The Use of Heuristics and Exposure Models in Improving Exposure Judgment Accuracy

A Dissertation

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DEDICATION

This dissertation is dedicated to my family, especially my husband, Steve. It's been an incredible journey and so much more so because you were a part of it.

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CHAPTER 1 INTRODUCTION – INVESTIGATING INPUTS TO ACCURATE DECISION MAKING

BACKGROUND AND SIGNIFICANCE

Low accuracy of professional judgments relating to exposure:

Exposure assessments provide the foundation for determining whether occupational and environmental exposure risks are efficiently and effectively managed. Most exposure assessment strategies require the workforce to be categorized into similar exposure groups or SEGs. The American Industrial Hygiene Association's (AIHA) strategy is well-known and provides a simple yet elegant framework for exposure assessments (Jahn et al., 2015; Ignacio and Bullock, 2006; Mulhausen and Damiano, 1998). Judgments are made by identifying the exposure control category in which the 95th percentile of the exposure distribution is most likely located for a given job or task (Table 1-1). Acceptability is commonly evaluated by comparing the true group 95th percentile to the occupational exposure limit (OEL), and based on this comparison the exposure is classified into one of four categories: "highly-controlled", "well controlled", "controlled", or "poorly controlled". A judgment can be documented for each SEG, which can represent a single task that may be short in duration or may represent a group of tasks that comprise a full-shift exposure. Qualitative and quantitative exposure assessments are performed after a thorough review of available information and data related to the workforce, jobs, materials, worker interviews, exposure agents, exposure limits, work practices, engineering controls and protective equipment.

Table 1-1 AIHA Exposure Category Rating Scheme

A SEG is assigned an exposure rating by comparing the 95th percentile exposure distribution (X0.95) with the full-shift time-weighted average (TWA), Occupational Exposure Limit (OEL) or Short-Term Exposure Limit (STEL) to determine in which category it most likely falls.

AIHA Exposure Rating	Proposed Control Zone Description	General Description	AIHA-Recommended Statistical Interpretation
1	Highly Controlled (HC)	95th percentile of exposures rarely exceeds 10% of the limit.	X0.95 < 0.10 OEL
2	Well Controlled (WC)	95th percentile of exposures rarely exceeds 50% of the limit.	0.10 OEL < X0.95 < 0.5 OEL
3	Controlled (C)	95th percentile of exposures rarely exceeds the limit.	0.5 OEL < X0.95 < OEL
4	Poorly Controlled (PC)	95th percentile of exposures exceeds the limit.	OEL < X0.95

Exposure judgments are commonly used in a wide range of situations, including retrospective exposure assessments for epidemiology studies (e.g. Esmen et al., 1999; Ramachandran, 2001; Ramachandran et al., 2003; Friesen et al, 2003) and current and prospective exposure assessments for managing exposures related to consumer use and manufacturing operations, (e.g. Hawkins and Evans, 1989; Teschke et al., 1989; Macaluso, 1993; Friesen et al., 2003; Ramachandran et al., 2003). When there are limited sampling data, occupational hygienists (OHs) use a combination of professional judgment, personal experience with a given operation, and review of exposures from similar operations to assess the acceptability of exposures for managing engineering controls, medical surveillance, hazard communication and personal protective equipment programs (Teschke et al., 1989; de Cock et al., 1996; Burstyn & Teschke, 1999; Friesen, 2003; Kolstad, et al., 2005; Logan et al., 2009; 2011; Vadali et al., 2011; 2012). In the context of this work, a decision is represented by a chart showing the hygienist's assessment of the probabilities that the 95th percentile lies in each of the four categories (Figure 1-1).

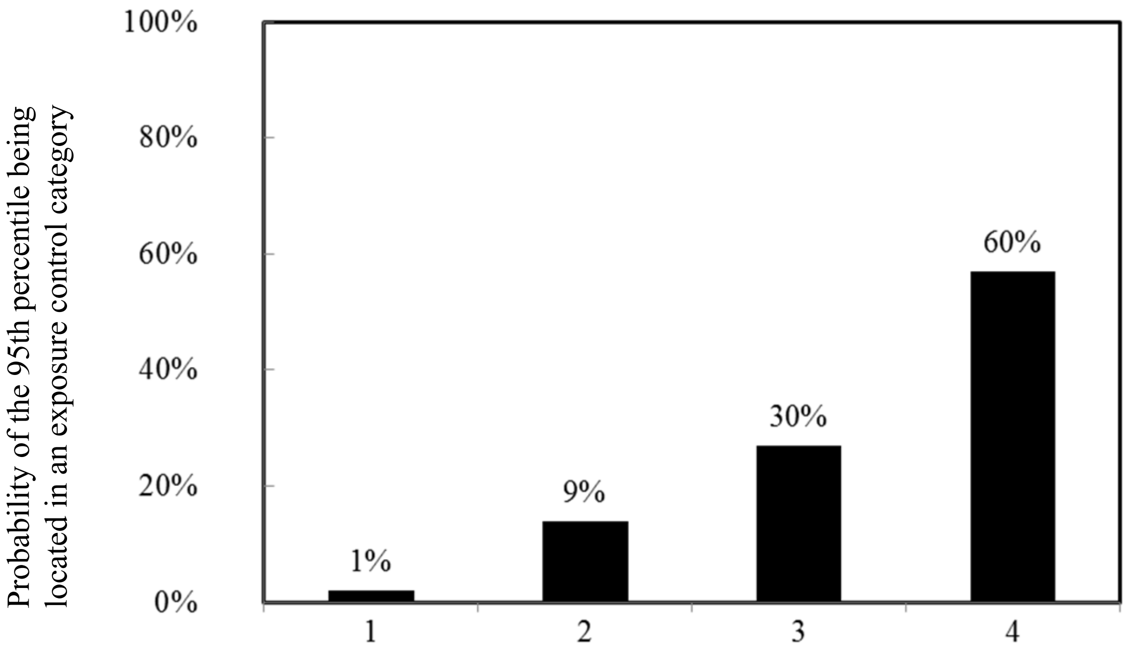

Figure 1-1 Example qualitative exposure judgment chart illustrating an occupational hygienist's exposure judgment given the information and data available

This chart shows that the hygienist is highly confident the 95th percentile falls into Category 4 – >100 of the OEL (Arnold and Ramachandran, 2015)

A number of studies have been published on the accuracy of professional judgments (Kahneman et al., 1982; Kromhout, et al., 1987; Glaser & Chi, 1988; Teschke, et al., 1989; Hawkins & Evans, 1989; Macaluso et al., 1993). Recent studies (Logan et al., 2009; Logan et al., 2011; Vadali, et al. 2011; Vadali et al., 2012) involved both desktop assessments (where participating OHs viewed videos of tasks, task information and sampling data) and walkthrough assessments (where they directly observed the task). The key findings relating to quantitative judgments (made using monitoring data) shown in Figure 1-2a and 1-2b are:

- The accuracy of exposure judgments made by hygienists when monitoring data are available is low (<50% correct judgments) but still better than random chance (25%).
- There is a significant underestimation bias in the exposure judgments, i.e., there is marked tendency to assign a lower exposure category than the correct one, thus increasing occupational risk to workers.
- The low accuracy is likely due to cognitive biases in understanding skewed lognormal distributions. A training focused on heuristics relating to lognormal statistics significantly improves accuracy to ~70%.
- Several factors relating to cumulative professional experience, training, certification, and educational level of the hygienists, as well as task-specific experience were significant predictors of judgment accuracy.

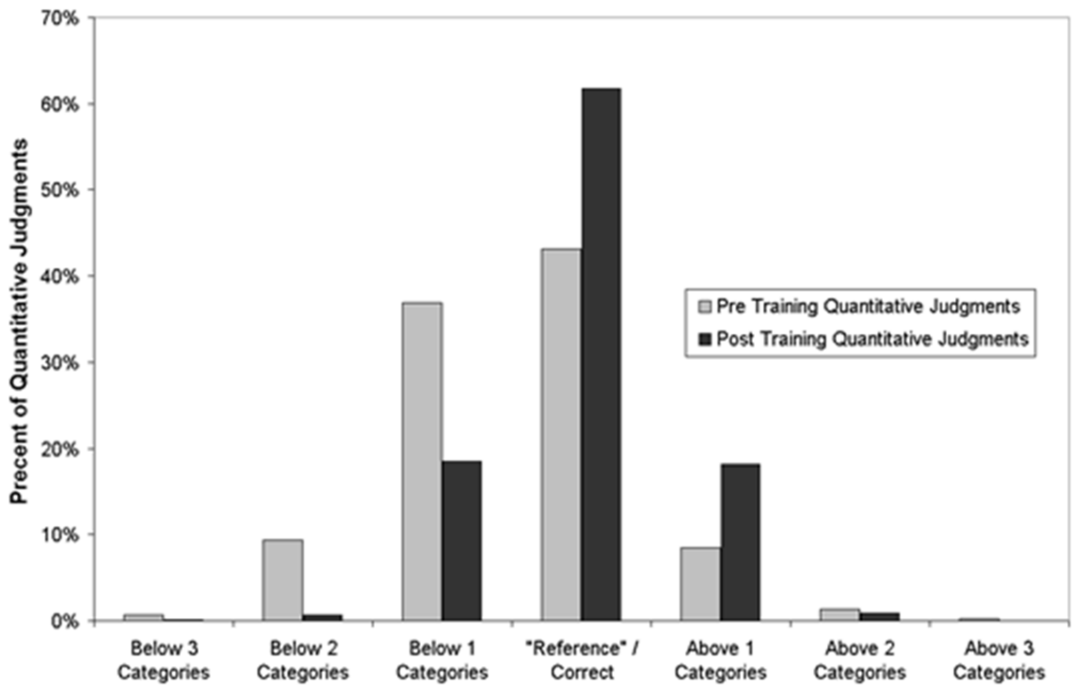

Figure 1-2 *(a)* Percentage of all pre- and post-training quantitative task judgments above, below and reference categories for (a) desktop study, N = 3834, (Logan et al., 2009)

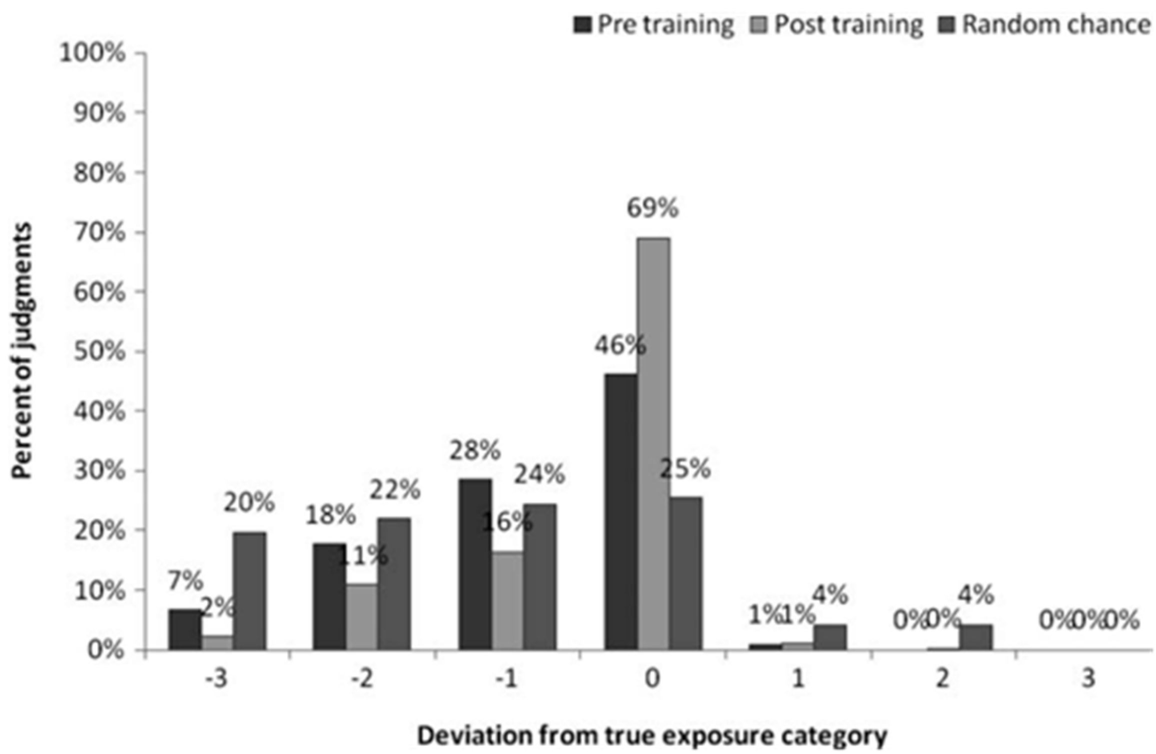

Figure 1-2*(b)* Percentage of all pre- and post-training quantitative task judgments above, below and reference categories for walkthrough study, N = 2142

This figure shows the deviation of participants' quantitative judgments pre and post training from random chance, (Vadali et al., 2012b).

The findings related to qualitative judgments (when no monitoring data are available) shown in Figures 3a and 3b are:

• The accuracy of exposure judgments made by hygienists when monitoring data are not available (30%) is not much different from random chance (25%).

• The underestimation bias is significant in this case as well.

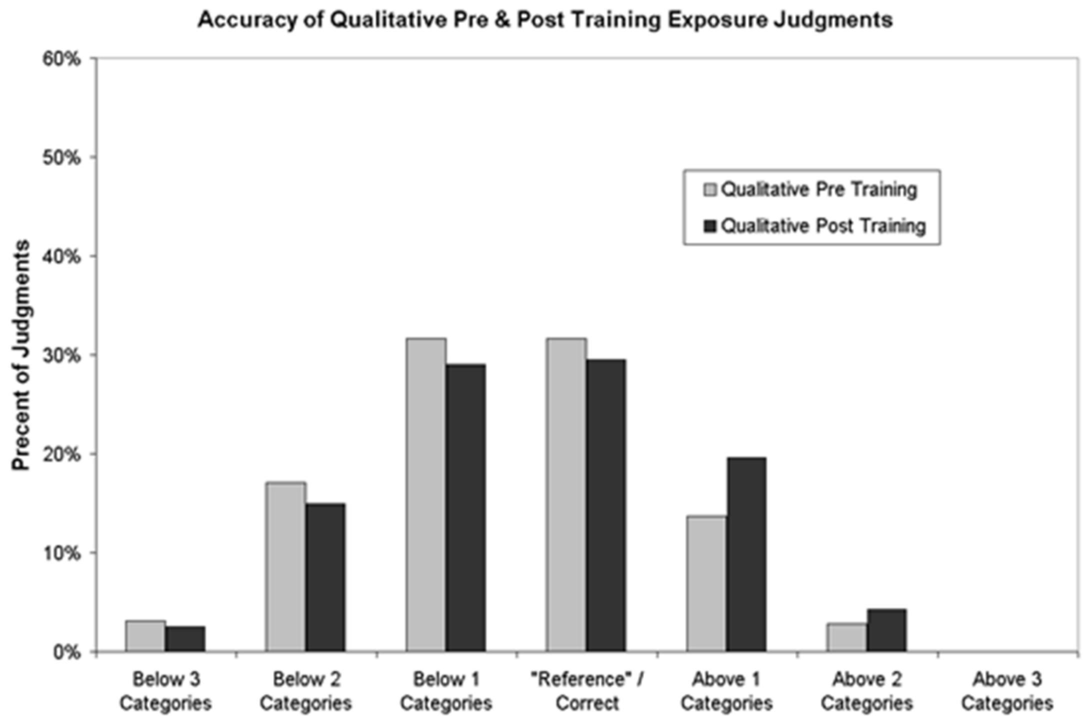

Figure 1-3 *(a):* Percentage of all pre- and post-training qualitative task judgments above, below and reference categories for (a) desktop study, N = 552, (Logan et al., 2009)

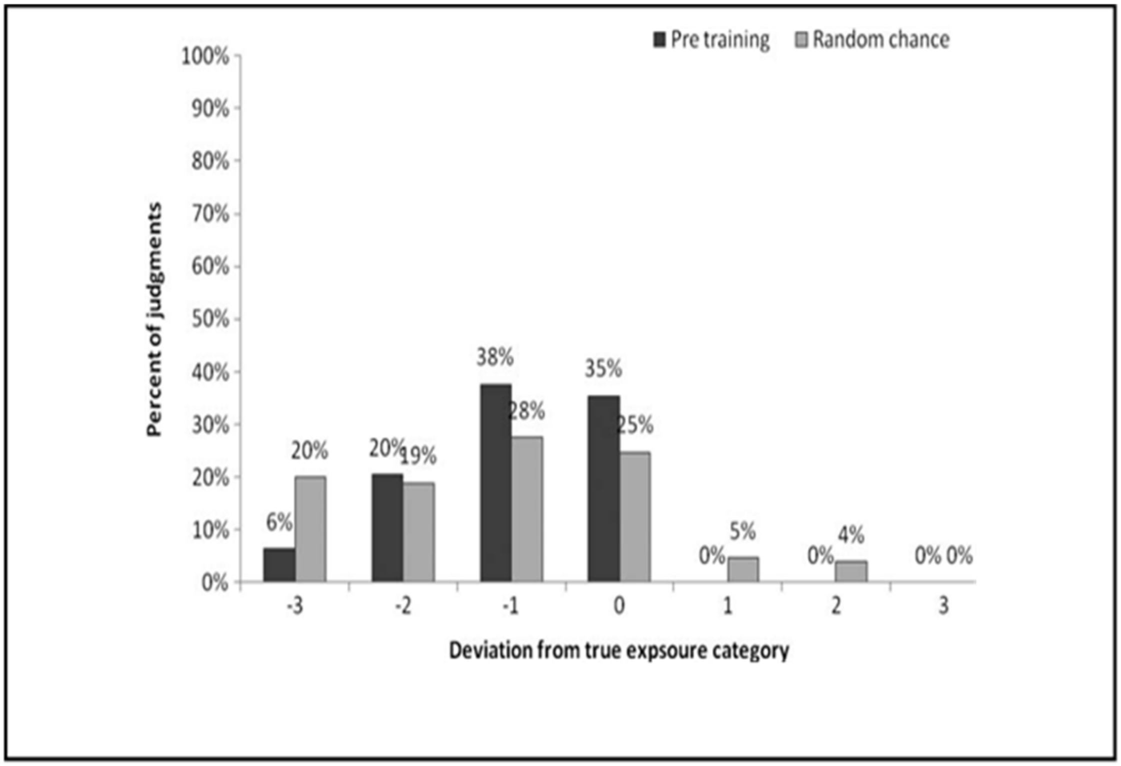

Figure 1-3 *(b)* Percentage of all pre- and post-training qualitative task judgments above, below and reference categories for workplace walkthrough study, N = 93.

This figure shows the deviation of participants qualitative' judgments pre-training from random chance, (Vadali et al., 2012b).

It is this second set of findings relating to qualitative judgment accuracy (Figure 1-3a, b) that motivated this research, although the quantitative accuracy findings (Figure 1-2a, b) are related as well.

The vast majority of the exposure judgments made by practitioners are qualitative and in many cases even determine if any measurements should be made. The low accuracy of these judgments can therefore lead to incorrect follow-up activities, and is therefore a cause for concern. These findings suggest that the understanding of how workplace factors affect exposure needs to be significantly improved among practitioners (Burstyn and Teschke, 1999; Hawkins & Evans, 1989). Statistical training, being unrelated to decision-making when there are no data, did not improve accuracy. However, we hypothesized that there are other types of training that may be relevant and could improve accuracy, including Exposure Determinants Heuristics (EDH) and exposure modeling training.

Exposure Heuristics:

Mental shortcuts, known as heuristics, are often used when information or data are insufficient or absent, making the decision process efficient but can lead to errors in judgment and introduce bias. Using these heuristics leads to a pattern that, when faced with uncertain prospects, assigns weights to our decisions that differ from the true probabilities of these outcomes. Improbable outcomes are over-weighted, while almost-certain outcomes are under-weighted.

In their research on decision making, Kahneman et al., (1982) found these cognitive biases could frequently be attributed to three heuristics: availability, representativeness, and anchoring and adjustment. The availability heuristic reflects the tendency to equate the probability of an event with the ease with which an occurrence can be retrieved from our memory. The degree to which a person's experiences and memory matches the true frequency determines whether these judgments are accurate. Representativeness reflects assignment of an object or event to a specific group or class of events. If the decision maker lacks relevant experience, a surrogate (and less relevant) memory may be used, leading to erroneous conclusions. The anchoring and adjustment heuristic is a strategy for estimating uncertain quantities. When trying to determine the correct value, our minds 'anchor' on a value, and then adjust to accommodate additional information. The degree to which our final answer is anchored to the initial value can be influenced by many factors. For example, when tired or when our mental resources are spent, we tend to stay closer to the initial value. Within the realm of industrial hygiene decision making, there are many situations where these heuristics can be identified, such as judgments based solely on the "available" information in one's memory. The representativeness heuristic might be invoked when "eyeballing" exposure data, making a judgment modeled on a symmetrical (normal) distribution (which our minds more readily intuit) rather than the skewed, lognormal distribution that more closely reflects most exposure profiles. By modeling the data after a symmetrical, rather than a skewed distribution, the hygienist is likely to underestimate the decision statistic, and consequently underestimate the true exposure. Similarly, when a hygienist 'anchors on a single piece of information', neglecting to take into consideration the most critical factors before making an exposure judgment can lead to erroneous conclusions.

Objective, structured approaches, using simple algorithms and exposure modeling are more resistant to these vulnerabilities, focusing the decision maker on the decision making process, and on the critical inputs, while filtering out nonessential information. These approaches have been shown to improve decision making across a broad range of domains, including psychology (Kahneman, 2011 and Kahneman et al., 1982), drug delivery and development (Lipinski et al., 2001); redicting transdermal delivery and toxicity (Magnusson et al., 2004;) environmental exposure assessment (Fristachi et al., 2009); and aggregate exposure assessment (Cowan-Ellsberry and Robinson, 2009). These same objective approaches can be applied to occupational exposure assessment. In fact, decisions are most accurate in highly uncertain ‘low validity’ environments, i.e. situations with little or no data, when the final decision is generated from algorithms. The Apgar test is an excellent example. This algorithm, capturing a pattern of behaviors recognized by obstetrical anesthesiologist Virginia Apgar, considers just five basic inputs, with a score assigned to each. The sum of the scores corresponds to the baby’s health prognosis. First reported in 1952, this algorithm was better able to predict when medical assistance was needed than individual experts, (Apgar, 1958, Gawande, 2010) and is the still the standard in assessing a newborn’s transition to life outside the womb.

Aids to decision making: Use of algorithms (checklists) and models

Algorithms consider critical and consistent inputs and are consistently better at making accurate judgments, while experts try to out-finesse algorithms, thinking outside the box, considering complex combinations of inputs (Meehl, 1954). Humans, however, are inconsistent in making summary judgments of complex information and are therefore less consistent, and less accurate. (Kahneman, 2010) The algorithms may not be optimal or 100% accurate, but are close enough to be informative and ensure limited resources are used efficiently. Subjective intuitive qualitative judgments are, most of the time, no more accurate than random chance (Arnold et al., 2015; Logan, et al., 2011; Vadali et al., 2011; Vadali et al., 2012). Identifying and applying proven aids to decision making, is essential to ensuring these exposure judgments are highly accurate and health conservative.

One of the characteristics of algorithms and models contributing to consistent decision making is the consistent order in which information is processed. Checklists provide guidance on the order in which inputs are considered. These simple tools have been the cornerstone of safety excellence in the aviation industry for years. That is not to say that checklists and models do not replace knowledge and expertise, and pilots go through rigorous training before they are allowed to fly. The checklists ensure they follow the critical steps at the right time to ensure theirs, and their passengers' safety. Likewise, checklists may help OHs focus on the critical inputs to decision making in the right order, leading to consistent and accurate exposure judgments, protecting the health and safety of those in their care.

Exposure Models:

Models have been applied across a broad range of fields to improve decision making, from weather forecasting to medical diagnosis and treatment selections (Kahneman, 2011). Meehl (1954) asserted that models consistently produce significantly more accurate judgments than subjective expert judgments. The nearly 200 studies conducted since this evidence was first published support this assertion (Kahneman, 2011). The range of predicted outcomes has expanded to include economic indicators, career satisfaction of workers, questions of interest to government agencies and the future price of Bordeaux wines. Pharmaceutical researchers use simple models based on readily available inputs, identifying potential candidate compounds for transdermal drug

(Magnusson et al., 2004) and oral drug delivery (Lipinski et al., 2011). The Apgar test, a simple model comprised of five critical determinates has been helping save the lives of neonates since 1953 (Kahneman, 2011). These fields have in common a significant degree of uncertainty and unpredictability, which Kahneman (2011) refers to as 'low-validity'. The application of models to the low-validity field of occupational hygiene exposure risk assessment is a logical next step towards improving exposure judgments.

Exposure models have tremendous potential for improving the efficiency and effectiveness of risk assessment and management programs. They can be used to predict exposures for operations that have not yet been installed or to reconstruct exposures for processes that have long disappeared, or when monitoring data are impossible or expensive to generate. They can enrich and inform qualitative exposure judgments and offer potential for increasing judgment accuracy. The physical models employed today in occupational hygiene are typically based upon some simplifying assumptions about air-flow and contaminant transport pattern (Hemeon, 1963; Nicas, 1996; Keil et al., 2009). Predicting exposure in real settings is constrained by lack of quantitative knowledge of exposure determinants (Keil and Murphy, 2006; Arnold et al., 2009; Cherrie et al., 1999; Jones et al., 2011; Earnest and Corsi, 2013).

Selecting commonly used occupational exposure physical models

There are several deterministic models with varying levels of sophistication (Ramachandran 2005; Arnold, et al., 2009) and correspondingly varying costs due to the amount of information needed as model inputs. For example, the near field-far field model requires knowledge of room ventilation and contaminant generation rates in addition to a parameter known as the inter-zonal ventilation rate – involving a non-trivial investment. A sophisticated eddy diffusion model, which accounts for concentration gradients around pollution sources, requires even greater investments. While costs increase with the level of sophistication, more complex models can also yield more refined exposure estimates. Two commonly referenced physical models are briefly outlined here – a more complete listing is provided in Keil et al. (2009). These models are applicable to both gas/vapor as well as aerosol contaminants, by proper choice of some model parameters.

Box Models

The one-compartment model

This model assumes that (a) a source is generating an airborne pollutant at a rate G (mg/hour) in a room of volume V (m^3) with a ventilation rate Q (m^3/hour), and (b) the air in the room is perfectly mixed creating a uniform contaminant concentration throughout the room, irrespective of the distance from the source. A loss rate coefficient, k_L, governs mechanisms (other than ventilation) by which the pollutant is removed from the room. Examples of such mechanisms include adsorption of gases and vapors onto various surfaces (here k_L is an adsorption rate for the particular vapor and surface type) and particle deposition on surfaces by gravitational settling (k_L is now a function of terminal settling velocity for particles of a given diameter and density), impaction, and Brownian diffusion. Thus, k_L helps generalize this model to gaseous as well as particulate air contaminants. The differential equation describing this model is:

$$\frac{d}{dt}C(t) + \frac{Q+k_L}{V}C(t) = \frac{G+C_{IN}Q}{V}, \tag{1-1}$$

where C_{IN} is the concentration in the incoming air. The steady state concentration for this scenario is

$$C_{SS} = \frac{G}{Q+k_L V} \tag{1-2}$$

in mg/m^3.

Therefore, the input parameters required for this model are the generation and ventilation rates, the room volume, and the loss rate parameter that is a function of contaminant physical properties.

The two-compartment or two-zone model

The near field far field (or two-zone) model assumes that (a) a contamination source is present in the workplace, (b) the region very near and around the source is one well-mixed box, called the near field, while the rest of the room is another well-mixed box, called the far field, which completely encloses the near field box, (c) there is air exchange between the two boxes with airflow rate equal to β, (d) the contaminant's total mass is emitted at rate G, and (e) the supply and exhaust flow rates are both equal to Q. The k_L refers to contaminant loss by other mechanisms as described earlier.

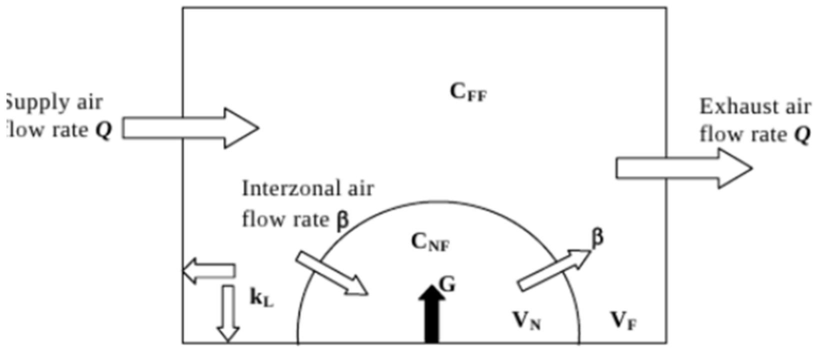

Figure 1-4 Schematic Diagram of the two-compartment or two-zone model

Figure 1-4 schematically depicts the system, where V_N and V_F denote the volumes at the near and far field, respectively. In this context, the occupational hygienist seeks to model the exposure concentrations at the near and far fields based upon observations collected over a period of time. The mass balance for the two zones, ignoring k_L since its contribution is *de minimis,* is given by:

$$V_{NF} \cdot dC_{NF} = [G \cdot dt + \beta \cdot C_{FF} \cdot dt] - \beta \cdot C_{NF} \cdot dt \qquad (1\text{-}3)$$

$$V_{FF} \cdot dC_{FF} = \beta \cdot C_{NF} \cdot dt - [\beta \cdot C_{FF} \cdot dt + Q \cdot C_{FF} \cdot dt] \qquad (1\text{-}4)$$

This gives a pair of coupled differential equations that can be solved to yield the near-field and far-field concentrations as a function of time. The solutions are of the form

$$C_{NF} = \alpha_1 \bullet \exp(\lambda_1 t) + \alpha_2 \bullet \exp(\lambda_2 t) \qquad (1\text{-}5)$$

$$C_{FF} = \alpha_3 \bullet \exp(\lambda_1 t) + \alpha_4 \bullet \exp(\lambda_2 t) \qquad (1\text{-}6)$$

where α_i is

$$\frac{G+C_{IN}Q}{V} \tag{1-7}$$

And λ_i is

$$\frac{Q+k_L V}{V}(t) \tag{1-8}$$

Traditionally, subjective judgments made with little transparency have driven most exposure judgments, (Logan and Hewett, 2009), while direct measurements have played a less conspicuous role. Recent studies (Logan et al., 2009; Vadali, et al. 2012; Vadali et al., 2012) have shown that the accuracy of judgments made by occupational hygienists (OHs), when small numbers of monitoring data are available is rather low (~40-45%). Exposure modeling, which has been shown to improve decision making across a broad range of domains, (Kahneman et al., 1982; Lipinski, et al., 2001; Magnusson et al.,, 2004; Fristachi et al. 2009; Cowan-Ellsberry & Robison, 2009; Jones et al., 2011; Kahneman, 2011) provides a systematic and transparent approach for making exposure judgments but has received little support from industry and government. Guidance directing OHs on which model would produce the most accurate exposure estimate under a defined set of conditions is needed – and for this, the models need to be systematically evaluated in both chamber and field environments. OHs also lack training opportunities providing immediate feedback on their judgment accuracy, allowing them to calibrate their judgment based on these exposure models. Lacking this training experience, OHs may undervalue models as tools for making accurate exposure judgments and therefore underutilize them. However, this situation is changing dramatically with the advent of the REACH regulations in the EU that requires assessing exposures in a variety of exposure scenarios where monitoring may not be feasible.

Exposure models seek to capture the underlying physical processes generating chemical concentrations in the workplace. An accurate representation will produce better concentration estimates and facilitate decision-making in exposure management. However, this is challenging because workplaces are notoriously complex and no physical model is likely to provide a complete representation. Thus, characterizing model parameters, and accounting for parameter and model uncertainty is crucial.

Impacts on occupational exposure assessment and Research-to-Practice (R2P):

The work conducted falls under the NIOSH Cross-Sectoral Program on Exposure Assessment. In addition, the exposure scenarios evaluated were in four main industry sectors –Manufacturing, Construction, Services and Pharmaceutical/Healthcare. Hence, it is relevant to these four NIOSH Sector Programs. The completed work contributes to the NIOSH r2p initiative in the following areas:

NIOSH has recently embarked on an initiative to update its Occupational Exposure Sampling Strategies Manual (Ramachandran, 2008). The findings from this research will be a very useful input to these efforts. There has been substantial interest in developing a comprehensive exposure assessment strategy that evaluates health risks from all substances for all workers for all days. Such a strategy would characterize exposure variability and produce data that can be used for baseline monitoring, and surveillance, deciding whether to start or discontinue specific exposure control measures and for epidemiology. Accurate professional judgment with modeling input is a key ingredient of any such strategy.

Occupational exposure data are often collected with minimal information about the workplace which can limit the effective use of the data for exposure assessment. Knowledge of these determinants of exposure can significantly improve our understanding of the variability in exposure measurements. Though the profession has for long been aware of the importance of a thorough knowledge of the determinants of exposure on the part of the hygienist, most companies do not collect such information routinely. Even basic data such as ventilation rates and pollutant generation rates are hard to come by in most situations. However, if hygienists did document each exposure judgment they made along with the rationale behind it, there would be a greater incentive to systematically measure them routinely, leading to a better understanding of these parameters.

Knowledge of exposure determinants can significantly improve our understanding of the variability in exposure measurements. If OHs documented each exposure judgment they made along with the rationale behind it, there would be a greater incentive to systematically document the determinants of exposure and measure them routinely. This will have two salutary effects: (a) it will improve the OHs understanding of their workplace, and thereby their judgments, and (b) knowledge of model input parameters will allow them to use readily available exposure models which, in turn, will also improve subjective exposure judgments.

Innovation:

This research contains several innovative elements. Evaluation of models in occupational settings is a challenge – not only do the model parameters need to be known, the models also need to predict the output with some degree of accuracy. Till now, little research has been conducted to evaluate the parameters used in physical models to assess model performance. Currently no standardized approaches exist for evaluating models and documenting results. In order for exposure models to reach their full potential, exposure models must be validated in a manner that sets boundaries around their use and gives confidence in their output. Model evaluation must be transparent, well documented, and include criteria that define specific model application conditions and outcome performance. Thus, there is a critical need to study the use of occupational exposure models in terms of model accuracy, determining whether: (a) models lead to accurate judgments under specific exposure conditions for various agents; (b) OHs select appropriate models and use them to make accurate exposure judgments. This research addressed, in part, this critical need to study these models. Finally, several tools and templates were developed by me in collaboration with other AIHCE workshop volunteers to facilitate consistent and transparent data collection that will be useful to OHs conducting exposure assessment.

Specific Aims of this Research

The overall goal of this research was to evaluate whether the application of environmental determinant heuristics, checklists and algorithms, and mathematical models make exposure judgments more accurate. Three major aims were completed to meet this objective.

Aim 1. Evaluate the impact of heuristics, checklists and algorithms on exposure judgment accuracy

> The impact of heuristics, checklist and algorithms, was evaluated using a qualitative checklist tool (Checklist) that was developed for the study. The tool provided a structured approach for applying and interpreting a collection of heuristics that were developed from fundamental physical chemical principles and refined, empirically. Exposure judgment accuracy of novice and practicing OHs was evaluated before and after receiving training on the heuristics and the tool.

The following hypotheses were tested in this work:

1. There is no statistically significant difference in exposure judgment accuracy of novice hygienists before and after applying the Checklist to guide exposure judgments.
2. There is no statistically significant difference in exposure judgment accuracy of practicing hygienists before and after applying the Checklist to guide exposure judgments.

To meet Aim 1, two main tasks were completed:

1. A dataset of 11 task-based and full shift exposure scenarios were developed from a wide variety of occupational exposure settings, agents and across different

magnitudes of exposure.

2. A series of exposure judgments were elicited for these exposure scenarios from OHs, capturing their decisions using a Bayesian Decision framework.

   The details of this research are discussed in Chapter 2.

Aim 2. Evaluate model performance of the Well Mixed Room and Near Field Far Field models under highly controlled conditions, in a chamber setting.

> Model performance of two widely applicable models, the Well Mixed Room (WMR) and Near Field Far Field (NF FF) were evaluated using two different evaluation schemes, ASTM Standard 5157: Standard Guide for Evaluation of Indoor Air Quality Models, and the AIHA Exposure Assessment Exposure Control Categories (ECC). High quality model inputs were generated in a controlled environment, generating more than 800 measured and modeled exposure pairs against which model performance was measured.

The following hypotheses were tested:

1. Categorical model accuracy based on the WMR model and using the Occupational Safety and Health Administration (OSHA) Permissible Exposure Limit (PEL) or the American Conference of Governmental Industrial Hygienists (ACGIH) TLV as the Occupational Exposure Limit (OEL) is no better than random chance.
2. Categorical model accuracy based on the WMR model and using the Action Limit (AL), as the Occupational Exposure Limit (OEL) is no better than random chance.

3. Categorical model accuracy based on the NF FF model modeling NF exposures and using the OSHA PEL or ACGIH TLV as the OEL is no better than random chance.

4. Categorical model accuracy based on the NF FF model modeling NF exposures and using the AL as the OEL is no better than random chance.

5. Categorical model accuracy based on the NF FF model modeling FF exposures and using the OSHA PEL or ACGIH TLV as the OEL is no better than random chance.

6. Categorical model accuracy based on the NF FF model modeling FF exposures and using the AL as the OEL is no better than random chance.

7. The Well Mixed Room model meets all the ASTM Criteria for all the scenarios in the chamber study.

8. The Near Field Far Field model meets all the ASTM Criteria for all the scenarios in the chamber study.

To meet Aim 2, the following major tasks were completed:

1. A full size exposure chamber was constructed, providing an environment where the generation and ventilation rates and contaminant concentrations could be

measured and controlled.

2. 162 chamber studies were completed, resulting in a rich database of exposure scenarios containing exposure and exposure determinant data under controlled (chamber) conditions.
3. Model evaluation of the Well Mixed Room and Near Field Far Field models was completed using this study data.

Details of the chamber study are discussed in Chapter 3.

Aim 3. Evaluating model performance of the Well Mixed Room and Near Field Far Field models under field (real workplace) conditions

Field studies comprised of 10 contaminant-scenarios from five diverse workplaces were conducted, evaluating exposure scenarios similar to those used in the chamber studies, characterizing exposure determinant data under real world (field) conditions, capturing parameter variability and uncertainty. Model performance was evaluated using these scenarios and applying the same criteria identified in Aim 2.

The following hypotheses were

1. Categorical model accuracy based on the WMR model and using the Occupational Safety and Health Administration (OSHA) Permissible Exposure Limit (PEL) as the Occupational Exposure Limit (OEL) is no better than random chance.
2. Categorical model accuracy based on the WMR model and using the Action Limit (AL), as the Occupational Exposure Limit (OEL) is no better than random chance.

3. Categorical model accuracy based on the NF FF model modeling NF exposures and using the OSHA PEL as the OEL is no better than random chance.

4. Categorical model accuracy based on the NF FF model modeling NF exposures and using the AL as the OEL is no better than random chance.
5. The Well Mixed Room model meets all the ASTM Criteria for all the scenarios in the field study.

6. The Near Field Far Field model meets all the ASTM Criteria for all the scenarios in the field study.

The following tasks were completed to meet Aim 3:

1. Workplace tasks were identified across a broad range of industry types, tasks and agents, and basic characterizations completed for each one, using the Industrial Hygiene Exposure Scenario Tool (IHEST), developed for this research.
2. Measurements were made of the contaminant concentrations and model inputs were either measured directly if possible, or estimated using a submodel or guidance from a range of sources. Both models were used to model exposures for each scenario.
3. Measured and modeled exposures were compared and model performance evaluated using the same criteria that was applied in the chamber study.

Details of the Field Study are presented in Chapter 4.

CHAPTER 2. USING CHECKLISTS AND ALGORITHMS TO IMPROVE QUALITATIVE EXPOSURE JUDGMENT ACCURACY

INTRODUCTION

The vast majority of assessments conducted within comprehensive exposure assessment programs are qualitative, i.e., without monitoring data. This is by design and necessity, as the number of exposure scenarios in a workplace may be in the tens or hundreds of thousands, all of which will eventually be assessed under a comprehensive program, in which conducting quantitative exposure assessments (i.e., using monitoring data with sufficient samples to support valid decision making) for every scenario is not feasible. The American Industrial Hygiene Association (AIHA) exposure assessment strategy calls for initial, qualitative assessments of exposures, relative to a reference exposure level, such as an Occupational Exposure Limit, (OEL), Emergency Planning Guideline (EPG) or Interim Exposure Limit (IEL), based on a No-Observed Adverse Effect Level (NOAEL), respectively. Industrial hygienists (IHs) assess these using a combination of their formal and informal education, professional judgment, personal experience with a given operation, and review of exposures from similar operations to determine the acceptability of exposures for managing engineering controls, medical surveillance, hazard communication and personal protective equipment programs. Since the type of follow-up that occurs, if at all, is determined by these initial qualitative judgments, their accuracy is essential.

Research suggests qualitative exposure judgment accuracy, based on subjective professional judgment is low, not statistically different from random chance, and tends to underestimate exposures (Logan et al., 2009; Vadali et al., 2012). These findings, indicating qualitative exposure judgments are not only wrong much of the time, but tend to underestimate true exposures are deeply concerning because they lead to ineffective (failing to adequately protect workers) and inefficient (misdirecting resources) exposure assessments, in turn leading to inefficient and ineffective comprehensive IH programs. Despite the urgent need for better approaches, and a body of literature from psychology, medicine, and aviation safety suggesting they may be helpful (Meehl, 1954; Billings et al., 1984; Magnusson et al,, 2004; Lipinski et al., 2001; Gawande, 2010), the influence of alternate, objective approaches to decision-making on exposure judgment accuracy has not been systematically investigated, .

Simple algorithms, requiring just a few inputs have improved health outcomes of neonates (Apgar, 1958), reduced infection rates (Pronovost et al., 2006), and increased airline safety (Billings and Reynard, 1984; Gawande, 2010). These algorithms, especially useful in low validity environments, i.e. situations with little or no data, and a high degree of uncertainty, focus the decision maker on the most critical inputs, filtering out details that would otherwise distract. In the field of industrial hygiene, simple rules or heuristics, applied consistently, have been shown to improve quantitative judgment accuracy (Logan et al., 2009).

We present a checklist (Checklist) that was developed to guide the application of a series of algorithms or heuristics, aiding qualitative exposure assessment judgments, i.e., judgments for which personal exposure measurement data is not available, so the assessment must be conducted using other inputs. The Checklist is applicable to vapor, aerosol, fiber and particulate exposure scenarios, and requires only four readily available pieces of information: the OEL, vapor pressure of the pure chemical (VP) in the case of a vapor, the observed or reported workplace control measures (ObsLC) and the required level of control (ReqLC). While the OEL and VP are truly objective, characterizing the ObsLC is more subjective and subject to interpretation by the IH. This tends to improve with clearly defined criteria coupled with examples to reduce uncertainty, and is further enhanced with diagrams and pictures of engineering controls. The ReqLC is determined as a result of a heuristic, as described later. This paper discusses the application of the checklist, and its influence on qualitative exposure judgment accuracy and inter-rater reliability (IRR).

METHODS

A qualitative exposure assessment Checklist was developed to guide the application of a set of heuristics developed from empirical observations that are based on physical-chemical principles to systematically improve qualitative exposure judgment accuracy and reliability. For this study, accuracy is defined as categorical agreement between the reference Exposure Control Category (ECC) and the participant's exposure judgment regarding the ECC. The ECC is the category to which the 95th percentile of the exposure distribution ($X_{0.95}$) most likely falls (Hewett et al., 2006). The boundaries of the four ECCs are presented in Table 2-1, found in Appendix I. Reliability is the probability that two or more assessors, evaluating the same scenario, come to the same assessment, i.e., select the same ECC. The Checklist has broad applicability and can be administered quickly, with minimal and readily available inputs. It includes three of the most widely applicable heuristics; the first two, the Rule of 10 and the Vapor Hazard Ratio, apply to scenarios involving pure or relatively pure volatile and semi-volatile compounds. The Particulate Hazard Ratio applies to aerosol, particulate and fiber scenarios (Stenzel, 2015). IHs using the Checklist follow these heuristics in a specific order. Though not included in this version of the tool, other heuristics addressing scenarios involving mixtures of chemicals, considering frequency and duration of exposure, quantity of agent, configuration of a vessel opening, system pressure, etc., have been developed and are being added to the next version of the Checklist. The current version is available through the Supplemental Materials which can be found online.

The Rule of 10

The Rule of 10 heuristic is premised on the incremental reduction in the maximum potential airborne concentration of a volatile chemical resulting from incrementally higher levels of control. For every step change in control (through the use of engineering controls), the maximum concentration for a scenario is reduced by a factor of 10. Engineering control types and their corresponding reduction of the airborne concentrations, expressed as a fraction of the Saturated Vapor Concentration (SVC) are presented in Table 2-2, in Appendix I. The SVC is calculated from the chemical's pure vapor pressure divided by the atmospheric pressure, in mm Hg, and multiplied by $10^6$to determine a saturation vapor concentration in parts per million (ppm) (Stenzel, 2015).

Vapor Hazard Ratio

The Vapor Hazard Ratio (VHR) heuristic is the ratio of the SVC, divided by the OEL. A VHR Scale ranging from 1 to 6, reflecting ranges of increasing VHRs is used to identify the ReqLC (Table 2-3 in Appendix I). This is the minimum level of control deemed necessary to adequately control the exposure (Stenzel, 2015).

Particulate Hazard Ratio

The Particulate Hazard Ratio (PHR) heuristic, similar to the VHR, assigns a PHR Scale value ranging from 1 to 6. The Scale value increases as the OEL value decreases as shown in Table 2-4 in Appendix I (Stenzel, 2015).

The Checklist

The Checklist (Table 2-5 in Appendix I) provides a prescribed step-by-step process for applying each heuristic. The first two heuristics are appropriate for scenarios involving pure or relatively pure volatile or semi-volatile chemicals. When assessing a volatile or semi-volatile, both heuristics are used independently. If the two heuristics predict ECCs that are not consistent with one another, the highest predicted ECC is used. Using the Rule of 10, the $C_{max;}$ the estimated concentration based on the saturation vapor concentration and taking into account the type of engineering control in place acts as a surrogate for the 95th percentile exposure and is compared directly to the OEL to identify the appropriate ECC. With the VHR, a decision logic is applied whereby ObsLC is compared to the ReqLC. If the ObsLC exceeds the ReqLC, then the exposure is most likely a Category 1. If the ObsLC is equivalent to the ReqLC, then the exposure is most likely a Category 2. If the ObsLC is less stringent than the ReqLC, the exposure is most likely a Category 4 (note that these heuristics bypass Category 3). This finding was validated both empirically over many years by Stenzel, and confirmed by the exposure data corresponding to the scenarios used in our study.

The third heuristic applies to scenarios involving aerosols, (droplets, fibers and particulates) and was derived from the performance based exposure limits used in the pharmaceutical industry. The PHR heuristic is used in the same manner as the VHR, and the same decision logic is used.

Eliciting IH exposure judgments using the Checklist

Practicing IHs (n = 39) were recruited for a study evaluating the influence of the Checklist on exposure judgment accuracy. Personal determinants (experience, training and education) were collected from this group. Novice IHs (n = 8 Master's degree students in Industrial Hygiene) were also recruited, and their personal determinants were recorded. Each group was assigned several exposure scenarios and asked to assess worker exposures, before and after receiving the Checklist training. Informed consent was obtained from all participants and human subject research approval for the study granted by the University of Minnesota Institutional Review Board (IRB Code 1212M25182).

Scenarios were developed from information and data voluntarily submitted by a number of companies and organizations. A novel tool, the Industrial Hygiene Exposure Scenario Tool (IHEST) was developed to facilitate consistent collection and reporting of exposure scenario details, determinants and personal exposure data. The tool is available through the Supplemental Materials. Each exposure scenario was described in a two-page narrative, systematically presenting exposure related information and providing details regarding the workplace, work tasks, chemical agent and OEL. An example of a scenario narrative is available in the Supplemental Materials and in Appendix I. A list of the scenarios developed for this study, the agent of interest, and ECC are presented in Table 2-6 in Appendix I. Quantitative personal exposure monitoring data were excluded from the narratives, and were used only to determine the reference ECC, against which exposures were compared. Reference ECCs were calculated from a minimum sample size of six personal exposure measurements to ensure a reasonable degree of confidence in these reference values. The measurements were used in the IHDA Lite software (oesh.com) in which uniform priors were assumed and the ‘likelihood’ decision chart produced by this Bayesian Decision Analysis software was used as the Reference ECC. Specifically, the ECC with the highest probability was identified as the Reference ECC. In two separate workshops, practicing IHs were randomly assigned four scenarios from a database comprising 11 exposure scenarios: five vapor-related scenarios and six involving aerosols, fibers and particulates. Each IH evaluated two scenarios at the beginning of the study, before training was conducted, providing data on the participant’s exposure assessment proficiency from which baseline accuracy was determined. Seven very enthusiastic study participants assessed more than the two pre-training scenarios that were assigned to them, providing additional baseline exposure judgments. These were included in the baseline analysis. A one-hour training session was conducted, explaining each of the three sections in the Checklist and providing instructions on how to apply them. A case study (Scenario 7) was used to illustrate the application of the Excel-based Checklist tool, developed specifically for the study. The Checklist tool is included in the Supplementary Materials. Following training, in addition to reassessing the two baseline scenarios, IHs evaluated two new scenarios. Judgments were expressed probabilistically, with hygienists expressing their beliefs about the true group 95th percentile belonging to each ECC, and assigning the highest probability to the ECC to which the true group 95th percentile most likely belonged. A (hypothetical) example of this probabilistic expression is illustrated in Figure 1. While participants gave their signed consent prior to participating in the study, some participants were either not comfortable providing all of their judgments or were unable to complete the four assigned scenarios in the time provided. A total of 61 baseline judgments were collected (5 participants provided 1 judgment = 5 judgments; 17 participants provided 2 judgments = 34 judgments; 6 participants provided 3 judgments = 18 judgments; 1 participant provided 4 judgments = 4 judgments; for a total of 61 judgments from 29 participants).

Post-training judgments were provided by 30 participants and totaled 115 participant-judgments. (1 x1 + 1 x 2 + 1 x 3 + 26 x 4 + 1 x 5 from 30 participants providing 115 post-training judgments).

Novice IHs were asked to assess three scenarios at the beginning of the study, prior to training, providing 24 baseline judgments. Following Checklist training, they were instructed to re-assess the same three scenarios, and assigned seven more new scenarios. This group was allowed to take the materials home to complete their assessments, submitting their judgments one week later. A total of 80 post-training exposure judgments were submitted.

Evaluating Exposure Judgments

Exposure judgment accuracy was calculated by comparing the participant's predicted ECC ($ECC_{PRED)}$ to the reference ECC ($ECC_{REF)}$ for each scenario.

$$Accuracy = ECC_{PRED} - ECC_{REF} \tag{2-1}$$

For example, if the reference ECC indicated that the exposure most likely belonged to category 2, and the hygienist assigned the highest probability to ECC 2, the judgment was deemed categorically accurate. The difference between the proportion of accurate baseline judgments and the number of accurate post-training judgments (of all participants) was evaluated using χ^2- analysis.

If the scenarios had been balanced such that there was an equal distribution of scenarios belonging to each of the four ECCs, then the probability of a participant correctly making a judgment by randomly picking a category would have been 25%, the probability of under-predicting or over-predicting by one category would be 18.75%, by two categories would be 12.5%, and by three categories would be 6.25%. If the scenarios are not equally balanced among the four categories, the probabilities of being incorrect by one, two, or three categories would be different (although the probability of being correct would still be 25%). Since the scenarios were not equally distributed among the four categories, a Monte Carlo simulation with 10,000 iterations where an ECC is selected randomly for each of the ten scenarios, representing an exposure judgment for each of those scenarios. The number of times the random selection turns out to be correct across all scenarios, i.e., matches the reference ECCs is calculated, along with the number of times the random selection under- or over-predicts by one, two of three categories. Thus, the random chance probability of being correct or incorrect by a specific number of categories was calculated.

Judgment bias was calculated for baseline and Checklist judgments from the following equation:

$$Bias_k = \text{Average Assessed } ECC_k - \text{Reference } ECC_k \tag{2-2}$$

where the Average Assessed ECC = average of all predicted ECC judgments for the k^{th} scenario, and Reference ECC_j = Reference ECC for the k^{th} scenario

For the k^{th} scenario, the standard deviation (SD) is defined as:

$$SD_k = \sqrt{\sum_{i=1}^{N} \frac{\left(ECC_{i,k} - Average\,Assessed\;ECC_k\right)^2}{N-1}} \tag{2-3}$$

where $ECC_{i,k}$ is the i^{th} participant's judgment about scenario k and N = number of participants providing judgments, and *Average Assessed* ECC_k is the Average of all Assessed ECC judgments for the k^{th} scenario.Pair-wise inter-rater reliability (IRR), a measure of agreement between two assessors making judgments about the same scenario, was calculated for each group, using Cohen's κ (Cohen, 1960). Weighted and unweighted κ were calculated, where weighted κ reflect scores generated by assigning differential penalty weights accounting for the magnitude of disagreement between the two judgments; larger weights reflect greater disagreement. Fleiss' κ providing an aggregate κ for novice IHs (n=8) assessing the same ten scenarios was also calculated (Fleiss, 1971). A third IRR metric, G(q,k) (Putka et al., 2008) evaluating practicing IHs' IRR was calculated, taking into account the non-fully-crossed study design used to assign exposure scenarios. Specifically the design produced some overlap between raters evaluating a specific scenario, but not every practicing IH assessed every scenario. This alternate measure of IRR explicitly models the variance components (Scenario main effect, Rater main effect and Scenario-Rater interaction and residuals) and applies a multiplier, q to scale the contribution of the Rater main effect to the observed score variance. The expected value of the observed variance in judgments that have been scaled across *k* raters per scenario is calculated using Brennan's (1992) formulation:

$$\sigma_Y^2 = \sigma_T^2 + q\sigma_R^2 + \frac{\sigma_{TR,e}^2}{\hat{k}} \qquad (2\text{-}4)$$

where σ_Y^2 =Expected observed variance, σ_T^2 = Scenario main effects, σ_R^2 = Raters main effects, $\sigma_{TR,e}^2$ = combination of rater x rate interaction and residual effects, $\hat{k}$ =harmonic mean number of rates per scenario, and q=multiplier

These values were then used to calculate the inter-rater reliability, G(q,k):

$$G(q,k) = \frac{\hat{\sigma}_T^2}{\hat{\sigma}_T^2 + \left(q\hat{\sigma}_R^2 + \frac{\hat{\sigma}_{TR,e}^2}{\hat{k}}\right)} \qquad (2\text{-}5)$$

Statistical analysis was conducted using R, version 3.03. The package lmer was used to calculate the variance components for G(q,k), and for Cohen's kappa, the cohen.kappa (psych) package was used.

RESULTS

A total 85 baseline exposure judgments (61 + 24),described above, in Methods, were collected and analyzed. Baseline exposure judgment accuracy was low: 32.9% overall; 29.5% for practicing IHs, 41.7% for novice IHs, and not statistically significantly different from random chance (25.1%). Baseline judgments collected from practicing IHs were negatively biased, with 50.8% underestimating the 'true' exposure by one (34.4%), two (9.8%) or three (6.6%) ECCs (Figure 2). Additional details are provided in the Supplemental Material, Tables SIIIa and SIIIb in Appendix I.

The post-training evaluations reported here include both re- evaluation of scenarios and evaluation of new scenarios. Since the accuracy rates are similar for the scenarios evaluated twice and the scenarios evaluated only after training/checklist use, we report only the results of the pooled evaluations. Judgment accuracy increased significantly, (χ^2 (1) = 25.36, $p < 0.001$) when decisions were guided by the Checklist. The percent of accurate judgments increased from pre-training baseline (28/85), to post-training (123/195). Judgments that were categorically accurate are shown in the center columns of the graph, labelled “Accurate”. The reduction in the number of exposure judgments underestimating the true ECC for practicing IHs when their decisions were guided by the Checklist can also be seen in Figure 2. Judgment accuracy based on random chance, for baseline and Checklist judgments are presented in Figure 3. A detailed breakdown of judgment accuracy for novice and practicing IHs is provided in the Supplemental Materials (Tables SIa and SIb found in Appendix I).

The negative bias observed in the baseline judgments of practicing IHs was attenuated in Checklist-guided judgments such that the absolute magnitude of bias was reduced. Precision, measured using the standard deviation, also improved for both groups, although not in all cases. The values for bias and precision are presented in Table 2-7a Baseline and Checklist Judgment Bias and Precision: Novices and Table 2-7b practicing IHs. These tables are in Appendix I.

Fleiss' κ, measuring interrater agreement of novice assessors, evaluating the same 10 scenarios was $\kappa = 0.39$, $p < 0.001$. Fleiss' κ represents an aggregate value for inter-rater agreement indicating in this case, that the intra-novice IH group judgment agreement was far greater than would be observed by chance alone ($\kappa = 0$). The pair-wise evaluation is shown in Table SIIa in Appendix I. While there is no one widely accepted interpretation of values for Fleiss' κ, Landis and Koch (1977) suggest values of 0.2 to 0.4 represent fair agreement and values of 0.4 to 0.6 represent moderate agreement. Cohen's (1960) weighted and unweighted κ, scores were calculated for the novice IH (0.77 and 0.81) and practicing IHs (0.93 and 0.89). These values represent good to excellent agreement (Landis and Koch, 1977). G(q,k), calculated for practicing IHs only, was 0.76 and would similarly indicate good agreement. The pair-wise evaluation is shown in Table SIIb in Appendix I.

DISCUSSION

In disciplines where increasing complexity has led to specialization, sub-specialization and super specialization, expertise alone may not guarantee acceptable performance. Many fields, including exposure assessment are too complex, with the amount of information exceeding the capacity of the pre-frontal cortex (PFC), the area of the brain where decision-making occurs. This overload makes the brain vulnerable to flaws of memory, distraction and thoroughness, inviting bias and over-confidence in our decisions (Kahneman, 2010; Gawande, 2010). It also leads to inconsistent summary judgments: given the same scenario, experts, rarely come to the same conclusion twice, and two experts may not come to the same conclusion (Kahneman, 2010).

Simple algorithms typically perform better than ‘expert professional judgment’. Expressed as checklists, they ensure that the critical steps in a process are followed in order every time. Effective checklists contain only the essential inputs or steps, so they are not forgotten when the mind is occupied by multiple tasks. “Under conditions of complexity, not only are checklists a help, they are required for success. There must always be room for judgment, but judgment aided – and even enhanced – by procedure” (Gawande, 2010). Checklists free the practitioner from having to focus cognitive energy on the mundane but critically important tasks, maximizing the energy available for innovation and for dealing with non-routine events (Meehl, 1954). First adopted by the aviation safety industry, the use of checklists led to an impressive safety track record that continues till today (Gawande, 2010). Checklists are also impacting medical performance measures, reducing errors and health complications associated with its inherently complex and uncertain environment (Apgar, 1958; Luby et al., 2005; Pronovost et al., 2006).

Qualitative exposure judgments, like many of the decisions in aviation safety and medicine, are inherently complex and frequently require decision-making under pressure, with minimal data. The low baseline judgment accuracy observed in this study, consistent with previously reported low subjective-intuitive qualitative exposure judgment accuracy (Logan, 2009; Vadali, 2012) reflect these complexities and uncertainties, and the inability of our cognitive systems to handle them. It is interesting that the novice IHs were more accurate and less biased in their baseline judgments. Without prior experience in conducting exposure assessments or collecting exposure measurements, this cohort could not draw upon 'professional judgment' and instead, applied their academic training in IH, as determined by follow-up conversations. The students had attended several lectures on IH statistics, including characteristics of the (skewed) lognormal distribution that typifies exposure measurement data, and two lectures on exposure modeling during the semester. In contrast, ~ 70% of the practicing IH group reported limited expertise in IH statistics and modeling, but >50% had extensive experience conducting exposure assessments and had considerable expertise collecting exposure measurement data. Of this group, 70% reported having conducted ≤10 exposure assessments following the AIHA Strategy. This suggests, based on our understanding of the conventional approach to exposure assessment, that the vast majority of data sets upon which the practicing IHs based their decisions and calibrated their professional judgment were small, most likely n =0, 1 or 2.

Moreover, the data were probably not subjected to any statistical treatment, resulting in erroneous feedback.

To illustrate why these behaviors might lead hygienists to underestimate the true exposure, consider the following examples. In case study 1, three exposure measurements are collected for a scenario in which the true exceedance fraction is 25%. From Table 2-8 we can see the percentage of time the measurements, collected based on N = 1, 2, 3, 4 or 5, will all fall below the OEL for a scenario in which the OEL = 10 ppm, for various Exceedance Fractions when the Geometric Mean (GM) = 10, and the Geometric Standard Deviation (GSD) = 2.5). With n = 3 samples collected, there is a 42% probability that the three samples will all be below the OEL, meaning that the hygienist will not realize the exposure is unacceptable, 25% of the time. Consequently, the hygienist's professional judgment may be miscalibrated by this erroneous feedback and further reinforced each time only a few measurements are collected. In case study 2, the benchmark is the Action Limit (AL). Using the same parameters as before, i.e., exceedance fraction = 0.25, n = 3 samples but using the AL as the benchmark, we can see from Table SIV there is a 10% probability that these three samples would all be below the AL. The feedback loop, even when using the more conservative AL may be faulty, reinforcing biased decision making.

Checklist based judgments improved qualitative judgment accuracy significantly, increasing them by a factor of 2. Novice IHs produced judgments that were just as accurate as their more experienced colleagues, suggesting that this objective approach is equally helpful for hygienists of all experience levels. Further, the level of accuracy observed in this study using the Qualitative Exposure Assessment Checklist tool was comparable to the results observed in quantitative studies (Logan et al., 2009; Vadali et al., 2012). For scenarios involving specialized engineering controls, such as the glutaraldehyde in scenario 1 (using general mechanical and local exhaust ventilation), and mannitol in scenario 2 (a clean room environment using primary and secondary containment), IHs underestimated the true exposure by 1 ECC, possibly because most of them were not familiar with this specialized work environment and engineering controls, leading to a misclassification of the level of controls used ('ObsLC'). The effectiveness of the local exhaust ventilation (LEV) was highly dependent upon work practices in the methylene chloride scenario (scenario 11), a fact that many practicing and almost all novice IHs did not take into account (nor did the training provided by the investigators suggest it). Most IHs overestimated the true exposure for bystander asbestos (scenario 7) and acetone (scenario 8) by 1 ECC, which could reflect the fact that the agents were present as mixtures, not pure or relatively pure chemicals. The algorithms in the current version of the tool do not account for the lesser magnitude of exposure, and therefore tend to overestimate in these cases. The next version of the Checklist tool will take mixtures into account.

Judgments made by practicing IHs using the Checklist were also less biased compared to when they did not use the Checklist. In fact, maximal accuracy for practicing IHs and novice IHs was achieved when the exposure judgments were based on the Checklist algorithms. This suggests that judgments guided by objective methods and based on only the critical inputs produce exposure judgments that are superior (because they are more accurate) to decisions based solely on subjective professional judgment. Intuition adds value if, and only if, it follows disciplined collection of objective information with robust scoring and analysis, i.e., if the judgment has been carefully calibrated with immediate, clear and accurate feedback. Judgments reflect true expertise when the environment is sufficiently regular to be predictable AND the expert has had time and the opportunity to learn these regularities through practice AND the expert can express a judgment accurately in probabilistic terms. Algorithms outperform experts because experts try to think 'outside the box', considering complex combinations of inputs (Meehl, 1954; Ashenfelter, 2008; Kahneman, 2010). This may help explain why baseline exposure judgments made by novice IHs, lacking professional experience, did not exhibit the same bias towards underestimating the true exposure as was observed by 'expert' practicing hygienists. It may also explain why the novice IH group's Checklist judgments were more precise, as they were less likely to try to outsmart the algorithms.

IRR helps discriminate between variance in observed judgment accuracy due to variance in the true accuracy (scores) after the variance due to measurement error between raters has been removed (Hallgreen, 2012). Since each metric is based on different assumptions, using several measures is recommended (Taylor and Watkinson, 2007). Cohen's κ (1960) tends to give lower estimates of reliability although in this study, unweighted values for practicing IHs were relatively high. This may be due to the non-fully crossed study design, resulting in rater pairs sometimes overlapping for only one or two scenarios; if the two raters agreed in their judgments, $\kappa = 1$ so Cohen's κ for the practicing IHs may be somewhat artificially inflated. The value for $G(q, k) = 0.80$ is very similar to the Cohen's κ (unweighted) score observed with the novice IHs' judgments that were produced using a fully-crossed design. G (q, k) explicitly accounts for the rater main effect component of the variance (σ_R^2). G (q, k) uses the q multiplier to scale the contribution of σ_R^2 to the observed judgment variance, based on the amount of overlap between the sets of raters evaluating each scenario. Inter-rater agreement was consistently good to excellent (Landis and Koch, 1977) and while the results should be interpreted conservatively given the study size, they suggest that the Checklist contributes to greater inter consistency in qualitative exposure judgments.

Checklist judgments may prove useful in a broader context. The Checklist provides one approach to developing accurate, informative priors in Bayesian exposure assessments which, used in conjunction with maximum likelihood estimates (calculated from exposure measurements, for as few as n = 1), produce more confident or precise posterior judgments, making Bayesian Decision Analysis more powerful. In other words, by facilitating accurate, informative priors, exposure measurements can serve a validation role, producing highly confident and accurate judgments with fewer measurements. This could and should motivate a major shift in exposure assessment practice.

There are several important limitations to this study. One is that personal exposure data were used to characterize the reference ECC, thereby suggesting quantitative measurement data is the gold standard. We defined a minimum of six personal samples to ensure a reasonably high level of confidence in these ECCs. However, when insufficient samples are collected or the data are not analyzed appropriately, using relevant statistical metrics, quantitative measurements, and conclusions drawn from such data can be highly misleading. Secondly, a systematic approach was used in conducting the basic characterization for each scenario, and the information collected was presented to participants logically and consistently. This may have impacted the degree to which Checklist guided judgments agreed with the reference ECCs. Lacking this kind of systematic and thorough characterization, the IH may have come to different, less accurate conclusions. Finally, as with any small study, selection bias may occur. The decision by some participants to potentially refrain from submitting their judgments which were likely less accurate, may have favorably biased the results.

CONCLUSIONS

Qualitative exposure judgments form the foundation upon which most comprehensive exposure assessments are based. Their accuracy is critical to ensuring appropriate exposure and risk assessment and risk management outcomes. The widely prevalent practice of conducting qualitative assessments based on subjective professional judgment not only fails to meet this imperative, it often leads to negatively biased exposure judgments in which the true exposure and risk is underestimated.

Judgments aided by the Checklist, on the other hand, significantly improved judgment accuracy, producing ~ 60% judgments categorically accurate, and ~ 70 - 74% accurate or overestimating by one ECC. This approach, applying algorithms consistently through the use of a checklist and other objective methods, offers a pathway to more accurate decisions.

To maximize the Checklist's value and impact, further evaluation against additional scenarios is recommended. Scenarios should be developed for specific industry types and task environments, and include sufficient personal sampling data to generate reasonably confident reference ECCs . These additional studies, conducted across a broader spectrum of exposure scenarios will further illuminate the bounds within which the tool contributes to accurate exposure judgments, and the limits beyond which it will not. Additional studies should also be conducted with novice assessors, to determine the generalizability of the results reported here. Lastly, continuous feedback, provided through additional research and from those using the tool is necessary to improve the Checklist and identify other useful objective approaches to improving qualitative exposure judgment accuracy.

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CHAPTER 2 EVALUATING WELL MIXED ROOM AND NEAR FIELD FAR FIELD MODEL PERFORMANCE UNDER HIGHLY CONTROLLED CONDITIONS

INTRODUCTION

When decisions regarding the acceptability of occupational exposure are based on professional judgment informed by subjective inputs, they are accurate ~30 % of the time and tend to underestimate the true exposure. (Logan et al., 2009; Vadali et al., 2012, Arnold et al., 2015). However when professional judgment is informed by structured, objective inputs such as statistical analyses of exposure monitoring data (Logan et al., 2009) or algorithms and checklists (Arnold et al., 2015), they tend to be significantly more accurate.

Anecdotal reports suggest that the use of exposure models such as deterministic physical-chemical models contribute to accurate decision making, but these models are not widely used in practice. Possible reasons for this might be that these models have not been systematically evaluated, scant guidance on how to select them, and a lack of model input values to apply the models. Models tend to be under-valued and under-utilized, especially in the practice of occupational hygiene. Models have been applied across a broad range of fields to improve decision making, from weather forecasting to medical diagnosis and treatment selections (Kahneman, 2011). Meehl (1954) asserted that models consistently produce significantly more accurate judgments than subjective expert judgments. The nearly 200 studies conducted since this evidence was first published support this assertion (Kahneman, 2011). The range of predicted outcomes has expanded to include economic indicators, career satisfaction of workers, questions of interest to government agencies and the future price of Bordeaux wines. Pharmaceutical researchers use simple models based on readily available inputs, identifying potential candidate compounds for transdermal drug (Magnusson et al., 2004) and oral drug delivery (Lipinski et al., 2011). The Apgar test, a simple model comprised of five critical determinates has been helping save the lives of neonates since 1953 (Kahneman, 2011). These fields have in common a significant degree of uncertainty and unpredictability, which Kahneman (2011) refers to as 'low-validity'. The application of models to the low-validity field of occupational hygiene exposure risk assessment is a logical next step towards improving exposure judgments.

There are several deterministic models with varying levels of sophistication (Ramachandran 2005; Arnold, et al., 2009) and correspondingly varying costs due to the amount of information needed as model inputs. For example, the near field-far field model requires knowledge of room ventilation and contaminant generation rates in addition to a parameter known as the inter-zonal ventilation rate – involving a non-trivial investment. A sophisticated eddy diffusion model, which accounts for concentration gradients around pollution sources, requires even greater investments. While costs increase with the level of sophistication, more complex models can also yield more refined exposure estimates.

Two models, the Well Mixed Room (WMR) and Two Zone or the Near Field-Far Field (NF-FF) models, were evaluated in a series of studies conducted in a full-sized exposure chamber using criteria defined in ASTM 5157 and using categorical criteria defined in the AIHA Exposure Assessment Strategies framework (Mulhausen and Damiano, 1998; Jahn, Ignacio and Bullock, 2015). More than 800 measured and modeled concentration pairs ($C_{measured}$ and $C_{modeled}$) generated under highly controlled conditions and using three organic solvents across a range of experimental condition were generated for the evaluation.

METHODS

A series of chamber studies were conducted to evaluate model performance under highly controlled conditions. Experimental conditions in the chamber were changed systematically so that model performance could be evaluated under a range of environmental conditions. The highly controlled environment also facilitated evaluation of different models under similar conditions, providing insight into whether one model provides a more accurate exposure estimate for a given set of conditions. The WMR and NF-FF models were selected for evaluation, having broad applicability in assessing both occupational and non-occupational exposures. These models, described in detail elsewhere (Nicas, 1996; Ramachandran, 2005; Keil et al., 2009) and briefly presented in Appendix II, assume that the chemical released into the air is instantaneously well mixed in one or two boxes. The WMR model, illustrated in Figure 3-1 assumes a one-box geometry and is useful for estimating the average exposure when the emission is released from a large or non-point source. It assumes that air entering the room (Qin) is instantaneously well mixed, so that the contaminant concentration (C_A) is uniformly dispersed throughout the room. The model also assumes that the rate at which air enters the room is the same as the rate at which it is exhausted, so that given sufficient time, the contaminant concentration would reach steady state levels. The NF-FF model, shown in Figure 3-2 assumes a box-within-a-box geometry, accounting for spatial differences in magnitude of exposure associated with point source emissions. It assumes that the air and contaminant concentration within each box is well mixed, with the same assumption regarding the rate at which air enters and is exhausted from the room. The model is premised on an additional assumption regarding the rate at which the contaminant concentration in the NF moves to and from the FF. It is defined as the interzonal airflow rate, ß. The chamber setup in this work was arranged to account for these fundamental assumptions.

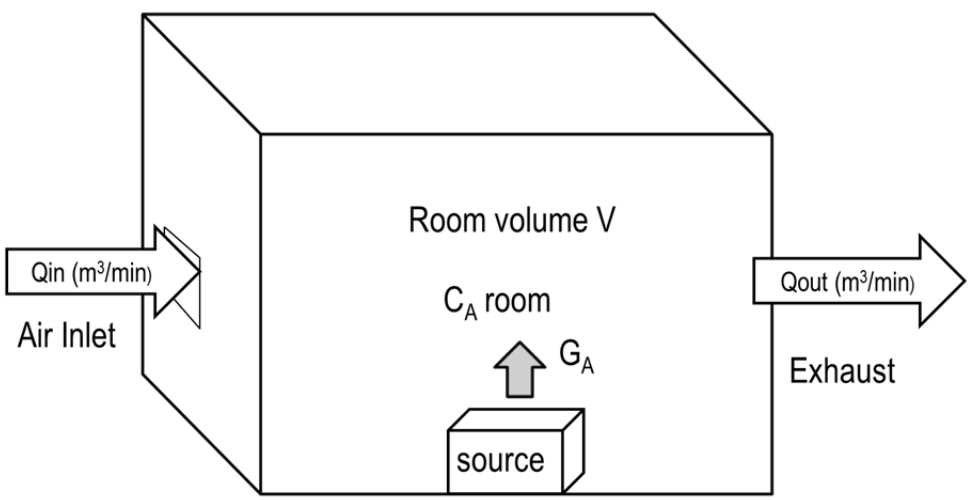

Figure 2-1a Schematic of WMR model

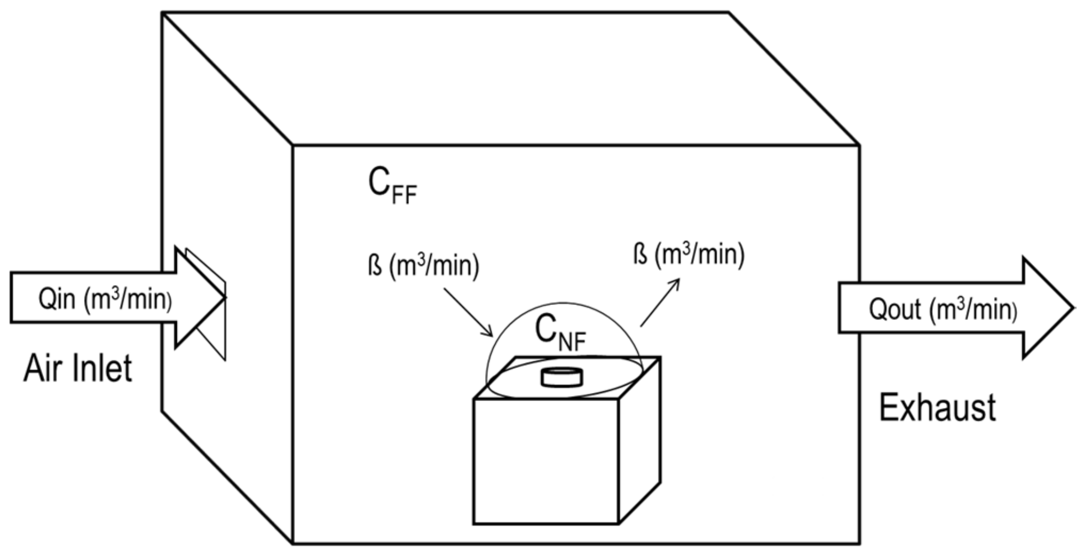

Figure 2-1b *Schematic of NF-FF model*

Chamber Design and Construction

A full size exposure chamber (2.0 m x 2.8 m x 2.1 m) constructed of 80/20® framing and black Omega-Lite aluminum-faced composite panels was used to conduct the chamber studies. These materials were selected for their strength, durability and resistance to corrosion and reactivity with a broad range of chemicals. The chamber was fitted with a filter bank on the air-inlet side to filter incoming air. Inside the chamber, a mesh screen was installed over the filter bank to reduce directional airflow and encourage eddy currents. Air was exhausted through a 6 m (20 ft.) length of flexible duct that was attached to a 0.15 m (6 inch) elbow duct located near the back corner of the chamber on one of the long-walls. The flexible duct was perforated so that air could be removed from multiple locations in the chamber, minimizing advective effects. The ventilation duct was connected to the lab exhaust, which is in turn connected to the building general mechanical ventilation system, exhausting air directly to the building exterior. With this system, air exchange rates up to 5 ACH could be achieved. A glass panel was installed in the chamber ceiling, allowing fluorescent lighting located above to illuminate the chamber. A second glass panel was installed along one of the long walls so that activity in the chamber could be viewed from outside.

Chamber Study Design

Three industrial solvents - toluene, 2-butanone and acetone - were selected due to their widespread industrial application and range of vapor pressures.

Table 2-1 Solvent Properties of the three solvents used in the chamber study

Solvents	MW	Vapor Pressure **@ 25 degrees C**	Density
Toluene	92.11	28 mm Hg	0.864
2-Butanone	84.93	71 mm Hg	0.805
Acetone	58.08	200 mm Hg	0.791

A factorial study design was used to evaluate the WMR model across a range of emission and ventilation rates. Solvent injection rates (of 0.05 ml/min, 0.1 ml/min and 0.15 ml/min) were selected to accommodate instrument sensitivity, delivery capacity and time required to approach steady state concentrations. Three ventilation rates (Q) of 0.3, 1.3 and 3 ACH corresponding to 0.059 m^3/min, 0.258 m^3/min and 0.595 m^3/min, respectively, representing ranges relevant to residential and industrial settings were used. Each set of chamber studies was repeated 3 times. Thus for each solvent, 3 generation rates x 3 ventilation rates x 3 repetitions = 27 studies were conducted. Generation and ventilation rates are shown in Table II.

Table 2-2Generation Rates and Ventilation Rate Ranges

Generation rates corresponding to delivery volumes 0.05, 0.1 and 0.15 ml/min

Solvent	Generation Rate, G (mg/min)			Ventilation Rate, Q (m3/min)		
	low	med	high	Low	med	high
Toluene	43.18	86.36	129.54	0.04 - 0.07	0.23 - 0.27	0.47- 0.77
2-Butanone	40.25	80.5	120.75			
Acetone	39.55	79.1	118.65			

Precise generation rates G (mg/min), were achieved by releasing a solvent into the chamber using a Harvard Apparatus® Pump, Series 11 Elite, (Harvard Apparatus, Holliston, MA) equipped with a Becton Dickenson 30 ml or 50 ml glass syringe (East Rutherford, NJ). Because of the relatively high vapor pressures, the solvents evaporated almost immediately upon delivery, emitting the solvent vapor at a known and consistent generation rate.

The chamber volume is 2.0 m x 2.8 m x 2.1 m = 11.9 m^3. Ventilation rates, Q (m^3/min), were set by installing an orifice corresponding to the desired range of air changes per hour (ACH) into the orifice housing located in the exhaust duct and adjusting a damper, which is located between the orifice and the exhaust fan. Concentration decay data, measuring the concentration in the chamber after the generation rate went to zero and as the contaminated air was replaced with fresh air, was collected at the conclusion of every test at each of the six sample locations, (Table III).

Table 2-3 Sampling locations in the chamber relative to the contaminant source for the WMR tests

Sampling Location	Position Relative to Source	Distance from Source, m		
		X direction	Y direction	Z direction
1	Upstream	0.03	1.27	0.52
2		0.61	1.14	0.20
3		0.67	0.25	0.41
4	Downstream	0.03	0.2	0.41
5		0.00	0.74	0.39
6		0.06	1.3	0.58

The corresponding slope of the curve was obtained by plotting the rate of decay, . (Figure 3-2) and since V is known, an accurate estimate of Q can be determined:

$$-\ln\left(\frac{C}{C_0}\right) = \frac{Q}{V} \times t \qquad (3\text{-}1)$$

Where

C is the concentration at time, t (mg/m^3)

C0 is the initial concentration at start of decay period (mg/m^3)

Q is the ventilation rate (m^3/min)

V is the room volume (m^3)

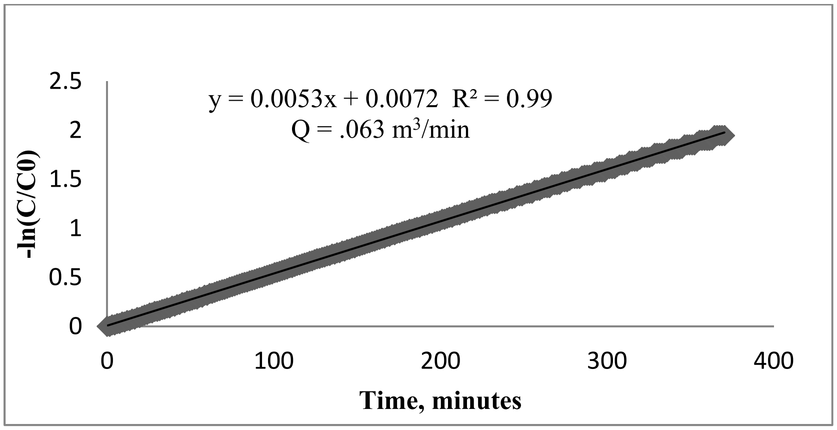

Figure 2-2 Measuring Q from concentration decay data

A Magnehelic® differential pressure gauge (Dwyer Instruments Inc., Michigan City, IN) was used to measure the pressure differential across the orifice located in the ventilation duct and thus ensure relatively consistent air exchange rates across tests.

To induce good mixing in the chamber, two Air King adjustable-height 3-speed fans equipped with tilting heads (W.W. Grainger, Inc., www.grainger.com) were placed in opposite corners of the chamber facing the corners and set on the lowest fan speed.

Solvent vapor concentrations, hereafter referred to as $C_{measured}$, were measured in real-time using two Dräger X-am 7000 Multi-Gas Monitors (MGM) equipped with Smart PID® sensors (Dräger Safety AG & Co. KGaA). Each instrument was calibrated according to the manufacturer's instructions using a standard calibration gas of 100 ppm isobutylene (IBUT) (Dräger Safety AG & Co. KGaA). To ensure the most accurate results, additional calibration studies were conducted with each MGM, verifying the response factor for the three solvents. For toluene, in addition to the fresh air test in which the zero baseline was set, two standard calibration gases of 20 ppm and 200 ppm were used, following instructions found in the MGM Technical Manual. Since standard calibration gases for the other two solvents were not readily available, area TWA air samples were collected in the chamber as steady state conditions were reached using sorbent tubes for a period of 20 minutes. The TWA 2-butanone concentrations were compared to the 20-minute average concentrations reported as IBUT, using the MGMs. These studies were conducted at three air exchange rates, ~ 0.059 m^3/min, 0.258 m^3/min, and 0.595 m^3/min to generate a calibration curve. TWA samples were collected following NIOSH Method 2500 using Anasorb 747 sorbent tubes (SKC Model 226-81A, SKC, Inc. Pittsburgh, PA). Sample analysis was conducted by an AIHA Accredited laboratory following NIOSH Method 2500. Similarly, response factors for acetone were determined following NIOSH Method 1300 using charcoal sorbent tubes (SKC model 226-01, SKC, Inc. Pittsburgh, PA).

The Response Factor was calculated by comparing the desired concentration by the observed concentration:

$$\text{Response Factor} = \frac{\text{Desired concentration}}{\text{Observed concentration}} \tag{3-2}$$

Table 2-4 Reported (Dräger Safety AG & Co. KGaA) and observed Response Factors

	Response Factors (RF)	
	Reported RF	**Measured RF**
Toluene	0.7	0.7
2 Butanone	0.64	0.91
Acetone	1.15	1.3

(RF)

In the WMR studies, real-time contaminant measurements ($C_{measured}$) were collected at six locations in the chamber (Table 3-3 and Figure 3-3) – three upstream and three downstream. Two MGMs, both located outside the chamber were connected to a multiplexer, an instrument fitted with switch valves and controlled using software to control which valves are open at any given time, for how long and at with what frequency. On the other side of the multiplexer six lengths of copper tubing were connected, each one fed through a dedicated port in the chamber wall and positioned in the chamber at various locations, (Figure 3-3). For the WMR studies, measurements were collected concurrently at one location upstream and downstream of the source, with each instrument capturing three 10-second average measurements before the valves controlling those locations closed and a new set of valves opened, allowing the next locations (one upstream and one downstream) to be sampled. Following this pattern, each location was sampled every 1.5 minutes. The sampling distances from the source for each location are shown in Table III.

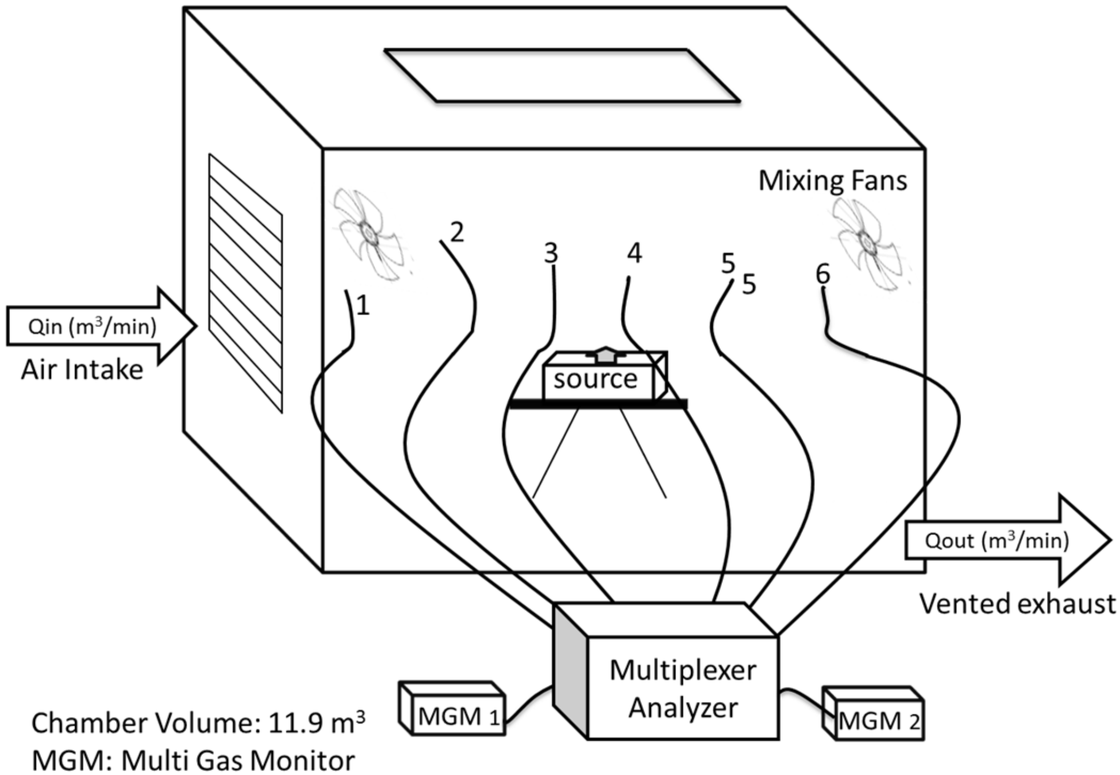

Figure 2-3 Full size exposure chamber arrangement for WMR studies

The initial contaminant concentration (C_0) and contaminant concentration in the incoming air, C_{in} were also measured directly using the MGMs. Since the incoming air was clean air, i.e. it did not contain detectable levels of the solvents used in this study, C_{in} was set to zero. When the initial concentration was greater than zero, C_0 was adjusted accordingly.

The WMR model includes a loss term, k_L, that is useful for accounting for sample loss due to mechanisms such as sample degradation or adhesion to surfaces such as the chamber walls or copper tubing surfaces. To determine whether any contaminant losses occurred as the sample moved through the copper tubing and multiplexer on its way to the MGM sensor, a series of tests were conducted across the 3 ventilation rates used in the model performance tests. One MGM (MGM #1) was located inside the chamber next to the source, and a second instrument (MGM #2) was connected remotely, sampling the chamber air as described above with the copper tubing positioned beside MGM #1. The concentration measured inside the chamber was regressed over the concentration measured remotely, and using standard linear regression methods k_L was determined to be < 0.01 min^{-1}.

Chamber Study Design for the NF-FF Model Evaluation

The NF-FF model assumes the Near Field (NF), the area encompassing the source is a well-mixed box situated within a larger well mixed box, the Far Field (FF). While the NF is typically a conceptual space and not necessarily defined by physical barriers, we constructed a NF box from perforated wire mesh. Open on all six sides, this (.51 x .51 x .41 m = .105 m^3) box was sized to ensure the differences in the magnitude of exposure were large enough to be detected by the MGM. The FF volume is the chamber volume minus the NF volume = 11.79 m^3. The NF with the source inside of it was placed 0.6 m downstream of the air inlet with one of the MGM placed 0.2 m from the source inside the NF box. Since the instrument was placed inside the chamber, only one sample was collected in the NF for each test. FF measurements were collected in the same manner as the WMR studies, at the same locations. Thus for the FF, three samples were collected for each test (Figure 3-4).

The same ventilation rates used in the WMR studies were also used for the NF-FF model evaluation. Decay data was collected following the same protocol to measure Q at each sample location.

Air within the NF and FF is assumed to be instantaneously well mixed, but air movement between the two zones is assumed to be limited. The rate at which air, and any contaminant in the air, moves from the NF to the FF and vice versa is called the inter-zonal airflow rate, ß. Unlike the other model inputs, β cannot be measured directly and is estimated by accounting for the effects of the NF geometry and local air speed.

$$\beta = \tfrac{1}{2} \times FSA \times S \qquad (3\text{-}3)$$

where FSA is the Free Surface Area of the NF (m^2), and S is the random local air speed (m/min)

Since the NF in these studies was a box with all six sides deemed open to air movement, the free surface area was calculated by summing the area across the six sides of the box. The FSA was 1.34 m^2.

Local air speed measurements were collected every 30 seconds along the x and y-axes in the chamber during each test and data-logged, using two TSI Velocicalc® model 9545 thermal anemometers (TSI Inc., Shoreview, MN). Data were downloaded at the end of each test day. The standard deviations of the air speed measurements along each of the x- and y-axes were taken to be the random air speeds along those axes (Jones, 2008). Since the Velocicalc did not measure along the z-axis, the standard deviations along the x- and y-axis were averaged to estimate the air speed along the z-axis. An overall average local air speed was calculated from the square root of the summed squares of Sx, Sy and Sz.

$$S_{x,y,z} = \sqrt{s_x{}^2 + s_y{}^2 + s_z{}^2} \qquad (3\text{-}4)$$

Thus values for β varied according to the variability in the local air speed for each test and ranged from 0.24 to 1.24 m^3/min.

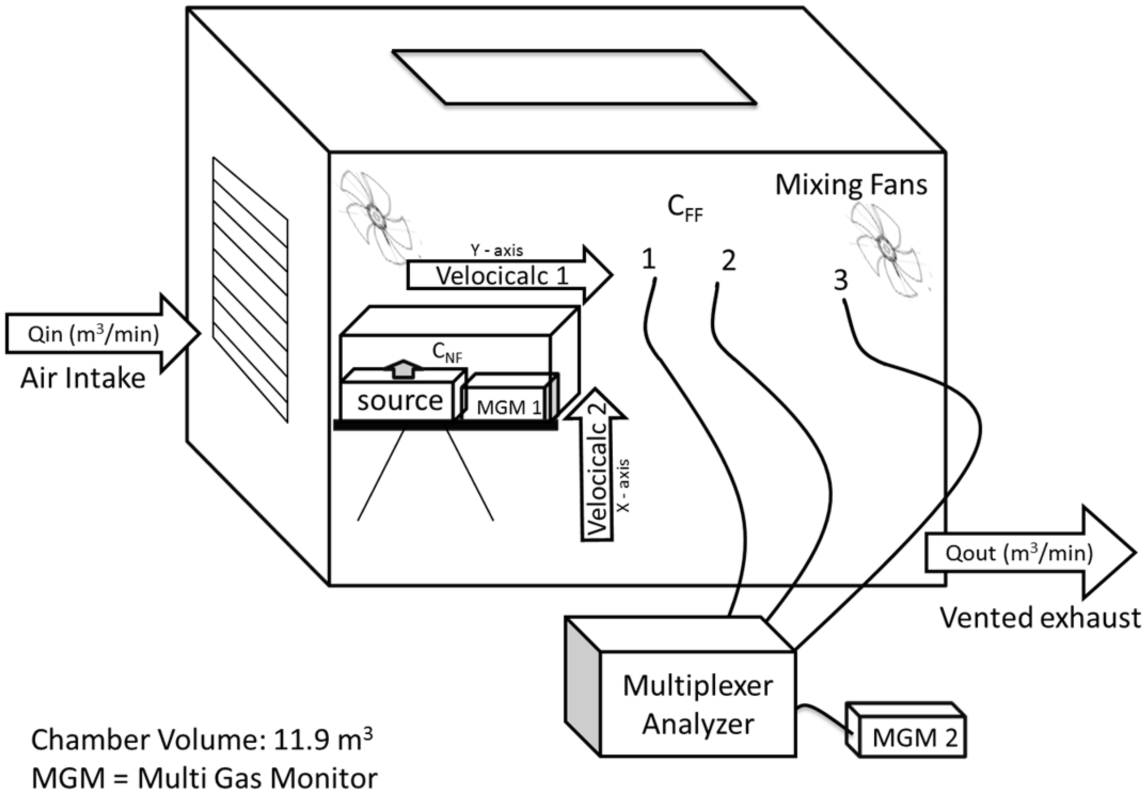

Figure 2-4 Exposure Chamber – NF/FF Configuration showing arrangement in the chamber for the NF-FF model. FF sampling locations correspond to WMR sampling locations 4, 5 and 6, respectively.

Model Evaluation Criteria

To compare model performance of each model under a range of conditions and compare performance of the two models for a specific set of conditions, ASTM 5153-97 criteria were used. General concordance between measured and modeled time-varying concentrations for each model was evaluated using the correlation coefficient, *r*, and the line of regression. The degree of concordance ranges from -1 to 1. A value of 1 indicates a strong, direct relationship; a value of 0 indicates no relationship, and a value of -1 indicates a strong, inverse relationship.

$$r = \frac{\sum_{i=1}^{n}[(C_{oi}-\bar{C}_o)(C_{pi}-\bar{C}_p)]}{\sqrt{\sum_{i=1}^{n}[(C_{oi}-\bar{C}_o)^2]\left[\sum_{i=1}^{n}(C_{pi}-\bar{C}_p)^2\right]}} \tag{3-5}$$

where C_{oi} is the $C_{observed}$ for the i[th] test, C_{pi} is the i[th] $C_{modeled}$ for the i[th] test, $\bar{C}_o$ *and* $\bar{C}_p$ are averages, for example, $\bar{C}_o = \sum_i^n \frac{C_{oi}}{n}$, where *n* is the number of observed values.

A line of best fit, with slope *b* and intercept *a*, were calculated. Ideally, the measured and modeled exposures will agree across all pairs of C_o and C_p, as indicated by a slope, *b* equal to 1 and intercept, -*a* equal to 0. Intercepts were evaluated using t-tests to determine if they were statistically significantly different from 0.

$$b = -\frac{\sum_{i=1}^{n}[(C_{oi}-\bar{C}_o)(C_{pi}-\bar{C}_p)]}{\sum_{i=1}^{n}[(C_{oi}-\bar{C}_o)^2]} \tag{3-6}$$

$$-a = \bar{C}_p - [(b)(\bar{C}_o)] \tag{3-7}$$

The degree of prediction error was quantified by the magnitude of the Normalized Mean Square Error, *NMSE*. When there is perfect concordance, the *NMSE* will equal 0. Higher values of *NMSE* indicate greater magnitudes of discordance between C_o and C_p.

$$NMSE = \frac{\left(\overline{C_p - C_o}\right)^2}{[(\bar{C}_o)(\bar{C}_p)]} \tag{3-8}$$

Bias, assessed as the Normalized or Fractional Bias, *FB*, was calculated for each test as the mean bias of all C_o - C_p pairs. The FB will ideally have a value of 0 when all pairs of C_o and C_p match. The degree to which they do not agree will be evident by the magnitude of departure of *FB* from zero . Temporal patterns of bias were investigated by plotting FB against time for the duration of the study.

$$FB = 2 \times \left[\frac{\overline{C_p} - \overline{C_o}}{\overline{C_p} + \overline{C_o}}\right] \tag{3-9}$$

Model performance was also evaluated categorically, using the Exposure Control Categories (ECC) defined in the AIHA Exposure Assessment Strategies framework (Table 3-5) (Mulhausen and Damiano, 1998; Ignacio and Bullock, 2006; Jahn, Ignacio, and Bullock 2015).

Table 2-5 Framework showing AIHA Exposure Control Categories (ECC) and recommended statistical interpretation

AIHA Exposure Control Category (ECC)	Proposed Control Zone Description	General Description	AIHA-Recommended Statistical Interpretation
1	Highly Controlled (HC)	95th percentile of exposures rarely exceeds 10% of the OEL	$X_{0.95} \leq 0.10$ OEL
2	Well Controlled (WC)	95th percentile of exposures rarely exceeds 50% of the OEL	0.10 OEL $\leq X_{0.95} \leq$ 0.50 OEL
3	Controlled (C)	95th percentile of exposures rarely exceeds the OEL	0.50 OEL $\leq X_{0.95} \leq$ OEL
4	Poorly Controlled (PC)	95th percentile of exposures exceeds the OEL	OEL $\leq X_{0.95}$

TWA exposures were calculated from the measured and modeled exposure data for each test. Thus from each set of 3 replicate tests for each condition, two sets of assessments were developed; one based on exposure measurement data and a parallel set of assessments derived from modeled exposure data. For the WMR model evaluation, 27 scenarios were assessed based on measured and modeled concentrations with each scenario comprised of 3 replicate tests x 6 sample locations generating scenarios with n = 18 measurements. For the NF-FF model, 27 scenarios were assessed; one location in the NF was sampled so the NF assessments comprised 3 replicate tests x 1 location, producing n = 3 measurements. The FF scenarios comprised 3 replicate tests x 3 sample locations generating n = 9 measurements. The group 95th percentile for each scenario was then calculated and compared against the selected Occupational Exposure Limit (OEL) to determine the ECC to which it belonged. Two types of OELs were used in the analysis, the Occupational Health and Safety Administration Time Weighted Average Permissible Exposure Limit (OSHA PEL-TWA) and the Action Limit (AL) defined as ½ the OSHA PEL. In some cases, companies use the AL instead of the PEL as the benchmark that drives exposure and risk management actions, so it was included along with the PEL in this analysis. The ECC to which the scenario belonged (based on the measurement data alone) was deemed the Reference ECC. The ECC to which the scenario belonged based on modeled exposures was then evaluated for concordance with the Reference ECC. If they were the same, then categorical agreement was achieved. If the modeled ECC was one category higher than the Reference ECC, it was identified by +1, indicating it overestimated the correct ECC by 1 category.

Lastly, the scenarios and the ECCs to which they belonged were used to evaluate the impact of using the wrong model. For example, to investigate model performance of the NF-FF model in predicting exposures occurring in a well-mixed room environment, the ECC corresponding to modeled NF was compared to the Reference ECC derived from measurements in the WMR tests.

RESULTS

Model Evaluation – WMR model

For each test and sampling location, a dataset of $C_{measured}$ values and a corresponding set of $C_{modeled}$ values were generated. For the WMR model evaluation, six pairs of $C_{measured}$ and $C_{modeled}$ comparisons were generated from each test replicate. The similarity in $C_{measured}$ values across the six locations was consistent with a well-mixed environment. (Figure 3-5).

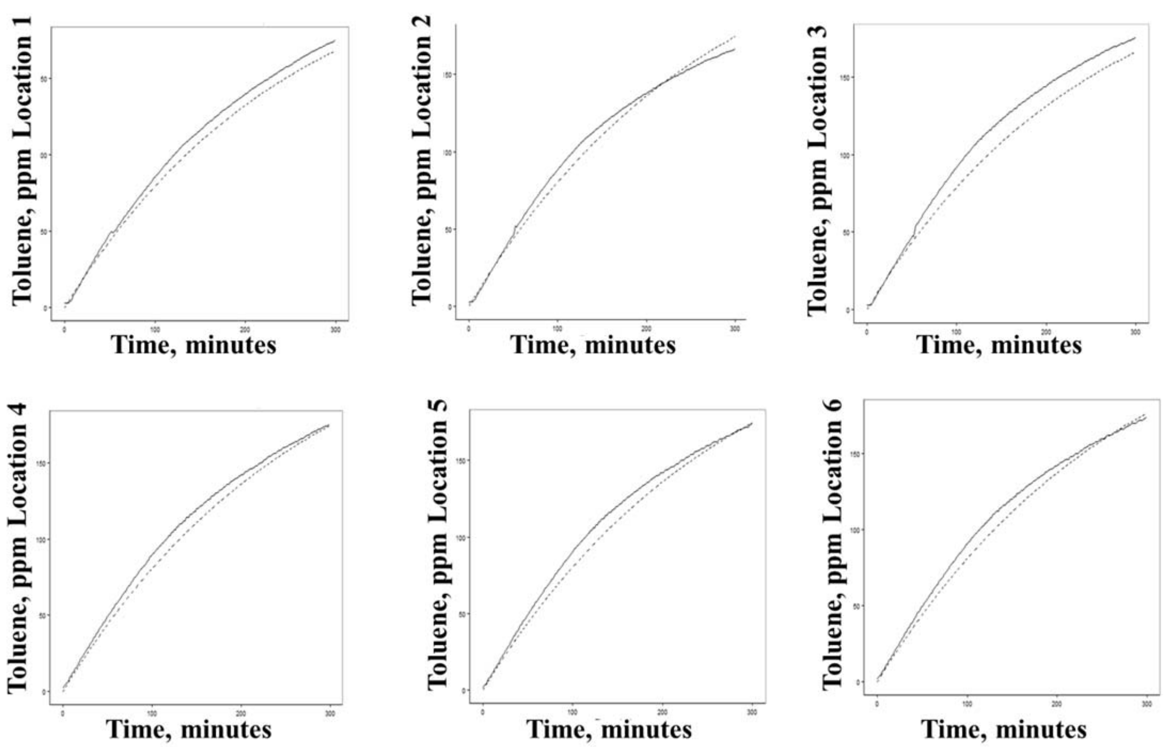

Figure 2-5 Measured and modeled toluene concentrations for the WMR model , corresponding to the six sampling locations in the chamber from which the concentrations were measured when G = 43.2 mg/min and Q = 0.05 m^3/min.

WMR model performance was evaluated in accordance with ASTM 5157 using 486 pairs of $C_{measured}$ and $C_{modeled}$ exposures from three different solvents. Since samples were collected at 6 locations in the chamber in each of the toluene and acetone studies, 162 pairs were obtained. During one of the 2-butanone tests however, one of the MGM failed to collect the data, reducing the data recovered to 3 instead of 6 sampling locations. Consequently the total number of 2-butanone pairs was 159. Results, showing the mean values calculated across all pairs and the percent for each chemical group, i.e., based on 162 pairs, falling within the acceptable ranges are presented in Table VI.

Table 2-6 Evaluation of the WMR model using ASTM 5157 Criteria.

WMR Model Performance Evaluation			
ASTM 5157 Criteria	Results		
Correlation coefficient, r (≥ 0.9)	Toluene	2 Butanone	Acetone
Mean	0.99	1	1
% acceptable	**100%**	**100%**	**100%**
slope, b (0.75 - 1.25)			
Mean	1.01	1.15	0.94
% acceptable	**99%**	**88%**	**97%**
intercept, a (≤ 25% C average)			
Mean/$C_{0.25}$	<0.07	<0.04	<0.001
Intercept p-value	0.28	.18	0.98
% acceptable	**100%**	**100%**	**100%**
NMSE (≤ 0.25)			
Mean	0.01	0.03	0.02
% acceptable	**99%**	**100%**	**99%**
FB (≤ 0.25)			
Mean	0.06	0.13	0.02
% acceptable	**97%**	**95%**	**99%**
Acceptable (all criteria)	**97%**	**88%**	**97%**

Acceptable values or ranges are shown in parenthesis. NMSE: Normalized Mean Square Error; FB: Fractional Bias

Model performance was deemed adequate when all criteria were met, in accordance with ASTM 5157. The WMR model performance was adequate in, 96% of the toluene tests, 88% in the 2-butanone tests and 97% of the acetone tests. The intercepts were not significantly different from zero. Since FB was calculated for $C_{measured}$ and $C_{modeled}$ pairs recorded every 1.5 minutes for the duration of each study, temporal patterns of bias were also investigated for each set of replicate tests. In the case of FB, the greatest bias was observed at the beginning of each test and may reflect less than instantaneous mixing in the chamber when the contaminant generation first started, resulting in $C_{modeled} > C_{measured}$. FB decreased as the tests progressed and as steady state conditions were approached (Figures 3-6 (a) – (c)).

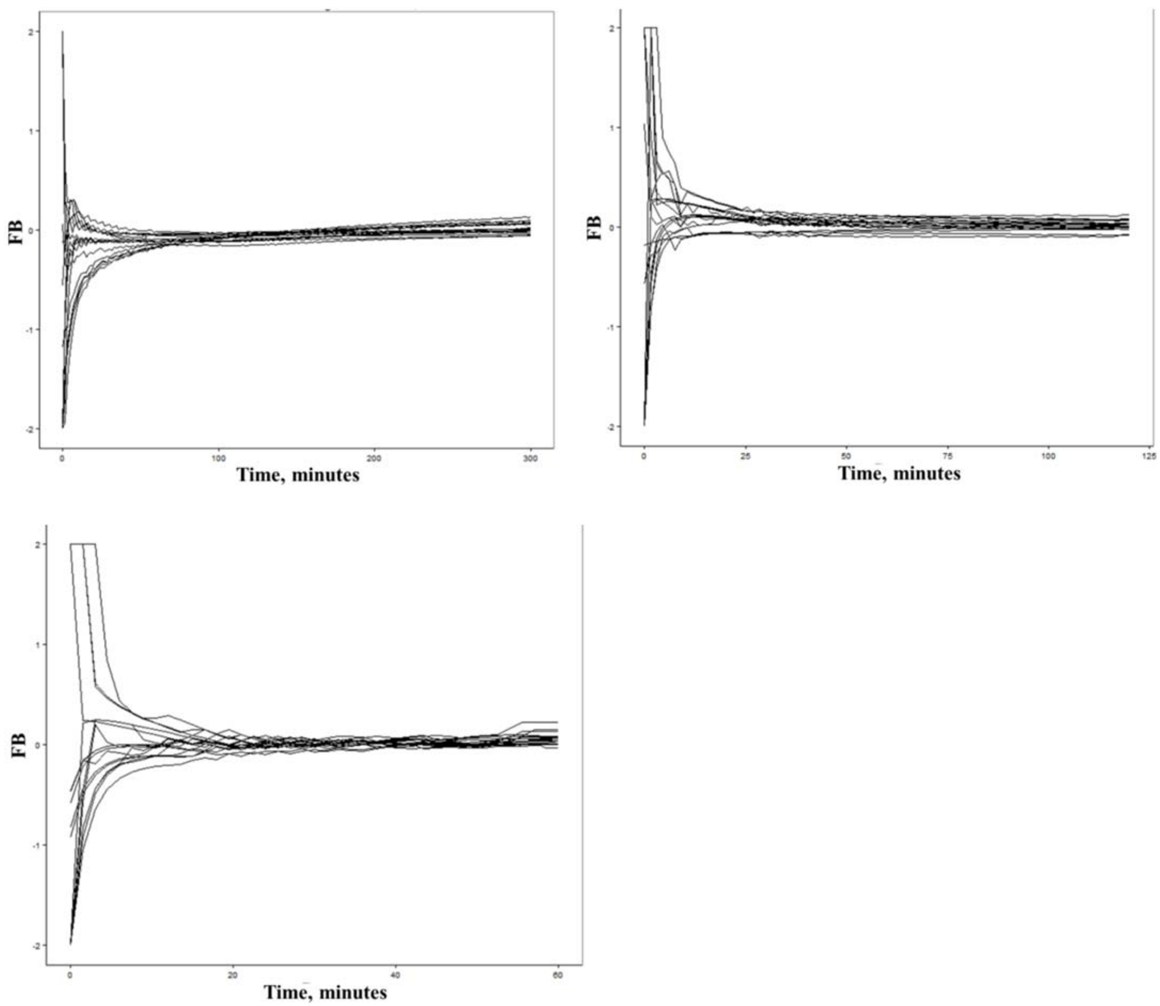

Figure 2-6 WMR Fractional Bias (toluene) and showing convergence at FB = 0 (a): Low Q, t = 300 minutes (0.06 m^3/min)b): Medium Q, t = 120 minutes (0.24 m^3/min)(c): High Q, t = 60 minutes (0.52 mg/m^3)

Categorical accuracy was evaluated using two benchmarks, the OSHA PEL-TWA and the AL. The decision statistic upon which the ECC classification is based is the 95th percentile of the distribution of exposures, for each of SEGs of measured and modeled exposures. Since each SEG was comprised of 18 measured or modeled exposure estimates, 27 scenarios, rather than 162 pairs were evaluated. Using the PEL as the benchmark, the WMR model was categorically accurate for 26/27 scenarios. When the

AL was used as the benchmark, the model was categorically accurate for 25/27 scenarios. Results are presented in Table VII which shows the number of categorically accurate tests by ECC, for each scenario. For example when the OSHA PEL was the benchmark OEL, for the tests using toluene, there was one scenario that was a Category 1 exposure. The WMR model correctly predicted a Category 1 exposure for that scenario and is reported as 1/1.

Table 2-7 Categorical Evaluation of WMR Model

WMR Categorical Accuracy						
ECC	Toluene PEL = 200 ppm	2-Butanone PEL =200 ppm	Acetone PEL = 250 ppm	Toluene AL = 100 ppm	2-Butanone AL = 200 ppm	Acetone AL = 125 ppm
1	1/1	1/1	1/1			
2	5/5	4/6	4/4	4/4	3/4	4/4
3	2/2	1/1	2/2	2/2	1/3	1/1
4	1/1	1/1	2/2	3/3	2/2	4/4
Total	**9/9**	**7/9**	**9/9**	**9/9**	**6/9**	**9/9**

ECC: Exposure Control Category; PEL: OSHA Permissible Exposure Limit; AL: Action Limit

Model Evaluation – NF-FF Model

Measured and modeled NF and measured and modeled FF pairs were compared to evaluate model performance. Generally good concordance was observed, as shown in Figure 3-7. The modeled NF and FF concentrations were higher than the measured and modeled concentrations.

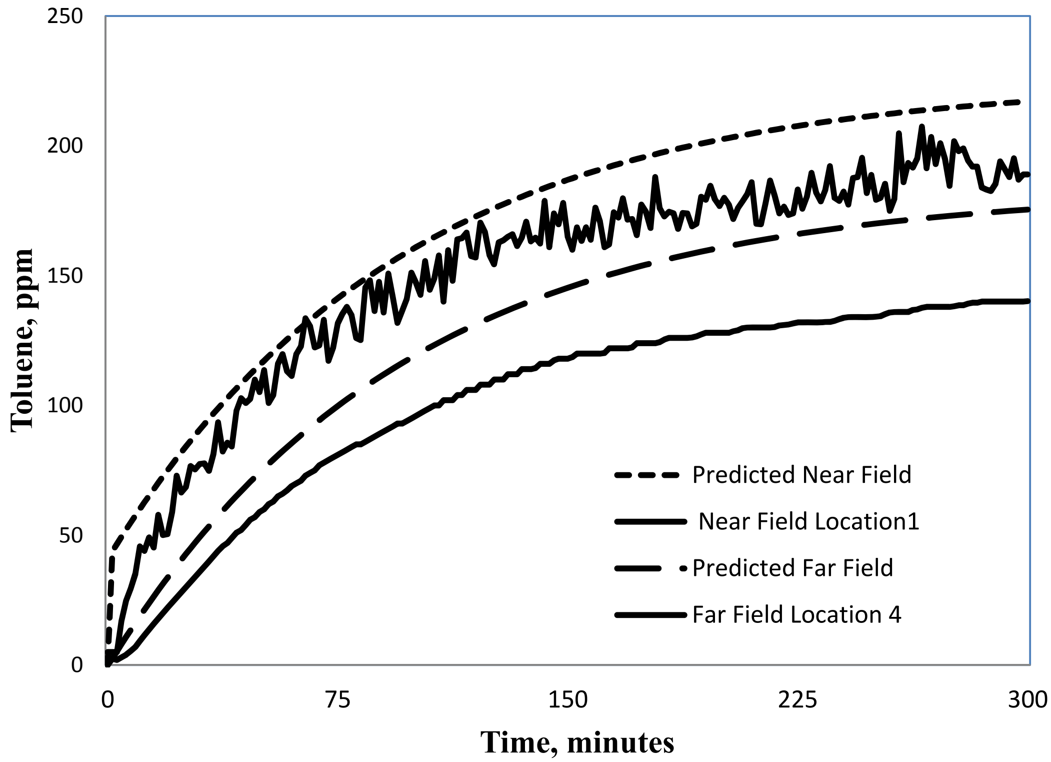

Figure 2-8 Measured and modeled toluene concentrations showing reasonable concordance between the measured and modeled pairs, in the chamber Near and Far Field.

The NF-FF model was evaluated against the ASTM criteria using 81 pairs of NF and 243 pairs of FF exposures = 324 pairs of $C_{measured}$ and $C_{modeled}$ exposures across three different solvents. Reasonable to excellent concordance was observed for the slope, NMSE and FB. However, since all criteria must be met for the model performance to be deemed adequate, the NF-FF Model (Near Field) performance was deemed adequate in only 33%, 19% and 11% of tests across the 3 solvents. The NF-FF model (Far Field) performance was deemed adequate for 69%, 91% and 97% of the tests.

Results are presented in Table VIII.

Table 2-8 Evaluation of the NF-FF model using ASTM 5157 Criteria

NF-FF Model Performance Evaluation						
ASTM 5157 Criteria	Solvent					
	Toluene		2 Butanone		Acetone	
Correlation coefficient, r (≥ 0.9)	NF	FF	NF	FF	NF	FF
Mean	0.95	0.99	0.91	0.91	0.93	0.91
% acceptable	**81%**	**100%**	**67%**	**99%**	**99%**	**100%**
Slope, b (0.75 - 1.25)						
Mean/$C_{0.25}$	1.35	0.04	0.93	1.12	0.9	0.94
% acceptable	**89%**	**69%**	**96%**	**91%**	**81%**	**97%**
Intercept, a (≤ 25% C average)						
Mean	25.1	3.39	1.86	-0.12	2.04	0.02
% acceptable	**44%**	**100%**	**19%**	**98%**	**11%**	**100%**
NMSE (≤ 0.25)						
Mean	0.18	0.11	0.2	0.06	0.23	0.03
% acceptable	**89%**	**99%**	**78%**	**94%**	**94%**	**96%**
FB (≤ 0.25)						
mean	0.36	0.24	0.35	0.01	0.42	-0.06
% acceptable	**33%**	**75%**	**26%**	**93%**	**15%**	**100%**
Acceptable (all criteria)	**33%**	**69%**	**19%**	**91%**	**11%**	**96%**

.

Acceptable values or ranges are shown in parentheses. NMSE: Normalized Mean Square Error; FB: Fractional Bias

Categorical analysis of the NF-FF model was used to evaluate performance using the OSHA PEL or ACGIH TLV and AL as the benchmarks. The model predicted the correct ECC for 21/27 NF scenarios and 20/27 NF scenarios when benchmarked against the PEL and AL, respectively. These results were highly statistically significant ($p < 0.001$). For Far Field exposures, the NF-FF model correctly predicted the ECC for 26/27 FF scenarios for both benchmarks. These results were also highly statistically significant ($p < 0.001$). Categorical analysis of the NF FF - NF model is presented in Table VIIIa by chemical and benchmark and for the FF categorical analysis, results are shown in Table VIIIb.

Table 2-9a Categorical Evaluation of NF-FF Model – Near Field

NF-FF Categorical Accuracy – Near Field						
ECC	Toluene PEL = 200 ppm	2-Butanone PEL =200 ppm	Acetone TLV = 250 ppm	Toluene AL = 100 ppm	2-Butanone AL = 200 ppm	Acetone AL = 125 ppm
1						
2	3/4	4/6	3/5	2/2	0/1	1/2
3	4/4	2/2	2/3	1/2	4/5	1/3
4	1/1	1/1	1/1	4/5	3/3	4/4
Total	**8/9**	**7/9**	**6/9**	**7/9**	**7/9**	**6/9**

ECC: Exposure Control Category; PEL: OSHA Permissible Exposure Limit; AL: Action Limit; TLV: ACGIH TLV

Table 9b Categorical Evaluation of NF-FF Model – Far Field

NF-FF Categorical Accuracy – Far Field						
ECC	Toluene PEL = 200 ppm	2-Butanone PEL =200 ppm	Acetone TLV = 250 ppm	Toluene AL = 100 ppm	2-Butanone AL = 200 ppm	Acetone AL = 125 ppm
1	1/1	1/1				
2	6/6	6/6	6/6	4/4	4/4	2/2
3	1/2	2/2	3/3	3/3	3/3	3/4
4				2/2	2/2	3/3
Total	**8/9**	**9/9**	**9/9**	**9/9**	**9/9**	**8/9**

ECC: Exposure Control Category; PEL: OSHA Permissible Exposure Limit; AL: Action Limit; TLV: ACGIH TLV

Thus far, model performance was evaluated by comparing modeled exposures propagated from model inputs generated under conditions that were aligned to the model's assumptions with exposures measured in the chamber when chamber conditions were similarly aligned to the model's assumptions. To evaluate the impact of model selection, measured and modeled exposures were compared under different conditions. Specifically, for a given set of chamber conditions, the model whose assumptions did not match was used to model the exposures, and these exposures were compared to the measured exposures. The 95th percentile measured and modeled exposure data, was used to identify the exposure control categories to which the measured and modeled exposures, respectively, most likely belonged. Model selection evaluation was then conducted using the categorical data. In the first case, the NF-FF model was used to predict exposures occurring in a well-mixed environment. Specifically, the predicted NF 95th percentile concentration was compared to the measured 95th percentile FF concentration, which is essentially equivalent to WMR conditions. The model overestimated exposures in 25/27 scenarios, by up to 281%. Categorically, the model overestimated exposures by one to two ECCs and the magnitude with which the model overestimated exposure increased as the ventilation rate in the chamber increased. Scenarios reflecting less than well mixed environmental conditions for which the WMR model is used were also evaluated categorically. Measured NF exposures were compared to modeled FF exposures, using the 95th percentile estimate in both cases. The model underestimated exposures for 22/27 scenarios by as much as 71%. However, this numerical underestimation had varying impacts: 13/27 were still categorically accurate, while 8/27 exposures were underestimated by one ECC and 1/27 were underestimated by two ECCs.

DISCUSSION

Two sets of criteria were applied to evaluate model performance in this study. The ASTM 5157 Standard provided a generic set of objective measures useful for gaining an overall sense of model concordance and potential bias which are important for understanding the bounds within which models are useful, as well as for comparing the performance of two or more models. This was especially useful because the WMR and NF FF models have not been systematically evaluated until now and this general performance knowledge is important. More practically relevant to industrial hygiene is the categorical criterion applied to measure model performance. Since the type of exposure or risk management that occurs, if any, is highly influenced by the ECC to which an exposure belongs, ensuring that the modeled exposure matches the measured exposure categorically is critical to the model's utility and value.

The WMR model performance using the ASTM 5157 criteria can be characterized as excellent, with ≥ 88% of the 483 pairs of $C_{measured}$-$C_{modeled}$ pairs deemed adequate. Categorically, the WMR model correctly predicted the correct ECC for 93% of the 27 scenarios. There were no observable trends associated with changing the generation or ventilation rates across the three solvents, suggesting the model is stable within the ranges of G and Q used in the study. Since the mechanism by which all three solvents become airborne is the same, i.e. rapid evaporation, it is not surprising that changing the solvent did not significantly impact the results.

Evaluating model performance under highly controlled conditions likely favors good performance, given the ability to control environmental conditions, and measure all model inputs with a reasonable degree of accuracy and precision. Thus these results probably represent the best case. They strongly suggest that when conditions are likely to meet the model's fundamental assumptions, using the WMR model to guide decisions about the magnitude and acceptability of exposure will increase the likelihood of making accurate decisions.

Model performance of the NF-FF model, based on the ASTM standard was not as strong as for the WMR model, with only 11 to 33% of the $C_{measured}$ and $C_{modeled}$ NF pairs deemed adequate. This seemingly poor performance is largely driven by the estimates of the intercept and to a lesser degree, the fractional bias (FB) values that were outside the acceptable ranges defined in ASTM Standard 5157. Indeed, model performance based on the other three criteria was much higher and more consistent with the WMR model performance. Despite sizing the NF to create spatial differences in the magnitude of exposure, the size of the chamber was still a limiting factor for this study.

Model performance for the FF was stronger than the NF, with 163 of the 243 $C_{measured}$ and $C_{modeled}$ FF pairs (67 %) deemed adequate. When the intercept and FB are not included, model performance is similar to the WMR model performance. Ideally, the FF should be a perfectly mixed box but the size of the chamber and difficulties overcoming advection, especially at the higher ventilation rates may have contributed to the higher intercept and FB values.

Categorically, model performance of the NF-FF model was good to excellent for the NF and FF scenarios, with the model predicting the correct ECC for 20/27 NF (~74%)scenarios and 26/27 FF scenarios (~96%). The categorical differences in NF ECCs are probably attributable to chamber conditions that reflect a WMR environment rather than a NF-FF environment; modeled NF exposures consequently exceeded measured NF exposures. Despite the limitations associated with the chamber size in achieving the ideal air dispersion patterns, model performance results support the use of the NF-FF model for guiding professional judgment when assessing scenarios for which the NF-FF model's fundamental assumptions are met and the following hypotheses were rejected:

1. Categorical model accuracy based on the WMR model and using the Occupational Safety and Health Administration (OSHA) Permissible Exposure Limit (PEL) or the American Conference of Governmental Industrial Hygienists (ACGIH) TLV as the Occupational Exposure Limit (OEL) is no better than random chance.
2. Categorical model accuracy based on the WMR model and using the Action Limit (AL), as the Occupational Exposure Limit (OEL) is no better than random chance.

3. Categorical model accuracy based on the NF FF model modeling NF exposures and using the OSHA PEL or ACGIH TLV as the OEL is no better than random chance.

4. Categorical model accuracy based on the NF FF model modeling NF exposures and using the AL as the OEL is no better than random chance.

5. Categorical model accuracy based on the NF FF model modeling FF exposures and using the OSHA PEL or ACGIH TLV as the OEL is no better than random

chance.

6. Categorical model accuracy based on the NF FF model modeling FF exposures and using the AL as the OEL is no better than random chance.

While most of the scenarios met the ASTM criteria, some did not and therefore the following hypotheses were also rejected:

7. The Well Mixed Room model meets all the ASTM Criteria for all the scenarios in the chamber study.

8. The Near Field Far Field model meets all the ASTM Criteria for all the scenarios in the chamber study.

Matching a model's assumptions to the scenario is an important consideration in modeling. When a model is selected that is based on assumptions that are inconsistent with environmental conditions, modeled exposure estimates may not agree with the true exposures. When environmental conditions differ only modestly from a model's assumptions, using the wrong model may not matter as much. Indeed, in industrial hygiene, differences that do not result in categorical misclassification may be inconsequential. The impact of selecting the wrong models was investigated under two different sets of conditions. Using the NF from the NF-FF model to predict exposures when the environment is well mixed resulted in the majority of modeled exposures overestimating the true exposures. In 18/27 cases these differences did not result in categorical misclassification, but in 8/27 scenarios exposures were overestimated by one category. In one scenario, the modeled exposure overestimated the true exposure by two exposure categories. Thus, using the NF-FF model to predict exposures in well-mixed environments is likely to over-estimate the true exposure, leading to unnecessary follow-up activities 33% of the time. Using the WMR model to predict exposures occurring in a NF-FF environment leads to more serious errors. The WMR model underestimated the true exposure for 22/27 scenarios, with differences between the measured and modeled exposure sufficiently large to cause categorical misclassification for 10/27 of the scenarios. In most cases, the model underestimated the true exposure by one category. There was one scenario for which the true exposure was underestimated by two categories. Thus, using the WMR model to assess NF FF scenarios could result in insufficient follow up 33% of the time, based on the chamber study data. However, it is likely that the impact will be even greater in real world environments, where there is more variability in environmental conditions and more model input uncertainty. Since this could lead to inappropriate decision making and follow-up, careful attention in selecting the right model for a given scenario and set of conditions is essential. Thus, model selection and use guidance will be a critical component of modeling occupational and non-occupational exposures.

CONCLUSION

The WMR and NF-FF model performance, evaluated across more than 800 $C_{measured}$ and $C_{modeled}$ pairs support their use for estimating the magnitude and acceptability of occupational and non-occupational exposures to chemicals. However, the model selected must be based on assumptions that are likely to be consistent with the exposure scenario and for this, model selection and application guidance is needed. More research is needed to develop databases of model input values and scenarios for these models to be fully utilized and valued.

ACKNOWLEDGMENTS

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CHAPTER 3 EVALUATION OF FUNDAMENTAL EXPOSURE MODELS IN OCCUPATIONAL SETTINGS

INTRODUCTION

Decisions regarding the acceptability of occupational exposure impacts real people. Making the right decision about a scenario for which the exposure is truly unacceptable drives appropriate exposure and risk management, and protects the health and safety of those people. When these decisions are based solely on professional judgment guided by subjective inputs, they are more than likely wrong, and biased such that they underestimate exposure (Logan et al., 2009; Vadali et al., 2012, Arnold et al., 2015). Consequently, the exposures and risks are not 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, yet they are undervalued and underutilized. This is likely due to several factors; previously, they had not been systematically evaluated, there is a scarcity of model parameter data and lack of guidance on how to select and apply models. 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.

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 highly controlled conditions in an exposure chamber, (Arnold and Ramachandran, 2015, Submitted for publication) in which concordance between measured and modeled airborne concentrations of three solvents under a range of conditions was excellent. Unlike the chamber, conditions in real workplaces can be controlled to a very limited degree; and factors possibly influencing exposures cannot be removed or known precisely or may be very hard to measure, contributing to model uncertainty. In this second phase of a broader systematic evaluation, the same two models were evaluated under field conditions in real work places. The evaluation included ten diverse exposure scenarios at five workplaces involving four 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

Model Description

Two models commonly used to assess occupational and non-occupational exposures, the Well Mixed Room (WMR) and Near Field Far Field NF-FF models, were evaluated under real world conditions. Ten contaminant-scenario pairs from five diverse workplaces were modeled. Whereas the chamber evaluation of model performance allowed for direct measurement of almost all model inputs with a reasonable degree of confidence, (Arnold and Ramachandran, 2015), the field evaluation 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.

The WMR and NF-FF models were evaluated using information and exposure data from ten contaminant-scenarios collected in five different workplaces and for a range of physical and chemical agents. 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 simulate the work tasks and the 95th percentile exposure obtained from the distribution of modeled exposures. Personal time weighted average (TWA) exposure measurements were collected from individuals performing tasks with the chemical agent. The 95th

percentile of the distribution of the TWA exposure measurements was used as the decision metric against which modeled exposures were compared.

The Models

The Well Mixed Room and NF-FF models are described in detail elsewhere (Nicas, 1996; Ramachandran, 2005; Keil et al., 2009) and briefly discussed here.

The WMR model (Figure 4-1) assumes a one-box geometry and is useful for estimating the average exposure when the emission is released from a large or non-point source. A key assumption of this model is that air in the room is completely and instantaneously well mixed; a physically unrealistic but useful construct for estimating the average concentration when the contaminant is generated from a large or non-point source. (Ramachandran, 2005) The constant source form of this model assumes that a contaminant concentration builds from an initial concentration towards a steady state concentration as the duration of contaminant generation increases.

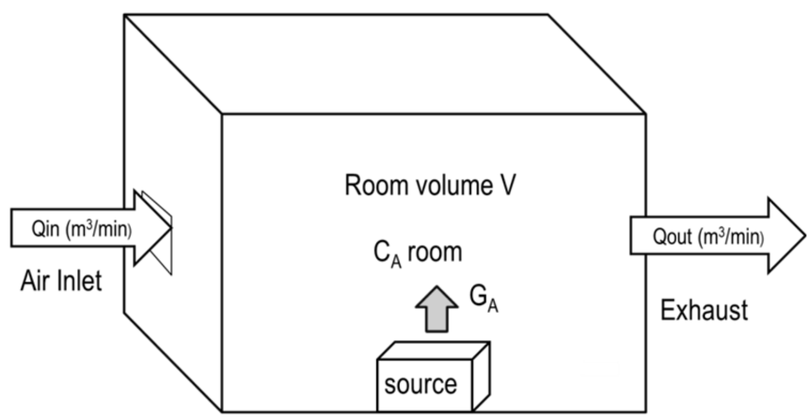

Figure 3-1 Schematic of the WMR Model, with a non-point source generating an airborne concentration and air that is well mixed so that the contaminant concentration in the air is uniform throughout the room.

This model requires only a few inputs, most of which can be readily obtained. One exception is the generation rate, which is especially challenging to characterize in field environments and usually has to be estimated indirectly. Model inputs for the Well Mixed Room model are listed in Table II

The time varying equation for the WMR model is expressed as:

$$C(t) = \frac{G + C_{in} \times Q}{Q + k_L \times V}\left[1 - exp\left(-\frac{Q + k_L \times V}{V} \times t\right)\right] + C(0) \qquad (4\text{-}1)$$

$exp\left(-\frac{Q + k_L \times V}{V} \times t\right)$ (4-1)

Where

C(t) is the concentration at time, t (min)
G is the generation rate (mg/min)
C_{in} is the contaminant concentration in the incoming air (mg/m^3)
Q is the ventilation rate (m^3/min)
k_L is the loss factor (min^{-1})
V is the room volume (m^3)

The NF-FF model assumes a box-within-a-box geometry, accounting for spatial differences in magnitude of exposure associated with point source emissions. This model assumes a two box construct, with the air within each box well mixed. The area close to and around the source is the Near Field (NF) and can be described using a range of geometries, such as a box, sphere, hemisphere, etc. The geometry is defined on a scenario by scenario basis. The rest of the room is the Far Field (FF). The supply and exhaust flow rates are assumed to be the same, and denoted by Q (m^3/min), consistent with the WMR model. Air movement from one box to the other is called the interzonal airflow rate and is denoted by the symbol β (m^3/min). Inputs for NF-FF model, in addition to those required for the WMR model are shown in Table II.

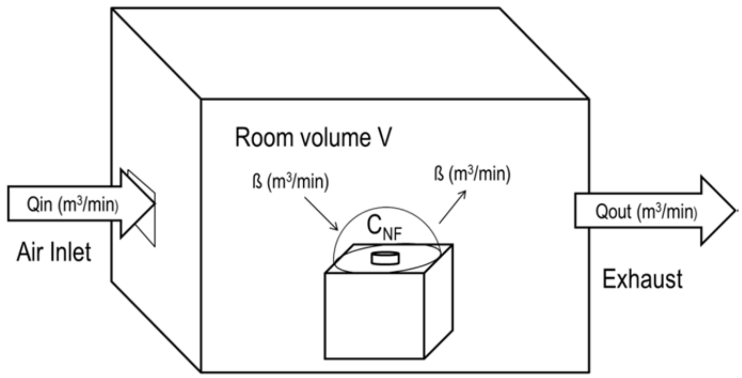

Figure 3-2 Schematic of the NF-FF Model with a point-source generating an airborne contaminant concentration, resulting in a concentration that is greater immediately surrounding the source. Air in each of the NF and FF are well mixed, but air moving between the two boxes, denoted by ß is limited.

The time varying NF and FF equations are:

$$C_{NF}(t) = \frac{G}{Q} + \frac{G}{\beta} + G \times \left[\frac{\beta \times Q + \lambda_2 \times V_{NF}(\beta + Q)}{\beta \times Q \times V_{NF}(\lambda_1 - \lambda_2)}\right] \times \exp(\lambda_1 \times t) - G \times \left[\frac{\beta \times Q + \lambda_1 \times V_{NF}(\beta + Q)}{\beta \times Q \times V_{NF}(\lambda_1 - \lambda_2)}\right] \times \exp(\lambda_2 \times t) \quad (4\text{-}2)$$

$$C_{FF}(t) = \frac{G}{Q} + G \times \left[\frac{\lambda_1 \times V_{NF} + \beta}{\beta}\right] \times \left[\frac{\beta \times Q + \lambda_2 \times V_{NF}(\beta + Q)}{\beta \times Q \times V_{NF}(\lambda_1 - \lambda_2)}\right] \exp(\lambda_1 \times t) - G \times \left[\frac{\lambda_2 \times V_{NF} + \beta}{\beta}\right] \times \left[\frac{\beta \times Q + \lambda_1 \times V_{NF}(\beta + Q)}{\beta \times Q \times V_{NF}(\lambda_1 - \lambda_2)}\right] \exp(\lambda_2 \times t) \quad (4\text{-}3)$$

Where $\lambda_1 = 0.5 - \left[\frac{\beta \times V_F + V_N(\beta + Q)}{V_{NF} \times V_{FF}}\right] + \sqrt{\left[\frac{\beta \times V_F + V_N(\beta + Q)^2}{V_{NF} \times V_{FF}} - 4\left[\frac{\beta \times Q}{V_{NF} \times V_{FF}}\right]\right]}$ (4-4)

and

$$\lambda_2 = 0.5 - \left[\frac{\beta\times V_F + V_N(\beta+Q)}{V_{NF}\times V_{FF}}\right] - \sqrt{\left[\frac{\beta\times V_F + V_N(\beta+Q)^2}{V_{NF}\times V_{FF}} - 4\left[\frac{\beta\times Q}{V_{NF}\times V_{FF}}\right]\right]} \qquad (4\text{-}5)$$

Measurement of Model Inputs and Exposure Data

Table 3-1 Model inputs and output for the WMR and (additional) inputs required for the NF-FF model.

Model	Model Input	Description
WMR	Generation rate, G (mg/min)	Characterizes the contaminant source emission of mass per unit time
	Ventilation rate, Q (m^3/min)	Characterizes rate at which air moves through the room using either natural or mechanical sources of energy
	Concentration in incoming air, C_{in} (mg/m^3)	Characterizes contaminant mass per unit volume in the incoming airstream
	Initial concentration, C_0 (mg/m^3)	Characterizes the contaminant concentration at time t = 0
	Room Volume, V (m^3)	Volume of well mixed room
	Time, t (minutes)	Duration of exposure which may or may not be the same as the duration of source generation
	Loss factor, k_L (%)	Fraction of contaminant mass in air lost per minute due to adsorption, absorption, decomposition or particle settling
NF-FF	Additional model inputs	
	Near Field Volume, NF vol, (m^3)	Characterizes the area around the worker's breathing zone
	Far Field Volume, FF vol, (m^3)	The total room volume minus the NF volume
	Free Surface Area, FSA, (m^2)	Characterizes the NF surface area
	Local air velocity, s (m/min)	Local velocity in the x,y,z planes at or near the Near and Far field interface
	Interzonal airflow rate, β (m^3/min)	Characterizes the rate at which air moves from the NF to the FF, and vice-versa
	Model Output	Description
	Concentration, C (mg/m^3)	Contaminant concentration, can be a TWA or time-varying C.

A detailed basic characterization of each scenario was conducted and information recorded using the Industrial Hygiene Exposure Scenario Tool (IHEST). This tool was developed specifically for this application and is freely available. It is included in the online Supplemental Materials. Information collected included 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.

A range of methods were used to define model input values. A general explanation is provided here, with more 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 for estimating G 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.

$$G = C \times Q \tag{4-6}$$

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 instrumentation and personal exposure measurements were used to measure the time weighted average (TWA) contaminant concentration, C. 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. Using this approach in the field, the contaminant concentration is measured at the source, essentially capturing the contribution of all sources of G. Sometime the work environment is too complex or dynamic, and 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 generation rate was generated by point source, source sampling was conducted by collecting concentration measurements in the NF and the total airflow accounted for in solving for G.

Another method for estimating G was 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 rate at which a fluid enters or is transferred to a vessel is proportional to the 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 also very useful because the inputs needed to apply it typically readily obtained or estimated.

$$G = \mathrm{vol/time}\left({}^{\mathrm{m}^3}\!/_{\mathrm{min}}\right) \times \mathrm{headspace\ conc'n}\left({}^{\mathrm{mg}}\!/_{\mathrm{m3}}\right) \qquad (4\text{-}7)$$

where

G is the Generation rate, mg/min

Vol is the volume of the drum

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., (2015). Briefly, by plotting the natural log of the rate of concentration decay over time when there is no source emitting the contaminant and knowing the room volume, Q can be estimated from the slope of the line of best fit.

$$-\ln\left(\frac{C}{C_0}\right) = \frac{Q}{V} \times t \tag{4-8}$$

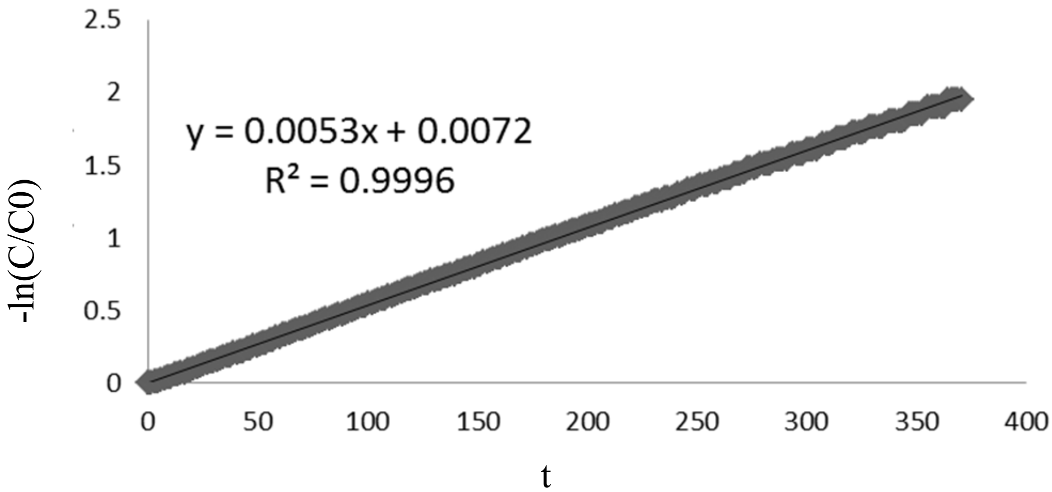

Figure 3-3 Measuring Q from concentration decay data

Q was estimated in some cases 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

$$Q = vA \tag{4-9}$$

where

v is the average velocity measured at the duct or hood face

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

and r is the duct radius

Contaminant concentrations were measured using direct reading instruments for seven of the ten scenarios.

Acetone was measured 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 at the foundry using a TSI DustTrak (Model 8520) aerosol monitor with a respirable inlet and a 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. All other aspects of sample collection for respirable dusts were the same.

Personal time weighted average (TWA) exposure measurements were collected using 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 were comprised of 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.

Local air dispersion patterns and random air speed were characterized using a TSI Velocicalc thermal anemometer (TSI, Inc., Shoreview, MN). Details surrounding measurements collected for each scenario and the application of this information to define model input values are provided in the scenario narratives in the online Supplemental Materials.

Scenarios

Ten scenarios involving four contaminants were used for this evaluation. Briefly, scenarios ranged from tasks conducted during medical parts manufacturing in a clean area to sanding drywall in a hospital under construction. Exposures to acetone, methylene chloride, respirable dust and respirable silica (quartz) were measured and modeled. The scenarios are summarized in Table I.

Table 3-2 Summary Describing Field Scenario Tasks, Agents and Exposure Limits included in the 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.
Agents:	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.
Agents:	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:	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:	ACGIH TLV 8 hour TWA for Quartz = 0.025 mg/m^3

Scenario 5.	Weighing Lithium Cobalt Oxide powder from a bulk container
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:	Cobalt. ACGIH TLV 8 hour TWA: 0.02 mg/m^3

Scenario 6.	Mixing and cleaning in clean room environment
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:	Cobalt. ACGIH TLV 8 hour TWA: 0.02 mg/m^3

Scenario 7.	Making sand mold in iron foundry using a phenolic resin
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:	Phenol. ACGIH TLV 8 hour TWA 5 ppm

Scenario 8.	Removing nail polish and cleaning nails with acetone in a nail salon

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:	Acetone. ACGIH TLV 8 hour TWA: 250 ppm
Scenario 9	Collecting a liquid methylene chloride sample from manufacturing vessel
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 ~ 15 minutes.
Agent:	Methylene chloride. OSHA PEL STEL: 125 ppm
Scenario 10	Cleaning Morehouse mixer in clean room environment
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:	Acetone. ACGIH TLV STEL: 500 ppm

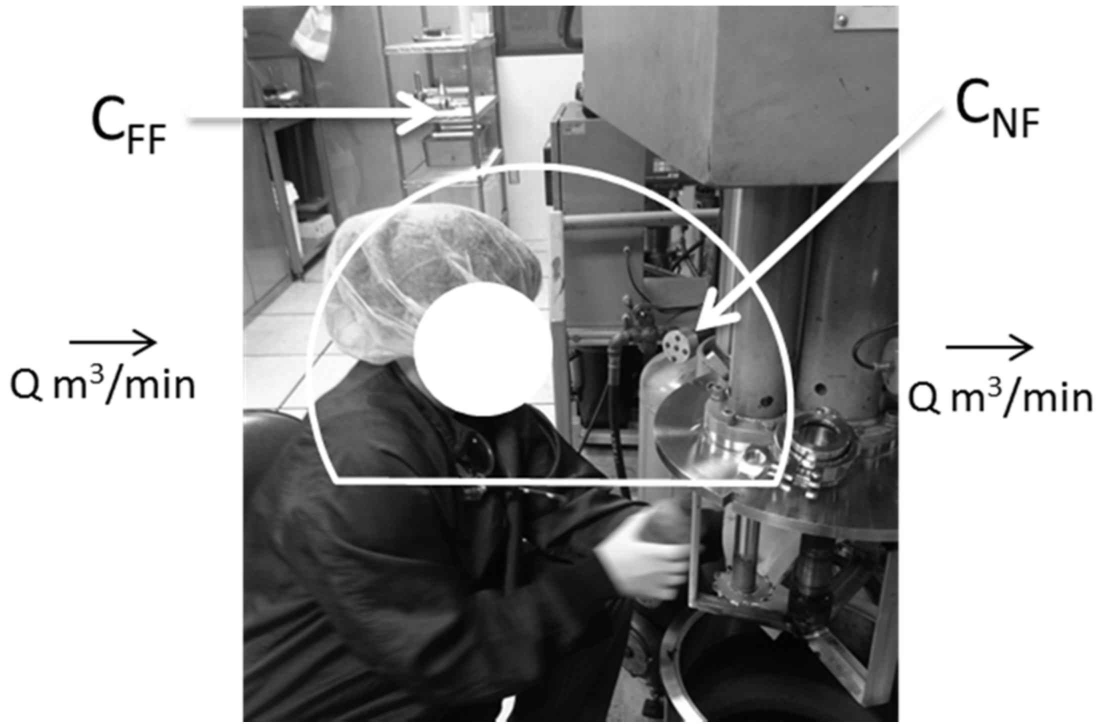

Figure 3-4 Application of the NF FF model to the slurry pot lid cleaning task defining the NF as a hemisphere, encompassing the source and the technician's breathing zone.

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. For the generation rates, multiple contaminant concentration measurements were made, from which multiple generation rates were estimated so that a mean and standard deviation, geometric mean (GM) and geometric standard deviation (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 including the slurry pot lid cleaning task, shown in Figure 4-4. For this scenario, 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. An underlying assumption of log normality was tested using the Filliben's (improved) goodness of fit test. If the assumption was deemed reasonable with the Filliben's test score exceeding the critical R value, a log normal distribution was used to characterize the generation rate. When there was insufficient data or information to identify a parametric distribution, ranges of values, expressed as a uniform distribution were used. In such cases, professional judgment, informed by input from hygienists or the technicians performing the tasks was applied to identify the lower and upper bound values.

Simulations of 10,000 iterations were run with each model and a 95th percentile exposure was obtained from the distribution of modeled exposure 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 inputs are presented in Table III. Detailed explanations for each of the model inputs are provided in the Supplemental Materials

Table 3-3 Model inputs for each scenario, including distributions and ranges used to apply models probabilistically. LN: Log normal distribution with (Geometric Mean, GM, and Geometric Standard Deviation, GSD). U: Uniform distribution with (minimum, maximum) values.

Scenario	Description	Generation Rate, G (mg/min)	Ventilation Rate, Q(m3/min)	Random Air Speed, S (m/min)	Room Volume (m3)	NF Volume (m3)	FF Volume (m3)	Beta (m3/min)
1	Iron foundry RD	LN(82.1, 1.67)	80 to 100	0.45	1200	4.2	1196	LN(34, 1.5)
2	Iron foundry RS	LN(82.1, 1.67)*U(0.5, 15)	80 to 100	0.45	1200	4.2	1196	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	4.2	855.8	LN(5.0, 1.6)
4	Drywall finishing RS	LN (2.13, 1.58)*U(3, 5) * U(1.2, 2.4)	U(1.4 to 4.3)	2.13	860	4.2	855.8	LN(5.0, 1.6)
5	Weighing and transferring powder	U(.002, 1.77)	U(2.68 to 4.02)	7.7	126	1.1	124.4	LN(7.8, 2.1)
6	Mixing powder and clean up	U(.002, 006)	U(70.5 to 105.7)	7.7	126	1.1	124.4	LN(7.8, 2.1)
7	Collecting sample from vessel	LN(220, 4)	U(94-136)	3 to 6	379	0.9	379	U(3.5 to 7.1)
8	Iron foundry Shell Core phenol	LN(13.6, 2)	U(8.33 - 10.4)	30	125	4.2	120.8	LN(94, 1.1)
9	Salon manicure using acetone	LN(16.3, 2.68)	U(6.2, 7.7)	15	31	1.0	29.97	LN(23, 1.1)
10	Cleaning mixer using acetone	LN(1600, 1.37)	U(10.8, 15.1)	7.7	126	1.1	124.4	LN(15, 1.5)

Model Evaluation Criteria

Time varying measured and modeled time exposure estimates were compared and model performance evaluated using ASTM 5157 (ASTM D5157-97(2014)) for six of the ten scenarios for which time-varying measurements were made. Measured and modeled TWA exposure estimates were evaluated categorically, comparing the 95th percentiles using the AIHA Exposure Assessment Exposure Control Categories (ECC) framework. The ASTM standard is intended to help assess the overall performance of indoor air quality models and identify areas of model deficiency. This standard applies a set of strict criteria, providing insight to the general concordance between measured and modeled exposures and the potential for systematic bias. 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 the same kind of exposure and risk management as would be recommended based on a robust set of personal exposure measurements.

General concordance between measured and modeled concentrations for each model was evaluated using the correlation coefficient, *r* between observed and model-predicted values. The degree of concordance ranges from -1 to 1. A value of 1 indicates a strong, direct relationship; a value of 0 indicates no relationship, and a value of -1 indicates a strong, inverse relationship.

$$r = \frac{\sum_{i=1}^{n}\left[(C_{oi}-\bar{C}_o)(C_{pi}-\bar{C}_p)\right]}{\sqrt{\sum_{i=1}^{n}[(C_{oi}-\bar{C}_o)^2]\sum_{i=1}^{n}\left[(C_{pi}-\bar{C}_p)^2\right]}} \tag{4-10}$$

where C_{oi} is the $C_{observed}$ for the ith test, C_{pi} is the ith $C_{modeled}$ for the ith test, $\bar{C}_o$ *and* $\bar{C}p$ are averages, for example, $\bar{C}_o = \sum_i^n \frac{C_{oi}}{n}$, where n is the number of observed values. A line of best fit between observed and modeled values, with slope, b and intercept a, were calculated. Ideally, the measured and modeled exposures will agree across all pairs of C_{oi} and C_{pi}, as indicated by a slope, b equal to 1 and intercept, -a equal to 0. A t-test evaluated whether non-zero intercepts differed statistically from zero.

$$b = -\frac{\sum_{i=1}^{n}[(C_{oi}-\bar{C}_o)(C_{pi}-\bar{C}_p)]}{\sum_{i=1}^{n}[(C_{oi}-\bar{C}_o)^2]} \tag{4-11}$$

$$-a = \bar{C}_p - [(b)(\bar{C}_o)] \tag{4-12}$$

The degree of prediction error was quantified by the magnitude of the Normalized Mean Square Error, *NMSE*. When there is perfect concordance, the *NMSE* will equal 0. Higher values of *NMSE* indicate greater magnitudes of discordance between C_{oi} and C_{pi}.

$$NMSE = \frac{\left(\overline{C_p - C_o}\right)^2}{[(\bar{C}_o)(\bar{C}_p)]} \tag{4-13}$$

Bias, assessed as the Normalized or Fractional Bias, *FB*, was calculated for each test as the mean bias of all C_{oi} - C_{pi} pairs. The FB will ideally have a value of 0 when all pairs of C_o and C_p match. The degree to which they do not agree will be evident by the trend of *FB* away from zero, depending on the magnitude of C_p and C_o, respectively. Temporal patterns of bias were investigated by plotting FB against time for the duration of the study.

$$FB = 2 \times \left[\frac{\overline{Cp}-\overline{Co}}{\overline{Cp}+\overline{Co}}\right] \tag{4-14}$$

Model performance was also evaluated categorically, using the Exposure Control Categories (ECC) defined in the AIHA Exposure Assessment Strategies framework (Mulhausen and Damiano, 1998; Ignacio and Bullock, 2006; Jahn, 2015). 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 corresponding to 95th percentile modeled exposure was identified and compared to the Reference ECC. If the two ECCs matched, then categorical accuracy was achieved.

Table 3-4 Framework showing AIHA Exposure Control Categories (ECC) and recommended statistical interpretation for each category. Using this framework, model performance was evaluated categorically.

AIHA Exposure Control Category (ECC)	Proposed Control Category Description	General Description	AIHA-Recommended Statistical Interpretation
1	Highly Controlled (HC)	95th percentile of exposures rarely exceeds 10% of the OEL	$X_{0.95} \leq 0.10$ OEL
2	Well Controlled (WC)	95th percentile of exposures rarely exceeds 50% of the OEL	0.10 OEL $\leq X_{0.95} \leq$ 0.50 OEL
3	Controlled (C)	95th percentile of exposures rarely exceeds the OEL	0.50 OEL $\leq X_{0.95} \leq$ OEL
4	Poorly Controlled (PC)	95th percentile of exposures exceeds the OEL	OEL $\geq X_{0.95}$

RESULTS

Scenarios for which time-varying exposure data was collected were evaluated, comparing concordance with both models, using the ASTM Standard 5157 criteria. For scenarios 3 and 4, real time data was collected for a single work shift. Time varying measurements were made for six salon manicures (scenario 8) and on multiple days for scenarios 5, 6, and 10 and for these scenarios, results shown in Table IV reflect the average performance.

Table 3-1 Performance evaluation criteria and scores in accordance with ASTM 5157 using time-varying measured and modeled exposure estimates from the WMR and NF FF models, respectively for six scenarios.

Acceptable Criteria		3. Respirable dust		4. Quartz		5. Cobalt		6. Cobalt		8. Acetone		10. Acetone	
		WMR	NF FF	WMR	NF FF	WMR	NF FF	WMR	NF FF	WMR	NF FF	WMR	NF FF
r	(≥ 0.9)	-0.11	-0.10	-0.11	-0.10	0.25	0.11	0.33	0.25	0.10	0.14	0.68	0.35
b	(0.75 - 1.25)	-0.03	-0.05	-0.08	-0.09	0.01	0.01	0.001	0.01	1.16	0.04	0.35	0.13
a	(≤ 25% C average)	2.99	3.99	0.07	0.10	0.01	0.0003	0.0005	0.01	9.88	1.74	45.97	68.38
NMSE	(≤ 0.25)	0.4	0.35	0.62	1.06	16.23	10.52	568.9	16.23	324.6	5.35	2.47	0.84
FB	(≤ 0.25)	-0.02	0.04	0.61	0.68	0.91	-1.28	-0.94	0.91	1.66	1.75	0.01	0.44
Acceptable (all criteria)		0	0	0	0	0	0	0	0	0	0	0	0

Scenario-contaminant

Collecting measurements several months apart for some scenarios provided insight into day-to-day and inter-worker variability. For example, in the slurry pot cleaning scenario, slight differences in work practices were observed and reflected in the contaminant concentration dispersion patterns. Consequently, concordance between measured and modeled exposures was better on some days than on others. Concordance between measured and modeled exposure estimates for the WMR and NF FF models from day 4 are shown in Figures 4-5a and b.

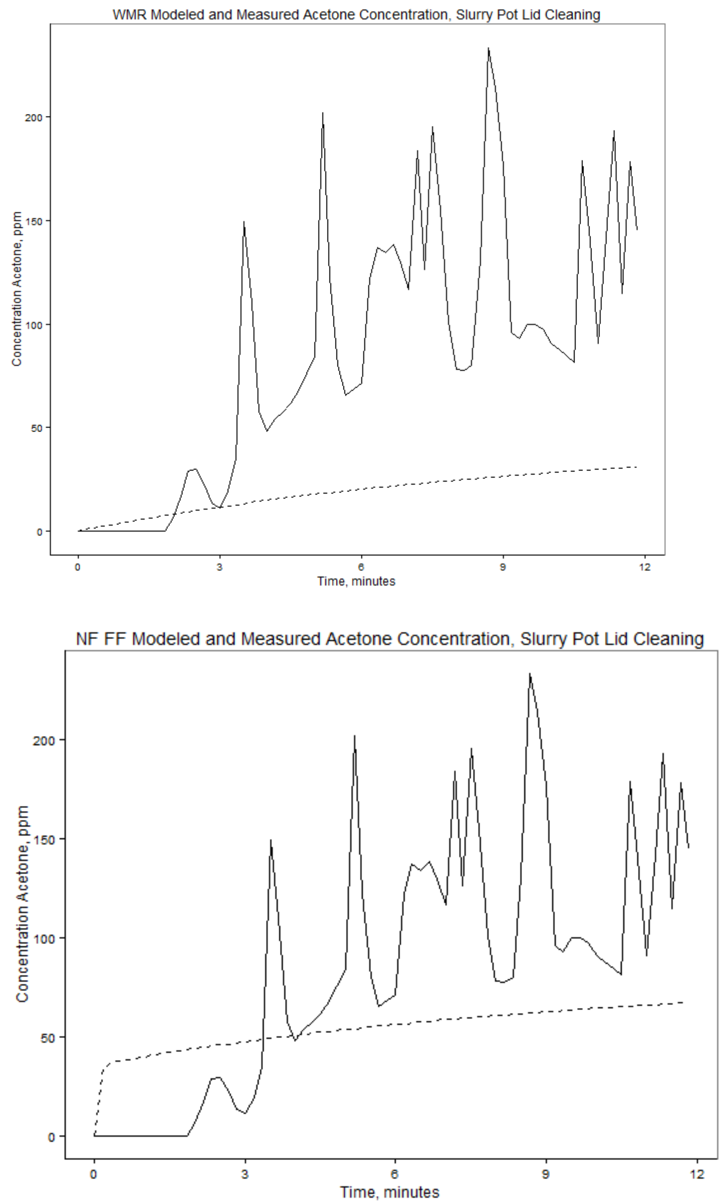

Figure 3-1a and b Measured and modeled time varying acetone concentration from slurry pot lid cleaning collected on day 4, using the WMR andNF FF models.

Performance criteria for the Day 4 measured and modeled exposure estimates, displayed in Figure 4-6 are shown in Table V.

Table 4-6 ASTM 5157 criteria and scores for model performance for Day 4 showing scores closer to, but still outside the acceptable ranges.

		Day 4	
		WMR	NF FF
r	(≥ 0.9)	0.78	0.71
b	(0.75 - 1.25)	0.11	0.13
a	(≤ 25% C average)	8.98	43.37
NMSE	(≤ 0.25)	4.79	0.87
FB	(≤ 0.25)	-0.67	0.01

Categorical analysis of each scenario was also conducted, comparing model performance for both the WMR and NF FF models from TWA 95th percentile exposures. Results are presented in Table VI.

Table VII. Evaluating categorical accuracy for each model by 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. $C_{measured}$ and $C_{WMR,}$ $C_{NF\text{-}FF}$ are 95th percentile values. [a] Short Term Exposure Limit (STEL)

Scenario-contaminant	OEL (mg/m^3)	$C_{observed}$ (mg/m^3)	Reference ECC	C_{WMR} (mg/m^3)	C_{WMR} ECC	$C_{NF\text{-}FF}$ (mg/m^3)	$C_{NF\text{-}FF}$ ECC
1. Respirable dust	3	3.27	4	2.13	3	8.98	4
2. Quartz	0.025	0.38	4	0.23	4	0.96	4
3. Respirable dust	3	6.35	4	8.06	4	8.67	4
4. Quartz	0.025	0.15	4	0.16	4	0.17	4
5. Cobalt	0.02	0.42	4	0.53	4	0.78	4
6. Cobalt	0.02	0.09	4	0.02	4	0.03	4
7. Methylene Chloride	434	674	4	18.41	1	452	4
8. Phenol	19	2.27	1	1.70	1	1.90	1
9. Acetone	595	0.62	1	11.88	1	15.68	1
10.Acetone	1190.5[a]	731	3	503	3	1043	4
Categorical accuracy					8/10 p <0.001		9/10 p <0.001

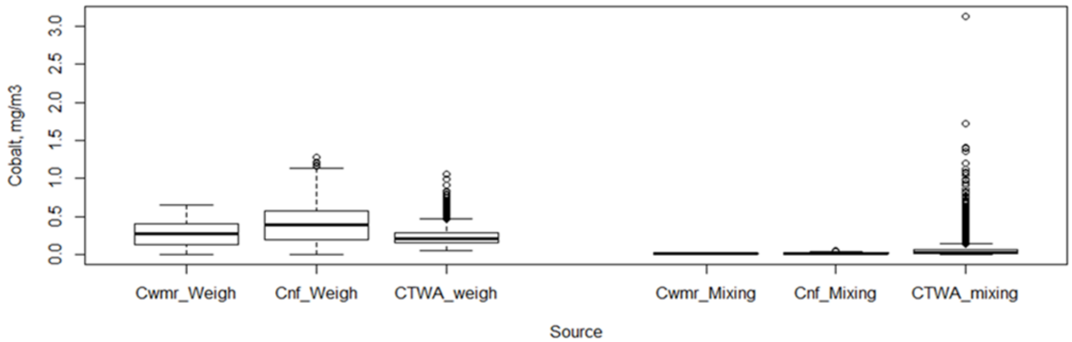

Figure 3-2 Comparison of Modeled and measured Cobalt (mg/m^3) for weighing and mixing tasks, respectively.

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.

Categorical accuracy was compared to random chance by first calculating the probability, given *this* set of 10 scenarios that the model would correctly predict the category that matched the reference ECC, underestimated it by 1, 2 or 3 categories, or overestimated the ECC by 1,2,or 3 categories. For each of the ten scenarios, a simulation of 10,000 iterations was conducted, randomly selecting one of the four categories and for each iteration, the random number represented an exposure category. That exposure category was compared to the reference ECC. If the correct category was selected by random chance, i.e., the difference between the reference ECC and random chance predicted ECC was zero. If the random chance ECC underestimated the ECC by one category, it was -1 and if it overestimated the ECC, the difference was +1and so on. For each simulation, these values were summed and divided by 10,000, Thus, the random chance probability of being correct or incorrect by a specific number of categories was calculated for each scenario and then summed for the ten scenarios.

Categorical accuracy for each model, relative to model accuracy based on random chance alone is presented in Figure 4-8.

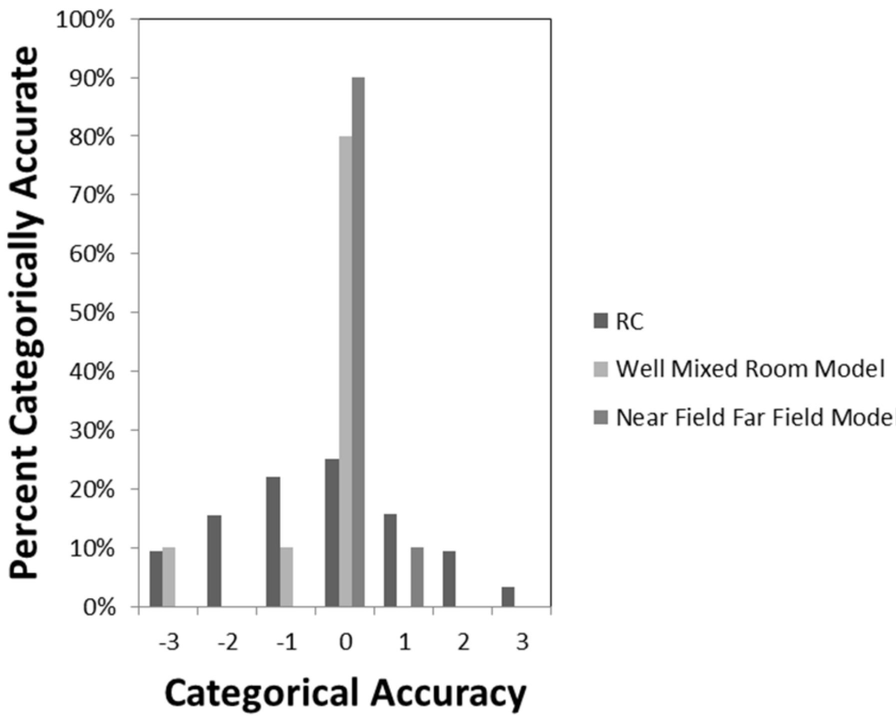

Figure 3-3 Categorical accuracy of each model relative to random chance.

"0" represents categorically accurate predicted exposures. "-1" indicates the exposure was underestimated by 1 category; "-2" indicates it was underestimated by 2 categories and " -3" indicates it was underestimated by 3 categories. "+1" represents the exposure was overestimated by 1 category; "+2" indicated it was overestimated by 2 categories and "+3" indicates it was overestimated by 3 categories.

DISCUSSION

Modeling real-world exposures requires a full understanding of the underlying model assumptions and mathematical constructs so that the models can be applied appropriately. When scenarios differed from these underlying model assumptions, a significant effort was required to account for them. To better explain some of the challenges encountered in this study, selected scenarios and their nuances are discussed in more detail.

In seven of the ten scenarios, when the generation rate could not be determined directly, source sampling was used to back-calculate from C to solve for G. Since these scenarios all involved point sources, the NF-FF model was deemed the more appropriate candidate, thus solving for G required first estimating the ventilation rate near the source. In the phenol scenario, TWA measurements captured near the source were used to estimate C, with the total near-source ventilation rate estimated using professional judgment based on the experience of several IHs measuring ventilation rates in similar workplaces and recommended ventilation rates stated in the Industrial Ventilation Manual (ACGIH, 1995). Specifically, the phenolic resin in this scenario was used in an area where there was a relatively constant flow of air due to two area fans directed towards the shell core work area and the presence of an exterior door next to the work area that was opened on a regular basis, providing an influx of fresh air. In the foundry respirable dust and quartz scenarios, the total near-source ventilation was estimated by measuring the face velocity of the ducts and measuring the area of each duct. This ventilation rate was the product of the face velocity and area. The ventilation rates and source sampling measurements were used to solve for G at each source location. A generation rate for each source was then estimated from the source sampling data and estimated ventilation rates, and an overall G calculated by aggregating the four generation rates.

For the weighing and mixing and cleaning tasks involving cobalt, a similar approach was used to estimate the total near-source ventilation rate, measuring the face velocity for each slot and its respective area. In this case, however, since the slots collectively removed contaminant generated from one source, a total ventilation rate was calculated from the sum contribution of each slot. G was estimated from the source sampling concentration data and ventilation rate.

Assessing exposures under such dynamic conditions encountered in a new construction environment is inherently challenging, but this is especially true when attempting to model them. The use of direct reading instruments providing a record of the time varying contaminant concentration was valuable for selecting the model that best represented work place contaminant dispersion patterns. In this case, the environment was found to be relatively well mixed, thus the WMR model was the model applied. Characterizing the generation rate in the field was deemed infeasible, so a simulated dry wall finishing study was conducted in an exposure chamber, under much less complex and much more controlled conditions. Eleven tests were conducted, measured the time varying contaminant concentration with direct reading instruments and controlling the chamber ventilation rate. Similar to the source sampling approach, G was estimated for each test from C and Q, and an overall average G calculated. A bulk sample of drywall dust was collected and submitted for quartz analysis, providing the weight percent fraction of quartz. Thus the generation rate for quartz was estimates as the product of the respirable dust g and the weight percent quartz. These generation rates, representing the contribution from one source-worker were then used to estimate the respirable dust and quartz exposures, respectively, in the real drywall finishing environment. A scaler was applied to each G, accounting for multiple drywall finishers sanding drywall when the personal and direct reading measurements were collected. In the Monte Carlo analysis, a range of 3 to 5 workers was applied to account for movement of workers, breaks, etc.

The ventilation rate at the hospital was estimated in consultation with the construction foreman and safety personnel, indicating the mechanical ventilation system was shut off during drywall sanding activities to prevent dust entrainment that could compromise patient well-being. Thus a range of plausible ventilation rates, based on this knowledge and supported by ventilation rates reported in the publicly available literature for ambient air flow rates (Hanzawa et al., 1987) was developed.

Direct reading MGMs were used to measure the rate of contaminant concentration decay for the acetone scenarios. Knowing the room volume, Q could be estimated from the slope of the decay curve. This was a very practical approach providing a reasonably accurate estimation of Q without requiring specialized tracer gases or expensive analytical equipment. Using these estimates of Q, the source sampling data collected from the same instruments was used to solve for G. Since source sampling was conducted on multiple occasions for these scenarios, multiple values for G were estimated, from which a mean G, standard deviation, GM and GSD were calculated. The variability and distribution characteristics were used to estimate the distribution and values for G in the Monte Carlo analysis. In the salon scenario, a small amount of acetone was placed in an open container on a work surface the day before the exposure data was collected. One of the MGMs was placed in the NF and set to data log the concentration of acetone. In the clean room area, the rate of decay was measured as the residual acetone concentration was removed from the area following completion of the cleaning tasks.

In the methylene chloride scenario, the contaminant generation was similar in behavior to that of a drum filling scenario, where the rate at which the contaminant was emitted from the vessel is roughly equivalent to the rate at which the sampler is lowered into it. Site personnel confirmed that the contents were at ambient temperatures and the vessel was not pressurized; both are important assumptions as these would impact the generation rate. The site hygienist and area supervisor provided details and relevant data regarding the sampling rates, general mechanical ventilation rates and local exhaust ventilation (LEV) rates as well as the specific type and dimensions of the LEV. Room volume and vessel capacity and dimensions were also provided. The sampling rates and ventilation rates were provided as ranges which were then used in the Monte Carlo analysis.

Model performance was evaluated using two different types of criteria. Performance measured against the ASTM Standard criteria, evaluating concordance between the time-varying measured and modeled exposure estimates was outside the acceptable range; none of the six scenarios for which these criteria were applied met the definition of acceptability. This is not surprising given that applying the WMR and NF-FF models to non-ideal scenarios are more likely to provide a reasonable estimate of the average concentration, not necessarily represent minute by minute changes in contaminant concentrations. Indeed, the contaminant concentrations in the study scenarios tended to exhibit peak exposures followed by steep declines, sometimes falling to zero before peaking again whereas the model assumes a constant increase in contaminant concentration, approaching steady state concentrations. In some cases, exposures did trend upward temporally, as in the example shown in Figure 4-6, and on these occasions the models tracked more closely with the measured exposures. Performance scores were accordingly better than on average (Table V).

Despite the predominant lack of close concordance between time-varying measured and modeled exposures, the models were sufficiently accurate to achieve categorical concordance, most of the time. 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, (scenarios five and six) are presented in Figure 4-7. These findings can be interpreted as indicating the models are sufficiently accurate from a practical perspective, correctly predicting the ECC to which the exposures belong and therefore guiding decision making that would drive 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.

In this nascent science, 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 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. Category 1 - 4, for any given scenario, and a total of 27 scenarios assessed. So based on random chance alone, the models would predict the correct ECC for 6.25/27 scenarios. As reported earlier, accuracy for both models was much higher and thus the following test hypotheses were all rejected.

1. Categorical model accuracy based on the WMR model and using the Occupational Safety and Health Administration (OSHA) Permissible Exposure Limit (PEL) as the Occupational Exposure Limit (OEL) is no better than random

chance.

2. Categorical model accuracy based on the WMR model and using the Action Limit (AL), as the Occupational Exposure Limit (OEL) is no better than random chance.
3. Categorical model accuracy based on the NF FF model modeling NF exposures and using the OSHA PEL as the OEL is no better than random chance.

4. Categorical model accuracy based on the NF FF model modeling NF exposures and using the AL as the OEL is no better than random chance.

Since the ASTM criteria were met for only some of the scenarios in this study, the following hypotheses were rejected:

5. The Well Mixed Room model meets all the ASTM Criteria for all the scenarios in the field study.

6. The Near Field Far Field model meets all the ASTM Criteria for all the scenarios in the field study.

The NF-FF model over-estimated the 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 the methylene chloride sample scenario. The WMR model-predicted 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 towards improving exposure judgment accuracy.

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.

One implication of this work is that ASTM Standard 5157 applies criteria that is too strict and is not especially useful for evaluating models intended for assessing occupational exposures. Therefore it is not recommended for this purpose.

Several areas that require additional research were identified from this work. Selecting and applying the models consistently will require guidance in the form of a structured checklist. This checklist will need to be evaluated using the same approach that was employed to evaluate the qualitative exposure assessment checklist and for this, more exposure scenarios need to be developed. The database model input values represents a significant contribution to the field and needs to be expanded so that the models can be applied across a broader range of tasks and work environments.

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.

Acknowledgments

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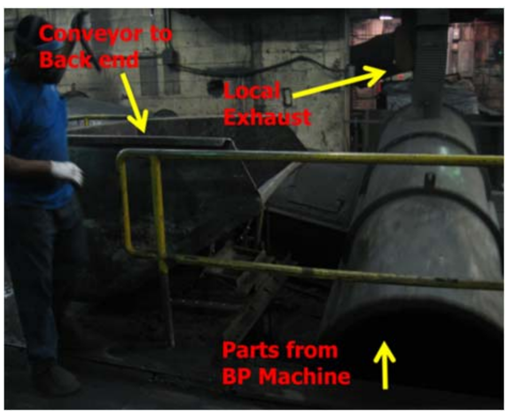
CHAPTER 4 SCENARIOS

Scenarios 1 and 2: Using physical chemical models to estimate respirable dust and silica in an iron foundry

Operator moves cope and drag to conveyor, aided by a pulley system



Parts unloaded from cope and drag are conveyed to the back

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. Mold and parts from the Continumatic area (a casting area with an auto conveyor, following the "BP machine") move under the walkway to the conveyor, and are moved to the back end, as well. Operators work in the front and back end of the shake-out area. 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 by a second (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, tossing them into a bin.

1. Ventilation rate:
   a. The Near Field ventilation rate, ß(m^3/min) was estimated for each emission source
   b. Local air velocity was measured at each source, measuring the face velocity at nine points to calculate an average velocity. Three replicate sets of measurements were collected.
   c. The area of each source was calculated by measuring the diameter of each circular source and for rectangular sources, the width (m) and length (m)
   d. The area of a rectangle is $A(m^2) = \text{length(m)} \times \text{width(m)}$
   e. The area of a circle is $A(m^2) = \pi r^2$
   f. $\beta\left({m^3}/{min}\right) = v\ ({m}/{sec}) \times A(m^2\ )$

Table 4-1S Calculating the Near Field flow rate from the face velocity and area measurements

	G1 (round)			G2 (round)			G3 (rectangular)			G4 (round)		
Sample	1	2	3	1	2	3	1	2	3	1	2	3
Dimensions	1.04	1.04	1.04	1.04	1.04	1.04	2.24 *1.65	2.24 *1.65	2.24 *1.65	1.27	1.27	1.27
Area (m^2)	0.85	0.85	0.85	0.85	0.85	0.85	3.70	3.70	3.70	1.27	1.27	1.27
velocity (m/s)	0.29	0.40	0.80	0.38	0.31	0.32	0.29	0.19	0.25	0.74	0.46	0.31
ß, flowrate (m^3/min)	27.4	37.7	75.4	35.8	29.2	30.1	27.3	17.9	23.6	69.7	43/3	29.2

2. Generation rate:
    a. Respirable Dust:
        i. Four sources contributed to the respirable dust and silica exposures in this area. These were
            1. Front end:
                a. unloading the cope and drag using a pulley
                b. moving them onto the shaker which vibrated, causing the sand mold and metal part to separate
                c. Transport of parts from another area onto a conveyor located under the walkway.
            2. Back end:
                a. Operator breaks molded iron pieces into individual parts. Pieces are picked up and dropped onto table, then tossed into bins as parts moved up the line onto the shaker table
    b. The generation rate was estimated by solving for G, using the average respirable dust concentrations measured using direct-reading instruments at 4 locations. The relationship between C and G is:
        i. $G = C \times \beta$

        Where

        G is the Generation rate (mg/min)

C_{NF} is the concentration (mg/m3)

β is the interzonal air flow rate (m^3/min)

Table 4-2S Calculating an average G for each source from C measured at each source. An overall average G is calculated from these average values.

Generation rate	G1 (round)			G2 (round)			G3 (rectangular)			G4 (round)		
Sample	1	2	3	1	2	3	1	2	3	1	2	3
Dimensions	1.04	1.04	1.04	1.04	1.04	1.04	2.24 *1.65	2.24 *1.65	2.24 *1.65	1.27	1.27	1.27
Area (m^2)	0.85	0.85	0.85	0.85	0.85	0.85	3.70	3.70	3.70	1.27	1.27	1.27
velocity (m/s)	0.29	0.40	0.80	0.38	0.31	0.32	0.29	0.19	0.25	0.74	0.46	0.31
ß, flowrate (m3/min)	27.4	37.7	75.4	35.8	29.2	30.1	27.3	17.9	23.6	69.7	43.3	29.2
C_Respirable (mg/m^3)	0.78	3.31	0.32	1.12	1.71	1.48	2.15	6.16	2.29	0.67	1.75	1.39
G_Respirable (mg/min)	11.52	67.37	12.96	21.68	26.97	24.13	138.40	259.63	126.90	37.50	61.29	32.66

Table 4-3S An average G is calculated for each of the four sources, as well as an overall average G.

Average G (mg/min)	G1	G2	G3	G4
G_Respirable	61.2	48.5	174.9	43.8

(b) **Average Respirable Dust G** = 82.1 mg/min

(c) To facilitate Monte Carlo analysis, the generation rate is characterized using a lognormal distribution with a geometric mean (GM) and a geometric standard deviation (GSD):
   (i) G = LN(82.1, 1.67)

(d) Generation rate for **Silica (Quartz)**
   (i) Silica is a component in the respirable dust, present at 0.5 to 15% according to the msds.
   (ii) The generation rate is estimated by multiplying the Respirable Dust G by this fraction
      1. $G\ (mg/min) = \ 82.1\ \times .05\ = 4.1 mg/min$
      2. $G\ mg/min = \ 82.1\ \times .15\ = 12.3\ mg/min$
      3. For Monte Carlo analysis, G is described as a lognormal distribution:
         a. LN(82.1,1.67)*U(min =0.05, max=0.15)

(2) Room volume :
   (i) Comprised of Shake Out front and back end
   (ii) Dimensions $Volume = 2\ \times (5m\ \times 12m\ \times 10m) = 1200m^3$

(3) The Near Field Volume is calculated from the volume of a hemisphere, Where
   (a) Volume of a hemisphere: $2/3\pi r^3$
      (i) Radius, r = 0.8 m, representing arms' length between the operator and the respective source.
      (ii) NF volume = 4.2 m^3

(4) The Far Field Volume is the total room volume – NF volume
   (a) FF volume = 1200 m^3 – 4.2 m^3 = 1196 m^3

(5) Time
   (a) This was a full shift activity. Time = 480 minutes.

Applying a Monte Carlo approach, the 95th percentile CNF exposure =8.98 mg/m^3.

The ACGIH TLV for Respirable Dust (3 mg/m^3) is used as the exposure benchmark. Using the AIHA Exposure Control Categories, the predicted NF concentration falls into Category 4.

The 95th percentile exposure based on 8 personal samples was 3.27 mg/m^3. The reference exposure category is Category 4.

The 95th percentile CNF for Silica (Quartz) exposure based on Monte Carlo analysis = 0.96 mg/m^3.

The ACGIH TLV for Quartz (0.05 mg/m^3) is used as the exposure benchmark. Using the AIHA Exposure Control Categories, the predicted NF concentration falls into Category 4.

The 95th percentile exposure based on 8 personal samples was 0.38 mg/m^3. The reference exposure category is Category 4.

Scenarios 3 and 4. Using physical chemical models to estimate respirable dust and silica from sanding drywall in new construction environment

Dryall finishers sanding new drywall using pole (Left) and Block (right) methods and in Chamber

Drywall sanding generates a lot of dust, some of which is in the respirable range. Drywall also contains crystalline silica (quartz) which can cause lung function impairment, silicosis and cancer. Drywall finishers use a range of methods to sand drywall in a large hospital suite under construction. To characterize the generation rate for this scenario, a series of simulations were conducted under highly controlled conditions, in an exposure chamber. Measuring C and Q relatively accurately, a reasonably accurate generation rate was calculated.

3. Ventilation rate (Chamber):
    a. The ventilation rate in the chamber was set to 0.26 ACH for each test. The chamber volume is 11.9 m^3 corresponding to a ventilation rate = 0.05 m^3/min.

4. Generation rate (Chamber):
    a. Respirable Dust:
        i. Real time instruments were used to measure the respirable dust concentration in the exposure chamber, where drywall sanding was simulated under well mixed conditions.
    b. The generation rate was estimated by solving for G, knowing C and Q. The relationship between C and G is:
        i. $G = C \times Q$

            Where

G is the Generation rate (mg/min)

C_{NF} is the concentration (mg/m3)

Q is the air flow rate (m^3/min)

c. Simulations were conducted in the chamber using pole and block sanding methods. Conditions approached steady state after approximately 10 minutes so TWA concentrations were calculated from the last 5 minutes of each test.

Table 4-4S Calculating G for each test by back-calculating from the concentration generated under highly controlled conditions.

Estimating G from the Time Weighted Average Respirable Dust Concentrations											
	#1	#2	#3	#4	#5	#6	#7	#8	#9	#10	#11
5-min TWA(mg/m^3)	23.69	30.78	37.96	60.55	31.01	17.46	43.43	56.73	63.75	59.68	69.89
Q(m^3/min)	0.052										
G(mg/m^3) for respirable dust	1.22	1.59	1.96	3.12	1.60	0.90	2.24	2.93	3.29	3.08	3.60
Sanding Method	Pole 150			Hand 120			Pole 220				

d. An average G is calculated for each test, and from these values an overall average G is calculated.

e. **Average Respirable Dust G** = 2.50 mg/min which represents the generation rate for 1 drywall finisher.

5. There were 5 finishers sanding drywall, so to estimate G for the construction scenario, the average G was multiplied by 5.
   a. **G Respirable Dust for this scenario = 5 x 2.5 = 12.5 mg/min**
   b. To facilitate Monte Carlo analysis, the generation rate is characterized using a lognormal distribution with a geometric mean (GM) and a geometric standard deviation (GSD):
      1. G = LN(2.13, 1.58) per drywall finisher
      2. G = LN(2.13, 1.58)*(3-5 finishers)

   c. Generation rate for **Silica (Quartz)**
      1. Silica is a component in the respirable dust, and from a bulk sample analysis determined to be present at 1.2 to 2.4%.
      2. The generation rate is estimated by multiplying the Respirable Dust G by this fraction, to get a minimum and maximum G for Quartz.
      3. $\text{G minimum} = 2.5 \times .012 = .03 \text{ mg/min}$
      4. $\text{G maximum} = 2.5 \times .024 = .06 \text{ mg/min}$

5. For Monte Carlo analysis, G is described as a lognormal distribution:
6. LN(2.13,1.58)*U(min =0.012, max=0.24)

6. Ventilation rate (Construction environment):
   a. The ventilation rate in the hospital suite was estimated, knowing that the mechanical ventilation system was turned off and covered to prevent entrainment of construction dust.
   b. Q is estimated to be between 0.1 and 0.3 ACH = 1.4 to 4.3 m^3/min
   c. For the Monte Carlo analysis, a uniform distribution was defined using these estimates as the lower and upper bound, respectively.

7. Interzonal airflow rate:
   a. Local air velocity measurements were taken approximately every 3 m across the suite at the beginning and midway through the work shift. Six 10-second samples were measured at each location, producing 88 sets of velocity measurements. The average velocity at each location was calculated and then used to calculate an overall average velocity for the suite.
   b. The average local velocity, s = 5.6 m/min
   c. Using a hemispherical geometry with a radius of 0.8 m, the Free Surface Area (FSA) = $2\pi r^2$ = 4.02 m^2

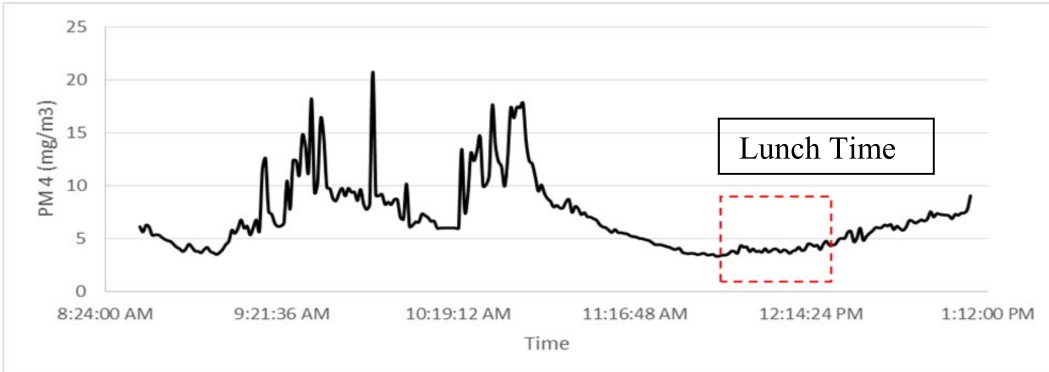
5. $\beta = \frac{1}{2}FSA \times s = \frac{1}{2}(4.02\ m^2) \times 5.6\ {}^{m}/_{min} = 11.3\ {}^{m^3}/_{min}$
6. Room volume :
   (i) Calculated from measurements of each room and hallways
   (ii) Room volume = 860 m^3
7. The Near Field Volume is calculated from the volume of a hemisphere, Where
   a. Volume of a hemisphere: $2/3\pi r^3$
      (i) Radius, r = 0.8 m, representing arms' length between the operator and the respective source.
      (ii) NF volume = 4.2 m^3

8. The Far Field Volume is the total room volume – NF volume
   a. FF volume = 860 m^3 – 4.2 m^3 = 875.8 m^3

(6) Time:
   (a) This was a full shift activity. Time = 480 minutes

(7) Background respirable dust and silica:
   (a) Real time measurements were used to quantify background levels in this very dusty environment, attributable to multiple days of sanding, a variety of work tasks going on concurrently, real time data. Background was quantified during the lunch break when all sanding stopped for approximately 30 minutes.

(b) The ambient respirable dust = 1.78 mg/m^3



(c) In the model, this was accounted for by setting C_{IN} = 1.78

Applying a Monte Carlo approach, the modeled C WMR 95th percentile exposure =8.06 mg/m^3.

The ACGIH TLV for Respirable Dust (3 mg/m^3) is used as the exposure benchmark. The 95th percentile respirable dust exposure, based on the real time data is 6.35 mg/m^3. The reference ECC is also a Category 4.

For quartz, the 95th percentile modeled C WMR exposure based on Monte Carlo analysis = 0.16 mg/m^3.

The ACGIH TLV for Quartz (0.05 mg/m^3) is used as the exposure benchmark. The 95th percentile quartz exposure, based on the real time data is 0.15 mg/m^3. The reference ECC is also a Category 4.

Scenario 5. And 6. Using physical chemical models to estimate cobalt exposure while weighing Lithium Cobalt Oxide powder, and mixing through cleaning tasks in a clean room area.

Ingredients are weighed before being transferred to a blender for mixing. After mixing, the slurry is transferred to another pan and moved to the staging area for the next step in the manufacturing process. The blender and surrounding areas are cleaned using a HEPA vacuum.

Weighing was treated as a separate task and modeled separately. Mixing and cleanup tasks were treated as one SEG for personal monitoring and modeling purposes.

Technician weighs Lithium Cobalt Oxide powder into a pan placed on a scale

Technician adds powder to a blender to be mixed.

1. Weighing Lithium Cobalt Oxide:
    a. Generation rate:
        i. The Near Field acetone concentration was measured during weighing and mixing through cleaning tasks. The time weighted average

concentration used to solve for the generation rate. This relationship between C and G is:

ii. $G = C_{NF} \times Q$

1. Where
2. G is the Generation rate (mg/min)
3. C_{NF} is the Near Field concentration (mg/m3)
4. Q is the near field ventilation rate (m^3/min)

(d) A generation rate was estimated from measurements collected in the near field on multiple occasions using a TSI DustTrak. The mean and standard deviation were calculated, and producing an overall average generation rate. On one occasion, measurements were collected directly above the source. This data was used to estimate an upper bound generation rate. The average generation rate is .044 mg/min.

Table 4-5S Calculating the Generation rate from the Near Field Concentration, the value obtained directly over the source (G4) to estimate the upper bound G

	G1	G2	G3	G4
Concentration ppm	.002	.002	.001	1.36
Q (m3/min)		3.35		
G (mg/min)	.007	.006	.004	4.56
Correction Factor = $C_{TWA}/C_{DustTrak}$		0.39		
G (mg/min)	.003	.003	.002	1.77

(e) To facilitate Monte Carlo analysis, the generation rate is characterized using a uniform distribution.
   (i) G = U(minimum = .002, maximum = 1.77)

(3) Room volume :
   (b) The room dimensions were measured, and the volume calculated.
      (i) Width = 7.9 m; Length = 5.5 m; Height = 2.9 m
      (ii) Volume = 7.9 x 5.5 x 2.9 = 125.9 m^3

(5) The Near Field Volume is calculated from the volume of a hemisphere, Where
   (a) Volume of a hemisphere: $2/3\pi r^3$
      (i) Radius, r = 0.8 m, reflecting the close proximity of the salon professional to the source

(ii) NF volume = 1.07 m

(6) The Far Field Volume is the total room volume – NF volume
    (a) FF volume = 125.9 m^3 – 1.07 m^3 = 124.4 m^3

(7) Ventilation rate:
    a) Weighing and mixing tasks were conducted in a clean room area where contaminants were removed by a large slot hood. The velocity was measured at several points across the face of each of the five slots in the slot hood. The area of each slot was also measured. The distance from the scale to the hood was approximately .1 m.

$$Q = v \times A$$

Where
(i) Q (m^3/min) is the ventilation rate
(ii) v (m/min) is the velocity
(iii) A is the area of the slot (m^2).
(iv) The average ventilation rate is 3.35 m^3/min
(v) For Monte Carlo Analysis, a uniform distribution was used to characterize Q. The area is a clean room area where a high degree of control over the process and environment are required, thus minimum and maximum are set ± 20% of the average Q.
    1. $Q_{minimum}$ = 2.68 m^3/min
    2. $Q_{maximum}$ = 4.02 m^3/min

(8) Interzonal airflow rate:
    (a) The interzonal airflow rate (ß) is estimated using the following formula:
        i. $ß = \frac{1}{2}\ Free\ Surface\ Area\ \times s$
    (b) where $FSA = 2\pi r^2$. The FSA is estimated using a hemisphere to describe the near field, with a radius r = 0.8 m, reflecting the less-than arms' length distance between the source and the salon professional.
    (c) ½ free surface area = 2.01 m^2
    (d) where s = local air velocity and is estimated at 15 m/minute.
    (e) $\beta = 2.01\ m^2 \times 3.9\ m/\min = 7.8\ {m^3}/{min}$
    (f) For Monte Carlo analysis, ß is characterized by a lognormal distribution. The GSD is based on the variability observed in local velocity measurements.
    (g) ß = LN(7.8, 2.1)

(9) Time

(a) The average time to weigh the Lithium Cobalt Oxide powder was 17 minutes.

Applying a Monte Carlo approach and incorporating the upper bound estimate of G, the 95th percentile exposure for the weighing task = 0.78 mg/m^3.

The measured 95th percentile exposure for the weighing task is 0.42 mg/m^3, based on 7 personal exposure measurements. The OEL is 0.02 mg/m^3, thus the reference ECC is Category 4.

Mixing and Cleaning:

8. Generation rate:
   a. The same approach was used as for the weighing task. The Near Field acetone concentration was measured during mixing through cleaning tasks. The time weighted average concentration used to solve for the generation rate. This relationship between C and G is:
      i. $G = C_{NF} \times Q$

         Where

         G is the Generation rate (mg/min)

         C_{NF} is the Near Field concentration (mg/m3)

         Q is the near field ventilation rate (m^3/min)

   (c) A generation rate was estimated from measurements collected in the near field on multiple occasions. Cleaning tasks including vacuuming were captured on two occasions, and these values were used to characterize the distribution for G, providing minimum and maximum values for G. The average G is 4.5 mg/min.

Table 4-6S Estimating G from Source Sampling

	G1		G2
Concentration ppm	.002		.004
Q (m3/min)			3.35
G (mg/min)	.08		.14
Correction Factor = $C_{TWA}/C_{DustTrak}$		0.39	
G (mg/min)	.03		.06

(d) To facilitate Monte Carlo analysis, the generation rate is characterized using a uniform distribution.

(i) G = U(minimum = .03, maximum = 0.06)

(4) Room volume :

(b) The room dimensions were measured, and the volume calculated.

(i) Width = 7.9 m; Length = 5.5 m; Height = 2.9 m

(ii) Volume = 7.9 x 5.5 x 2.9 = 125.9 m^3

(8) The Near Field Volume is calculated from the volume of a hemisphere, Where

(a) Volume of a hemisphere: $2/3\pi r^3$

(i) Radius, r = 0.8 m, reflecting the close proximity of the salon professional to the source

(ii) NF volume = 1.07 m^3

(9) The Far Field Volume is the total room volume – NF volume

(a) FF volume = 125.9 m^3 – 1.07 m^3 = 124.8 m^3

(10) Ventilation rate:

The velocity was measured at several points across the face of each of the five slots in the slot hood. The area of each slot was also measured. The distance from the scale to the hood was approximately .1 m.

$$Q = v \times A$$

Where

(i) Q (m^3/min) is the ventilation rate

(ii) v (m/min) is the velocity

(iii) A is the area of the slot (m^2).

(iv) The average ventilation rate is 3.35 m^3/min

(v) For Monte Carlo Analysis, a uniform distribution was used to characterize Q. The area is clean room areas where a high degree of control over the process and environment are required, thus minimum and maximum are set ± 20% of the average Q.

3. $Q_{minimum}$ = 2.68 m^3/min
4. $Q_{maximum}$ = 4.02 m^3/min

(10) Interzonal airflow rate:

(a) The interzonal airflow rate (ß) is estimated using the following formula:

ii. $ß = \frac{1}{2}\, Free\ Surface\ Area\ \times s$

(b) where $FSA = 2\pi r^2$. The FSA is estimated using a hemisphere to describe the near field, with a radius r = 0.8 m, reflecting the less-than arms' length distance between the source and the salon professional.
(c) ½ free surface area = 2.01 m^2
(d) where s = local air velocity and is estimated at 15 m/minute.
(e) $\beta = 2.01\, m^2 \times 3.9\, m/\min = 7.8\, {m^3}/{min}$
(f) For Monte Carlo analysis, ß is characterized by a lognormal distribution. The GSD is based on the variability observed in local velocity measurements.
(g) ß = LN(7.8, 2.1)

(11) Time
(a) The average time for mixing, including cleanup is approximately 120 minutes.

Applying a Monte Carlo approach, the 95th percentile CNF exposure = .027 mg/m^3.

The measured 95th percentile exposure for the mixing and cleaning tasks is 0.09 mg/m^3, based on 7 personal exposure measurements. The OEL is 0.02 mg/m^3, thus the reference ECC is Category 4.

Scenario 7. Using physical chemical models to estimate exposure to methylene chloride:

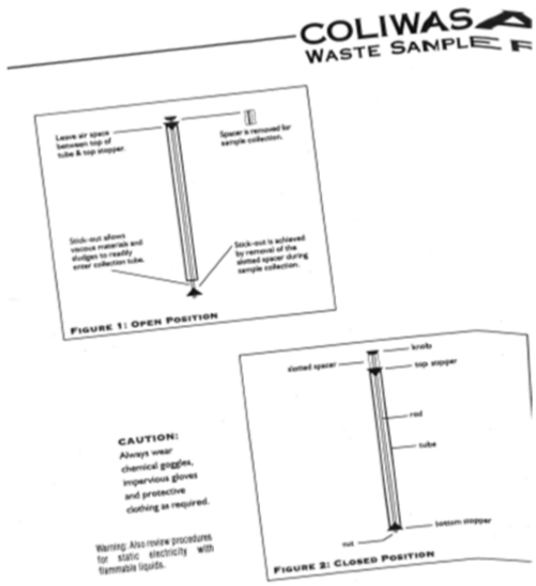


Diagram of a Colowasa sampler

Stainless steel vessel

The Near Field Far Field model is a good candidate model for this scenario, since the operator is standing close to the vessel portal when collecting the sample.

1. Generation rate: The Colowasa sampler resembles a large ladle. Dipping the sampler through the portal, into the vessel is analogous to drum filling, where air containing the chemical vapor is displaced into the workplace air, and the rate of displacement is proportional to the rate at which the sampler is lowered into the vessel. This is useful for estimating the Generation rate, G. The following information is needed to use this approach:
   a. Volumetric fill (and displacement) rate:
      i. The sampler has a volumetric capacity of 460 ml. This volume of air is displaced when the sampler is lowered into the vessel over ~ 2 minute period. The volumetric fill rate is the volume/unit time:
         1. $Vol\ fill\ rate = \frac{460\ ml}{2\ min} = 230 \frac{ml}{\min \times \frac{m^3}{10^6\ ml}} = 0.00023\ {m^3}/{min}$
   b. Headspace (methylene chloride) concentration
      i. Using the vapor pressure of methylene chloride, we can calculate the saturated vapor concentration expected to occupy the headspace of the vessel.

1. VP $_{\text{methylene chloride}}$ = 350 mm Hg
2. Saturated vapor concentration = $\frac{350\ mm\ Hg}{760\ mm\ Hg} \times 10^6\ ppm$
3. Headspace concentration = saturated vapor conc'n = 460526.32 ppm

ii. Converting from ppm to mg/m^3 so units are compatible with IHMOD:

1. $\frac{mg}{m^3} = 460525.32\ ppm\ \times \frac{84.93\ g/mol}{24.45\ g{-}mol/k}$ = 1.6 x 10^6 mg/m^3

c. Generation rate:

i. Combining *a* and *b* to estimate the Generation rate, G, in mg/min:

1. $G = vol/time\ \left({m^3}/{min}\right) \times headspace\ conc'n\ \left({mg}/{m3}\right)$
2. $G =\ 0.00023\ {m^3}/{min} \times\ 1.6\ \times 10^6\ {mg}/{m^3}\ =\ 367.93\ {mg}/{min}$
3. The range stated in the scenario, (304 – 457 mg/min) reflects uncertainty around the rate at which the sampler is lowered into the vessel by the operator.
4. For Monte Carlo analysis, G is defined using a lognormal distribution, with GM = 220 and GSD = 4.

2. Room volume
   a. As stated in the scenario, = 379.4 m^3

3. Ventilation rate:
   a. The general ventilation rate, calculated from the room volume and stated ACH, = 118 m3/min.
   b. LEV is also used, and in the near field will contribute to the rate at which vapors are removed. Q $_{\text{LEV}}$ is calculated using the ventilation rate information and area of the duct:
      i. Q = VA
      ii. $Q_{LEV} = 100\ fpm\ \times 6.2\ ft^2 = 628\ cfm\ \times 0.0283\ \frac{m^3}{ft^3} = 17.8\ {m^3}/{min}$
   c. The total ventilation rate is the sum of the general and local ventilation rates.
      i. $Q_{total} = 118\ {m^3}/{min} + 17.8\ {m^3}/{min} =\ 136.03\ {m^3}/{min}$
      ii. For Monte Carlo analysis, Q is defined using a uniform distribution, minimum = (0.8 x 118 m^3/min = 94 m^3/min), maximum = (1.2 x 118 m^3/min = 140 m^3/min)

4. Interzonal airflow rate:
   a. The interzonal airflow rate (ß) is estimated using the following formula:
      i. $ß = \frac{1}{2}\ free\ surface\ area\ \times s$
         1. free surface area = 1.2 m^2
         2. where s = local air velocity and is estimated at 3 – 6 m/minute
         3. $ß = 3.5\ to\ 7.1\ {m^3}/{min}$
         4. For Monte Carlo analysis, a uniform distribution is defined using these values the upper and lower bound estimates.

The modeled CNF 95th percentile exposure based on Monte Carlo analysis = 194.1 ppm.

The OEL = 125 ppm so the predicted ECC = category 4.

The reference exposure control category is category 4, with 69% probability, based on n = 10 and using the IH Data Analyzer software.

Scenario 8. Using physical chemical models to estimate phenol exposure while making sand molds containing a phenolic resin

Operator files rough edges off mold

Operator fills mold

In this scenario, the operator fills the molds with the sands/phenolic resin, which are heated in the mold press 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. The 2 Zone model is a good candidate reflecting the close proximity of the operator to the source while making the molds.

1. Interzonal airflow rate:
   a. The interzonal airflow rate (ß) is estimated using the following formula:
   b. $ß = \frac{1}{2}\ Free\ Surface\ Area\ \times s$
      Where
      i. $FSA = 2\pi r^2$
      ii. The FSA is estimated using a hemisphere to describe the near field, with a radius r = 1 m, reflecting the less-than arms' length distance between the source and the salon professional.
      iii. ½ free surface area = 3.14m^2
      iv. where s = local air velocity and is estimated at 30 m/minute, based on local air velocity measurements. Two fans ensure constant and relatively consistent air movement in this area.

v. $\beta = 3.14\, m^2 \times 30\, m/\min = 94\ {m^3}/{min}$

vi. For Monte Carlo analysis, ß is characterized by a lognormal distribution. The GSD reflects the relatively moderate variability in local air velocity.

vii. ß = LN(94, 1.8)

2. Generation rate:
   a. An average Near Field concentration was calculated from personal TWA phenol measurements collected over a five day period. This average was used to solve for the generation rate. This relationship between C and G is:
   b. $G = C_{NF} \times \beta$

   Where

   i. G is the Generation rate (mg/min)

   ii. C_{NF} is the Near Field concentration (mg/m3)

   iii. β is the interzonal air flow rate (m^3/min)

   iv. From the TWA data C average = 0.196

   v. β = 94 m^3/min

   vi. Average G (mg/min) = 18.4

   vii. To facilitate Monte Carlo analysis, the generation rate is characterized using a lognormal distribution with a geometric mean (GM) and a geometric standard deviation (GSD):

   viii. G = LN(13.1, 2.3)

3. Room volume :
   a. The shell core area is approximately 5 x 5 x 5 m (125 m^3)

4. The Near Field Volume is calculated from the volume of a hemisphere,

   Where
   a. Volume of a hemisphere: $2/3\pi r^3$
   b. Radius, r = 0.8 m, reflecting the close proximity of the salon professional to the source
   c. NF volume = 4.2 m

5. The Far Field Volume is the total room volume minus the NF volume
   a. FF volume = 125.9 m^3 – 1.07 m^3 = 120.8 m^3

6. Ventilation rate:
   a. The ventilation rate was estimated using professional judgment, informed by the knowledge that an exterior door located next to the middle shell core machine

opens and closes repeatedly throughout the day. The building is in general very old and not well sealed, further promoting air movement. Based on this information, the ventilation rate is estimated to be 4 to 5 ACH.

b. $Q = 125\, m^3 \times {}^{4\,ACH}\Big/{}_{60\,min/hr} = 8.33$

c. $Q = 125\, m^3 \times {}^{5\,ACH}\Big/{}_{60\,min/hr} = 10.4$

d. For Monte Carlo Analysis, a uniform distribution was used to characterize Q using these estimates as the minimum and maximum values.

e. Q = U(8.33, 10.4)

7. Time
   a. This was a full shift activity. Time = 480 minutes.

Converting from mg/m^3 to ppm, and applying a Monte Carlo approach, the modeled 95th percentile CNF exposure = 0.8 ppm.

The ACGIH TLV (5 ppm) is used as the exposure benchmark. Using the AIHA Exposure Control Categories, the predicted NF concentration falls into Category 2.

The reference exposure category is Category 2, with a 100% probability based on 8 personal samples.

Scenario 9. Using physical chemical models to estimate a salon professional's exposure to acetone in a nail salon:

Waterless manicures were given to five clients throughout the day using acetone to clean nail surfaces. The services were offered in a new building with large, well ventilated suites in a commercial loft setting.

Salon Professional (right) gives client a waterless manicure using acetone to clean nails

Products used during manicure and nail painting. Acetone is used as a polish remover and non-aqueous cleaner.

The 2 Zone model is a good candidate reflecting the close proximity to which the salon professional works with acetone while giving the client a manicure.

1) Generation rate: The salon professional works across the table from the client and uses a squirt bottle to wet a cotton pad with acetone, which is then used to clean the client's nails as part of a waterless manicure. Acetone on the nails evaporates quickly, providing a clean, dry nail surface. Some of the acetone evaporates when the cotton pad is wetted and continues to evaporate from the cotton pad until it is disposed of in a trash can and the trash can lid closed. Typically, the cotton pad is placed in the trash can as soon as this task is completed. This is the first and only source of acetone exposure unless the client chooses to have nail polish applied. When nail polish is being applied, the nails are wiped with acetone again after the bond aid, or dehydrator is applied and before the base coat is applied. For some manicures in which only buffing and shaping were done, acetone was not used and thus the generation rate for these manicures was equal to zero.

a) The Near Field acetone concentration was measured during each manicure and used to back-calculate, solving for the generation rate. This relationship between C and G is:

$$G = C_{NF} \times \beta$$

Where

G is the Generation rate (mg/min)

C_{NF} is the Near Field concentration (mg/m3)

β is the interzonal air flow rate (m^3/min)

b) A generation rate was estimated for each manicure, from which the mean and standard deviation were calculated, producing an overall generation rate. The average generation rate was 21 mg/min.

Table 4-7S Calculating G from C for each manicure.

	G1	G2	G3	G4	G5
Concentration ppm	0	0.58	0.47	0	0.10
Concentration mg/m3		1.38	1.11		0.23
Beta (m3/min)		23.10	23.10		23.10
G (mg/min)		31.98	25.75		5.25

c) To facilitate Monte Carlo analysis, the generation rate is characterized using a lognormal distribution with a geometric mean (GM).

i) G = LN(16.3, 2.68)

2) Room volume :

a) The room dimensions were measured, and the volume calculated.

i) Width = 2.7 m; Length = 3.0 m; Height = 3.8 m

ii) Volume = 2.7 x 3. 0 x 3.8 = 31 m^3

3) The Near Field Volume is calculated from the volume of a hemisphere,

Where

i) Volume of a hemisphere: $2/3\pi r^3$

ii) Radius, r = 0.7 m, reflecting the close proximity of the salon professional to the source, (less than arm's length)

iii) NF volume = 1.03 m

4) The Far Field Volume is the total room volume minus NF volume

a) FF volume = 31 m^3 – 1.03 m^3 = 29.9 m^3

5) Ventilation rate:
   a) A decay study was conducted using real time instruments to measure the concentration as the acetone was removed from the salon to estimate the ventilation rate.
   b) Acetone was placed in an open, flat container in the salon and allowed to evaporate. A Drager X-am 7000 direct reading instrument equipped with a Smart PID® sensor (Dräger Safety AG & Co. KGaA) was used to measure the concentration every 10 seconds, as the acetone evaporated. The decay rate was calculated from the declining the concentration and from it, the ventilation rate was determined. The relationship between the removal rate of acetone, ventilation rate and room volume is shown in the equation below:

$$-\ln\left(\frac{C}{C_0}\right) = \frac{Q}{V} \times t$$

Where

(i) C_0 (mg/m^3) is the initial concentration measured at time t = 0. This was the time at which the acetone has evaporated from the container.

(ii) C (mg/m^3) is the concentration measured at each 10 second time interval

(iii) Q (m^3/min) is the ventilation rate

1. V (m^3) is the room volume and is known (measured).

b. By plotting $-\ln\left(\frac{C}{C_0}\right)$ against t, the slope can be used to deterirmine Q, since the room volume is known.

c. From the curve, y = 0.2318x - 0.1306, Q $= \frac{0.2318}{\text{min}} \times 31\text{m}^3 = 7.19\ {m^3}/{min}$ or 13.9 ACH.

d. For the Monte Carlo Analysis, a uniform distribution was used to characterize Q. Professional judgment was used to estimate minimum and maximum values, knowing the building was newly constructed and ventilated with a variable air volume system.

Where

(ii) $Q_{minimum}$ = 12 ACH = 6.2 m^3/min

(iii) $Q_{maximum}$ = 15 ACH = 7.7 m^3/min

4) Interzonal airflow rate:
   a. The interzonal airflow rate (ß) is estimated using the following formula:

$$ß = \frac{1}{2}\,Free\ Surface\ Area\ (FSA)\ \times s$$

Where

(i) $FSA = 2\pi r^2$. The FSA is estimated using a hemisphere to describe the near field, with a radius r = 0.7 m, reflecting the less-than arms' length distance between the source and the salon professional.
(ii) ½ free surface area = 1.54 m^2
(iii) where s = local air velocity and is estimated at 15 m/minute.
(iv) $\beta = 1.54\, m^2 \times 15\, m/\min = 23.1\ {m^3}/{min}$

b. For Monte Carlo analysis, ß is characterized by a lognormal distribution. The GSD is based on professional judgment and represents low variability.
c. ß = LN(23.1, 1.1)

5) Time
   a. While the time varied from client to client depending on the service provided, the average time for a manicure was 35 minutes.

From the Monte Carlo approach, the 95th percentile exposure = 11.9 ppm for a single manicure. A time weighted average concentration is calculated assuming each manicure lasts 35 minutes, there are five manicures and there are no other exposures to acetone for the remaining work shift.

$$TWA\ Acetone = \frac{5 \times (11.9\, ppm \times 35\, minutes)}{480\, minutes} = 4.33\, ppm$$

.

The ACGIH TLV (8 hour TWA = 250 ppm) is used as the exposure benchmark. Using the AIHA Exposure Control Categories, the predicted NF concentration falls into Category 1.

The measured TWA 95th percentile exposure to acetone = 9.75 ppm. The reference exposure category is Category 1, with a 100% probability based on 10 personal samples.

Scenario 10. Using physical chemical models to estimate acetone exposure while cleaning the lid and blades of a Morehouse mixer

Technicians cleaning slurry pot lid and blades, alternately squirting the surfaces with acetone and wiping them off with paper wipes

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. The 2 Zone model is a good candidate given the close proximity of the technician to the source while cleaning the mixer.

1. Generation rate:
    a. The Near Field acetone concentration was measured while the lid and blades were cleaned and the time weighted average concentration used to solve for the generation rate. This relationship between C and G is:
        i. $G = C_{NF} \times \beta$

Where

ii. G is the Generation rate (mg/min)

iii. C_{NF} is the Near Field concentration (mg/m3)

iv. β is the interzonal air flow rate (m^3/min)

b. Near Field concentration measurements were made on several days, from which the mean and standard deviation were calculated, producing an overall generation rate.

Table 4-8S Back calculating from C to estimate G. The average generation rate was 1638.2 mg/min.

	G1	G2	G3	G4
Concentration ppm	62.7	127.8	96.8	72.7
Concentration mg/m3	149.3	289.9	229.8	173.1
Beta (m3/min)	7.8			
G (mg/min)	1161.7	2367.4	1788.0	1346.7

c. To facilitate Monte Carlo analysis, the generation rate is characterized using a lognormal distribution with a geometric mean (GM).

d. G = LN(1600, 1.37)

2. Room volume :
    a. The room dimensions were measured, and the volume calculated.
    b. Width = 7.9 m; Length = 5.5 m; Height = 2.9 m
    c. Volume = 7.9 x 5.5 x 2.9 = 125.9 m^3
3. The Near Field Volume is calculated from the volume of a hemisphere, Where
    a. Volume of a hemisphere: $2/3\pi r^3$
    b. Radius, r = 0.8 m, reflecting the close proximity of the salon professional to the source
    c. NF volume = 1.07 m

4. The Far Field Volume is the total room volume – NF volume
    a. FF volume = 125.9 m^3 – 1.07 m^3 = 124.8 m^3

5. Ventilation rate:
    a. A Drager X-am 7000 direct reading instrument equipped with a Smart PID® sensor (Dräger Safety AG & Co. KGaA) was used to measure the concentration every 10 seconds, as the acetone evaporated after all cleaning tasks were finished. The decay rate was calculated from the declining the

concentration and from it, the ventilation rate was determined. The relationship between the removal rate of acetone, ventilation rate and room volume is shown in the equation below:

$$-\ln\left(\frac{C}{C_0}\right) = \frac{Q}{V} \times t$$

Where

C_0 (mg/m^3) is the initial concentration measured at time t = 0. This was the time at which the acetone has evaporated from the container.

C (mg/m^3) is the concentration measured at each 10 second time interval

Q (m^3/min) is the ventilation rate

V (m^3) is the room volume and is known (measured).

By plotting $-\ln\left(\frac{C}{C_0}\right)$ against t, the slope can be used to deterirmine Q, since the room volume is known.

From the curve, y = 0.1025x + 1.194, $= \frac{0.1025}{\text{min}} \times 126\ \text{m}^3 = 12.8\ {m^3}/{min}$ or 6.2 ACH.

For Monte Carlo Analysis, a uniform distribution was used to characterize Q. The area is a clean room area where a high degree of control over the process and environment are required, thus minimum and maximum values corresponding to 5 and 7 ACH respectively represent a conservative estimate of the expected variability in the system.

$Q_{minimum}$ = 10.1 m^3/min

$Q_{maximum}$ = 15.1 m^3/min

Interzonal airflow rate:

The interzonal airflow rate (ß) is estimated using the following formula:

$$ß = \frac{1}{2}\ free\ surface\ area\ \times s$$

where $FSA = 2\pi r^2$. The FSA is estimated using a hemisphere to describe the near field, with a radius r = 0.8 m, reflecting the less-than arms' length distance between the source and the salon professional.

½ free surface area = 2.01 m^2

where s = local air velocity and is estimated at 15 m/minute.

$$\beta = 2.01\, m^2 \times 15\, m/\min = 15.6\ {m^3}/_{min}$$

For Monte Carlo analysis, ß is characterized by a lognormal distribution. The GSD is based on professional judgment and represents low variability.

ß = LN(15, 1.1)

Time

The average time to clean the lid and blades was 20 minutes.

Applying a Monte Carlo approach, the 95th percentile modeled CNF exposure = 439 ppm.

The ACGIH TLV (STEL = 500 ppm) is used as the exposure benchmark. Using the AIHA Exposure Control Categories, the predicted NF concentration falls into Category 3.

The reference exposure category is Category 3, with a 100% probability based on 6 personal samples.

CHAPTER 5 CONCLUSIONS AND FUTURE DIRECTION

OVERALL CONCLUSIONS

Exposure judgments are used in a wide range of situations, including retrospective exposure assessments for epidemiology studies (e.g. Esmen, 1979; Ramachandran 2001; Ramachandran et al., 2003; Friesen, 2003) and current as well as prospective exposure assessments for managing exposures related to consumer use and manufacturing operations (e.g. Hawkins and Evans 1989; Teschke et al. 1989; Macaluso et al., 1993; Friesen et al., 2003; Ramachandran et al., 2003; Jones et al., 2014). When there are limited or no sampling data available, hygienists use a combination of professional judgment, personal experience with a given operation, and review of exposures from similar operations to assess the acceptability of exposures for managing engineering controls, medical surveillance, hazard communication and personal protective equipment programs (Teschke et al., 1989; de Cock et al., 1996; Burstyn & Teschke, 1999; Friesen, 2003; Kolstad, et al., 2005; Logan et al., 2009; Logan, et al., 2011; Vadali et al., 2012a; Vadali et al., 2012b). In many cases, there is not an opportunity to collect quantitative measurements prior to making an exposure assessment judgment. For example, hazard communications triggered by an exposure assessment must be made prior to the introduction of the agent into the workplaces similarly; a theoretical technical basis is often the only thing available to define adequate engineering controls related to the introduction of new processes or changes in existing processes. The term “qualitative” refers to judgments or decisions made in the absence of quantitative personal exposure data. This term can be further subdivided according to the type of inputs from which the judgments are synthesized; subjective qualitative judgments are based on intuition or 'personal experience' that is derived from unstructured inputs and is not overtly defined. Objective qualitative judgments are produced using structured, more transparent approaches.

Research has shown that subjective, unstructured qualitative exposure judgments tend to be no more accurate than random chance, with a significant underestimation bias, i.e., there is marked tendency to assign a lower exposure category than the correct one, thus increasing occupational risk to workers (Logan et al. 2009; Vadali et al., 2012; Arnold et al., 2015). The low accuracy could be due to several factors. OHs receive little, if any formal training on how to conduct a basic characterization. If this step of the exposure assessment is not conducted in a systematic way, using physical and chemical principles, and collecting the relevant exposure determinant information, the hygienist may not investigate the exposure that presents the highest exposure potential with sufficient detail, leading to low judgment accuracy. Another factor may be cognitive biases in understanding skewed lognormal distributions (Logan, 2009). Mental shortcuts, known as heuristics, are often used, making the decision process efficient but can lead to errors in judgment and introduce bias. Using these heuristics leads to a pattern that, when faced with uncertain prospects, assigns weights to our decisions that differ from the true probabilities of these outcomes. Improbable outcomes are over-weighted, while almost-certain outcomes are under-weighted.

Objective, structured approaches, using simple algorithms and exposure modeling are more resistant to these vulnerabilities, focusing the decision maker on the decision making process, and on the critical inputs, while filtering out nonessential information. These approaches have been shown to improve decision making across a broad range of domains, including psychology (Kahneman, 2011 and Kahneman et al.,, 1982), drug delivery and development (Lipinski, et al., 2001); predicting transdermal delivery and toxicity (Magnusson et al., 2004;) environmental exposure assessment (Fristachi, et al., 2009); and aggregate exposure assessment (Cowan-Ellsberry & Robison, 2009). These same objective approaches can be applied to occupational exposure assessment. In fact, decisions are most accurate in highly uncertain 'low validity' environments, i.e. situations with little or no data, when the final decision is generated from algorithms.

One of the characteristics of algorithms and models contributing to consistent decision making is the consistent order in which information is processed. Checklists provide guidance on the order in which inputs are considered. These simple tools have been the cornerstone of safety excellence in the aviation industry for years. To be sure, checklists and models do not replace knowledge and expertise, and pilots go through rigorous training before they are allowed to fly. The checklists ensure they follow the critical steps at the right time to ensure theirs, and their passengers', safety. Likewise, checklists help hygienists focus on the critical inputs to decision making in the right order, leading to consistent and accurate exposure judgments (Arnold et al., 2015), protecting the health and safety of those in their care.

Exposure models seek to capture the underlying physical processes generating chemical concentrations in the workplace. An accurate representation will produce better concentration estimates and facilitate decision-making in exposure management.

However, this is challenging because workplaces are notoriously complex and no physical model is likely to provide a complete representation. Thus, characterizing model parameters, and accounting for parameter and model uncertainty is crucial. Guidance on selecting and applying the models appropriately is also essential. Without these, hygienists may select the wrong model or use model input values that are inappropriate and misleading. Further, without guidance on how to interpret the model output relative to making decisions about the acceptability of an exposure, the hygienist may draw conclusions that are not consistent with the 'true' magnitude of exposure.

This research was conducted to evaluate the use of several structured, objective approaches, namely the use of checklists and heuristics and exposure models in improving qualitative exposure judgment accuracy. Three major studies were investigated to meet this objective, with each study generating a manuscript. Chapter 2 discusses the development and application of a foolproof checklist for using heuristics and algorithms. It has already been accepted for publication (JOEH, 2015). Chapter 3 and 4 discuss evaluation of the Well Mixed Room (WMR) and Near Field Far Field (NF FF) models, conducted in a way that is analogous to the way in which a NIOSH method is validated, identifying the bounds within which the models are useful, as well as their limitations. Specifically, Chapter 3 discusses model evaluation under highly controlled conditions, in which model parameters are known and well controlled, providing near-ideal model conditions. In Chapter 4, model evaluation under less controlled conditions, using scenarios from real workplaces is discussed. The impact of selecting the wrong model is also discussed in Chapter 4. Chapters 3 and 4 will be submitted to the Annals of Occupational Hygiene in the near future.

The primary conclusions of these papers are:

1. Previously published research suggested that when hygienists make decisions regarding the acceptability of exposure based on professional judgment guided by unstructured, subjective inputs, their exposure judgment accuracy is low, and not statistically significantly different from random chance. Moreover, the data indicated a negative bias in these decisions, resulting in a tendency to underestimate exposures, with a consequent risk of inadequately managing unacceptable exposures and risks.

   A study was conducted in which a database of exposure scenarios were developed, capturing reasonably well defined model input values and including a minimum dataset of six personal exposure measurements. The personal exposure data was used to characterize the reference exposure control category (ECC), representing the 'true' exposure and against which qualitative exposure judgment accuracy was measured. A new tool, the Qualitative Exposure Assessment Checklist was constructed for this research, comprised of heuristics and algorithms that were developed from physical and chemical principles but refined empirically, over many years. These heuristics were presented in a structured format; a checklist requiring only a few inputs that guided the hygienist through the selection, application and interpretation of the results. Using this tool, exposure judgment accuracy was evaluated by collecting exposure judgments from novice and practicing hygienists that were made with and without guidance from the tool.

2. Exposure judgment accuracy of exposure judgments made by practicing hygienists without the benefit of personal exposure measurement data and based on professional judgment guided by subjective inputs were ~ 30% accurate, no better than random chance and tended to underestimate the true exposure. These results were consistent with the study results reported by previous investigators (Logan et al., 2009; Logan et al., 2011; Vadali, et al. 2011; Vadali et al., 2012). Exposure judgment accuracy made by novice hygienists in the absence of personal exposure data was slightly higher than those of their more experienced colleagues but not statistically significantly different from random chance. However, the novices' judgments did not exhibit the same negative bias; they were equally balanced between over and underestimating the true exposure. When exposure judgments were guided by the Checklist, a statistically significant increase in judgment accuracy was observed with both practicing and novice hygienists. In fact, exposure judgment accuracy increased by a factor of 2 to ~ 65% and was highly statistically significant ($p < 0.001$). Moreover, the negative bias observed in judgments made by practicing hygienists was reduced. Thus the main conclusions of this research is that exposure judgments made in the absence of robust personal exposure measurement data, but based on professional judgment that is guided by structured, objective inputs are likely to be more accurate than random chance and significantly more accurate than judgments

guided by unstructured, subjective inputs. The checklist format for applying the heuristics is essential to improving exposure judgment accuracy as it ensures the heuristics are applied in consistently and appropriately and that the output is interpreted correctly. Exposure models, such as the Well Mixed Room (WMR) and Near Field Far Field (NF FF) models have been found to be useful for estimating exposures to chemicals across a range of situations. The literature is scattered (Esman et al., 1999; Ramachandran 2001; Ramachandran et al., 2003; Friesen, 2003, Hawkins and Evans 1989; Teschke et al. 1989; Macaluso 1993) anecdotal case study reports indicating these models are useful for predicting exposures in retrospective epidemiological studies to facilitate dose reconstruction, for guiding product stewardship recommendations for best work practices aimed at minimizing exposure, when it is not feasible to collect a robust dataset of personal exposure measurements and in prospective exposure studies to guide scale up from pilot to manufacturing activities. However, models tend to be undervalued and underutilized by hygienists. Several factors may influence this trend, including a lack of model selection and application guidance and the scarcity of model input values needed to use the models. Another possible reason they have not been more readily adopted in practice is that their performance relative to accurately predicting exposure had not been systematically evaluated.

A study was conducted to test whether these models works well under controlled conditions where the models' underlying assumptions are met. These tests were conducted in an exposure chamber in which three chemicals were used to evaluate model performance of the WMR and NF FF models across a range of conditions. The chamber allowed conditions to be controlled so that they could be changed one at a time and measured with a reasonable degree of confidence. This generated high quality model inputs and measured contaminant concentration data and consequently produced over 800 modeled and measured exposure pairs, against which model performance was measured. Two sets of criteria, the ASTM Standard 5157, providing insight regarding general concordance across the time-varying spectrum of exposures and identifying potential for systematic bias, and the AIHA Exposure Assessment categorical criteria providing insight the model's ability to predict the TWA exposure and thus predict the correct ECC.

Model performance of the WMR model across all three chemicals and chamber conditions was excellent, with ≥ 82% of the 483 of $C_{measured}$-$C_{modeled}$ pairs deemed adequate, meeting all ASTM performance criteria. Categorically, the WMR model predicted the correct ECC for 93% of the 27 scenarios. In comparing categorical accuracy of the WMR model to accuracy attributable to random chance alone, the WMR model accuracy was highly statistically significant ($p < 0.001$). Model performance for the NF FF model was impacted by the physical limitations of the chamber in generating a true NF FF environment, so model performance of the NF modeled exposures relative to the ASTM 5157 performance criteria was low, with only 11 to 33% of the $C_{measured}$ and $C_{modeled}$ NF pairs deemed adequate. Categorically, and more relevant to their use to hygienists, model performance was much higher and highly statistically significant (p

<0.001), with the model predicting the correct ECC for 20/27 NF scenarios (~74%). Model performance of the FF modeled exposures stronger than the NF based on the ASTM 5157 performance criteria, with 163 of the 243 $C_{measured}$ and $C_{modeled}$ FF pairs deemed adequate (~ 67 %) and categorically, producing excellent concordance, with 26/27 FF scenarios (~96%) predicting the correct ECC. These results, relative to model accuracy based on random chance alone were highly statistically significant (p <0.001).

There are several important implications of this study:

1. The models are designed to provide a reasonable estimation of the average concentration in a room, and when environmental conditions parallel the underlying assumptions of the model, model performance of both models is strong. Moreover, when the contaminant concentration is generated by a source whose behavior parallels the assumptions of the model in its relevant form, e.g., time-varying, model performance is excellent.
2. The AIHA categorical criterion is a better performance metric that the very strict ASTM 5157 for models that will be used to assess occupational exposures.
3. Characterizing the generation rate with a reasonable degree of certainty was instrumental in achieving the observed performance levels.

Model performance under field (work place) conditions may differ from performance evaluated under highly controlled conditions. Two types of uncertainty will come into play in such studies; (1) parameter uncertainty, when we do not know the parameter values under these field conditions precisely, and (2) model uncertainty, when it is not abundantly clear which model should be used. Selecting the best candidate model likely is an important component of generating accurate estimates of the exposure, but the choice is not always obvious and selecting the wrong model can result in categorical ly misclassifying the exposure. For all these reasons, it is important to understand model performance under real work place conditions.

A study was conducted under these less than ideal conditions to evaluate model performance by evaluating ten scenarios from a diverse range of workplaces and tasks, involving four chemical agents. Personal exposure measurements were collected following a similar protocol to the approach used in the chamber study and were used to define the reference ECC for each scenario. Model input values were measured directly whenever possible, and estimated using submodels or professional judgment guided by input from site hygienists and work area experts. Time varying measurements, necessary for applying the ASTM 5157 criteria were collected for six of the scenarios. Categorical performance criteria were applied to all ten scenarios, based on the 95th percentile measured and modeled exposures.

Model performance based on the ASTM criteria was low, with none of the six scenarios achieving scores within the defined ranges for all parameters using the WMR or NF FF models. Categorically, however, performance was excellent, with the WMR model predicting the correct ECC in 8/10 scenarios, and the NF FF model predicting the correct

ECC in 9/10 scenarios. Model performance accuracy for both models, relative to random chance was both highly statistically significant ($p < 0.001$).

Implications of this research are three-fold:

1. Model performance was heavily influenced by the ability to generate reasonably high quality generation rates. The efforts invested were not trivial but are valuable beyond the specific scenarios for which they were developed. These generation rates will be useful in assessing other scenarios involving the same agent under similar conditions, thus the generation rates have portability.
2. Categorical model performance was highly statistically significant, even when model performance as defined by ASTM Standard 5157 was poor. Thus, this standard, with its strict criteria is not recommended for evaluating performance of models intended to be used to guide decisions regarding the acceptability of occupational exposure.
3. Selection and application of the models also required a significant intellectual investment and required judicious professional judgment. Thus a checklist is needed to provide guidance for the systematic selection and application of the models.

Limitations of the Study and Future Directions

This research produced several novel tools, evidence to support the use of models in guiding exposure judgments, especially when personal exposure data are not available or insufficient. A data base of model input values was generated under highly controlled (chamber) conditions and less controlled, (field) conditions that was previously were not available. Several practical field methods for characterizing model inputs were applied that were found to produce reasonably accurate estimates. Future research, expanding on this foundation could include:

Chamber Studies:

1. Expanding the chamber study conditions to further explore the bounds in which the models are useful to hygienists
2. Evaluating different types of exposure scenarios, including exposures resulting from the use of consumer products
3. Expanding the chamber studies to evaluate the impact of aerosols on model performance
4. Evaluating additional models, such as the turbulent eddy diffusion model

Field Studies:

1. Developing a checklist to guide hygienists in selecting and applying the models and interpreting model output appropriately and consistently.
2. Developing a library of generation rates for standard industrial tasks, e.g. sanding, cutting, drum filling of solvents, etc.

Model Application Studies

1. Validating the modeling checklist, demonstrating that hygienists can select and apply the best model candidate and interpret the model output appropriately when guided by the checklist.

2. In conjunction with validating the modeling checklist, a database of exposure scenarios needs to be developed to support model checklist validation workshops.

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APPENDIX I

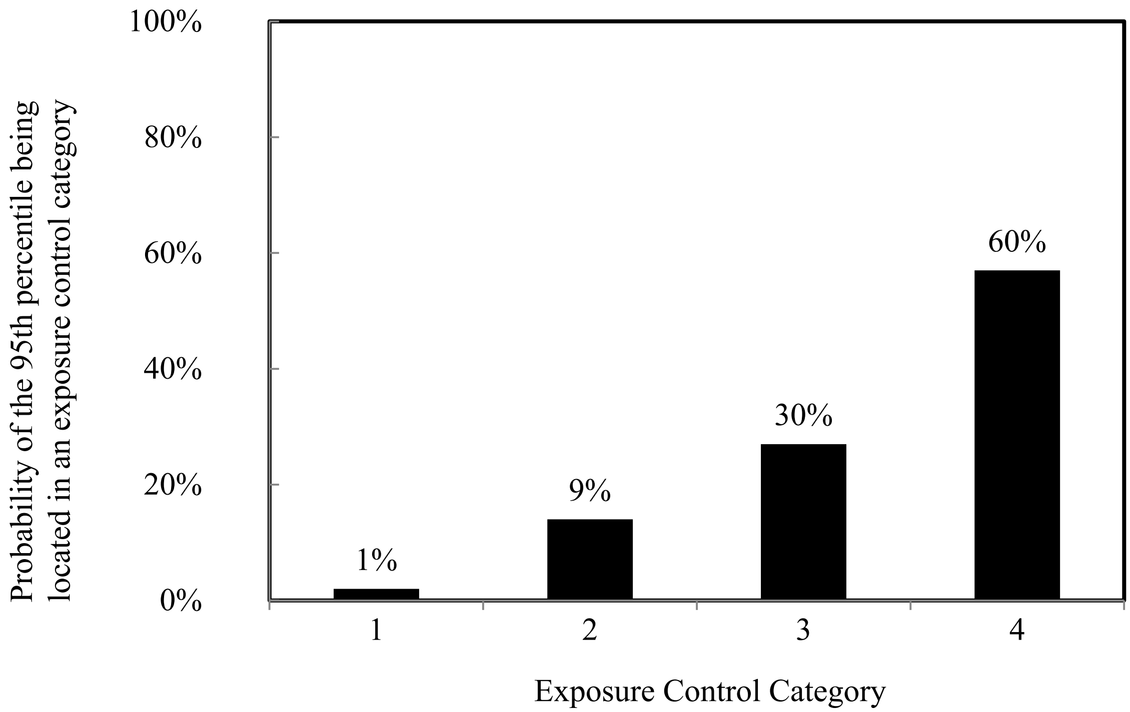

Figure 5-1 Bayesian Decision Chart, showing the IHs belief that the 95th percentile of the exposure distribution for a given scenario most likely belongs to Exposure Control Category (ECC) 4.

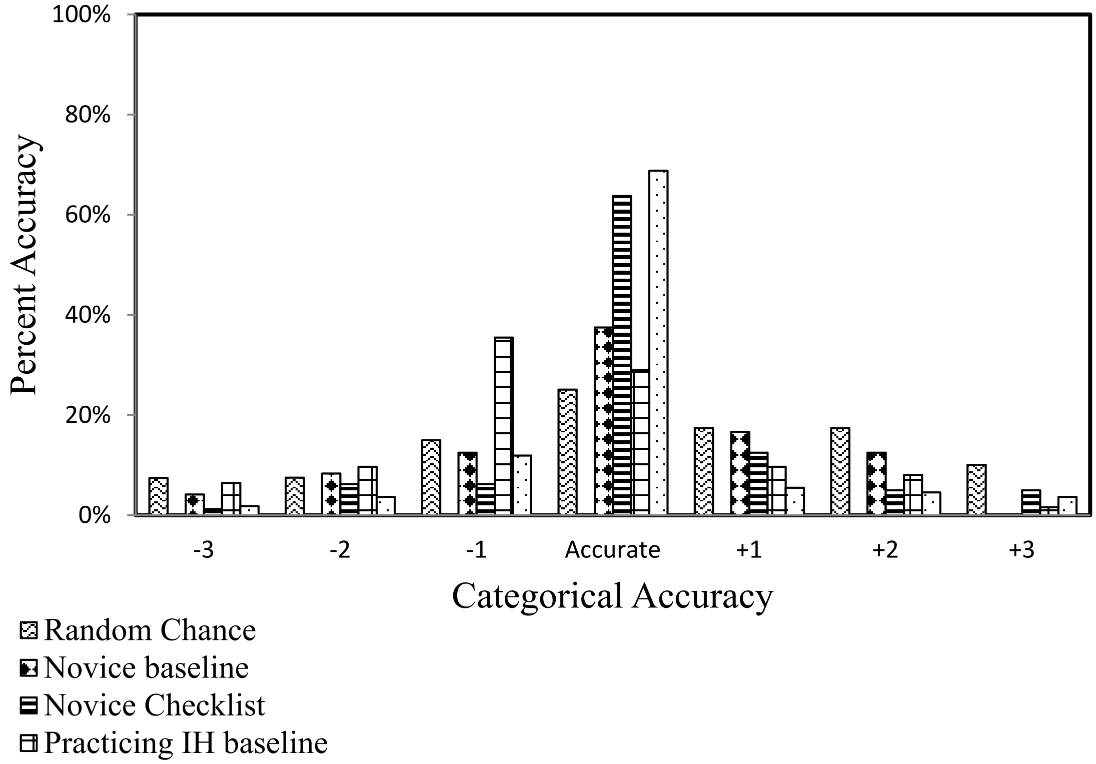

Figure 5-2 Categorical Judgment Accuracy, showing accuracy attributable to random chance pre-training (Baseline), post-training Checklist-guided judgment accuracy for Novices and practicing IHs.

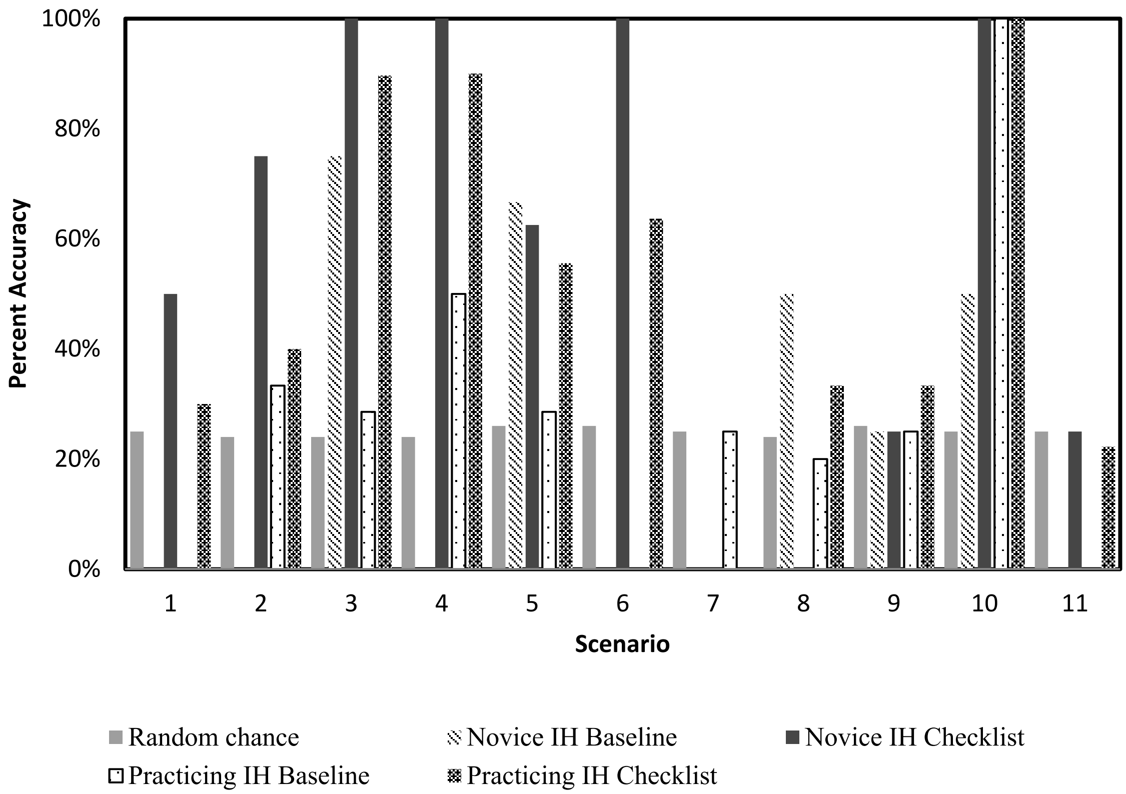

Figure 5-3Baseline and Checklist based judgment accuracy for Novice IHs and practicing IHs respectively, broken out by scenario

Table 5-1 AIHA Exposure Control Categories (ECC) with criteria for interpretation

Exposure Control Category (ECC)	**Criteria for Statistical Interpretation**
1	$X_{0.95} \leq 0.1 \times OEL$
2	$0.1 \times OEL < X_{0.95} \leq 0.5 \times OEL$
3	$0.5 \times OEL < X_{0.95} \leq OEL$
4	$X_{0.95} > OEL$

Table 5-2 Rule of 10 Engineering Control Matrix

Level of Control	Fraction of the Saturation Vapor Concentration (SVC)
Confined Space – Virtually no circulation	1/10th of Saturation
Poor – Limited Circulation	1/100th of Saturation
Good – General ~ 6 Air Changes/Hour	1/1,000th of Saturation
Capture	1/10,000th of Saturation
Containment	1/100,000th of Saturation

Table 5-3 Vapor Hazard Ratio (VHR) Engineering Control Matrix

Vapor Hazard Ratio (VHR)	VHR Scale	Required Level of Control (ReqLC)
< 0.05	1	General Ventilation ~ 3 to 6 air changes /hr.
0.05 to < 1	2	Good general ventilation ~ 6 to 12 air changes/hr. (GGV)
1 to < 25	3	GGV with capture at emission points
25 to < 500	4	Capture at points of emission with containment wherever practical
500 to < 3000	5	Containment
> 3000	6	Primary and Secondary Containment

Table 5-4 Particulate Hazard Ratio (PHR) Engineering Control Matrix

OEL Range (mg/m^3)	PHR Scale	Required Level of Control (ReqLC)
5	1	General ventilation ~ 2 to 4 air changes/hr.
≤ 5 to 1	2	Good – General + fans ~ 4 to 6 air changes/hr.
≤ 1 to 0.1	3	Good – General + fans ~ 6 to 8 air changes/hr.
≤ 0.1 to 0.01	4	Capture
≤ 0.01 to 0.001	5	Containment
≤ 0.001	6	Secondary containment

Table 5-5 The Checklist - an ordered approach to applying the three heuristics

Rule of 10	1. Select the appropriate Occupational Exposure Limit (OEL) 2. Determine the Vapor Pressure & Saturated Vapor Concentration (SVC) 3. Identify the Observed Or Reported Level of Control (ObsLC) 4. Estimate the fraction of the SVC 5. Calculate the maximum concentration (C_{max}) 6. Compare the C_{max} to the OEL 7. Determine the predicted Exposure Control Category (ECC)
Vapor Hazard Ratio (VHR)	1. Divide VP/OEL to determine VHR Score 2. Identify Required Level of Control (ReqLC) from VHR matrix 3. Compare ReqLC with ObsLC 4. Determine ECC: If ObsLC > ReqLC= 1 If ObsLC = ReqLC = 2 If ObsLC < ReqLC = 4 5. If the ECC's based on Rule of 10 & VHR differ, use the highest ECC
Particulate Hazard Ratio (PHR)	1. Identify OEL 2. Identify ReqLC from PHR matrix 3. Compare ReqLC with ObsLC 4. Determine ECC: If ObsLC > ReqLC = 1 If ObsLC = ReqLC = 2 If ObsLC < ReqLC = 4

Table 5-6 Exposure Scenario Details, showing the Scenario number, agent of concern (Chemical Agent), the relevant OEL , the primary task or work process from

which the exposure occurred (Process), the number of personal exposure samples collected, from which the Reference ECC was calculated (Reference ECC data set) and the corresponding Reference ECC.

Scenario	Chemical Agent	OEL	Process	Number of measurements in Reference ECC data set (n)	ECC
1	Glutaraldehyde	Cal OSHA ceiling: 0.05 ppm	Neutralizing, dumping and pouring liquid	6	2
2	Mannitol	NIOSH REL: 8 hour TWA: 0.25 µg/m^3	Potent compound transfer	6	2
3	Trichloro-ethylene	ACGIH TLV TWA: 5 ppm	Spray cleaning degreaser	11	4
4	Asbestos	OSHA PEL: 8 hour TWA: 0.1 f/cc	Locomotive steamline repair	9	2
5	Isopropanol	OSHA PEL: 8 hour TWA 400 ppm	Cleaning printing presses	8	2
6	Hexavalent chromium	OSHA PEL: 8 hr. TWA: 0.5 mg/m3	Repair – welding railroad frog	8	4
7	Asbestos	OSHA PEL: 30 min. excursion limit: 1 f/cc	Bystander exposure in locomotive repair shop	29	1
8	Acetone	OSHA PEL: 8 hour TWA: 1000 ppm	Cleaning printing presses	8	1
9	Phenol	ACGIH TLV: TWA: 5 ppm	Foundry shell core – mold making	8	1
10	Quartz	ACGIH TLV TWA for α-quartz = 0.025 mg/m^3	Foundry shake out – breaking molded parts	8	4
11	Methylene chloride	OSHA PEL: 15 min. STEL: 125 ppm	Collecting a sample from a vessel	10	4

Table 5-7a Results from novice IHs' exposure judgments, showing bias (the difference between the average predicted ECC and reference ECC), and Precision (standard deviation) for each scenario (n = 8)

Scenario	**Bias**		**Precision**	
	Baseline	Checklist	Baseline	Checklist
1	0.5	-.13	0.84	0.98
2	0.3	-.25	0.64	0.46
3	-0.5	0	0.76	0
4	-3	0	0	0
5	0.3	0.8	0.64	1.04
6	-1	0	0	0
7	0.5	1.6	0.84	0.92
8	1.3	1.3	1.2	1.16
9	-1	0	1.19	0
10	-1	-1.6	1.19	1.06

Table 2-7b Results from practicing IH exposure judgments, showing bias, (the difference between the average predicted ECC and reference ECC), and Precision (standard deviation) for each scenario by .

Scenario	n		Bias		Precision	
	Baseline	Checklist	Baseline	Checklist	Baseline	Checklist
1	2	10	0	-0.7	NA	0.48
2	3	10	1	-0.6	1.00	0.52
3	30	29	-1.1	-0.1	0.94	0.33
4	2	10	-0.5	-0.3	0.71	.95
5	7	9	-0.7	0.3	0.57	0.87
6	4	11	-1.5	-0.5	1.0	1.00
7	4	3	1.2	1.2	0.5	1.17
8	6	6	1.5	1.7	1.0	1.32
9	2	9	0	0	0	0
10	2	9	-2	1.4	NA	1.01

Table 5-8 Exposure Scenario using the OEL as the benchmark, OEL = 10 ppm, GSD = 2.5

EF	GM	95^{th} % (ppm)	Distribution < AL	Probability (%) that All Indicated Measurements of Dataset Size N (N = 1,2,3, 4 or 5) Will Fall Below the OEL				
				N = 1	N = 2	N = 3	N = 4	N = 5
0.5	10	45.15	0.5	50	25	12.5	6.25	3.13
0.25	5.39	24.32	0.75	75	56.3	42.2	31.6	23.7
0.1	3.09	13.95	0.9	90	81	72.9	65.6	59.1
0.05	2.22	10	0.95	95	90.3	85.7	81.5	77.4
0.02	1.52	6.87	0.98	98	96	94.1	92.2	90.4

APPENDIX II

Well Mixed Room Model

The Well Mixed Room (WMR) model considers exposures as a factor of air movement into, through and out of a room and the generation rate of a contaminant within the room. A key assumption of this model is that air in the room is completely and instantaneously well mixed; a physically unrealistic but useful construct for estimating the average concentration when the contaminant is generated from a large or non-point source. (Ramachandran, 2005)

While there are various forms of the model depending on the contaminant source, the constant emission source will be described here since it is the form used in this study. Several terms are invoked to apply the conservation of mass principle, accounting for the movement of contaminant mass. . In a room of volume, V (e.g. m^3) with a constant ventilation rate, Q (m^3/min), air entering the room has a contaminant concentration of Cin (mg/m^3), and a contaminant source in the room, C (mg/m^3) generating an airborne concentration at a constant generation rate, G (mg/min). Thus, as air enters the room and the source contributes contaminant to the room air the contaminant concentration in the room increases.

Air enters and exits the room, either actively, via mechanical ventilation systems or passively, through doors and windows or cracks and spaces around them. We assume that the rate at which air enters is the same as when air exists the room, i.e., $Q_{in} = Q_{out}$ and thus drop the subscripts.

When air leaves the room, it removes some of the contaminant. Contaminant mass may also be removed by other mechanisms, for example, vapor and gases may adsorb onto surfaces in the room and aerosols of certain size ranges may be lost due to gravitational settling. These loss mechanisms are summed up into one loss term, denoted by k_L. Thus, the contaminant concentration in the room is reduced as these mechanisms remove the contaminants from the room air.

The general equation for the WMR model as a function of time is expressed as:

$$C(t) = \frac{G + C_{in} \times Q}{Q + k_L \times V}\left[1 - exp\left(-\frac{Q + k_L \times V}{V} \times t\right)\right] + C(0)exp\left(-\frac{Q + k_L \times V}{V} \times t\right) \quad \text{(A-1)}$$

At steady state, the expression compresses to

$$C(SS) = \frac{G}{Q} \quad \text{(A-2)}$$

Near Field Far Field Model

When a person is located close to a contaminant source, the WMR model will underestimate that person's exposure. The Near Field Far Field (NF FF) model is designed to account for this deficiency, but at a cost of added complexity, and the non-trivial investment in acquiring data to characterize the additional model inputs.

This model assumes a two box construct, with the air within each box well mixed. The area close to and around the source is the Near Field (NF) and can be described using a range of geometries, such as a box, sphere, hemisphere, etc. The geometry is defined on a scenario by scenario basis. The rest of the room is the Far Field (FF).

The supply and exhaust flow rates are the same, and denoted by Q (m^3/min), consistent with the WMR model. Air movement from one box to the other is called the interzonal airflow rate and is denoted by the symbol ß (m^3/min). Q can be measured directly in many cases, but quantifying ß is more complicated. The most common approach to estimate ß is to determine the product of the random air speed at the NF FF boundary and one half the free surface area (FSA) of the NF.(Ramachandran, 2005). Thus, ß is somewhat dependent on the geometry used to define the NF.

$$\beta = \frac{1}{2FSA} \times s \quad \text{(A-3)}$$

The ½ accounts for the fact that as ß flows into the NF through one half the FSA, ß flows out of the NF through the other half of the FSA.

The NF and FF equations are

$$C_{NF}(t) = \frac{G}{Q} + \frac{G}{\beta} + G \times \left[\frac{\beta\times Q + \lambda_2\times V_{NF}(\beta+Q)}{\beta\times Q \times V_{NF}(\lambda_1-\lambda_2)}\right] \times \exp(\lambda_1 \times t) - G \times \left[\frac{\beta\times Q + \lambda_1\times V_{NF}(\beta+Q)}{\beta\times Q \times V_{NF}(\lambda_1-\lambda_2)}\right] \times \exp(\lambda_2 \times t) \quad \text{(A-4)}$$

$$C_{FF}(t) = \frac{G}{Q} + G \times \left[\frac{\lambda_1\times V_{NF}+\beta}{\beta}\right] \times \left[\frac{\beta\times Q + \lambda_2\times V_{NF}(\beta+Q)}{\beta\times Q \times V_{NF}(\lambda_1-\lambda_2)}\right] \exp(\lambda_1 \times t) - G \times \left[\frac{\lambda_2\times V_{NF}+\beta}{\beta}\right] \times \left[\frac{\beta\times Q + \lambda_1\times V_{NF}(\beta+Q)}{\beta\times Q \times V_{NF}(\lambda_1-\lambda_2)}\right] \exp(\lambda_2 \times t) \quad \text{(A-5)}$$

Where $\lambda_1 = 0.5 - \left[\frac{\beta\times V_F + V_N(\beta+Q)}{V_{NF}\times V_{FF}}\right] + \sqrt{\left[\frac{\beta\times V_F + V_N(\beta+Q)^2}{V_{NF}\times V_{FF}} - 4\left[\frac{\beta\times Q}{V_{NF}\times V_{FF}}\right]\right]}$ (A-6)

And $\lambda_2 = 0.5 - \left[\frac{\beta\times V_F + V_N(\beta+Q)}{V_{NF}\times V_{FF}}\right] - \sqrt{\left[\frac{\beta\times V_F + V_N(\beta+Q)^2}{V_{NF}\times V_{FF}} - 4\left[\frac{\beta\times Q}{V_{NF}\times V_{FF}}\right]\right]}$ (A-7)

At Steady State, these equations shrink considerably to:

$$C_{NF}(SS) = \frac{G}{Q} + \frac{G}{\beta} \quad \text{(A-8)}$$

$$C_{FF}(SS) = \frac{G}{Q} \quad \text{(A-9)}$$