes standing on stilts and sanding above another finisher. This is a full shift task.
Agent and Exposure Limit:	Respirable Dust and Quartz (present at 5 – 20% respirable dust). ACGIH TLV 8 hour TWA for respirable dust = 3 mg/m^3
Scenario 4	**Dry wall finishing in a new construction environment - Respirable Silica (Quartz)**
Description:	Five dry wall finishers sand dry wall during construction of a new hospital suite. Drywall dust is generated. Respirable dust is comprised of, among other things, 1–2% respirable silica (quartz).
Tasks:	Drywall finishers use pole and block (hand) sanding methods to sand drywall in a large hospital suite. Multiple finishers work in the same area, sometimes standing on stilts and sanding above another finisher. This is a full shift task.
Agent and Exposure Limit:	ACGIH TLV 8 hour TWA for Quartz = 0.025 mg/m^3
Scenario 5	**Weighing a powder from a bulk container - Lithium Cobalt Oxide**
Description:	Powders and liquids are mixed under highly controlled conditions in a clean room area of a medical device manufacturing facility. The area is cleaned after mixing is completed.
Tasks:	A technician scoops Lithium Cobalt Oxide (LiCo) powder from a bag inside a pail to a tray positioned on a scale. The pan is set to the side, and a lid is placed on it. After all ingredients are weighed and ready to be mixed, the LiCo is transferred to a v-blender located in an enclosed hood.
Agent and Exposure Limit:	Cobalt. ACGIH TLV 8 hour TWA: 0.02 mg/m^3
Scenario 6	**Mixing and cleaning in clean room environment - Lithium Cobalt Oxide**
Description:	Powders and liquids are mixed under highly controlled conditions in a clean room area of a medical device manufacturing facility. The area is cleaned after mixing is completed.
Tasks:	A technician scoops Lithium Cobalt Oxide (LiCo) powder from a bag inside a pail to a tray positioned on a scale. The pan is set to the side, and a lid is placed on it. After all ingredients are weighed and ready to be mixed, the LiCo is transferred to a v-blender located in an enclosed hood.
Agent and Exposure Limit:	Cobalt. ACGIH TLV 8 hour TWA: 0.02 mg/m^3
Scenario 7	**Collecting a liquid sample from manufacturing vessel (Methylene Chloride)**
Description:	Manufacturing technicians remove a batch sample through a sampling port located on top of an 800 liter reactor on the second floor of the manufacturing suite. The chemical of interest is methylene chloride. This facility is well maintained and has an effective housekeeping program in place.
Tasks:	Technicians collect a sample by removing the liquid methylene chloride from a vessel through a sampling port, using a sampling device called a Colowasa sampler and place the liquid into a graduated cylinder. This process is repeated three or four times until approximately 120 - 150 ml is collected. The sample is then covered and carried to the lab for testing. This task takes $\sim$ 15 minutes.
Agent and Exposure Limit:	Methylene chloride. California OSHA PEL STEL: 125 ppm

(Continued on next page)

Table 1. *(Continued)*

Scenario 8	Making sand mold in iron foundry using a phenolic resin - Phenol
Description:	Phenolic resins are combined with a sand mixture under pressure to make a sand mold that will be used to shape metal parts in a foundry operation. Phenol is released from the hot molds.
Tasks:	The operator fills the molds with the sands/phenolic resin, which are heated to form the shell core. After a few minutes, he takes the shell core out and modifies its shape, as necessary; changing the mold or repairing as necessary, by holding the shell core in one hand, and using the other hand, files it with a hand file. This task is repeated for the entire 8 hour shift
Agent and Exposure Limit:	Phenol. ACGIH TLV 8 hour TWA 5 ppm
Scenario 9	**Removing nail polish and cleaning nails in a nail salon - Acetone**
Description:	A Salon professional manicures her clients' nails, cleaning, shaping and forming the nails and applying nail polish in a professional salon.
Tasks:	Acetone is used as a nail polish remover and non-aqueous cleaner as part of the manicure process. The Salon professional wets a cotton pad with acetone from a squirt bottle before applying it to the client's nails. The cotton pad is then disposed of in a trash can, and the trash can lid is closed
Agent and Exposure Limit:	Acetone. ACGIH TLV 8 hour TWA: 250 ppm
Scenario 10	**Cleaning Morehouse mixer in clean room environment - Acetone**
Description:	A slurry pot is cleaned using solvents to remove slurry residue. The lid and blades are cleaned first, followed by the pot and lastly the lines are flushed with solvent. For this scenario, cleaning the slurry pot lid is modeled.
Tasks:	The slurry pot lid and blades are cleaned by alternately applying acetone, from a squirt bottle and wiping the blades and lid with a paper wipe. Some of the acetone evaporates immediately; some falls or drips from the blades into the slurry pot and the remainder is wiped off using the paper wipes, which are then deposited in an uncovered trash can.
Agent and Exposure Limit:	Acetone. ACGIH TLV STEL: 500 ppm

corresponding to 95th percentile modeled exposure was identified and compared to the Reference ECC. If the two ECCs matched, then categorical accuracy was achieved.

Results

For each Scenario, a comparison of means and a categorical analysis was conducted, comparing model performance for both the WMR and NF FF models with mean and TWA 95th percentile exposures. Results are presented in Tables 3 and 4.

Discussion

The WMR and NF FF models are expected to provide reasonable estimates of the average airborne concentration of a contaminant, thus it was appropriate to compare mean measured and modeled exposure estimates. For 7/10 scenarios, the WMR model was within a factor of ~ 2.5 in predicting the mean concentration, underestimating the exposure for 4/7 ESs. The NF model predicted mean exposure values within a factor of ~ 2.5 in 9/10 ESs, overestimating exposures in 7/9 ESs. Both models overestimated mean exposures for the foundry-phenol ESs by

Table 2. Model inputs for each scenario, including distributions and ranges used. LN: Log normal distribution with (Geometric Mean, GM, and Geometric Standard Deviation, GSD). U: Uniform distribution with (minimum, maximum) values. RD: Respirable Dust; RS: Respirable Silica; $G_{RD:}$ Foundry Respirable Dust G; Co: Cobalt; MC: Methylene Chloride; P: Phenol, A: Acetone.

Scenario	Description	Generation Rate, G (mg/min)	Ventilation Rate, Q(m3/min)	Median Random Air Speed, S (m/min)	Room Volume (m3)	NF Volume (m3)	FF Volume (m3)	Beta (m3/min)
1	Iron foundry RD	LN(43.7, 2.64)	U(80 to 100)	18.9	1200	1.1	1199	LN(34, 1.5)
2	Iron foundry RS	LN(43.7, 2.64)* U(0.5, 15)	U(80 to 100)	18.9	1200	1.1	1199	LN(34, 1.5)
3	Drywall finishing RD	LN (2.13, 1.58)* U(3,5)	U(1.4 to 4.3)	5.6	860	1.1	858.9	LN(11.3, 1.6)
4	Drywall finishing RS	LN G_{RD}* U(1.2, 2.4)	U(1.4 to 4.3)	5.6	860	1.1	858.9	LN(11.3, 1.6)
5	Weighing, transferring - Co	U(.002, 1.77)	U(2.68 to 4.02)	3.9	126	1.1	124.5	LN(7.8, 2.1)
6	Mixing powder, clean up - Co	U(.03, 06)	U(2.68 to 4.02)	3.9	126	1.1	124.5	LN(7.8, 2.1)
7	Collecting sample -MC	LN(220, 4)	U(94 to 140)	3 to 6	379	1.1	378.3	U(3.5 to 7.1)
8	Sand Mold in foundry - P	LN(13.1, 2.3)	U(8.33 to 10.4)	30	125	2.1	123.8	LN(94, 1.8)
9	Salon manicure - A	LN(16.3, 2.68)	U(6.2 to 7.7)	15	31	1.0	29.9	LN(23, 1.1)
10	Cleaning mixer -A	LN(1600, 1.37)	U(10.1 to 15.1)	7.7	126	1.1	124.8	LN(15, 1.5)

*G_{RD} represents the Geometric mean generation rate for respirable dust, accounting for multiple emission sources (workers)

Table 3. Comparison of means for each model by scenario and contaminant showing mean measured and modeled concentrations using the WMR and NF FF models.

Scenario-contaminant	$C_{observed}$ (mg/m^3)	C_{WMR} (mg/m^3)	C_{NF-FF} (mg/m^3)	Ratio WMR/$C_{observed}$	Ratio NF/$C_{observed}$
1. Iron foundry - RD	1.89	1.03	3.98	0.54	2.11
2. Iron foundry - RS	0.16	0.10	0.39	0.63	2.44
3. Dry wall finishing - RD	1.78	3.67	4.19	2.06	2.35
4. Dry wall finishing - RS	0.11	0.07	0.08	0.64	0.73
5. Weighing, transferring - Co	0.23	0.27	0.51	1.17	2.22
6. Mixing powder, cleanup - Co	0.04	0.01	0.02	0.25	0.50
7. Collecting sample - MC	141.3	4.93	115.4	0.03	0.82
8. Iron foundry - Phenol	0.19	1.41	1.57	7.42	8.26
9. Salon manicure -Acetone	3.57	3.78	4.96	1.06	1.39
10. Cleaning mixer - Acetone	199.6	131.0	253.1	0.66	1.27

factors of ∼8. This could reflect both a larger degree of uncertainty in several of the model inputs for this scenario as well as the more complex phenolic resin from which the phenol emissions originated. The WMR model underestimated the mean and 95th percentile methylene chloride exposure in the sampling ES by a factor of ∼ 29 and 37, respectively. In this ES, despite good general ventilation and the availability of local exhaust ventilation (LEV), improper placement of the LEV resulted in the technician sometimes standing between the sampling port and LEV, very close to the contaminant source. Thus, the WMR failed to account for the spatial difference in exposure intensity during this short-term sampling event, underestimating the true exposure.

Categorically, the WMR model-predicted exposures matched the measured exposures for 8/10 scenarios. The NF-FF model-predicted exposures categorically matched the measured exposures for 9/10 scenarios. Concordance between the measured and modeled TWA exposures for the cobalt weighing and mixing tasks, (ES 5 and 6 in Table 3) are presented in Figure 1. Additional figures are included in the Supplemental Materials. These findings can be interpreted as indicating that the models are sufficiently accurate from the perspective of correctly predicting the ECC to which the exposures belong and, therefore, guiding appropriate decision making, and the correct type and level of exposure and risk management. More simply stated, these two models, when used appropriately will be helpful for improving exposure judgment accuracy.

The effort required to characterize model inputs, especially the generation and ventilation rates is not trivial, but once these inputs are known or reasonably estimated, they can be applied to other, similar types of scenarios. In this sense, they can become very portable. This is also true for model inputs generated from simulations, with these inputs being useful across a wide range of other scenarios under similar conditions. The use of real-time instruments to conduct source sampling in the field proved useful in estimating generation rates that were sufficiently accurate for achieving categorical accuracy.

The results of this study suggest that the source sampling approach is sufficient to guide industrial hygiene decision-making regarding conclusions of exposure acceptability that drive appropriate follow up, but when a more precise exposure estimate is needed, more refined methods may be needed. Scenarios for which a greater level of accuracy and precision are needed may require model inputs characterized under more controlled conditions in an exposure chamber.

The majority of the scenarios used in this study were Category 4 exposures, reducing the possibility of over-estimating the exposure to just three of the ten

Table 4. Evaluating categorical accuracy for each scenario and contaminant showing categorical accuracy for 8/10 scenarios when the WMR model was used, and categorical accuracy for 9/10 scenarios when the NF-FF model was used. [a]Short-term Exposure Limit (STEL) $X95_{measured}$ and $X95_{WMR}$, C_{NF-FF} are 95th percentile values.

Exposure Scenario-contaminant	OEL(mg/m^3)	$X95_{observed}$ (mg/m^3)	Reference ECC	$X95_{WMR}$ (mg/m^3)	$X95_{WMR}$ ECC	$X95_{NF-FF}$ (mg/m^3)	$X95_{NF-FF}$ ECC
1. Iron foundry - RD	3	3.27	**4**	2.13	3	8.98	**4**
2. Iron foundry - RS	0.025	0.38	**4**	0.23	4	0.96	**4**
3. Dry wall finishing - RD	3	6.35	**4**	8.06	4	8.67	**4**
4. Dry wall finishing - RS	0.025	0.15	**4**	0.16	4	0.17	**4**
5. Weighing, transferring - Co	0.02	0.42	**4**	0.53	4	0.78	**4**
6. Mixing powder, cleanup - Co	0.02	0.04	**4**	0.02	4	0.02	**4**
7. Collecting sample - MC	434	674	**4**	18.41	1	452	**4**
8. Iron foundry - Phenol	19	2.27	**1**	1.70	1	1.90	**1**
9. Salon manicure -Acetone	595	0.62	**1**	11.88	1	15.68	**1**
10. Cleaning mixer - Acetone	1190.5[a]	731	**3**	503	3	1043	**4**
Categorical accuracy					8/10		9/10

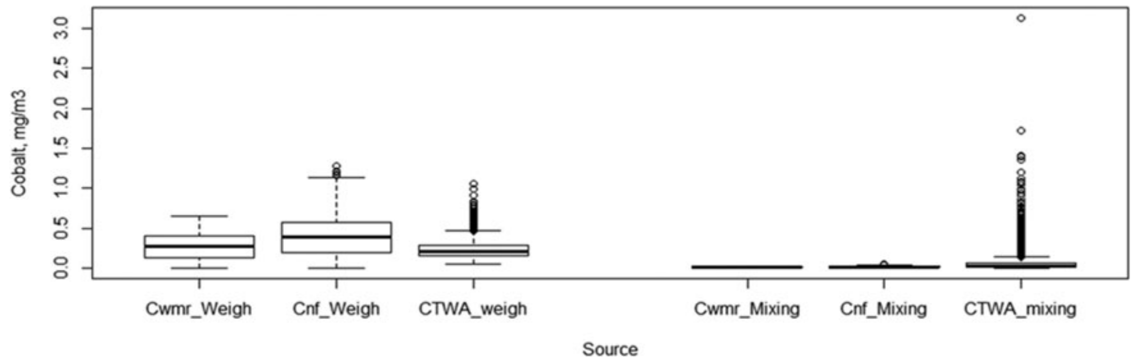

Figure 1. Comparison of modeled and measured Cobalt (mg/m^3) for weighing and mixing tasks. Cwmr_Weigh is the weighing task exposure estimate based on WMR model. Cnf_Weigh is the NF weighing task exposure estimate based on the NF FF model and CTWA_weigh is the TWA Cobalt exposure calculated from personal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

scenarios. Nevertheless, categorical accuracy of both models was highly statistically significantly better than random chance, ($p < 0.001$) regardless of which OEL was used. Random chance reflected the probability of selecting the correct ECC given four possible choices, i.e.,Categories 1–4, for any given scenario, and a total of 27 scenarios assessed. Therefore, based on random chance alone, the models would predict the correct ECC for 6.25/27 scenarios.

The NF-FF model over-estimated the 95th percentile exposure in one scenario, with the predicted exposure exceeding measured exposure by a factor of 1.3. Categorically, the NF-FF model predicted an ECC that was one category higher than the reference ECC for this scenario. In practical terms, this kind of categorical error could cause resources to be directed to an exposure scenario where they are not truly needed.

Conversely, in a true NF-FF scenario, and especially where ß is small such that the concentration in the FF is much lower than the NF concentration, the consequence of erroneously using the WMR model would result in a predicted exposure that underestimates the true exposure. The practical significance is that exposures that are underestimated fail to get the resources needed to mitigate the exposure and health risk. In this study, this effect is seen with Scenario, 7, the methylene chloride sample scenario. The WMR model-predicted 95th percentile exposure underestimated the measured exposure by a factor of 36, and categorically characterized the exposure three ECCs below the Reference ECC. These findings suggest that model selection is essential for ensuring modeled exposure estimates guide professional judgment toward improving exposure judgment accuracy. Both models predicted exposures that greatly exceeded the measured exposure for Scenario 9, the salon scenario. This was likely due to the models' assumptions of a constant mass emission rate as opposed to the short term, intermittent application of acetone. The models do not accurately predict or account for short-term peak exposures but neither were they designed to do so.

This work produced a dataset of model inputs for a broad range of scenarios useful for modeling exposures with similar environmental conditions. Several important points regarding model selection and used guidance can also be gleaned from this analysis. Model selection is a very important factor in achieving categorical accuracy, even though the two models appear to be rather robust most of the time, selecting the best candidate impacts the exposure estimate both directly and indirectly. For example, when using source sampling to solve for G, the model selected dictates the how ventilation rate is estimated that in turn determines the value for G. Source sampling using real time instruments is a useful and relatively robust approach that is applicable across a wide range of contaminant generation types. Similarly, using real time instruments to estimate decay rates in the work environment provide a reasonably accurate estimate of the average airflow rate.

Conclusion

This research provides objective evidence that the WMR and NF FF models, when selected and applied appropriately, accurately predict occupational exposures with sufficient precision to drive appropriate exposure and risk management decision making. There is also a non-trivial learning curve to becoming proficient in selecting and applying these models that will be facilitated as additional guidance is developed. A range of approaches for measuring or estimating model inputs are provided with contextual details to support modeling of other scenarios under similar conditions. More research is needed to identify additional practical and flexible approaches to estimating the generation rate, and to develop more robust databases providing model input values for a broad range of scenarios.

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