VALIDATION OF TWO QUALITATIVE OCCUPATIONAL EXPOSURE ASSESSMENT MODELS FOR PARTICULATES AND VAPORS

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ABSTRACT

To ensure industrial workers are not overexposed to hazardous chemicals, it is necessary to evaluate the magnitude of occupational exposures. Small and medium sized companies usually do not employ industrial hygienists or other professionals trained in occupational exposure evaluations. Thus, traditional quantitative air sampling methods are usually not feasible due to resource and budgetary limitations.

Qualitative exposure assessment models have gained in popularity because they are simple, inexpensive, and less time consuming than quantitative methods. Models are available which predict exposure concentrations or categorize exposures as acceptable or unacceptable. Unfortunately, most models have not been validated or previous studies have shown models perform differently in different exposure conditions.

The primary purpose of this study was to validate the Control of Substances Hazardous to Health (COSHH) Essentials model and the Qualitative Exposure Assessment (QLEA) model in low, medium, and high occupational exposure conditions involving particulates and vapors.

COSHH Essentials was developed by the United Kingdom and predicts a range of possible concentrations based on the usage quantity and volatility (or dustiness) of the chemical substance. The QLEA Model was developed by a global manufacturing company. It classifies an exposures as acceptable, unacceptable, or uncertain using four
predictor variables: duration of exposure, toxicity for inhalation, airborne risk, and controls present.

This study compared model predictions with retrospective exposure measurements obtained from National Institute of Occupational Safety and Health (NIOSH) Health Hazard Evaluation (HHE) Reports for 199 similar exposure groups (SEGs). SEGs were stratified based on the magnitude of the measured exposure (low, medium, high) and the physical state of the chemical substance (particulate or vapor).

This study illustrated that both models are vastly over-protective in low level exposure situations. Thus, prior to widespread adoption of these models, the rational concerning each model’s design should be critically evaluated and potentially modified to lessen the magnitude of over-prediction.
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CHAPTER 1
INTRODUCTION

Industrial hygiene is the science and art, dedicated to the anticipation, recognition, evaluation, and control of environmental factors arising in or from the workplace that may result in injury, illness, impairment, or affect the well-being of workers and members of the community (Plog, 1996). Central to this effort is the anticipation and recognition of occupational exposures to chemical agents, evaluation of exposures utilizing various exposure assessment methods, and control of exposures through the implementation of administrative, behavioral, and engineering controls (Mulhausen and Damiano, 2003).

Exposure to chemical contaminants in the occupational environment is typically unavoidable. Therefore, evaluation of the magnitude of exposures is critical to protect the health of industrial workers. Not only is it a best management practice for employers to evaluate occupational exposures, it is also a regulatory requirement under the OSHA Act (Leidel, Busch, and Lynch, 1977).

Occupational Exposure Assessment

Exposure assessment is the evaluation (quantitative, semi-quantitative, or qualitative) of the magnitude, frequency, duration, and route of exposure. When
conducting an occupational exposure assessment, the first step is to define the purpose and scope of the evaluation. Exposure assessments can be performed for various reasons.

For instance, exposure assessments may be used to evaluate compliance with Occupational Safety and Health Administration (OSHA) standards, comprehensively evaluate exposures in a specific work area, respond to employee complaints, or evaluate the effectiveness of engineering controls (Milz, Conrad, and Soule, 2003). Once the purpose and scope of the exposure assessment is defined, basic information characterizing the workplace, the workforce, and the work environment is gathered. Examples of information needed include job titles, task descriptions, process information, chemicals agents used, potential adverse health affects, toxicological information, and controls present (Stewart and Stenzel, 2000). After all preliminary information is gathered, a quantitative, semi-quantitative, or qualitative exposure assessment can be conducted to provide an estimate of the exposure concentration.

Once the occupational exposure assessment is completed, the exposure estimate is compared to an Occupational Exposure Limit (OEL). Several countries including the United States, the United Kingdom, Canada, Germany, etc. have established mandatory and recommended OELs (Lu and Kacew, 2002). These limits “represent conditions under which it is believed nearly all workers may be repeatedly exposed, day after day, without adverse health effects” (ACGIH, 2001, p. i). It’s important to keep in mind that while some OELs are based on extensive laboratory and epidemiological data, others are based solely on analogies and professional judgment (Lu and Kacew, 2002). One must weigh the facts and decide whether to use the regulatory limit [OSHA Permissible Exposure Limit (PEL)] or select a more conservative limit from among the American
Conference of Governmental Industrial Hygienists (ACGIH) Threshold Limit Values (TLV), National Institute of Occupational Safety and Health (NIOSH) Recommended Exposure Limits (REL), American Industrial Hygiene Association (AIHA) Workplace Environmental Exposure Limits (WEEL), or an in-house exposure limit (Klonne, 2003).

The final phase of the exposure assessment is to determine whether the evaluated exposure is acceptable, unacceptable, or uncertain. Both uncertainty in the exposure estimate and the OEL should be taken into consideration. Exposure estimates less than the OEL are considered acceptable. Acceptable exposures are associated with a low risk and do not require further action other than periodic review. Exposure estimates greater than the OEL are considered unacceptable. It is often easier to determine if an exposure is unacceptable than acceptable. Unacceptable exposures are associated with a high risk and should be controlled immediately. Lastly, if the exposure estimate is in close proximity to the OEL and can not confidently be classified as acceptable or unacceptable, the evaluated exposure is considered uncertain. Exposures may be uncertain due to lack of data, inadequate characterization of the work processes, or the inability to select an OEL due to limited health hazard information and the lack of established limits. Additional information concerning the workplace, workforce and/or the toxicity of the chemical agent must be collected to resolve uncertain exposures (Mulhausen and Damiano, 1998).

**Exposure Assessment Methods**

Depending on the purpose of the exposure assessment and the level of certainty desired, different methods can be utilized to assess occupational exposures. Exposure
assessment methods include quantitative, semi-quantitative, and qualitative approaches. Different approaches provide varied levels of certainty and have different limitations. In addition, the degree of industrial hygiene knowledge required to accurately utilize a particular exposure assessment method differs among methods. Normally, exposures are initially prioritized for further analysis using qualitative evaluations. Then, based on the level of certainty required, semi-quantitative (mathematical modeling) or quantitative (air sampling) techniques may be utilized (Milz, Conrad, and Soule, 2003).

Quantitative Methods

The “gold standard” for evaluating occupational exposures has traditionally been quantitative air sampling (Keil and Murphy, 2006). Samples can be collected using direct reading instruments, which give immediate results concerning the concentration of airborne contaminants, or collected on media that is subsequently analyzed by a scientific laboratory to yield the airborne concentration (Huey, 1996). Conventionally, quantitative air sampling methodology has utilized a compliance monitoring approach which focused efforts on “maximum risk employees”. If “maximum risk employees” were shown to have exposures below the OEL, it was reasonable to deduce that other employees were also not overexposed (Leidel et al., 1977).

Recently, focus has shifted from compliance monitoring to comprehensive exposure assessments, which involves the characterization of potential exposures to all workers on all days, not just maximum risk employees (Mulhausen and Damiano, 1998). Because the evaluation of daily exposures for every employee is virtually impossible, employees are combined into similar exposure groups (SEGs). SEGs consist of
employees who perform similar tasks using similar frequencies, materials, processes, and techniques, and thus have the same general exposure profile (Stewart and Stenzel, 2000). The exposure of a small portion of the group is randomly assessed, and the results of the assessment are considered representative of the entire group (Mulhausen and Damiano, 1998).

Two methods can be used to define SEGs: the observational approach and the sampling approach. The observational approach places workers in SEGs based on their daily activities (e.g. process, job, task, and environmental agent). Various hierarchical strategies have been suggested for establishing SEGs such as: classifying by process and environmental agent; classifying by process, job, and environmental agent; and classifying by process, job, task, and environmental agent (Mulhausen and Damiano, 1998).

Industrial operations are generally divided into administrative departments corresponding to distinct processes. Thus, administrative departments are often considered equivalent to the process element of the SEG. Unfortunately, categorization of workers at the process level rarely represents an SEG. Therefore, specific jobs within each process are compared to define multiple SEGs within a process. Occasionally, classification schemes are further defined by identifying tasks or specific work elements. However, it is often impractical to identify all tasks in an industrial operation. Therefore, task characterization is only necessary when such detail will have a significant contribution to understanding exposure (e.g. assessing peak exposures is inherently task-related).
The sampling approach utilizes statistically analyzed monitoring data to group workers in SEGs. An accepted quantitative measure is to determine the long-term arithmetic mean exposure of each worker in an SEG; 95% of the workers in the SEG should have a maximum difference between their long-term average exposures no greater than a factor of two as illustrated in Figure 1 (Mulhausen and Damiano, 1998). The sampling approach lacks the potential for errors in professional judgment, which is advantageous. However, a large number of measurements are necessary to accurately utilize the sampling approach and rarely this prerequisite is feasible and cost efficient. Ultimately, industrial hygienists generally utilize the observation approach to initially form SEGs and accept the risk of potentially miss-categorizing some employees (Mulhausen and Damiano, 1998).

Figure 1. Maximum different between AM exposures no greater than a factor of two for 95% of workers in SEG

Regardless of how carefully the sampling procedure and subsequent analysis are performed, quantitative air sampling only provides an estimate of the true average
concentration that exists in the environment. Some uncertainty will exist due to random
error caused by random fluctuations in pump flow rates, random analytical method errors
due to variability in chemical laboratory procedures, and random intraday and interday
fluctuations in airborne concentrations. A contaminant’s airborne concentration often
varies between days and among workers due to changes in the physical process that
generates the contaminant and spatial and temporal changes in an employee’s work habits
(Leidel et al., 1977). These random errors are sometimes called statistical errors since
they can be accounted for using statistical analysis.

Experience has shown that most occupational exposure data are best described by
a lognormal distribution because occupational exposure concentrations cover a wide
range of values; zero is the physical lower limit for possible values, large values
occasionally occur, and the processes that generate or control exposures tend to interact
in a multiplicative manner (Liedel et al., 1977; Hewett, 2007). Lognormally distributed
data (i.e. the logarithms (base $e$) of the data are approximately normally distributed) are
positively skewed, as shown in Figure 2, and are defined by the geometric mean (GM)
and the geometric standard deviation (GSD). The GM is an estimate of the median of the
exposure distribution and is calculated as the antilog of the averaged logtransformed data.
The GSD is a measure of the degree of dispersion in the data and is calculated as the
antilog of the standard deviation of the logtransformed data. A GSD of 1.0 indicates no
variation in the data (Liedel et. al, 1977). A GSD $\leq 1.5$ indicates low exposure variability,
a GSD between 1.5 and 2.5 indicates moderate exposure variability, and a GSD $> 2.5$
indicates high exposure variability (Hewett, 2007). As a guiding principle, an exposure
profile with a GSD greater than 3 should be evaluated to see if dissimilar workers or activities have erroneously been combined or if too few data exist (Hewett, 2007).

![Lognormal distribution](image)

**Figure 2. Lognormal distribution**

Although the lognormal distribution is defined by the GM and GSD, the arithmetic mean (AM) of a lognormal exposure distribution, not the GM, is the best descriptor of long term average exposure (Rappaport, 1991). For a normal distribution, the estimated AM is equivalent to the sample mean. However, for a lognormal distribution, the AM differs from the sample mean and must be estimated. Several methods exist for estimating the AM. However, the minimum variance unbiased estimator (MVUE) is the preferred point estimate of the true mean when the sample size is small and/or the sample GSD is large. The MVUE is difficult to compute by hand, thus a computer or programmable calculator is often utilized (Hewett, 2007).

Although occupational exposure data are presumed to be lognormally distributed, prior to conducting statistical analysis, the assumption of lognormality should be
confirmed. Data that are not lognormally distributed prompts review of the original categorization of workers into SEGs (Hewett, 2007).

Although quantitative air sampling is considered the “gold standard” for exposure assessment, it has some inherent limitations. The costs associated with sampling in terms of equipment (pumps, calibration devices, sampling media) and subsequent analysis can be quite expensive. In addition, quantitative sampling can be very time consuming. To obtain a representative sample, randomization is necessary. Therefore, quantitative sampling may require several weeks or several months to complete. Additionally, when conducting quantitative sampling and analyzing sampling results a certain level of expertise is required. Small and medium sized companies usually do not employ industrial hygienists or other trained professionals such as engineers, safety managers, etc. who are involved in occupational exposure evaluations. Therefore, it is usually not feasible for small and medium sized companies to conduct quantitative sampling due to budgetary and resource limitations.

*Semi-quantitative Methods*

A second approach to exposure assessment involves the use of semi-quantitative methods or mathematical models. Mathematical models can be used to estimate the concentration or predict the behavior of air contaminants in the workplace (Burton, 2004). Most models are based on the principle of the conservation of mass and use parameters such as the generation rate of a contaminant, vapor pressure of a contaminant, room volume, room ventilation rate, process temperature, etc. to describe the physical-chemical system that produces an exposure (Keil, 2000c; Keil, 2000b).
A wide variety of mathematical models exist ranging in complexity. These different levels of complexity are sometimes referred to as modeling “tiers”. Lowered tiered models are simple to use and include input variables that are readily available, such as vapor pressure of the contaminant and process temperature. Higher tiered models are more complex and often difficult to use because they require more precise input variables such as the generation rate of pollutants and room ventilation rates. Models become even more complex when the variability in generation rates and room mixing patterns due to mechanical ventilation are considered (Keil, 2000c). Lowered tiered models generally result in uncertain exposure predictions due to the conservative assumptions made by the models. In contrast, higher tiered models can provide predictions with much less uncertainty; however, their use is often limited by the availability and understanding of the input variables required (Keil, 2000b).

When determining which mathematical model to use, a tiered approach is useful. If lower tiered models result in an exposure estimate well below the OEL, it is generally unnecessary to apply more complex models. However, if lower tiered models result in an exposure estimate that is considered unacceptable or uncertain, it may be useful to apply higher tiered models (Keil, 2000c). A few mathematical models are briefly discussed below to provide an example of the tiered approach to modeling.

**Zero ventilation model.** The simplest mathematical model is the zero ventilation model. As indicated by the name, this model assumes there is no mechanical ventilation in the room. The concentration of a contaminant in air, C(mg/m³) is calculated by assuming that the entire mass of the chemical enters the air instantaneously and the
predicted concentration is assumed to be homogeneous throughout the room. The mass of contaminant available for evaporation is expressed in milligrams (mg), and the volume of the room, \( V \) is expressed in cubic meters (m\(^3\)). Because of the assumptions, the zero ventilation model typically overestimates exposures, especially in ventilated rooms. The model’s equation is shown in equation 1 (Keil and Murphy, 2006).

\[
C = \frac{\text{mass available for evaporation}}{V}
\]  

(1)

**Saturation vapor pressure (SVP) model.** The saturation vapor pressure (SVP) model uses the vapor pressure of the contaminant to calculate the worst case estimate of airborne concentration. Vapor pressure (VP) is defined as the pressure exerted when a pure solid or liquid is in equilibrium with its own vapor (Reinke, 2000b). The SVP model makes several assumptions. For instance, it is assumed that the liquid contaminant is allowed to evaporate for a long period of time, and sufficient liquid is present to allow the entire room to reach an equilibrium concentration. The model also assumes that the room is totally enclosed with no ventilation, the temperature remains constant, and Dalton’s law of partial pressures and the Ideal gas law are valid (Reinke, 2000b).

The Ideal gas law states that at constant temperature and volume, pressure is only a function of the number of molecules present. Therefore, the pressure of an ideal gas in a mixture is equal to the pressure it would exert if it occupied the same volume alone at the same temperature. As a consequence, Dalton’s law of partial pressures states that the
The total pressure of a mixture of ideal gases is equal to the sum of the partial pressures of the individual gases in the mixture (Reinke, 2000b).

The SVP model calculates the concentration of the contaminant in air in parts per million (ppm) according to equation 2, using the VP of the contaminant and atmospheric pressure, $P_{\text{atm}}$ in equivalent units. Due to the assumptions made by the SVP model, the calculated concentration is highly overestimating. In fact, the model has been shown to overestimate airborne concentrations by 1 to 4 orders of magnitude in some cases (Reinke, 2000b).

$$C(\text{ppm}) = 10^6 \times \frac{\text{VP}}{P_{\text{atm}}} \quad (2)$$

The two main components of an indoor air model are the generation term and the dispersion term. The generation term in the SVP model is an evaporating liquid or subliming solid. The dispersion term is not necessary in the SVP model because the model assumes that the room is totally enclosed with no ventilation and the entire room reaches equilibrium.

**Well mixed room (WMR) model.** The Well Mixed Room (WMR) model is the simplest representation of dispersion. It models a room as a large box with very turbulent airflow (Reinke, 2000a). The WMR model assumes that the room, or “box”, is perfectly mixed and air is moving as if there were several fans pushing air around the room. In addition, the model assumes that the concentration of the contaminant is uniform throughout the room, the generation rate of the contaminant is constant and low.
compared to airflow rates in and out of the room, the contaminant can generate gas, vapor, or aerosol, and the contaminant is only removed through the exhaust or ventilation system (Reinke, 2000a).

Assuming that the initial concentration of the contaminant in the room is zero, and no contaminant is present in the incoming air, the WMR model calculates the concentration of contaminant in air, \( C(\text{mg/m}^3) \) using the generation rate of the contaminant, \( G(\text{mg/s}) \), the room ventilation rate, \( Q(\text{m}^3/\text{s}) \), the amount of time elapsed, \( t(\text{s}) \), and the room volume, \( V(\text{m}^3) \) according to equation 4 (Keil and Murphy, 2006; Reinke, 2000a).

\[
C = \frac{G}{Q} \left( 1 - e^{-\frac{Qt}{V}} \right)
\]

Steady state concentrations occur when the physical properties of a system do not change with time. The time required for a room or system to reach steady state varies depending on the situation. The WMR model’s steady state concentration, \( C_{ss}(\text{mg/m}^3) \) can be calculated from equation 4 by assuming that the system operates unchanged for a long period of time \((t \to \infty)\). When \( t \) approaches infinity, then \( e^{-\frac{Qt}{V}} \) approaches zero. Equation 4 shows the WMR model steady state equation (Keil and Murphy, 2006; Reinke, 2000a).

\[
C_{ss} = \frac{G}{Q}
\]
Previous sampling data have indicated that exposure intensity is higher near the contaminant emission source. Because the WMR model treats the concentration as uniform throughout the room, it usually provides an adequate estimate of exposures far from the source. However, it typically underestimates exposure intensity close to the source (Nicas, 2000)

*Two-zone model.* The two-zone model conceptually divides a room into two boxes termed the near-field and the far-field. The near-field contains the emission source and is sized to include the breathing zone of the worker. The remainder of the room is considered the far-field. The two-zone model assumes that air is well mixed within each box; however, air flow is limited between boxes. The model assumes that air flows in and out of the near-field at a constant rate denoted by the interbox airflow rate, \( \beta (\text{m}^3/\text{min}) \) (Nicas, 2000). If the contaminant lingers near the source, then \( \beta \) will be small; however, if the contaminant is quickly dispersed from the source, \( \beta \) will be large. The interbox airflow rate is calculated using the surface area of the near-field, \( SA (\text{m}^2) \) and the average random air speed, \( s (\text{m/min}) \) according to equation 5 (Nicas, 2000). Unfortunately, little guidance is available on how the average random air speed should be measured for use in the calculation. Another disadvantage of the two-zone model is that no guidance is available for determining the size and shape of the near field (Keil, 2000c).

\[
\beta = \frac{1}{2} \times \text{SA} \times s
\]  

(5)
Other assumptions of the model are that the room’s supply air flows in and out of the far-field at a constant rate, the contaminant is generated at a constant rate, and the contaminant is only removed from the near and far fields via airflow and mechanical ventilation, respectively (Nicas, 2000). The concentration of contaminant in the near field, \( C_N \) and the far field, \( C_F \) are calculated using equations 6 and 7, respectively (Nicas, 2000).

\[
C_N = \frac{G}{Q} \times \frac{G}{\beta} + G \left( \frac{\beta \times Q + \lambda_2 \times V_N (\beta + Q)}{\beta \times Q \times V_N (\lambda_1 - \lambda_2)} \right) \times e^{\lambda_2 t}
\]

(6)

\[
C_F = \frac{G}{G} + G \left( \frac{\lambda_2 \times V_N \times \beta}{\beta} - \frac{\lambda_1 \times V_N \times \beta}{\beta} \right) \times e^{\lambda_2 t}
\]

(7)

Where:

- \( V_N \) and \( V_F \) = the near-field and far-field volumes, respectively (m\(^3\))
- \( G \) = constant mass emission rate (mg/min)
- \( Q \) = room supply air rate (m\(^3\)/min)
- \( t \) = time (min)

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

(8)

\[
\lambda_2 = 0.5 \left[ - \left( \frac{\beta \times V_F + V_N (\beta + Q)}{V_N \times V_F} \right) - \sqrt{\left( \frac{\beta \times V_F + V_N (\beta + Q)}{V_N \times V_F} \right)^2 - 4 \left( \frac{\beta \times Q}{V_N \times V_F} \right)} \right]
\]

(9)

Oftentimes mathematically complex models, such as the two-zone model, are programmed into a spreadsheet like Microsoft EXCEL\textsuperscript{®} to aid in the calculations (Nicas,...
and Armstrong, 2003). Another option is to make necessary assumptions to simplify the calculations. In the two-zone model, the parameters $\lambda_1$ and $\lambda_2$ will be negative numbers for practically all realistic scenarios. Therefore, as $t$ gets large ($t \to \infty$) and steady state concentrations are reached in the near-field, $C_{N,SS}$ and the far field, $C_{F,SS}$ the terms $e^{\lambda_1 t}$ and $e^{\lambda_2 t}$ approach zero and equations 6 and 7 are simplified to calculate near and far field concentrations at steady state as shown in equations 10 and 11 (Nicas, 2000).

\[ C_{N,SS} = \frac{G}{Q} + \frac{G}{\beta} \]  

(10)

\[ C_{F,SS} = \frac{G}{Q} \]  

(11)

All of the mathematical models discussed to this point have either represented the indoor environment as either a perfectly mixed space or as multiple zones with each zone perfectly mixed. These approaches will result in an adequate estimate of contaminant concentration most of the time. However, a model designed to account for concentration gradients around the emission source would better characterize contaminant concentrations in the indoor environment (Keil, 2000a).

**Eddy diffusion modeling.** In the absence of a cross draft, an emission source will diffuse a contaminant in a spherical pattern (Keil, 2000a). In the workplace, however, air is never perfectly still. The motion of a room’s occupants or the decay of air flow from supply air diffusers results in small vortexes of air, referred to as “eddies” (Keil, 2000a).
Eddy diffusion modeling accounts for these small pockets of turbulent airflow using the eddy diffusion coefficient, $D (m^2/\text{min})$. The model works best in environments where air velocities are less than 15 m/min (Keil, 2000c). Eddy diffusion modeling assumes that a point source generates a contaminant at a constant rate with no initial momentum, and diffusion of the contaminant occurs in a spherical pattern into an infinite space (Keil, 2000a). The steady state equation for the eddy diffusion model is shown in equation 12.

$$C = \frac{G}{4\pi Dr}$$  \hspace{1cm} (12)

Where:
- $G =$ generation rate (mg/min)
- $D =$ eddy diffusion coefficient (m$^2$/min)
- $r =$ distances from source to worker (m)

Unfortunately, because eddy diffusion is a turbulence phenomenon, very little theoretical information is available to estimate the eddy diffusion rate, $D$ (Keil, 2000a). It is possible to experimentally determine the diffusion coefficient; however, such efforts are difficult and time consuming.

In general, most mathematical models are not well validated. This is in part due to the tiered approach to modeling. Lower tiered models are applied initially, and depending on the exposure estimate’s relationship to the OEL, more complex models may be applied. A small number of higher tiered models are available. However, they are more difficult to use due to uncertainty in selecting input parameters. Therefore, when mathematical modeling results in an uncertain estimate of exposure, air sampling is normally conducted rather than refining the mathematical model. While, air sampling
provides a direct measurement of the contaminant concentration in air, such recourse has delayed the development of mathematical modeling (Mulhausen and Damiano, 1998).

Mathematical modeling can potentially be a useful tool to estimate occupational exposures when trained industrial hygienists are employed. However, most small and medium sized businesses do not employ an industrial hygienist or other trained professional skilled in quantitative sampling techniques and/or knowledgeable in the physicochemical properties of chemical contaminants. Therefore, the acceptance and use of mathematical models as an exposure assessment tool by small business owners is unlikely.

**Qualitative Methods**

As a result, the use of qualitative exposure assessment models has gained in popularity over the past decade. Qualitative models are simpler to apply, less expensive, and less time consuming than quantitative monitoring and mathematical models. A variety of qualitative models are available which estimate exposure concentrations or classify exposures as acceptable or unacceptable using predictor variables such as vapor pressure, duration of exposure, chemical toxicity, etc. The most developed and widely used qualitative models are the Estimation and Assessment of Substance Exposure (EASE) and the Control of Substances Hazardous to Health (COSHH) Essentials models.

**EASE model.** The EASE model was developed in the 1990s by the Health and Safety Executive (HSE) of the United Kingdom (UK) and is a computer based artificial intelligence system for quantitative prediction of potential exposure (Cherrie et al., 2003).
EASE uses a structured logic tree which considers three parameters (tendency of substance to become airborne, method of use, and method of control) to predict exposure ranges using comparable exposure data taken from the UK National Exposure Database (NEDB). The NEDB contains data collected primarily between 1986 and 1993 (Cherrie et al., 2003).

_COSHH Essentials model._ The COSHH Essentials model was developed by the UK HSE in 1998 to provide small and medium-sized companies with a simple yet useful method to evaluate the risk of chemical exposures (NIOSH, n.d.b). COSHH Essentials is a control banding approach which focuses resources on engineering controls necessary to result in an acceptable risk. COSHH Essentials estimates an exposure concentration range and leads the user to an appropriate control approach by evaluating the toxicity of the chemical agent based on risk phrases (R-phrases) assigned by the European Union and the likelihood of exposure based on the quantity used, dustiness, and/or vapor pressure (NIOSH, n.d.b). The COSHH Essentials model is suited for a wide range of users because it offers a step-by-step approach to risk assessment utilizing checklists and color coding (Russell, Maidement, Brooke, and Topping, 1998).

R-phrases are used in the classification, packaging, and labeling of dangerous substances and are assigned according to toxicological criteria agreed on throughout the European Union (EU) (Brooke, 1998). R-phrases are designed to indicate the route(s) of exposure of primary concern, the nature of the health hazard, and if the health hazard is due to acute or chronic exposure (Brooke, 1998). Substances with existing R-phrases are listed in both Annex I to the Dangerous Substances Directive and the UK’s Approved
Supply List (Brooke, 1998). R-phrases are used internationally, not just in Europe, and there is an ongoing effort towards complete international harmonization. A list of R-phrases and their meanings are contained in Appendix A.

COSHH Essentials first assigns a chemical substance to one of five hazard bands (A-E), shown in Table 1, based on R-phrases (HSE, 2003). Bands A-D represents substances associated with a concentration range that corresponds to an acceptable level of control while band E represents substances with serious adverse health effects which require advice from a specialist (Russell et al., 1998). Substances with more than one R-phrase are assigned to the hazard band necessitating more stringent controls, and substances with well understood toxicological properties indicating no health hazards exist, and thus no R-phrase, are allocated to hazard band A (Brooke, 1998).

### Table 1. COSHH Essentials Risk Phrases, Concentration Ranges, and Hazard Groups

<table>
<thead>
<tr>
<th>Risk phrases</th>
<th>Target airborne concentration range</th>
<th>Hazard Group</th>
</tr>
</thead>
<tbody>
<tr>
<td>R36, R38, R65, R67 and all R phrases not otherwise listed</td>
<td>Dust: 1 to 10 mg/m$^3$</td>
<td>A</td>
</tr>
<tr>
<td></td>
<td>Vapor: 50 to 500 ppm</td>
<td></td>
</tr>
<tr>
<td>R20, R21, R22, (R68/20/21/22)</td>
<td>Dust: 0.1 to 1 mg/m$^3$</td>
<td>B</td>
</tr>
<tr>
<td></td>
<td>Vapor: 5 to 50 ppm</td>
<td></td>
</tr>
<tr>
<td>R23, R24, R25, R34, R35, R37, R41, R43, R48/20/21/22, (R39/23/24/25)</td>
<td>Dust: 0.01 to 0.1 mg/m$^3$</td>
<td>C</td>
</tr>
<tr>
<td></td>
<td>Vapor: 0.5 to 5 ppm</td>
<td></td>
</tr>
<tr>
<td>R26, R27, R28, R40, Carc cat 3, R60, R61, R62, R63, R64, R48/23/24/25, (R39/26/27/28)</td>
<td>Dust: &lt;0.01 mg/m$^3$</td>
<td>D</td>
</tr>
<tr>
<td>R68 Muta cat 3 (formerly R40 Muta cat 3), R42, R45, R46, R49</td>
<td>Seek specialist advice</td>
<td>E</td>
</tr>
</tbody>
</table>


The rationale for allocating each R-phrase into one of the hazard bands A-E considered whether or not a potentially safe threshold dose exists, the seriousness of the health effect, and the exposure levels at which toxic effects occur (Brooke, 1998). The system used to allocate R-phrases to hazard bands and its evaluation is detailed in a paper by Brooke (1998). Brooke selected 111 substances with health based OEL’s to evaluate the system used to allocate R-phrases to hazard bands. Substances were selected so that at least one example of every R-phrase was evaluated with the exception of R-phrases allocated to hazard band E. The appropriate hazard band was selected for each substance according to Table 1. The target airborne concentration from Table 1 was then compared to the OEL established by the UK. Brookes found that for dusts and vapors the proportion of substances whose OEL was within or higher than the target airborne concentration range was 100% and 97%, respectively. Overall, for 98% of the substances evaluated, the system used to allocate R-phrases to hazard bands led to the selection of a target airborne concentration range equivalent to or less than the substance’s OEL (Brookes, 1998).

Once a hazard band is selected, the potential for exposure to a substance is assessed by considering the substance’s physical properties and the amount used for a particular task. The authors of the model determined that the majority of hazardous substances used in industry are either solids or liquids (Maidement, 1998). For solids, dustiness is the key physical property and is qualitatively assessed by the user as low, medium, or high according to Table 2. Although this approach is subjective, it provides a simple method that can be easily applied by small and medium sized companies (Maidement, 1998). For liquids, volatility is the key physical property and the vapor
pressure at a reference temperature or the boiling point along with the process
temperature is used as shown in Table 2 and Figure 3, respectively (Russell, et. al., 1998).

Table 2. COSHH Essentials Exposure Potential: Physical Properties

<table>
<thead>
<tr>
<th>Physical Property</th>
<th>Dustiness</th>
<th>Volatility</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low</td>
<td>Pellets</td>
<td>&lt;500 Pa</td>
</tr>
<tr>
<td>Medium</td>
<td>Crystals or granules</td>
<td>500 – 25,000 Pa</td>
</tr>
<tr>
<td>High</td>
<td>Powders</td>
<td>&gt;25,000 Pa</td>
</tr>
</tbody>
</table>

Figure 3. COSHH Essentials graph for selecting volatility of liquids

When using the vapor pressure at a reference temperature different than the
process temperature, the vapor pressure at the process temperature is calculated using
equation 13, were Ln is the natural logarithm, $P_{atm}$ is the vapor pressure in atmospheres,
\( T_{bp} \) is the boiling point of the substance, and \( T \) is the process temperature both in Kelvin (HSE, 2003):

\[
\ln (P_{\text{atm}}) = -10.6 \times \frac{T_{bp}}{T} - 1
\]  
(13)

The vapor pressure at the process temperature is used to determine the volatility in Table 2. When the boiling point and process temperature are used, the graphical approach shown in Figure 3 is used. The graph is divided into three areas corresponding to low, medium, and high volatility. At room temperature (25°C), low volatility is defined as a boiling point greater than 150°C, medium volatility is defined as a boiling point between 50°C and 150°C, and high volatility is defined as a boiling point less than 50°C. For process temperatures other than room temperature, volatility is determined using equations 14 - 16 (Maidement, 1998).

High volatility = Boiling Point \( \leq 2 \times PT + 10 \)  
(14)

Medium volatility = 2 x PT + 10 < Boiling Point < 5 x PT + 50  
(15)

Low volatility = Boiling Point \( \geq 5 \times PT + 50 \)  
(16)

The amount of substance used for a particular task is then subjectively defined by the user as low medium or high according to Table 3. Low usage corresponds to small scale operations like laboratory processes. Medium usage corresponds to operations that involve substances in drums, or sacks which are more difficult to handle, and high usage corresponds to large scale operations like bulk processes (Maidement, 1998).
Table 3. COSHH Essentials Exposure Potential: Amount of Substance

<table>
<thead>
<tr>
<th>Amount</th>
<th>Solids</th>
<th>Liquids</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low</td>
<td>Grams</td>
<td>Milliliters</td>
</tr>
<tr>
<td>Medium</td>
<td>Kilograms</td>
<td>Liters</td>
</tr>
<tr>
<td>High</td>
<td>Tons</td>
<td>Cubic Meters</td>
</tr>
</tbody>
</table>

Substances are then placed in one of four exposure predictor bands (EP Bands) by combining the substance’s physical properties and amount used as shown in Table 4. The combination of these two variables into one band was done primarily to simplify the developmental phase of the model and make it easier to align the exposure potential with the appropriate control approach (Maidment, 1998). Selection of the control approach is the final step in the COSHH Essentials model. Although a large number of potential engineering controls exist, the model’s authors grouped all control approaches into four main categories shown in Table 5 (Maidment, 1998).

Table 4. COSHH Essentials Exposure Predictor (EP) Bands

<table>
<thead>
<tr>
<th>Solids EP Band</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Grams of low/medium dusty solid</td>
</tr>
<tr>
<td>2</td>
<td>Grams of high dusty solid, kilograms/tons of low dusty solid</td>
</tr>
<tr>
<td>3</td>
<td>Kilograms of medium/high dusty solid</td>
</tr>
<tr>
<td>4</td>
<td>Tons of medium/high dusty solid</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Liquids EP Band</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Milliliters of low vapor pressure (VP) liquid</td>
</tr>
<tr>
<td>2</td>
<td>Milliliters of medium/high VP liquid, liters/cubic meters of low VP liquid</td>
</tr>
<tr>
<td>3</td>
<td>Cubic meters of medium VP liquid, liters of medium/high VP liquid</td>
</tr>
<tr>
<td>4</td>
<td>Cubic meters of high VP liquid</td>
</tr>
</tbody>
</table>
Table 5. COSHH Essentials Control Approaches

<table>
<thead>
<tr>
<th>Control Approach</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>General Ventilation. Good standard of general ventilation and good working practices</td>
</tr>
<tr>
<td>2</td>
<td>Engineering Control. Local exhaust ventilation (e.g. single point extraction, partial enclosure, not complete containment)</td>
</tr>
<tr>
<td>3</td>
<td>Containment. Enclosed, but limited, small scale breaches may be acceptable</td>
</tr>
<tr>
<td>4</td>
<td>Special. Expert advice is needed in selecting control measures</td>
</tr>
</tbody>
</table>

Expert occupational hygienist used professional judgment to estimate the range of exposure concentration for each EP Band when each of the four control approaches was applied. The results are shown in Table 6 (Maidment, 1998).

Table 6. Development of the Risk Assessment Scheme for COSHH Essentials

(Predicted concentration ranges for dust-in air, mg/m$^3$)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.01 to 0.1 mg/m$^3$</td>
<td>0.1 to 1 mg/m$^3$</td>
<td>1 to 10 mg/m$^3$</td>
<td>&gt; 10 mg/m$^3$</td>
</tr>
<tr>
<td>2</td>
<td>0.001 to 0.01 mg/m$^3$</td>
<td>0.01 to 0.1 mg/m$^3$</td>
<td>0.1 to 1 mg/m$^3$</td>
<td>1 to 10 mg/m$^3$</td>
</tr>
<tr>
<td>3</td>
<td>&lt;0.001 mg/m$^3$</td>
<td>0.001 to 0.01 mg/m$^3$</td>
<td>0.01 to 0.1 mg/m$^3$</td>
<td>0.1 to 1 mg/m$^3$</td>
</tr>
</tbody>
</table>

(Predicted concentration ranges for vapor-in air, ppm)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>&lt;5 ppm</td>
<td>5 to 50 ppm</td>
<td>50 to 500 ppm</td>
<td>&gt;500 ppm</td>
</tr>
<tr>
<td>2</td>
<td>&lt;0.5 ppm</td>
<td>0.5 to 5 ppm</td>
<td>5 to 50 ppm</td>
<td>50 to 500 ppm</td>
</tr>
<tr>
<td>3</td>
<td>&lt;0.05 ppm</td>
<td>0.05 to 0.5 ppm</td>
<td>0.5 to 5 ppm</td>
<td>5 to 50 ppm</td>
</tr>
</tbody>
</table>

Experts then determined which control approach for each EP Band would result in exposures within the acceptable range for each Hazard Group (HSE, 2003). The appropriate control approach is selected based on the exposure potential and hazard group according to Figure 4.
Once a control approach is selected, COSHH Essentials provides the user with guidance sheets that contain general advice on how to comply with the control recommendations as well as operation-based guidance sheets when applicable (Russell et al., 1998). The guidance sheets were developed by an outside consultant with experience advising a wide range of small industries on control approaches. Through consultation and market research, preconceived notations of the target audience were considered during the writing of the guidance sheets, and a jargon-free style was used. Guidance sheets contain information on how to put specific controls into practice, suggestions concerning PPE, training requirements, good operational practices, and preventative maintenance (Russell et al., 1998).
The scheme for determining exposure predictions, shown in Table 6, and selection of the control approach, shown in Figure 4, was evaluated two different ways. First, exposure predictions, shown in Table 6, were compared with measured data. For appropriate comparison, measured data records had to contain information about the volatility, quantity of use, and controls present. Occupational exposure records do not usually contain this information; therefore, it was difficult to locate data for comparison. One source of data was the Criteria Documents for Occupational Exposure Limits published by the HSE (Maidment, 1998). Comparison of measured data from these documents with the model’s exposure predictions showed the model to be a good predictor of exposures under defined conditions. However, these data were biased towards large scale use of solvents in closed systems. For most of the exposure scenarios in Table 6, no suitable data was available for comparison (Maidment, 1998).

Due to a lack of suitable data, numerical validation of the model’s scheme was not possible. Therefore, an independent peer review process was used to evaluate the model’s logic and predictions. The British Occupational Hygiene Society (BOHS) and the British Institute of Occupational Hygienist (BIOH) each organized a group of specialist to evaluate the logic applied and the technical accuracy of predictions made by the model. Both groups approved of the model’s approach and technical content (Maidment, 1998).

**QLEA model.** In additional to the development of qualitative models by governmental organizations, it is also becoming increasingly popular for private industries to develop proprietary qualitative models for use in occupational exposure
assessments. One such example is the Qualitative Exposure Assessment Model (QLEA) model developed by a global manufacturing company (Elliott and Oestenstad, 2007). The primary goal of the QLEA model is to assist other trained professionals conduct risk assessments in the absence of industrial hygienists. The QLEA model categorizes exposures as acceptable, unacceptable, or uncertain based on the following variables: duration of exposure, chemical agent toxicity, the agent’s ability to become airborne, and engineering controls present.

The QLEA model uses the four predictor variables shown in Table 7 to calculate the inhalation risk according to equation 17. The model then categorizes the risk of inhalation as acceptable, unacceptable, or uncertain and assigns a final rating based on the calculated inhalation risk (Table 8).
Table 7. QLEA Predictor Variables

<table>
<thead>
<tr>
<th>Predictor Variable&lt;sup&gt;A&lt;/sup&gt;</th>
<th>Rank</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Duration</td>
<td>1</td>
<td>Less than 1 hour of exposure daily</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1 to 3 hours of exposure daily</td>
</tr>
<tr>
<td>Frequency (DF)</td>
<td>3</td>
<td>3 to 5 hours of exposure daily</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>5 to 7 hours of exposure daily</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>Over 7 hours of exposure daily</td>
</tr>
<tr>
<td>Hazard Rank for Inhalation (HI)</td>
<td>1</td>
<td>OEL in range 3.1 to 10 mg/m³ or &gt;1000 ppm</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>OEL in range 0.51 to 3 mg/m³ or 101 to 1000 ppm</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>OEL in range 0.01 to 0.5 mg/m³ or 10 to 100 ppm</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>OEL &lt;0.01 mg/m³ or &lt;10 ppm</td>
</tr>
<tr>
<td>Airborne Risk (AR)</td>
<td>0</td>
<td>No risk of airborne exposure</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>Low risk of airborne exposure</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Medium risk of airborne exposure</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>High risk of airborne exposure</td>
</tr>
<tr>
<td>Engineering Controls (EC)</td>
<td>1</td>
<td>Full engineering controls that have been validated</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Full engineering controls that have NOT been validated</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>Fixed-moderate engineering controls that have been validated</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>Fixed-moderate engineering controls that have NOT been validated</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>Non-fixed engineering controls</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>No engineering controls</td>
</tr>
</tbody>
</table>

<sup>A</sup>The use of Personal Protective Equipment is ignored when selecting ranks for predictor variables

Inhalation Risk = DF x HI x AR x EC.  \hspace{1cm} (17)

Table 8. QLEA Model Classification of Acceptable Risk

<table>
<thead>
<tr>
<th>Inhalation Risk</th>
<th>Classification</th>
<th>Final Rating</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt; 50</td>
<td>Acceptable <em>(no further action required other than periodic review)</em></td>
<td>1</td>
</tr>
<tr>
<td>50 – 199</td>
<td>Acceptable <em>(controls that may further reduce exposure should be implemented if feasible)</em></td>
<td>2</td>
</tr>
<tr>
<td>200 – 400</td>
<td>Uncertain</td>
<td>3</td>
</tr>
<tr>
<td>&gt; 400</td>
<td>Unacceptable <em>(process must be controlled immediately)</em></td>
<td>4</td>
</tr>
</tbody>
</table>
**QOEA model.** Another qualitative model discussed in a paper by Dunham, Bullock, and Oestenstad (2001) is the Qualitative Occupational Exposure Assessment (QOEA) model developed by a United States chemical company. The QOEA model utilizes seven unevenly weighted variables (use frequency, use time, lowest regulatory limit, number of employees exposed, etc.) to calculate exposure ratings for individual exposure scenarios. These exposure ratings are then used to ascertain which chemicals and tasks present the greatest probability of exposure and prioritize quantitative monitoring.

**Model Validation**

A model’s validity is defined by its ability to provide accurate predictions. Although several qualitative models are available, most have not been validated or previous studies have shown that qualitative models do not accurately predict exposure concentrations across differing exposure conditions (Bredendiek-Kamper, 2001; Cherrie and Hughson, 2005; Creely et al., 2005; Devillers, Domine, Binstein, and Karcher, 1997; Dunham et al., 2001; ECETOC, 1997; Elliott and Oestenstad, 2007; Jones and Nicas, 2006; Mulhausen and Damiano, 1998; Tischer, Bredendiek-Kamper, and Poppek, 2003; Vincent, Devillers, Binstein, Sandino, and Karcher, 1996). Even though validation is an integral part of model evaluation, the concept of validation is not clearly defined in the scientific community (Tischer et al., 2003). In general, two approaches to model validation can be taken - an internal approach or an external approach. Internal validation investigates whether the underlying assumptions of a model correspond with established theories and if valid parameters are considered. Whereas, external validation
determines the accuracy of a model by how well model estimates and monitoring data agree (Tischer et al., 2003). A small number of external validation studies have been published for existing exposure assessment models and a few of these studies are summarized below.

**EASE Model Validation**

The EASE model is the most widely validated exposure assessment model. Creely et al. (2005) summarized the results of six validation studies of the EASE model for inhalation exposures. The authors reported that three of the early evaluations of the EASE model (Devillers et al., 1997; ECETOC, 1997; Vincent et al., 1996) were qualitative and provided limited information on how EASE predictions were compared with measured exposure data, but that in general the model tended to overestimate exposures.

The remaining three validation studies (Bredendiek-Kämper, 2001; Cherrie and Hughson, 2005; Mark, 1999) provided systematic evaluation of EASE using existing exposure measurement data. Mark (1999) and Cherrie and Hughson (2005) both calculated the percentage of measurement data within the exposure concentration range predicted by EASE. If > 50% of the measured exposures were within the exposure range predicted by EASE, the authors concluded that the model was in good agreement with the measured data. Both Mark (1999) and Cherrie and Hughson (2005) concluded that EASE tended to overestimate exposures for both particulates and vapors. Bredendiek-Kämper (2001) compared EASE predictions with measured exposure data in 11 exposure scenarios involving six industries. The author stated there was agreement between the
EASE prediction and measurement data if the 25th and 75th percentile of the data for an exposure scenario overlapped the EASE endpoint range. Using this criterion, the author concluded that the EASE predictions were in good agreement in four of six industry groups. However, EASE overestimated exposures in one industry group and underestimated exposures in another.

Cherrie et al. (2003) conducted a study to examine the underlying structure and philosophy of EASE. The authors conclude that because EASE was developed in the UK, and used only NEDB exposure data from the late 1980s and early 1990s, the model reflects only the situation in the UK during that period. Furthermore, the authors stated that EASE output ranges were last updated in 1992. Because industrial practices differ from country to country, the application of EASE to situations in countries other than the UK must be considered with caution. The authors concluded that the first step in improving the model is actually updating the data set on which it is based. A new version of EASE (version 3.0) was developed. However problems arose with the interpretation of the model during user trials and version 3 has not been distributed (Cherrie et al., 2003).

**COSHH Essentials Model Validation**

Tischer et al. (2003) compared approximately 1,000 personal measured exposures taken by Bundesanstalt fur Arbeitsschutz and Arbeitsmedizin (German authority for risk assessment of new substances) with COSHH Essentials exposure prediction ranges for 18 industrial applications. The percentage of measured data that was within the exposure concentration range predicted by COSHH Essentials was calculated along with the
percentage of measured data above and below the predicted range. In most cases, measured exposures were within or below the predicted range. Tisher concluded that COSHH Essentials tended to correctly estimate or overestimate exposures. However, when liquids were used in small scale operations like laboratory processes (e.g. milliliter quantities), measured exposures were shown to sometimes exceed the predicted range (i.e. the model underestimated exposures). A primary limitation of this study is that the sample size was small, and no inferential statistical analyses were performed, rather interpretation of the data was limited to descriptive statistics. In addition, the study was limited in that most exposure scenarios evaluated were “medium” scenarios meaning there was medium use of the chemical and the chemical had a medium level of dustiness/volatility. Tisher concluded that further evaluation involving low, medium, and high exposure scenarios was needed.

Jones and Nicas (2006) used air monitoring data from NIOSH Health Hazard Evaluation (HHE) reports to evaluate the ability of COSHH Essentials to select suitable engineering controls for vapor degreasing and bag filling operations and the ability of the controls to sufficiently limit airborne concentrations. Two types of misclassification errors were identified. Under-controlled errors were instances in which the airborne concentration exceeded the upper limit of the exposure concentration range predicted by COSHH Essentials in the presence of engineering controls. Over-controlled errors were instances in which the airborne concentration was below the upper limit of the exposure concentration range predicted by COSHH Essentials in the absence of engineering controls, yet COSHH Essentials recommended the use of controls. Among 167 vapor degreasing air samples taken in the absence of engineering controls, 102 were below the
upper limit of the predicted range, yet COSHH Essentials recommended the use of controls. Among 179 vapor degreasing air samples taken in the presence of engineering controls, 139 were above the upper limit of the predicted range despite the application of control technology. Among 36 air samples collected for bag filling operations in the absence of engineering controls, 3 were below the upper limit of the predicted range, yet COSHH Essentials recommended the use of controls. Among 159 air samples collected for bag filling operations in the presence of engineering controls, 76 were above the upper limit of the predicted range despite the application of control technology.

Therefore, under-controlled errors were observed in 78% (139/179) and 48% (76/159) of vapor degreasing and bag filling operations, respectively. Over-controlled errors were observed in 61% (102/167) and 8% (3/26) of vapor degreasing and bag filling operations, respectively. Unfortunately, interpretation of under-controlled errors in the Jones and Nicas study is potentially biased since the authors only determined whether engineering controls were present and not whether they provided optimum capture or containment efficiency. In addition, the study was severely limited in that only two exposure scenarios were evaluated—vapor degreasers and bag filling operations.

To summarize, Tischer et al. (2003) evaluated the ability of COSHH Essentials to accurately predict exposure concentrations. They concluded that COSHH Essentials is a reasonably good predictor of airborne exposures for solid substances and large-scale use of liquid substances. In contrast, Jones and Nicas (2006) tested a different hypothesis by evaluating the ability of COSHH Essentials to select appropriate engineering controls. They concluded that COSHH Essentials lacks the ability to select adequate engineering controls to limit airborne exposures. Although two separate validation studies have been
performed using the COSHH Essentials model, each study evaluated a different hypothesis and resulted in dissimilar conclusions.

**QLEA Model Validation**

The author recently conducted a validation study using the QLEA model. Elliott and Oestenstad (2007) evaluated the accuracy of the QLEA model in low level exposures by comparing the model’s output with measured exposure data using contingency tables. Thirty-five low-level exposure scenarios at a United States manufacturing facility were assessed. The QLEA model accurately classified measured exposures in 51% of the exposure scenarios evaluated. When measured exposures were considered acceptable, there was a 53% probability that the model would accurately classify exposures as acceptable (sensitivity). Likewise, when measured exposures were considered unacceptable there was a 33% probability that the model would accurately classify exposures as unacceptable (specificity). A Spearman’s Rho Correlation found no significant correlation between the model’s risk factor and the maximum measured exposure ($r_s=0.119$, $p=0.496$), and a Fisher’s Exact Test found that the maximum measured exposure was independent of the model’s inhalation risk factor ($\chi^2=0.203$, $p=0.653$). Therefore, we concluded that the QLEA model generally resulted in an overestimation of exposure and thus was a poor predictor of the low level exposures seen in this particular study. However, only a small number of exposure scenarios from a single manufacturing facility were assessed, and the QLEA model was not evaluated in medium to high exposure scenarios. Therefore, further study in diverse industrial
environments with low, medium, and high exposure ranges is crucial in order to make a final statement concerning the model’s validity.

**QOEA model Validation**

Dunham et al. (2001) conducted a partial validation study of the QOEA model. The QOEA model was compared with the Modified Vapor Hazard Rating System (MVHRS) and Workplace Exposure Assessment (WORKBOOK) model to evaluate agreement with measured exposures and consistency among the models. The MVHRS model contains three variables. The degree of exposure (DE) describes the level of the exposure. The severity of response (SR) defines the chemical hazard potential, and the vapor hazard index (VHI) compares the vapor pressure of the chemical to the allowable limit. The WORKBOOK model is a computerized model that evaluates three primary categories including homogeneous exposure groups, workplace exposure assessments, and appropriate monitoring programs. The authors compared hazard rankings obtained from the three models to measured exposures for three exposure scenarios (toluene in a laboratory, dust in a production operation, and toluene in gasoline in a maintenance operation). The MVHRS model consistently gave the highest ranking, while the WORKBOOK model consistently gave the lowest rankings. The QOEA and WORKBOOK models were found to be better predictors in moderately high exposure scenarios, and the WORKBOOK model was the better predictor in low exposure scenarios. The authors found that the inter-model agreement was inconsistent when they compared the 95% confidence intervals for the ratios of the models’ rating for three exposure scenarios to the maximum potential rating for those scenarios. Linear regression
analysis found that the models’ rating/maximum rating ratios and the ratios of the measured concentrations and the occupational exposure limits (OELs) for the chemicals in question were highly correlated. However, correlation coefficients and measured concentrations were not reported, so the level of agreement among the models is not known, or over what range of concentrations the models could be applied.

George E. P. Box once stated that, “All models are wrong, but some are useful” (Jayjock, 2003, p.131). Clearly, qualitative models could prove advantageous for small and medium sized companies whose resource and budgetary restraints prevent them from conducting occupational exposure assessments using quantitative air sampling techniques. Unfortunately, previous validation studies have shown that qualitative models can perform differently when exposure conditions differ. As a result the use of model estimates in decisions that pertain to worker health involves uncertainty. For example, a qualitative model that underestimates exposure concentrations would result in workers who are exposed above the OEL being classified as exposed below the OEL. As a result, appropriate control methodologies would not likely be implemented and could result in employees’ deleterious health as well as financial hardship for the company due to increased workers’ compensation premiums. Likewise, a qualitative model that overestimates exposure concentrations could lead to unnecessary spending if the model is used to prioritize and implement costly control methodologies. Thus, it is crucial that we determine under which conditions qualitative models will be most accurate prior to their widespread application.
Small Business Industries in the United States

Small businesses are a vital component of the United States’ economy. In 2004, the United States (US) Census Bureau estimated that 55% (63 million) of the private industry workforce is employed by establishments with fewer than 100 employees at a single site. Approximately 7.4 million private industry establishments were operating in the US as of 2004. Of these, approximately 99% (7.3 million) employed fewer than 250 employees, 98% (7.2 million) employed fewer than 100 employees, and 86% employed fewer than 20 employees.

Small businesses are found in all sectors of industry. Up until recently, OSHA has often focused efforts, such as safety and health inspections and other enforcement strategies, on the 2% of private industry establishments with more than 100 employees (NIOSH, 1999). However, both OSHA and NIOSH have recently created programs which provide free on-site consultations for small business owners as well as simplified guides for specific OSHA standards, technical information resources, and other services specifically targeted towards small businesses.

The goal of this research was to validate exposure assessment methods that could be used by small business owners to evaluate occupation exposures and thus potentially improve the work environment of millions of Americans. Because most small businesses do not employ an industrial hygienist or other trained professional skilled in quantitative sampling techniques, the acceptance and use of mathematical models as an exposure assessment tool is unlikely. Therefore, this study focused on the validation and advancement of the COSHH Essentials model and QLEA model.
CHAPTER 2
RESEARCH DESIGN AND METHODS

Previous validation studies have relied on an external validation approach. Likewise, this study utilized an external validation approach. Specifically, quantitative data obtained from NIOSH HHE reports were compared with COSHH Essentials and QLEA model estimates. Airborne contaminants are generally classified according to their physical state. Specifically, contaminants can be present in the air as particulate matter, in the form of liquids or solids, or as gaseous material in the form of a gas or vapor (Leidel et al., 1977). The goal of this study was to evaluate the accuracy of COSHH Essentials and QLEA model estimates for particulates and vapors in low, medium, and high exposure situations.

This study was accomplished in three distinct phases as depicted in Figure 5. Phase 1 involved identification of applicable NIOSH HHE reports and subsequent extraction of quantitative exposure measurements as well as pertinent exposure scenario information necessary to apply the COSHH Essentials and QLEA models. All applicable exposure scenarios identified in Phase 1 were qualitatively assessed using the COSHH Essentials and QLEA models in Phase 2. The final phase of this study, Phase 3, compared model estimates obtained in Phase 2 with measured exposure data extracted from HHE reports in Phase 1.
Phase 1: Data Collection

This study relied on pre-existing air monitoring data available from NIOSH HHE Reports (NIOSH, n.d.a). The NIOSH HHE Reports were chosen as a source of data for several reasons: 1) HHE Reports are available electronically from NIOSH’s web-site, 2) reports include detailed descriptions of the job tasks and rationale for quantitative air sampling, and 3) NIOSH investigators employed standardized sampling and analytical methods.

Between 1976 and 2007, NIOSH performed over 3,000 HHEs. To initially be considered for inclusion in the study, reports had to be available electronically and contain personal and/or area samples for exposures involving particulates and/or vapors in industrial operations such as manufacturing, mining, construction, automotive repair,
chemical processing, agricultural, etc. HHE’s related to heat stress analysis, noise, indoor air quality, etc. were not considered in this study.

Once applicable reports were identified, information necessary to establish SEGs using the observational approach (i.e. classified by process, job, task, and chemical substance) and subsequently conduct qualitative exposure assessments was extracted. Specifically, information regarding the process, job, task, physical state of the chemical substance, usage quantity, duration of exposure, ability of the chemical substance to become airborne, and control methods were extracted and recorded in a spreadsheet. An example detailing the process used to establish SEGs and subsequently conduct qualitative exposure assessments is given in Appendix B.

HHE reports with missing information were evaluated on a case by case basis. In instances where incomplete information could not be reasonably concluded the corresponding SEG(s) was not included in the study. For example, some reports contained limited information concerning the quantity of the chemical substance used. In instances were the usage quantity was not explicitly stated, several criteria were considered collectively to estimate the quantity used including: facility size, number of employees involved in the process/task, number of shifts, amount of product produced per day/shift/machine, etc. As a final alternative, Toxic Release Inventory (TRI) data from Environmental Protection Agency’s (EPA) website were reviewed when available. However, in instances where the scale of use could not be confidently determined, the corresponding SEG was not included in the study.

Once SEGs were confidently established, measured exposure concentrations for each SEG were recorded. Specifically, raw data as well as the minimum, maximum,
sample mean, AM, GM, GSD, and 95th percentile of the measured exposures were documented. SEGs with less than three quantitative air samples were omitted from the study. Although occupational exposure data are presumed to be lognormally distributed, prior to conducting statistical analysis, the assumption of lognormality was confirmed using the Kolmogorov-Smirnov goodness-of-fit test (Daniel, 1999). SEGS in which data were not lognormally distributed were also omitted from the study. Previous studies have reported that the evaluation of models may be affected by high variability in the exposure data used for comparison (Stewart and Stenzel, 2000; Kromhout, et al., 1987). Thus, to ensure that SEGs with high exposure variability did not bias the results of model validation, SEGs with GSDs greater than 3.0 were also omitted from the study.

The remaining SEGs or “exposure scenarios” were categorized based on the magnitude of measured exposures (high, medium, low) and the physical state of the chemical substance (vapor or particulate). Exposure scenarios in which the AM (Rappaport, 1991) was ≥ 75% of the OEL were categorized as high. Exposure scenarios in which the AM was between 50% and 75% of the OEL were categorized as medium, and scenarios in which the AM was <50% of the OEL were categorized as low (Mulhausen and Damiano, 2003). Thus, the data were stratified into six groups, exposure scenarios involving vapors with high, medium, and low exposures (VH, VM, and VL) and exposure scenarios involving particulates with high, medium, and low exposures (PH, PM, and PL).
Phase 2: Exposure Assessments

Each of the exposure scenarios identified from the HHE reports were qualitatively assessed by the investigator using the COSHH Essentials and QLEA models.

*COSHH Essentials*

Recall that COSHH Essentials estimates an exposure concentration range and leads the user to an appropriate control approach by evaluating the toxicity of the chemical and the likelihood of exposure (NIOSH, n.d.b).

This study evaluated the exposure prediction portion of COSHH Essentials. Recall that COSHH Essentials utilizes two components to arrive at a predicted concentration range – the EP Band and controls present. Also recall that two components are utilized when placing an SEG in a specific EP Band – usage quantity and volatility/dustiness. Information concerning the volatility/dustiness of the chemical substance and usage quantity was extracted from HHE reports and used to allocate SEGs into one of four EP Bands shown in Table 4. The final output of the COSHH model is selection of the appropriate control approach that would result in an acceptable range of exposures (HSE, 2003). However, for the purpose of this study, the current control approach present along with the EP Band selected by the model was used to determine the predicted concentration range from Table 6.

*QLEA*

Recall that the QLEA model uses the four predictor variables shown in Table 7 to calculate the inhalation risk according to equation 17. Information concerning the total
duration of exposure, ability of the substance to become airborne and engineering controls present was extracted from HHE reports and used to select values for model variables DF, AR, and EC, respectively. The ACGIH TLV was utilized to select a value for the HI model variable. The QLEA model’s inhalation risk (equation 17) was then calculated and used to assign a final rating (1 – 4) from Table 8 which corresponds to the acceptability of the exposure (Acceptable, Uncertain, Unacceptable).

Phase 3: Model Validation and Data Analysis

The final phase of this study involved comparison of model estimates for each exposure scenario with corresponding measured exposure data extracted from the HHE report. Tests of significances were conducted at alpha (α) = 0.05.

COSHH Essentials

For each exposure scenario, the COSHH Essentials model predicts a range of possible concentrations. The data were stratified into six groups (PH, PM, PL, VH, VM, and VL) based on the physical state of the chemical substance and the magnitude of the measured exposure. Pearson correlation analysis (Daniel, 1999) was used to determine if a significant linear relationship existed between the maximum measured exposure and the upper limit of the predicted concentration range as well as the minimum measured exposure and the lower limit of the predicted concentration range. Correlation coefficients calculated for each group were used to determine if the model was more accurate in predicting measured exposures under certain conditions. For the purpose of this study, the model was considered accurate if the correlation coefficient was ≥0.70 and
statistically significant at $\alpha=0.05$. In addition, the percentage of measured exposures that fell within, above, and below the model’s predicted concentration range were assessed, and the percentage of correct, underestimated, and overestimated exposures were calculated as was done by Tischer et al. (2003).

**QLEA**

The QLEA model is different from COSHH Essentials in that its final output is a classification of the acceptability of an exposure rather than a predicted exposure concentration. Therefore, in order to compare the model’s final output with measured exposure data, it was necessary to categorize measured exposures as acceptable, unacceptable, or uncertain. To be conservative in our approach, the maximum measured exposure was calculated as a percentage of the OEL. Measured exposures were then classified into four categories of acceptability and assigned a final rating (1 – 4) based on the percentage of the OEL in Table 9 (Mulhausen and Damiano, 2003). Note that this rating scheme corresponds with the model’s final classification of acceptability and final ratings shown in Table 8.

<table>
<thead>
<tr>
<th>Table 9. Measured Exposures Classification of Acceptable Risk</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Percentage of OEL</strong></td>
</tr>
<tr>
<td>&lt; 10%</td>
</tr>
<tr>
<td>10 – 50%</td>
</tr>
<tr>
<td>50 – 75%</td>
</tr>
<tr>
<td>&gt; 75%</td>
</tr>
</tbody>
</table>
Spearman correlation analysis (Daniel, 1999) was used to determine if a significant linear relationship existed between the final ratings for measured exposures and the model’s final rating. The data were stratified into the six groups, and correlation coefficients were calculated for each group to determine if the model was more accurate under certain conditions. For the purpose of this study, the model was considered accurate if the correlation coefficient was $\geq 0.70$ and statistically significant at $\alpha = 0.05$. As with our previous study (Elliott and Oestenstad, 2007), contingency tables were used to compare model ratings with measured exposure ratings. Kappa coefficients and Chi Square statistics (Daniel, 1999) were used to evaluate agreement between model ratings and measured exposure ratings. In addition, measurements of validity such as the efficiency, sensitivity, specificity, percentage of false low classification and percentage of false high classifications were calculated.
CHAPTER 3
RESULTS

Data Collection

Of the 3,000+ HHEs recorded on NIOSH’s website, 1,244 HHE reports were available electronically. All 1,244 reports were downloaded and reviewed for inclusion in the study. To initially be considered for inclusion in the study, reports had to contain personal and/or area samples for exposures involving particulates and/or vapors. Of the 1,244 reports reviewed, 345 were deemed applicable based on the initial criteria (i.e. 345 HHE Reports contained quantitative sampling data). These 345 applicable reports were carefully reviewed to determine if they contained adequate information necessary to confidently establish SEGs. Specifically, a detailed description of the job processes was necessary, along with the physical state of the chemical substance sampled, scale of use, ability of the substance to become airborne, and control technologies present. Of the 345 applicable reports, 277 reports had extremely limited information, making it impossible to confidently establish SEGs and subsequently apply the qualitative models. From the 68 reports which contained adequate information, 263 SEGs were initially identified using the observational approach, and measured concentrations for each SEG were recorded. For the purpose of this study, raw data as well as the minimum, maximum, sample mean, AM, GM, GSD, and 95th percentile of the measured exposures were documented.
SEGs with limited quantitative sampling data were not included in the study. Thus, of the 263 SEGs identified, 6 SEGs were omitted from the study due to small sample sizes (n<3). Although occupational exposure data are presumed to be lognormally distributed, prior to conducting statistical analysis, the lognormality assumption was confirmed using the Kolmogorov-Smirnov goodness-of-fit test (Daniel, 1999). SEGs in which the data were not lognormally distributed were omitted from the study; 5 SEGs were omitted because the sampling data were not lognormally distributed. Lastly, SEGs with high exposure variability (GSD>3.0) were not included in the study; 53 SEGs were omitted from the study due to high variability in the measured exposure data.

Thus, of the 263 SEGs initially identified, 199 SEGs met the criteria for inclusion in the study. SEGs in which the AM was \( \geq 75\% \) of the OEL were categorized as high. SEGs in which the AM was between 50% and 75% of the OEL were categorized as medium, and SEGs in which the AM was < 50% of the OEL were categorized as low (Mulhausen and Damiano, 2003). SEGs were labeled based on the magnitude of measure exposures (high, medium, low) and the physical state of the chemical substance (vapor or particulate). Thus, the data was stratified into the following six groups shown in Table 10.

<table>
<thead>
<tr>
<th>Particulates</th>
<th>Vapors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low</td>
<td>72</td>
</tr>
<tr>
<td>Medium</td>
<td>5</td>
</tr>
<tr>
<td>High</td>
<td>17</td>
</tr>
</tbody>
</table>

Table 10. Stratification of SEGs
COSHH Essentials

Recall that the COSHH Essentials model predicts a range of possible concentrations for an SEG based on the EP Band and current controls in place. Also recall that SEGs are assigned to a particular EP Band based on the usage quantity and the volatility/dustiness of the chemical substance.

Pearson Correlations

When evaluating the accuracy of the COSHH Essentials model, first Pearson correlation coefficients (Daniel, 1999) were calculated for each of the six groups (PH, PM, PL, VH, VM, and VL) to determine if the model was more accurate in predicting measured exposures under certain conditions. Specifically, correlation coefficients were used to determine if a significant linear relationship existed between the maximum measured exposure and the upper limit of the model’s predicted concentration range as well as the minimum measured exposure and the lower limit of the model’s predicted concentration range. Results are shown in Table 11.

<table>
<thead>
<tr>
<th>Table 11. COSHH Essentials Pearson Correlation Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Particulates</strong></td>
</tr>
<tr>
<td>Max Measured vs. Upper Limit</td>
</tr>
<tr>
<td>Low</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Medium</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>High</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>All</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

A Statistically significantly at α = 0.05
B Correlation coefficient not calculated
For SEG’s categorized as particulates (i.e. no stratification by the magnitude of the measured exposure), correlation coefficients were statistically significant for both the upper and lower concentration values. However, this relationship was considered weak. For SEG’s categorized as low level exposure to vapors (VL), correlation coefficients were also statistically significant for both the upper and lower concentration values. However, this relationship was also considered weak.

For SEG’s categorized as medium level exposures to vapors (VM), correlation analysis was not conducted because there were only two SEGs in this stratum. Correlation analysis between two data points would have resulted in a perfect linear correlation coefficient (1 or -1). For this category (VM), review of the raw data showed one SEG had a predicted lower concentration of 50 ppm with a corresponding minimum measured concentration of 3.7 ppm and a predicted upper concentration of 500 ppm with a corresponding maximum measured concentration of 20.9 ppm. The second SEG had a predicted lower concentration of 5 ppm with a corresponding minimum measured concentration of 80 ppm and a predicted upper concentration of 50 ppm with a corresponding maximum measured concentration of 315 ppm.

Percentages of Measured Exposures Above, Within, and Below Model’s Predicted Range

In addition to correlation analyses, the percentage of measured exposures that fell above, within, and below the model’s predicted concentration range were calculated as was done by Tischer et al. (2003). Results are shown in Tables 12 and 13 for particulates and vapors, respectively.
For particulate exposures, the COSHH Essentials model underestimated exposures in 8% of the cases assessed. The model correctly estimated or overestimated exposures in 11% and 81% of the cases assessed, respectively. For vapor exposures, the COSHH Essentials model underestimated exposures in 3% of the cases assessed. The model correctly estimated or overestimated exposures in 20% and 77% of the cases assessed, respectively.

Data were also stratified by the physical state of the chemical substance and the magnitude of exposure (PH, PM, PL, VH, VM, and VL) to determine if the model was more accurate in predicting measured exposures under certain conditions. For
particulates, regardless of data stratification, COSHH Essentials consistently overestimated exposures as can be seen in Figure 6 as well as Table 12. For vapors, COSHH Essentials consistently overestimated low-level exposures (VL) as can be seen in Figure 6 as well as Table 13. For high-level exposures to vapors (VH), COSHH Essentials overestimated or correctly estimated exposures. For medium-level exposures to vapors (VM), COSHH Essentials consistently underestimated exposures. However, it must be noted that only 2 SEGs containing 10 quantitative samples were included in this stratum.

![Figure 6: Percentage of exposures underestimated, correctly estimated, and overestimated by the COSHH Essentials model](image)

**General Linear Models**

Because the categories representing medium and high exposures to particulates and vapors (PM, PH, VM, VH) had small sample sizes (n≤17) we chose to focus further data analysis on low level exposures (PL and VL) only. Overall, the COSHH Essentials model led to an overestimation of exposure for both particulates (86%) and vapors (81%). Recall that two components, the EP Band and controls present, are used to arrive at a predicted concentration range.
A general linear model was constructed to determine which COSHH Essentials model component (i.e. EP Band or controls) led to the overestimation in exposure. The degree of overestimation was calculated for each SEG by subtracting the maximum measured concentration from the upper limit of the model’s predicted concentration range. This calculated variable was labeled “Difference”. Thus, if COSHH Essentials overestimated exposures, the “Difference” variable had a positive value. Likewise, if COSHH Essentials underestimated exposures, the “Difference” variable had a negative value. Further, the degree of overestimation was evident by the magnitude of the “Difference” variable.

The degree of overestimation was modeled as a function of EP Band, current controls, and the interaction between EP Band and current controls. For both particulates and vapors, the interaction term was statistically significant (F=42.930, p<0.0001 and F=576.484, p<0.0001, respectively) indicating that the model’s tendency to overestimate exposures was the result of a complex interaction between the EP Band variable and the controls variable. The mean difference between the maximum measured concentration and the upper limit of the model’s predicted concentration range, stratified by EP Band and current controls, is shown in Table 14. In general, anytime there are no mechanical engineering controls present (i.e. Controls = 1), COSHH Essentials overestimates exposure, and the magnitude of overestimation worsens as the EP Band gets higher.
Table 14. Mean Difference between Maximum Measured Exposure and Maximum Concentration Predicted by COSHH Essentials for EP Band*Control Interaction

<table>
<thead>
<tr>
<th>Control</th>
<th>Particulates</th>
<th>EP Band</th>
<th>Vapors</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S1</td>
<td>S2</td>
<td>S3</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A</td>
<td>0.48</td>
<td>9.58</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-0.36</td>
<td>0.77</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.91</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

A This level combination of factors is not observed.

Two components are considered when placing an SEG in a specific EP Band – quantity and vapor pressure/dustiness. Thus, a second general linear model was constructed to determine which component of the EP Band led to the overestimation in exposure. Overestimation was modeled as a function of quantity, vapor pressure/dustiness, and the interaction between quantity and vapor pressure/dustiness. For particulates, the interaction term was statistically significant (F=74.281, p<0.0001) indicating that the model’s tendency to Overestimate exposures was the result of a complex interaction between the quantity used and the dustiness. The mean difference between the maximum measured concentration and the upper limit of the model’s predicted concentration range, stratified by quantity and dustiness, are shown in Table 15. In general, COSHH Essentials consistently overestimates exposures for high dusty solids, and the magnitude of overestimation worsens as the quantity increases.
Table 15. Mean Difference between Maximum Measured Exposure and Maximum Concentration Predicted by COSHH Essentials for Dustiness*Quantity Interaction

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Low</th>
<th>Medium</th>
<th>High</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grams</td>
<td>0.32</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(n=2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Kilograms</td>
<td>0.33</td>
<td>6.67</td>
<td>5.43</td>
</tr>
<tr>
<td></td>
<td>(n=10)</td>
<td>(n=6)</td>
<td>(n=34)</td>
</tr>
<tr>
<td>Tons</td>
<td>0.99</td>
<td></td>
<td>93.80</td>
</tr>
<tr>
<td></td>
<td>(n=2)</td>
<td></td>
<td>(n=18)</td>
</tr>
</tbody>
</table>

* This level combination of factors is not observed

For vapors, the interaction term was not statistically significant (F=1.727, p=0.167). However, the main effect for vapor pressure was statistically significant (F=9.221, p<0.0001), and the main effect for quantity was marginally significant (F=2.802, p=0.066). For vapors, COSHH Essentials consistently overestimates exposures, and the magnitude of overestimation worsens as the vapor pressure increases, as shown in Table 16. The magnitude of overestimation also worsens as the usage quantity increases, as shown in Table 17.

Table 16. Mean Difference between Maximum Measured Exposure and Maximum Concentration Predicted by COSHH Essentials for Vapor Pressure Main Effect

<table>
<thead>
<tr>
<th>Vapor Pressure</th>
<th>Mean</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low</td>
<td>9.74</td>
</tr>
<tr>
<td></td>
<td>(n=16)</td>
</tr>
<tr>
<td>Medium</td>
<td>262.07</td>
</tr>
<tr>
<td></td>
<td>(n=77)</td>
</tr>
<tr>
<td>High</td>
<td>419.18</td>
</tr>
<tr>
<td></td>
<td>(n=5 )</td>
</tr>
</tbody>
</table>
Table 17. Mean Difference between Maximum Measured Exposure and Maximum Concentration Predicted by COSHH Essentials for Quantity Main Effect

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Mean</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>Milliliters</td>
<td>10.11</td>
<td>4</td>
</tr>
<tr>
<td>Liters</td>
<td>229.63</td>
<td>44</td>
</tr>
<tr>
<td>Cubic Meters</td>
<td>314.90</td>
<td>50</td>
</tr>
</tbody>
</table>

QLEA

Recall that the QLEA model calculates an inhalation risk factor and assigns a final rating (1 – 4) which corresponds to the acceptability of the exposure (Acceptable, Uncertain, Unacceptable). Thus, if the QLEA model’s inhalation risk factor is predictive of measured exposures, the model’s final rating (Table 8) should be correlated with measured exposure ratings (Table 9). The QLEA model was evaluated using nonparametric statistics. Specifically, Spearman correlations and contingency table analyses were used to assess how well the model agreed with measured exposures.

Correlations

Spearman correlation coefficients (Daniel, 1999) were calculated to determine if a significant linear relationship existed between the final ratings for measured exposures and the model’s final rating. Spearman correlation analysis found no significant association ($r_s=0.053$, $p=0.457$) between QLEA model ratings and measured exposures when analyzing the data collectively (i.e. no stratification by physical state and magnitude of exposure).

As was done when evaluating COSHH Essentials, data were stratified by the physical state of the chemical substance and magnitude of the measured exposure (PH,
PM, PL, VH, VM, and VL) to determine if the model was more accurate in predicting measured exposures under certain conditions. Unfortunately, spearman correlation coefficients (Daniel, 1999) could not be calculated for four of the six groups (PM, PH, VM, and VH) due to a constant (i.e. each case had a measured exposure rating of “4”). For the remaining groups, none of the correlation coefficients were statistically significant as shown in Table 18.

<table>
<thead>
<tr>
<th>Particulates</th>
<th>Vapors</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Low</strong></td>
<td></td>
</tr>
<tr>
<td>-0.0004</td>
<td>0.051</td>
</tr>
<tr>
<td>(p=0.997)</td>
<td>(p=0.617)</td>
</tr>
<tr>
<td><strong>Medium</strong></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>A</td>
</tr>
<tr>
<td><strong>High</strong></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>A</td>
</tr>
<tr>
<td><strong>All Groups</strong></td>
<td></td>
</tr>
<tr>
<td>0.069</td>
<td>0.049</td>
</tr>
<tr>
<td>(p=0.507)</td>
<td>(p=0.620)</td>
</tr>
</tbody>
</table>

\(^{A}\) Unable to calculate correlation coefficient due to constant

A concern was that the correlation analysis was biased due to the subjective schemes used to select QLEA model final ratings in Table 8 and measured exposure ratings in Table 9. To test if this may have been the case, the correlation analysis was repeated using the inhalation risk score from equation 17 and the maximum measured exposure expressed as a percent of the OEL. Pearson correlation coefficients are shown in Table 19. Results using both methods are similar. Therefore, it would appear that the selection of cut points for the OEL based rating scheme (Table 9) did not bias the correlation analysis. Note that for SEG’s categorized as medium level exposures to vapors (VM), correlation analysis was not conducted because there were only two SEGs in this stratum.
Table 19. QLEA Model Pearson Correlation Coefficients

<table>
<thead>
<tr>
<th></th>
<th>Particulates</th>
<th>Vapors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low</td>
<td>-0.009</td>
<td>0.069</td>
</tr>
<tr>
<td></td>
<td>(p=0.943)</td>
<td>(p=0.501)</td>
</tr>
<tr>
<td>Medium</td>
<td>-0.416</td>
<td>b</td>
</tr>
<tr>
<td></td>
<td>(p=0.486)</td>
<td></td>
</tr>
<tr>
<td>High</td>
<td>0.115</td>
<td>0.853</td>
</tr>
<tr>
<td></td>
<td>p=0.661</td>
<td>p=0.066</td>
</tr>
<tr>
<td>All Groups</td>
<td>0.110</td>
<td>0.116</td>
</tr>
<tr>
<td></td>
<td>(p=0.292)</td>
<td>(p=0.240)</td>
</tr>
</tbody>
</table>

*b Correlation coefficient not calculated

Contingency Table Analyses

Contingency tables were also used to compare model ratings with measured exposure ratings, and a Kappa statistic (Daniel, 1999) was calculated to test the significance of the agreement between the QLEA model and measured exposures.

Table 20 shows the relationship between QLEA model ratings and ratings based on measured exposures for the data collectively (i.e. no stratification by physical state and magnitude of exposure). The model ratings overestimated measured exposure ratings 70% of the time; 16% of model ratings coincide with measured exposure ratings, and model ratings underestimated measured exposure ratings 14% of the time. A Kappa statistic indicated there was no statistically significant agreement between model ratings and measured exposure ratings (κ = 0.030, p=0.194).
Table 20. Contingency Table Comparing QLEA Model Ratings and Measured Exposure Ratings for Data Collectively

<table>
<thead>
<tr>
<th>Measured Exposure Ratings</th>
<th>QLEA Model Ratings</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7</td>
<td>42</td>
<td>55</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>17</td>
<td>21</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>13</td>
<td>13</td>
<td>7</td>
<td></td>
</tr>
</tbody>
</table>

Table 21 shows the relationship between QLEA model ratings and ratings based on measured exposures for particulates only (i.e. no stratification by magnitude of exposure). The model ratings overestimated measured exposure ratings 58% of the time; 22% of model ratings coincide with measured exposure ratings, and the model underestimated measured exposure ratings 20% of the time. A Kappa statistic indicated there was no statistically significant agreement between model ratings and measured exposure ratings ($\kappa = 0.034$, $p=0.417$).

Table 21. Contingency Table Comparing QLEA Model Ratings and Measured Exposure Ratings for Particulates

<table>
<thead>
<tr>
<th>Measured Exposure Ratings</th>
<th>QLEA Model Ratings</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>24</td>
<td>8</td>
<td>14</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>12</td>
<td>2</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>10</td>
<td>8</td>
<td>7</td>
<td></td>
</tr>
</tbody>
</table>
Table 22 shows the relationship between the model ratings and ratings based on measured exposures for vapors only (i.e. no stratification by magnitude of exposure). The model ratings overestimated measured exposure ratings 81% of the time; 10% of model ratings coincide with measured exposure ratings, and the model underestimated measured exposure ratings 9% of the time. A Kappa statistic indicated there was no statistically significant agreement between model ratings and measured exposure ratings (κ < 0.0001, p=0.997).

Table 22. Contingency Table Comparing QLEA Model Ratings and Measured Exposure Ratings for Vapors

<table>
<thead>
<tr>
<th>Measured Exposure Ratings</th>
<th>QLEA Model Ratings</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
</tr>
</tbody>
</table>

Finally, the data were stratified into the 6 groups (PH, PM, PL, VH, VM, and VL) and contingency tables were used to calculate when the QLEA model overestimated, correctly estimated, and underestimated, measured exposures. The overall results of those analyses are shown in Table 23 and Figure 7. In general, the QLEA consistently overestimated low level exposures (PL and VL). For medium and high level exposures (PM, PH, VM, and VH) the QLEA consistently underestimated exposures. However, it must be noted that the sample size for these groups was extremely small (n≤17).
Table 23. Percentage of Exposures Underestimated, Correctly Estimated, and Overestimated by the QLEA Model

<table>
<thead>
<tr>
<th></th>
<th>n</th>
<th>Underestimated</th>
<th>Correctly Estimated</th>
<th>Overestimated</th>
</tr>
</thead>
<tbody>
<tr>
<td>PL</td>
<td>72</td>
<td>4% (n=3)</td>
<td>21% (n=15)</td>
<td>75% (n=54)</td>
</tr>
<tr>
<td>PM</td>
<td>5</td>
<td>80% (n=4)</td>
<td>20% (n=1)</td>
<td>0% (n=0)</td>
</tr>
<tr>
<td>PH</td>
<td>17</td>
<td>71% (n=12)</td>
<td>29% (n=5)</td>
<td>0% (n=0)</td>
</tr>
<tr>
<td>All Particulates</td>
<td>94</td>
<td>20% (n=19)</td>
<td>22% (n=21)</td>
<td>58% (n=54)</td>
</tr>
<tr>
<td>VL</td>
<td>98</td>
<td>2% (n=2)</td>
<td>11% (n=11)</td>
<td>87% (n=85)</td>
</tr>
<tr>
<td>VM</td>
<td>2</td>
<td>100% (n=2)</td>
<td>0% (n=0)</td>
<td>0% (n=0)</td>
</tr>
<tr>
<td>VH</td>
<td>5</td>
<td>100% (n=5)</td>
<td>0% (n=0)</td>
<td>0% (n=0)</td>
</tr>
<tr>
<td>All Vapors</td>
<td>105</td>
<td>9% (n=9)</td>
<td>10% (n=11)</td>
<td>81% (n=85)</td>
</tr>
<tr>
<td>All Data</td>
<td>199</td>
<td>14% (n=28)</td>
<td>16% (n=32)</td>
<td>70% (n=139)</td>
</tr>
</tbody>
</table>

Figure 7. Percentage of exposures underestimated, correctly estimated, and overestimated by the QLEA model

In order to calculate measurements of validity such as the efficiency, sensitivity, specificity, percentage of false low classification and percentage of false high classifications, the 4x4 contingency tables were collapsed into 2x2 tables. Since ratings
of one and two indicate acceptable exposures, they were combined into column and row one and labeled “Acceptable”. Because a rating of three indicates uncertainty, and a rating of four indicates unacceptable exposures, they were combined into column and row two and labeled “Uncertain/Unacceptable”.

The 4x4 contingency table comparing the final ratings for the data collectively (no stratification by physical state or magnitude) [Table 20] was collapsed into a 2x2 contingency table. Results are shown in Table 24. Chi Square analysis indicated no statistically significant agreement between model ratings and measured exposure ratings ($\chi^2 = 0.009$, p=0.926).

<table>
<thead>
<tr>
<th>Measured Exposure Ratings</th>
<th>QLEA Model Ratings</th>
<th>Acceptable</th>
<th>Uncertain/Unacceptable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acceptable</td>
<td></td>
<td>67</td>
<td>97</td>
</tr>
<tr>
<td>Uncertain/Unacceptable</td>
<td></td>
<td>14</td>
<td>21</td>
</tr>
</tbody>
</table>

The model accurately classified measured exposures in 88 out of 199 cases (44%). Forty-one percent of the measured exposures classified as acceptable were correctly classified as acceptable by the model (sensitivity), while 60% of the measured exposures classified as uncertain/unacceptable were correctly classified as uncertain/unacceptable by the model (specificity). In addition, there was a 40% probability that the model would result in a false low classification and a 59% probability that the model would result in a false high classification.
The 4x4 contingency table for particulates only (i.e. no stratification by magnitude of exposure) [Table 21] was collapsed into a 2x2 contingency table to calculate measurements of validity. Results are shown in Table 25. Chi Square analysis indicated no statistically significant agreement between model ratings and measured exposure ratings ($\chi^2 = 1.389, p=0.239$).

### Table 25. 2x2 Contingency Table Comparing QLEA Model Ratings and Measured Exposure Ratings for Particulates

<table>
<thead>
<tr>
<th>Measured Exposure Ratings</th>
<th>QLEA Model Ratings</th>
<th>Acceptable</th>
<th>Uncertain/Unacceptable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acceptable</td>
<td></td>
<td>38</td>
<td>30</td>
</tr>
<tr>
<td>Uncertain/Unacceptable</td>
<td></td>
<td>11</td>
<td>15</td>
</tr>
</tbody>
</table>

The model accurately classified measured exposures in 53 out of 94 cases (56%). Fifty-six percent of the measured exposures classified as acceptable were correctly classified as acceptable by the model (sensitivity), while 58% of the measured exposures classified as uncertain/unacceptable were correctly classified as uncertain/unacceptable by the model (specificity). In addition, there was a 42% probability that the model would result in a false low classification and a 44% probability that the model would result in a false high classification.

The 4x4 contingency table for vapors only (i.e. no stratification by magnitude of exposure) [Table 22] was also collapsed into a 2x2 contingency table to calculate measurements of validity. Results are shown in Table 26. Chi Square analysis indicated
no statistically significant agreement between model ratings and measured exposure ratings ($\chi^2 = 0.038$, p=0.846).

Table 26. 2x2 Contingency Table Comparing QLEA Model Ratings and Measured Exposure Ratings for Vapors

<table>
<thead>
<tr>
<th>Measured Exposure Ratings</th>
<th>QLEA Model Ratings</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Acceptable</td>
<td>Uncertain/Unacceptable</td>
</tr>
<tr>
<td>Acceptable</td>
<td>29</td>
<td>67</td>
</tr>
<tr>
<td>Uncertain/Unacceptable</td>
<td>3</td>
<td>6</td>
</tr>
</tbody>
</table>

The model accurately classified measured exposures in 35 out of 105 cases (33%). Thirty percent of the measured exposures classified as acceptable were correctly classified as acceptable by the model (sensitivity), while 67% of the measured exposures classified as uncertain/unacceptable were correctly classified as uncertain/unacceptable by the model (specificity). In addition, there was a 33% probability that the model would result in a false low classification and a 70% probability that the model would result in a false high classification.

Due to small sample sizes, it was not worthwhile to calculate measurements of validity using 2x2 contingency tables for each of the six groups (PL, PM, PH, VL, VM, and VH). Further, because categories representing medium and high exposures to particulates and vapors had such small sample sizes ([PM (n=5), PH (n=17), VM (n=2), and VH (n=5)],) we chose to focus additional data analysis on low level exposures (PL and VL) only.
Spearman Correlations

In general, the QLEA model overestimates low-level exposures. As was done with the COSHH Essentials model, the degree of overestimation was calculated for each SEG by subtracting the measured exposure rating from the QLEA model rating. This calculated variable was labeled “Difference”. Thus, if the QLEA model overestimated exposures, the “Difference” variable had a positive value. Likewise, if the QLEA model underestimated exposures, the “Difference” variable had a negative value. Further, the degree of overestimation was evident by the magnitude of the “Difference” variable.

Recall that four variables, the duration frequency (DF), hazard rank for inhalation (HI), airborne risk (AR), and engineering controls (EC), are used to arrive at a final rating (1 – 4) characterizing the acceptability of risk. Spearman correlation analyses were utilized to determine which QLEA model variables (i.e. DF, HI, AR, and EC) were associated with an overestimation in exposure by calculating the correlation coefficient between the “Difference” variable and each QLEA model variable. Results are shown in Table 27.

Table 27. Spearman Correlation Coefficients between QLEA Model Predictor Variables and Degree of Overestimation

<table>
<thead>
<tr>
<th></th>
<th>Particulates</th>
<th>Vapors</th>
<th>All</th>
</tr>
</thead>
<tbody>
<tr>
<td>DF</td>
<td>0.151</td>
<td>0.249A</td>
<td>0.207A</td>
</tr>
<tr>
<td></td>
<td>p=0.205  p=0.014</td>
<td>p=0.007</td>
<td></td>
</tr>
<tr>
<td>HI</td>
<td>0.564A</td>
<td>-0.231A</td>
<td>0.203A</td>
</tr>
<tr>
<td></td>
<td>p&lt;0.0001 p=0.022</td>
<td>p=0.008</td>
<td></td>
</tr>
<tr>
<td>AR</td>
<td>0.515A</td>
<td>0.464A</td>
<td>0.445A</td>
</tr>
<tr>
<td></td>
<td>p&lt;0.0001 p&lt;0.0001</td>
<td>p&lt;0.0001</td>
<td></td>
</tr>
<tr>
<td>EC</td>
<td>0.261A</td>
<td>0.632A</td>
<td>0.476A</td>
</tr>
<tr>
<td></td>
<td>P=0.027  p&lt;0.0001</td>
<td>p&lt;0.0001</td>
<td></td>
</tr>
</tbody>
</table>

*Statistically significantly at α = 0.05
For particulates, the HI, AR, and EC variables were significantly correlated with an overestimation of exposure. Specifically, chemical agents that are considered to be more hazardous, as indicated by an increasing value for HI, are associated with a higher degree of overestimation ($r_s=0.564$, $p<0.0001$). SEGs that are subjectively assessed as having a higher risk of airborne exposures, as indicated by an increasing value for AR, are also associated with a higher degree of overestimation ($r_s=0.515$, $p<0.0001$). Finally, SEGs with less sophisticated engineering controls, as indicated by an increasing value for EC, are associated with a higher degree of overestimation ($r_s=0.261$, $p=0.027$). However, this association was relatively weak.

For vapors, all model variables were significantly correlated with an overestimation of exposure. SEGs in which the duration of exposure to a chemical agent is extended, as indicated by an increasing value for DF, are associated with a higher degree of overestimation ($r_s=0.249$, $p=0.014$). However, this association was relatively weak. For vapors, there is a negative correlation between chemical toxicity, as indicated by the HI variable, and overestimation. Specifically, chemical agents that are considered to be less hazardous are associated with a higher degree of overestimation ($r_s=-0.231$, $p=0.022$). However, this association was also considered weak. SEGs that are subjectively assessed as having a higher risk of airborne exposures, as indicated by an increasing value for AR, are also associated with a higher degree of overestimation ($r_s=0.464$, $p<0.0001$). Finally, SEGs with less sophisticated engineering controls, as indicated by an increasing value for EC, are associated with a higher degree of overestimation ($r_s=0.632$, $p<0.0001$).
When the data were analyzed collectively, all model variables were significantly correlated with an overestimation of exposure. SEGs in which the duration of exposure to a chemical agent is extended, as indicated by an increasing value for DF, are associated with a higher degree of overestimation ($r_s=0.207$, $p=0.007$). However, this association is relatively weak. Chemical agents that are considered to be more hazardous, as indicated by an increasing value for HI, are associated with a higher degree of overestimation ($r_s=0.203$, $p=0.008$). However, this association is also considered weak. SEGs that are subjectively assessed as having a higher risk of airborne exposures, as indicated by an increasing value for AR, are also associated with a higher degree of overestimation ($r_s=0.445$, $p<0.0001$). Finally, SEGs with less sophisticated engineering controls, as indicated by an increasing value for EC, are associated with a higher degree of overestimation ($r_s=0.476$, $p<0.0001$).

**Examination of Data Variability**

It is well documented that exposure concentrations can vary from day to day as well as between workers (Leidel et al., 1977; Perkins, 1997). Previous studies have reported that the evaluation of models may be affected by high variability in the exposure data used for comparisons (Stewart and Stenzel, 2000; Kromhout, et al., 1987). Hewett (2007) stated that true GSDs greater than 4 are unusual, particularly for individual workers, and suggested that as a rule-of-thumb, SEGs with GSDs of 3 or more be scrutinized to see if dissimilar workers or activities have been combined (e.g. indoor and outdoor activities), if there is seasonal variation, or if too few data exist. Therefore, to remain conservative in our approach and ensure that data variability did not bias the
results of COSHH Essentials and QLEA model validation, statistical analyses excluded SEGs with GSDs greater than 3.0.

As an addendum to the primary objectives of this study, we chose to briefly investigate the concept of data variability as it applies to model validation. Specifically, we wanted to investigate whether SEGs with high data variability would have biased the results of our statistical analyses. First, all statistical tests were repeated and SEGs with high data variability (i.e. GSD > 3.0) were included in the analyses. All results remained practically identical to results involving SEGs with low data variability (i.e. GSDs ≤ 3.0). For example the percentage of exposures overestimated by both the COSHH Essentials and QLEA models for each category (PL, PM, PH, VL, VM, and VH) remained virtually the same as can be seen in Figure 8. In addition, statistical tests (i.e. General Linear Models and Spearman Correlations) used to determine which model components were associated with an overestimation in exposure yielded the same conclusions. Thus, we concluded one of two explanations were possible: 1) Data variability did not bias the results of model validation in our study or 2) the sample size of SEGs with high data variability (n=53) was too small to significantly alter the results when grouped with SEGs with low data variability (n=199).
Therefore, to further investigate this phenomenon, statistical analyses were once again repeated. This time, however, only SEGs with high data variability (GSDs > 3.0) were analyzed. Clearly, due to the small sample size (n=53) and stratification of the data into six groups (PH, PM, PL, VH, VM, and VL) results from some analyses were debatable. Regardless, when the percentage of exposures underestimated, correctly estimated, and overestimated by both the COSHH Essentials and QLEA models were evaluated, results were strikingly similar to those for SEGs with low data variability (GSDs < 3.0) as can be seen by comparing Figures 6 and 7, with Figures 9 and 10 respectively. Thus, it appears that in our study, inclusion of SEGs with high data variability would not have biased the results of model validation.

Figure 8. Comparison of the percent of overestimation between SEGs with GSD < 3.0 and all SEGs by COSHH Essentials and QLEA models
Recall that when a sampling approach is utilized to statistically define an SEG it is suggested that 95% of workers in the SEG should have a maximum difference between their long-term average exposures no greater than a factor of two (Mulhausen and Damiano, 1998). This concept was originally proposed by Rappaport (1991) and can be quantified using equation 18. Equation 18 utilizes the percentiles of the distribution of
individual worker means \((\bar{x}_{97.5\%tile}, \bar{x}_{2.5\%tile})\) to calculate the maximum difference between the long-term average exposures for 95% of workers in an SEG (R).

\[
R = \frac{\bar{x}_{97.5\%tile}}{\bar{x}_{2.5\%tile}} \leq 2
\]  

(18)

Review of previous literature (Rappaport, 1991; Rappaport, Kromhout, and Symanski, 1993; Perkins, 1997; Mulhausen and Damiano, 1998) did not establish a clear connection between the overall GSD of an SEG and R (the maximum difference between the long-term average exposures for 95% of workers in an SEG). We chose to further our investigation by examining the relationship between the GSD of an SEG and R in our particular dataset. Note that, in our study, we cannot calculate the “true” R-value for an SEG since calculation of R requires knowledge of the percentiles of the distribution of individual worker means. Unfortunately, HHE reports did not contain personal identifiers for SEGs sampled. As a result, it was not possible to determine if the same individual was sampled multiple times or if multiple individuals were sampled a single time. Thus, we cannot examine the distribution of individual worker means. Rather we must examine the distribution of the sampling data as a whole and utilize percentiles from the raw data. In doing this, we make the assumption that each sample is from an individual worker, and the exposure concentration measured is equal to the long-term average exposure of that specific worker. Although such a calculation is not a “true” representation of R, it gives us an estimation of R.

First, we reviewed estimated R values for SEGs with a GSD \(\leq 3.0\), henceforth referred to as low-variability SEGs. Estimated values for R ranged from 1 to 89 with a
median value of 4. For SEGs with a GSD > 3.0, henceforth referred to as high-variability SEGs, estimated values for R ranged from 12 to 5492 with a median value of 56. Thus, inspection of estimated R values revealed that even when the GSD was relatively low (GSD ≤ 3.0), individual workers still experienced significant differences in exposures (on average, a difference of 7-Fold). Overall, for low-variability SEGs, 39% (78 of 199) had estimated values of R ≤ 2, while 19% (38 of 199) had estimated values of R ≥ 10.

Next, we plotted the GSD against estimated R values for both low-variability SEGs and high-variability SEGs. Plots for both low-variability SEGs and high-variability SEGs are shown in figures 11 and 12, respectively. Pearson’s correlation analysis revealed a statistically significant correlation between the GSD and R for both low-variability SEGs and high-variability SEGs (r=0.578, p<0.0001 and r=0.568, p<0.00001, respectively). For both groups, the correlation coefficient was approximately 0.6, indicating there is a statistically significant relationship between an SEG’s GSD and R value.
Figure 11. Plot of GSD versus R for low-variability SEGs

Figure 12. Plot of GSD versus R for high-variability SEGs
CHAPTER 4

DISCUSSION

Data Collection

One limitation of this study is that model validation relied on pre-existing exposure measurements. Specifically, the COSHH Essentials and QLEA model were used to estimate exposure concentrations for retrospective exposure scenarios identified from HHE reports. A more appropriate method for conducting a validation study would be to evaluate exposures prospectively. Specifically, it would be ideal to qualitatively evaluate exposure scenarios from a wide range of industries (e.g. manufacturing, chemical, construction, etc.) using both models while concurrently obtaining quantitative air samples. Several companies were contacted and asked to participate in a study of this nature. However, due to potential legal ramifications associated with possible non-compliance issues, corporate industries were not willing to participate. While relying on pre-existing data is not an ideal study design, this approach has been used extensively in previous model validation studies (Bredendiek-Kamper, 2001; Cherrie and Hughson, 2005; Jones and Nicas, 2006; Mark, 1999; Tischer et al., 2003).

Of the 345 HHE reports identified as applicable to our study, only a small percentage (20%) contained sufficient information to conduct exposure assessments using the COSHH Essentials and QLEA models. To be included in the study, HHE reports had to include information concerning the scale of use, volatility/dustiness, and
engineering controls present. Not surprisingly, the developers of COSHH Essentials encountered a similar challenge during early model development. During the model’s infancy, developers attempted to validate the model utilizing the Criteria Documents for Occupational Exposure Limits published by the HSE (Maidment, 1998). They found that for most exposure scenarios (Table 6), no suitable data was available for comparison since most occupational exposure records do not contain information regarding the usage quantity, volatility, and engineering controls present. In fact, Maidment (1998) stated that due to a lack of suitable data, numerical validation of the model’s scheme was not possible. Rather, the model’s logic was evaluated by specialists from the BOHS and BIOH. Unfortunately, these evaluations were never published.

An additional limitation of this study is that of the 199 SEGs identified, the majority (85%) involved low level exposures (i.e. AM < 50% of the OEL). Thus, COSHH Essentials and QLEA model performance was thoroughly evaluated in low level exposure scenarios only. Although a primary goal of this study was to evaluate the accuracy of the COSSH Essentials and QLEA models in low, medium, and high exposure situations involving particulates and vapors, only a small number of SEGs identified from HHE reports involved medium (4%) and high (11%) exposures. While statistical tests were still performed for SEGs involving medium and high exposures (PM, PH, VM, and VH), we can only make inferences based on the results of these analyses due to the small sample size limitation.
COSHH Essentials Model

Pearson Correlations

Recall that the COSHH Essentials model predicts a range of possible concentrations for an exposure scenario. A Pearson correlation coefficient (Daniel, 1999) was calculated to evaluate the linear relationship between both the maximum measured exposure and the upper limit of the model’s predicted concentration range as well as the minimum measured exposure and the lower limit of the model’s predicted concentration range. Data were stratified into six groups (PH, PM, PL, VH, VM, and VL) and correlation coefficients were calculated for each group to determine if the model was more accurate in predicting exposures under certain conditions. For the purpose of this study, the model was considered accurate if the correlation coefficient was $\geq 0.70$ and statistically significant at $\alpha=0.05$. None of the calculated correlation coefficients met the established criteria. Thus, by our own definition, regardless of the physical state of the chemical substance and the magnitude of the exposure, the COSHH Essentials model was not an accurate predictor of measured exposures.

Percentages of Measured Exposures Above, Within, and Below Model’s Predicted Range

In addition, the percentage of measured exposures that fell within, above, and below the model’s predicted concentration range was calculated as was done by Tischer et al. (2003). The model consistently overestimated exposures for both particulates and vapors when data were not stratified by the magnitude of exposure (i.e. low, medium, and high).
Results from our study were similar to, but not as favorable as, those found by Tischer et al. (2003). In general, for particulates, the model correctly estimated or overestimated exposures in 93% of all cases. Tischer and colleagues found that for particulates, COSHH Essentials correctly estimated or overestimated exposures in 99% of all cases. However, the frequency of overestimation in our study was greater than that found by Tischer et al. (2003). Tischer and colleagues found that for particulates, COSHH Essentials overestimated exposures in 40% of all cases while our study found COSHH Essentials overestimated exposures in 81% of all cases.

In general, for vapors, the model correctly estimated or overestimated exposures in 97% of all cases. Tischer and colleagues found that for vapors, COSHH Essentials correctly estimated or overestimated exposures in 96% of all cases. However, the frequency of overestimation in our study was once again greater than that found by Tischer et al. (2003). Tischer and colleagues found that for vapors, COSHH Essentials overestimated exposures in 50% of all cases, while our study found COSHH Essentials overestimated exposures in 78% of all cases.

Recall that a primary limitation of our study was that the majority of exposure scenarios involved low level exposures. In contrast, a primary limitation of Tischer’s study was that most exposure scenarios evaluated were “medium” scenarios meaning there was medium use of the chemical and the chemical had a medium level of dustiness/volatility. Thus, a likely explanation for the differences observed when comparing results from the current study to those of Tischer et al. (2003) is that each study utilized exposure scenarios which were biased towards a single magnitude of exposure. Such comparisons further confirm that qualitative models should be fully
evaluated among low, medium, and high exposure scenarios prior to drawing any concrete conclusions.

Further, in the current study, when data were stratified by the physical state and magnitude of exposure, the frequency of overestimation appeared to lessen as the magnitude of exposure increased. For instance, for particulates, COSHH Essentials resulted in an overestimation for 86% of low level exposures. For medium and high level exposures, COSHH Essentials resulted in an overestimation in 69% and 55% of cases, respectively. For vapors, COSHH Essentials resulted in an overestimation for 81% of low level exposures. For medium and high level exposures, COSHH Essentials resulted in an overestimation in 30% and 45% of cases, respectively. However, it must be noted that the sample size for medium and high exposure scenarios (PM, PH, VM, and VH) was small.

**General Linear Models**

As with previous validation studies (Tischer et al., 2003), this study found that in general, the COSHH Essentials model led to an overestimation of exposure. This is not surprising considering the model was designed to be overprotective (Russell et al., 1998). Russell et al. (1998) stated that during early model development, it was recognized that an over-protective model would lack credibility while an under-protective model would not protect worker health. After weighing both factors, it was decided that COSHH Essentials would take a conservation approach and be “slightly” overprotective. However, it is clear from this study that COSHH Essentials has the potential to be vastly overprotective.
A primary strength of this study is that we went beyond the approach used in previous studies and attempted to identify which model components led to the overestimation in exposure. Recall that the exposure prediction portion of COSHH Essentials utilizes two components to arrive at a predicted concentration range – the EP Band and controls present. Also recall that two components are utilized when placing an SEG in a specific EP Band – usage quantity and volatility/dustiness. General linear models were constructed to determine which components or which combination of components led to the overestimation in exposure. Unfortunately, one limitation of the general linear model analysis is that although the sample size for low level exposures to both particulates (n=72) and vapors (n=98) was considered adequate by most standards, due to the numerous combination of factors possible within COSHH Essentials, several combination of factors were simply not observed (Tables 14 and 15). Therefore, we can only make inferences regarding which model components lead to an overestimation of exposure.

For particulates, it was found that the model’s tendency to overestimate exposures was the result of multiple interactions among model components. General linear model analysis found a statistically significant interaction between the EP Band and controls present in addition to a statistically significant interaction between the usage quantity and dustiness of the substance. However, in general when no mechanical engineering controls were present, the model overestimated exposure, and the magnitude of overestimation worsened as the EP Band increased. The model also consistently overestimated exposures for high dusty solids, and the magnitude of overestimation worsened as the quantity increased.
For vapors, it was found that the model’s tendency to overestimate exposures was the result of a complex interaction between the EP Band and controls present. As with particulates, the model tended to overestimate exposures in the absence of engineering controls, and the magnitude of overestimation worsened as the EP Band increased. However, for vapors there was no statistically significant interaction between the usage quantity and the volatility of the substance. Rather, the magnitude of overestimation worsened as the vapor pressure and usage quantity increased independently.

Overall, it appears that the magnitude of overestimation increases exponentially as values for predictor variables increase (i.e. usage quantity increases from low to high; volatility increase from low to high; EP-Band increases from 1 to 4; etc.). In addition, although the model overestimates exposures for both particulates and vapors, statistical analyses indicate that different model components may lead to the overestimation for particulates versus vapors. Neither finding is unexpected considering the model’s design.

The COSHH Essentials model was designed using log-based (10-fold) concentration ranges (Brooke, 1998). The model’s developers utilized a log-based scale when selecting predicted concentration ranges for each EP-Band/Control combination (Table 6). For instance, when no engineering controls are present, the predicted concentration range for EP-Band S1 is 0.01 to 0.1 mg/m$^3$, the predicted concentration range for EP-Band S2 is 0.1 to 1 mg/m$^3$, the predicted concentration range for EP-Band S3 is 1 to 10 mg/m$^3$, etc. Thus, it is expected that if the model is designed to be over-predictive in general, the magnitude of over-prediction will increase exponentially as values for predictor variables increase.
In addition, to simplify the model’s scheme, a pragmatic approach was adopted and predicted concentration ranges for particulates and vapors were aligned, as shown in Table 6. For instance, whenever the predicted concentration range for particulates is listed as 1 to 10 mg/m$^3$, the predicted concentration range for vapors is listed as 50 to 500 ppm. Recall that the relationship between the ppm concentration of a substance and the mg/m$^3$ concentration is a function of a chemical substance’s molecular weight at normal temperature and pressure (25°C and 760 mm Hg) as shown in equation 19.

$$C(\text{mg } / \text{ m}^3) = C(\text{ppm}) \times \frac{MW}{24.45}$$  \hspace{1cm} (19)

Consider, for example, a substance of molecular weight 100; 1 ppm is equivalent to about 4 mg/m$^3$. If that substance was allocated to EP-Band 2 and Control Approach 1, the concentration of the particulate form of the substance (4 mg/m$^3$) would be greater than the range predicted by COSHH Essentials (0.1 to 1 mg/m$^3$). However, the concentration of the vapor form of the substance (1 ppm) would be less than the range predicted by COSHH Essentials (5 to 50 ppm). Thus, it is expected that the model could potentially perform differently when assessing particulates versus vapors.

**QLEA Model**

*Correlations*

Recall that the QLEA model calculates an inhalation risk factor and assigns a final rating ranging from 1 to 4 based on the value of the inhalation risk. Spearman correlation coefficients (Daniel, 1999) as well as Pearson correlation coefficients were
calculated to evaluate the linear relationship between the model ratings and measured exposures. Data were stratified into six groups (PH, PM, PL, VH, VM, and VL) based on the physical state of the chemical substance and magnitude of the measured exposure. Correlation coefficients were calculated for each group to determine if the model was more accurate in predicting measured exposures under certain conditions. For the purpose of this study, the model was considered accurate if the correlation coefficient was \( \geq 0.70 \) and statistically significant at \( \alpha = 0.05 \). None of the calculated correlation coefficients met the established criteria. Thus, by our own definition, regardless of the physical state of the chemical substance and magnitude of the exposure, the QLEA model was not an accurate predictor of measured exposures.

In our previous validation study involving the QLEA model (Elliott and Oestenstad, 2007), data were not stratified by physical state or magnitude of exposure. Therefore, to accurately compare our current results with those from our previous study, we must consider the data collectively. Both the current study as well as the previous study found no significant correlation between QLEA model ratings and measured exposures (\( r = 0.053 \), \( p = 0.457 \) and \( r = 0.119 \), \( p = 0.496 \), respectively).

**Contingency Table Analyses**

As was done in our previous study (Elliott and Oestenstad, 2007), model ratings and measured exposure ratings were compared using contingency tables. In our previous study, data were not stratified by physical state or magnitude of exposure. Therefore, to accurately compare our current results with those from our previous study, we again must consider the data collectively. It is important to note that in our previous study (Elliott
and Oestenstad, 2007) 91% (32 of 35) of SEGs assessed were considered low-level exposures (AM < 50% of OEL) while 85% (170 of 199) of SEGs assessed in the current study were considered low-level exposures. Regardless, results from both studies remain similar. The QLEA model overestimated exposures in 70% of cases in the current study and 77% of cases in the previous study. The model correctly estimated exposures in 16% of cases in the current study and 14% of cases in the previous study, and the model underestimated exposures in 14% of cases in the current study and 9% of cases in the previous study.

We concluded in our previous study (Elliott and Oestenstad, 2007) that the QLEA model was a poor predictor of low level exposures and generally resulted in an overestimation of exposure. However, since only a small number of exposure scenarios from a single manufacturing facility were assessed (n=35), we recommended the QLEA model be further evaluated in both medium and high exposure scenarios as well as diverse industrial environments. Thus, one goal of the current study was to determine if the model was more accurate in predicting measured exposures under different exposure conditions. Therefore, in addition to analyzing the data collectively, the current study compared model performance for particulates and vapors and stratified the data into six groups (PH, PM, PL, VH, VM, and VL) based on the physical state of the chemical substance and the magnitude of exposure. In general, the model consistently overestimated exposures for both particulates and vapors when the magnitude of the measured exposure was low (AM < 50% of OEL). However, when the magnitude of the measured exposure was medium (AM between 50% and 75% of the OEL) or high (AM ≥ 75% of the OEL), the model consistently underestimated exposures. Unfortunately, a
primarily limitation of the current study is the sample size for these groups (PM, PH, VM, and VH) was extremely small (n=5, n=17, n=2, and n=5, respectively). Regardless, this study indicates the QLEA model likely performs poorly in low, medium, and high exposure scenarios.

As was done in our previous study (Elliott and Oestenstad, 2007), 4x4 contingency tables were collapsed into 2x2 tables in order to calculate measurements of validity. Data were analyzed collectively, and particulates and vapors were analyzed separately. Due to the small sample size, further data stratification was omitted. When the data were analyzed collectively, the model accurately classified measured exposures in 44% of all cases (efficiency). Forty-one percent of the measured exposures classified as acceptable were correctly classified as acceptable by the model (sensitivity), while 60% of the measured exposures classified as uncertain/unacceptable were correctly classified as uncertain/unacceptable by the model (specificity). These results are similar to those found in our previous study (Elliott and Oestenstad, 2007) for efficiency (51%) and sensitivity (53%). Although in our previous study the QLEA model was found to have a specificity of 33% compared to 60% in the current study, this difference is likely due to the small number of medium and high exposure scenarios (n=3) included in the initial study. Overall, both the current study as well as the previous study found no statistically significant agreement between model ratings and measured exposure ratings ($\chi^2 = 0.009, p=0.926$ and $\chi^2=0.203, p=0.653$, respectively).

It should also be mentioned that in the current study, when particulates and vapors were analyzed separately, results were slightly different. The model’s efficiency was calculated at 56% for particulates and 33% for vapors. The model had 56% sensitivity
for particulates and 30% sensitivity for vapors. Finally, specificity was 58% for particulates and 67% for vapors.

Spearman Correlations

A primary strength of the current study is it went beyond our previous study (Elliott and Oestenstad, 2007) and attempted to identify which model components were correlated with an overestimation in low-level exposures. Recall that four variables (DF, HI, AR, and EC) are used to arrive at a final rating (1 – 4) which characterizes the acceptability of exposure risk (Acceptable, Uncertain, Unacceptable). Spearman correlation analysis showed all four model variables were significantly associated with an overestimation of exposure when data were analyzed collectively (i.e. no stratification by physical state of the chemical substance). In general as the value for the predictor variable increased, the magnitude of overestimation worsened. However, it must be noted that the strength of correlation coefficients ranged from weak to moderate.

These findings indicate that in general, the QLEA model is a poor predictor of occupational exposures. The QLEA model was shown to overestimate low-level exposures in both the current study and our previous study (Elliott and Oestenstad, 2007). Spearman correlation analysis indicated that all four variables were associated with an overestimation in exposure. In addition, although the sample size was small, contingency table analyses from the current study indicate the model likely underestimates medium and high level exposures. On average, the QLEA model correctly classified exposures 44% of the time which is roughly the equivalent of flipping a coin. Thus, it appears that
the QLEA model is based on flawed logic. Unfortunately, no explanation concerning the rationale behind the model’s design is available.

Examination of Data Variability

With respective to data variability, NIOSH reported that occupational environments will possess distributions with GSDs ranging from 1.5 to 3.5 (Leidel, Busch, and Crouse, 1975; Leidel et al., 1977). However, Perkins (1997) pointed out that GSDs may appear on both sides of this range. Rappaport and Selvin (1987) reported GSDs of 6 and greater in the petroleum industry, and Buringh and Lanting (1991) reported GSDs ranging from 1.2 to 10 in Dutch factories. In the current study only 10% (25 of 252) of the SEGs (i.e. both low-variability and high-variability) had GSDs greater than 4.0 (Hewett, 2007).

As previously stated, an ad hoc objective of this study was to investigate the concept of data variability as it applied to model validation. Specifically, we investigated whether inclusion of SEGs with high data variability (i.e. GSD > 3.0) biased the results of statistical analyses and altered study conclusions. Repeated statistical analyses confirmed that inclusion of SEGs with high data variability would not have affected the results of model validation in this particular study.

However, further scrutiny of the qualitative models evaluated in this study reveals a likely explanation for this phenomenon. Consider the COSHH Essentials model. Table 6 illustrates that the model uses a log-base scale when predicting exposure concentration ranges (i.e. COSHH Essentials predicted exposure concentration ranges cover a 10-fold range). Therefore, COSHH Essentials is actually designed to accommodate SEGs in
which 95% of workers have a maximum difference between their long-term average exposures of up to 10 (R ≤ 10). Overall, for all SEGs in this study (i.e. both low-variability and high-variability SEGs), 66% (166 of 252) had estimated values of R ≤ 10. Therefore, a likely explanation for the fact that inclusion of high-variability SEGs did not alter the results of the statistical analyses is the qualitative models evaluated in this study were actually designed to predict a wide range of potential exposures.

**Implications for Small and Medium Sized Industries**

As previously stated, in the US, 98% of businesses have fewer than 100 workers with more than half (55%) of the American workforce being employed by small and medium sized industries (US Census Bureau, 2004). Small businesses are found in all sectors of industry. The majority of small and medium sized companies do not employ industrial hygienists or other professionals knowledgeable in occupational exposures evaluations. Therefore, it is usually not feasible for small and medium sized companies to conduct quantitative sampling due to budgetary and resource limitations. Qualitative exposure assessment models, such as COSHH Essentials and QLEA, are easy to understand and implement and could prove advantageous for small business owners. However, questions have been raised as to their accuracy. This study showed that both models vastly overestimate exposures in low-level exposure scenarios. Further, although the sample size was small, this study indicates that the QLEA model potentially underestimates exposures in medium and high-level exposure scenarios.

Thus, if these models were marketed to small business owners in their current form, decisions pertaining to worker health based on model results would involve great
uncertainty. On occasions when the models overestimate exposure, unnecessary spending to prioritize and implement costly control methodologies is likely to occur. Further, on occasions when the models underestimate exposure, controls strategies may not be implemented and workers may be exposed to chemicals above OELs.

With respect to qualitative models, it has been argued that reliability and accuracy are often sacrificed for the sake of simplicity and transparency. Thus, in general, there is already a low degree of confidence associated with qualitative models (Tischer, 2003). Therefore, given the COSHH Essentials and QLEA models have been shown to be exceedingly overprotective in their current form, it is unlikely that small business owners would be receptive of them.
CHAPTER 5

CONCLUSIONS

Feasibility of using Retrospective Exposure Data in Model Validation Studies

The primary goal of this research was to validate two qualitative exposure assessment models. This study utilized an external validation approach involving retrospective exposure measurements obtained from NIOSH HHE reports. One goal of this study was to evaluate both models in high, medium, and low exposure scenarios involving particulates and vapors to determine if the models performed differently in different exposure conditions. Unfortunately, because this study relied on retrospective exposure measurements, the majority of exposure data available were for low-level exposures only. Hence, although pre-existing exposure data has been used extensively in numerous validation studies (Bredendiek-Kamper, 2001; Cherrie and Hughson, 2005; Jones and Nicas, 2006; Mark, 1999; Tischer et al., 2003), it is difficult, if not impossible, to meticulously validate qualitative models using this approach. Unfortunately, at the present time, superior data are not available to allow appropriate validation of qualitative models (Jones and Nicas, 2006; Money, 2003; Tischer et al., 2003; Kromhout, 2002; Maidment, 1998). Experts who have written about qualitative exposure assessment models confirm their potential value as a risk assessment tool in the workplace, but express caution about the need for systematic, critical evaluation of models before widespread adoption. This study further emphasizes the need for collection of data under
controlled scenarios to validate the predictions of qualitative models (i.e. prospective validation studies).

NIOSH has recently proposed that a National Control Banding working group be developed and charged with creating a validation process to properly evaluate existing qualitative models (NIOSH, n.d.b). A primary objective of the working group would be to develop a statistically supported strategy for collecting personal sampling data as well as identify specific exposure scenario information (i.e. usage quantity, volatility, controls present, etc.) that field industrial hygienist must document in order to validate models.

**Key Findings and Recommendations**

Despite limitations involving data availability, the current study was able to demonstrate that both the COSHH Essentials and QLEA model, in their current form, are vastly over-protective in low level exposure scenarios. Further, although the sample size was small, this study inferred that the QLEA model is likely under-protective in medium and high exposure scenarios.

In addition, this study investigated which model components led to the overestimation in low-level exposures. For COSHH Essentials, it was found that the model’s tendency to overestimate exposures was likely the result of multiple complex interactions among model components. Overall, it appeared that the magnitude of overestimation increased exponentially as values for predictor variables increased (i.e. usage quantity increases from low to high; volatility increase from low to high; EP-Band increases from 1 to 4; etc.). Recall that COSHH Essentials predicted concentration ranges were designed using a log-based (10-fold) scale (Brooke, 1998). Based on the
results of this study, we recommend that the use of a log-based scale for predicted concentration ranges be scrutinized and potentially altered considering the magnitude of over-prediction appears to increase exponentially as values for predictor variables increase. Unfortunately, it is well beyond the scope of this study to suggest an alternative scheme. Further study in a wide variety of industrial environments with a range of occupational exposures is necessary prior to altering the predicted concentration ranges.

A wealth of information is available concerning the logic used to develop the COSHH Essentials model. Unfortunately, for the QLEA model no information is available concerning the rationale behind the model’s design. Regardless, this study found that in low-level exposure scenarios, all four QLEA model variables were significantly associated with an overestimation in exposure, though the associations were moderate to weak. Since the QLEA model is over-protective in low exposure scenarios and likely under-protective in medium and high exposure scenarios it is probable that the model is based on flawed logic. Recall that the QLEA model was developed by a global manufacturing company (Elliott and Oestenstad, 2007) to assist other trained professionals conduct risk assessments in the absence of industrial hygienists. When contacted, the proprietors of the model stated that the parent company had recently discontinued their use of the QLEA model. Thus, further validation of the QLEA model is probably unwarranted.

Overall, qualitative exposure assessment models have gained in popularity over the past decade because they are simpler to apply, less expensive, and less time consuming than traditional quantitative air sampling techniques. Unfortunately, at the present time, questions have been raised concerning the reliability and accuracy of
qualitative models. This study suggests that the limitations associated with qualitative exposure assessment models, in their present form, still outweigh the benefits of their use. Therefore, prior to their widespread adoption, the rational concerning both the COSHH Essentials and QLEA model’s design should be critically evaluated and modified to lessen the magnitude of over-prediction. In addition, prospective validation studies should be conducted for both models.
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APPENDIX A

RISK PHRASES
Risk Phrases Assigned by the European Union

R1: Explosive when dry
R2: Risk of explosion by shock, friction, fire or other sources of ignition
R3: Extreme risk of explosion by shock, friction, fire or other sources of ignition
R4: Forms very sensitive explosive metallic compounds
R5: Heating may cause an explosion
R6: Explosive with or without contact with air
R7: May cause fire
R8: Contact with combustible material may cause fire
R9: Explosive when mixed with combustible material
R10: Flammable
R11: Highly flammable
R12: Extremely flammable
R14: Reacts violently with water
R15: Contact with water liberates extremely flammable gases
R16: Explosive when mixed with oxidising substances
R17: Spontaneously flammable in air
R18: In use, may form flammable/explosive vapour-air mixture
R19: May form explosive peroxides
R20: Harmful by inhalation
R21: Harmful in contact with skin
R22: Harmful if swallowed
R23: Toxic by inhalation
Risk Phrases Assigned by the European Union – cont.

R24: Toxic in contact with skin
R25: Toxic if swallowed
R26: Very toxic by inhalation
R27: Very toxic in contact with skin
R28: Very toxic if swallowed
R29: Contact with water liberates toxic gas.
R30: Can become highly flammable in use
R31: Contact with acids liberates toxic gas
R32: Contact with acids liberates very toxic gas
R33: Danger of cumulative effects
R34: Causes burns
R35: Causes severe burns
R36: Irritating to eyes
R37: Irritating to respiratory system
R38: Irritating to skin
R39: Danger of very serious irreversible effects
R40: Limited evidence of a carcinogenic effect
R41: Risk of serious damage to eyes
R42: May cause sensitisation by inhalation
R43: May cause sensitisation by skin contact
R44: Risk of explosion if heated under confinement
R45: May cause cancer
Risk Phrases Assigned by the European Union – cont.

R46: May cause heritable genetic damage
R48: Danger of serious damage to health by prolonged exposure
R49: May cause cancer by inhalation
R50: Very toxic to aquatic organisms
R51: Toxic to aquatic organisms
R52: Harmful to aquatic organisms
R53: May cause long-term adverse effects in the aquatic environment
R54: Toxic to flora
R55: Toxic to fauna
R56: Toxic to soil organisms
R57: Toxic to bees
R58: May cause long-term adverse effects in the environment
R59: Dangerous for the ozone layer
R60: May impair fertility
R61: May cause harm to the unborn child
R62: Possible risk of impaired fertility
R63: Possible risk of harm to the unborn child
R64: May cause harm to breast-fed babies
R65: Harmful: may cause lung damage if swallowed
R66: Repeated exposure may cause skin dryness or cracking
R67: Vapours may cause drowsiness and dizziness
R68: Possible risk of irreversible effects
Risk Phrases Assigned by the European Union – cont.

R14/15: Reacts violently with water, liberating extremely flammable gases
R15/29: Contact with water liberates toxic, extremely flammable gases
R20/21: Harmful by inhalation and in contact with skin
R20/22: Harmful by inhalation and if swallowed
R20/21/22: Harmful by inhalation, in contact with skin and if swallowed
R21/22: Harmful in contact with skin and if swallowed
R23/24: Toxic by inhalation and in contact with skin
R23/25: Toxic by inhalation and if swallowed
R23/24/25: Toxic by inhalation, in contact with skin and if swallowed
R24/25: Toxic in contact with skin and if swallowed
R26/27: Very toxic by inhalation and in contact with skin
R26/28: Very toxic by inhalation and if swallowed
R26/27/28: Very toxic by inhalation, in contact with skin and if swallowed
R27/28: Very toxic in contact with skin and if swallowed
R36/37: Irritating to eyes and respiratory system
R36/38: Irritating to eyes and skin
R36/37/38: Irritating to eyes, respiratory system and skin
R37/38: Irritating to respiratory system and skin
R39/23: Toxic: danger of very serious irreversible effects through inhalation
R39/24: Toxic: danger of very serious irreversible effects in contact with skin
R39/25: Toxic: danger of very serious irreversible effects if swallowed
Risk Phrases Assigned by the European Union – cont.

R39/23/24: Toxic: danger of very serious irreversible effects through inhalation and in contact with skin

R39/23/25: Toxic: danger of very serious irreversible effects through inhalation and if swallowed

R39/24/25: Toxic: danger of very serious irreversible effects in contact with skin and if swallowed

R39/23/24/25: Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed

R39/26: Very Toxic: danger of very serious irreversible effects through inhalation

R39/27: Very Toxic: danger of very serious irreversible effects in contact with skin

R39/28: Very Toxic: danger of very serious irreversible effects if swallowed

R39/26/27: Very Toxic: danger of very serious irreversible effects through inhalation and in contact with skin

R39/26/28: Very Toxic: danger of very serious irreversible effects through inhalation and if swallowed

R39/27/28: Very Toxic: danger of very serious irreversible effects in contact with skin and if swallowed

R39/26/27/28: Very Toxic: danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed

R42/43: May cause sensitisation by inhalation and skin contact

R48/20: Harmful: danger of serious damage to health by prolonged exposure through inhalation

R48/21: Harmful: danger of serious damage to health by prolonged exposure in contact with skin

R48/22: Harmful: danger of serious damage to health by prolonged exposure if swallowed

R48/20/21: Harmful: danger of serious damage to health by prolonged exposure through inhalation and in contact with skin
R48/20/22: Harmful: danger of serious damage to health by prolonged exposure through inhalation and if swallowed

R48/21/22: Harmful: danger of serious damage to health by prolonged exposure in contact with skin and if swallowed

R48/20/21/22: Harmful: danger of serious damage to health by prolonged exposure through inhalation, in contact with skin and if swallowed

R48/23: Toxic: danger of serious damage to health by prolonged exposure through inhalation

R48/24: Toxic: danger of serious damage to health by prolonged exposure in contact with skin

R48/25: Toxic: danger of serious damage to health by prolonged exposure if swallowed

R48/23/24: Toxic: danger of serious damage to health by prolonged exposure through inhalation and in contact with skin

R48/23/25: Toxic: danger of serious damage to health by prolonged exposure through inhalation and if swallowed

R48/24/25: Toxic: danger of serious damage to health by prolonged exposure in contact with skin and if swallowed

R48/23/24/25: Toxic: danger of serious damage to health by prolonged exposure through inhalation, in contact with skin and if swallowed

R50/53: Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment

R51/53: Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment

R52/53: Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment

R68/20: Harmful: possible risk of irreversible effects through inhalation

R68/21: Harmful: possible risk of irreversible effects in contact with skin

R68/22: Harmful: possible risk of irreversible effects if swallowed
**Risk Phrases Assigned by the European Union – cont.**

R68/20/21: Harmful: possible risk of irreversible effects through inhalation and in contact with skin

R68/20/22: Harmful: possible risk of irreversible effects through inhalation and if swallowed

R68/21/22: Harmful: possible risk of irreversible effects in contact with skin and if swallowed

R68/20/21/22: Harmful: possible risk of irreversible effects through inhalation, in contact with skin and if swallowed
APPENDIX B

ESTABLISHING SIMILAR EXPOSURE GROUPS
Establishing Similar Exposure Groups

To better illustrate how data were collected and how models were applied an example is shown below using NIOSH HHE Report 98-0117-2719 involving Jostens, Incorporated (Ewers, Mauer, & Mattorano, 1999). One exposure scenario identified in the report involved a lacquer finisher’s exposure to acetone. The following information was taken directly from the HHE report.

The facility is a jewelry manufacturer who uses a lacquer finishing process to “highlight the three-dimensional relief of jewelry (primarily rings) by adding color to recessed areas” (Ewers et al., 1999, p. 1). “The lacquer finishing process involves painting colored lacquers onto the metal surfaces of rings with small brushes. To remove excess lacquer, workers manually wiped the jewelry with a pad saturated in acetone” (Ewers et al., 1999, p. 1). Small teams of workers (<11) lacquered during first shift only at five locations within the plant. Stationary local exhaust ventilation (LEV) was available at two locations. However, upon inspection, LEV was shown to not be functioning adequately (airborne containments were not being captured). In fact, “workers did not appear to be aware that local ventilation was in operation, and they sometimes used the hood openings as a storage area for tools, a practice which further reduced the effectiveness of the ventilation” (Ewers et al., 1999, p. 7). The three remaining workstations were not equipped with engineering controls.
**Phase 1: Data Collection**

During Phase 1, information necessary to establish the SEG using the observational approach (i.e. classified by process, job, task, and chemical substance) and subsequently conduct qualitative exposure assessments was extracted and recorded in a spreadsheet. Specifically, information regarding the process/job/task, physical state of the chemical substance, ability of the chemical substance to become airborne, duration of exposure, scale of use, and current control methods were documented in an approach similar to the one shown in Table B1 using the example involving lacquer finishers exposure to acetone.

### Table B1. Information Recorded and Utilized to Define SEGs

<table>
<thead>
<tr>
<th>ID</th>
<th>SEG Description</th>
<th>Chemical Agent</th>
<th>Physical State</th>
<th>VP / Dustiness</th>
<th>Duration of Exposure</th>
<th>Scale of Use</th>
<th>Current Controls</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Lacquer Finish</td>
<td>A</td>
<td>Acetone</td>
<td>Liquid</td>
<td>180 mm Hg</td>
<td>&gt; 7 hrs daily</td>
<td>mL quantities</td>
</tr>
</tbody>
</table>

*a* Facility is a jewelry manufacturer who uses lacquer finishing processes to highlight the three-dimensional relief of jewelry (primarily rings) by adding color to recessed areas. The lacquer finishing process involves painting colored lacquers onto the metal surfaces of rings with small brushes, and then removing excess color from the elevated areas with solvent-saturated cotton pads. To remove excess lacquer, workers manually wiped the jewelry with a pad saturated in acetone. Small teams of workers (<11) lacquer during first shift only at five locations within the plant. Two locations were equipped with stationary LEV; however, upon inspection, the LEV was shown to not be functioning adequately (airborne containments were not being captured).

*b* Criteria considered when determine scale of use is as follows: number of employees (<11), size of facility (lacquering is conducted at 5 workstations during 1st shift only); amount of products processed per day/shift/machine etc. (the lacquering process is small-scale considering it involves painting colored lacquers onto the metal surfaces of rings with small brushes, and then removing excess color from the elevated areas with small cotton pads saturated in acetone).

*c* Three workstations had no mechanical ventilation present. Two workstations had mechanical ventilation present; however, it was not functioning properly (workers were not aware mechanical ventilation was in operation, and sometimes used hood openings as a storage area, which further reduced the effectiveness of the ventilation).

Once the SEG was established, measured exposure concentrations for the SEG were recorded. Specifically, raw data as well as pertinent IH statistics (minimum, maximum, sample mean, AM, GM, GSD, and 95th percentile) were documented in an approach similar to the one shown in Table B2. The assumption of lognormality was confirmed using the Kolmogorov-Smirnov goodness-of-fit test (Daniel, 1999), and the GSD was
confirmed to be less than 3.0. Recall that SEGs were categorized based on the magnitude of measured exposures (high, medium, low) and the physical state of the chemical substance (vapor or particulate). SEGs in which the AM (Rappaport, 1991) was $\geq 75\%$ of the OEL were categorized as high. SEGs in which the AM was between 50% and 75% of the OEL were categorized as medium, and SEGs in which the AM was <50% of the OEL were categorized as low (Mulhausen and Damiano, 2003). Thus, SEGs were categorized into one of six groups – SEGs involving vapors with high, medium, and low exposures (VH, VM, and VL) and SEGs involving particulates with high, medium, and low exposures (PH, PM, and PL).

Table B2. Data Recorded and Utilized to Calculate Descriptive Statistics for SEGs

<table>
<thead>
<tr>
<th>ID</th>
<th>Category</th>
<th>Raw Sampling Data</th>
<th>n</th>
<th>Min</th>
<th>Max</th>
<th>Mean</th>
<th>AM</th>
<th>GM</th>
<th>GSD</th>
<th>95 %-tile</th>
<th>Lognormal</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>VL(^A)</td>
<td>A</td>
<td>11</td>
<td>9.1</td>
<td>93</td>
<td>47.1</td>
<td>48.3</td>
<td>38.6</td>
<td>2.03</td>
<td>123.7</td>
<td>Yes</td>
</tr>
</tbody>
</table>

\(^A\) The physical state of the chemical substance is a liquid (i.e. vapor) and the AM (48.3 ppm) is 10\% of the OEL (500 ppm)

\(^B\) Raw sampling data (49, 74, 63, 23, 23, 93, 35, 87, 9.1, 38, and 24 ppm) were recorded in a separate spreadsheet. Spreadsheets containing raw sampling data were used to calculate pertinent IH statistics summarized in the table.

Phase 2: Exposure Assessment

During Phase 2, each SEG was qualitatively assessed by the investigator using the COSHH Essentials and QLEA models. Information extracted from HHE reports was utilized to select values for model variables. Using the example involving lacquer finishers exposure to acetone, COSHH Essentials model variables were selected and the model’s predicted concentration range was documented in an approach similar to the one shown in Table B3. Likewise, QLEA model variables were selected and the model’s final classification of exposure was documented in an approach similar to the one shown in Table B4.
Table B3. Example COSHH Essentials Model Assessment

<table>
<thead>
<tr>
<th>ID</th>
<th>SEG</th>
<th>Chemical Agent</th>
<th>Volatility</th>
<th>Scale of Use</th>
<th>EP Band</th>
<th>Current Controls</th>
<th>Predicted Low Conc.</th>
<th>Predicted High Conc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Lacquer Finish</td>
<td>Acetone</td>
<td>Medium</td>
<td>mL</td>
<td>Band 1</td>
<td>5 ppm</td>
<td>5 ppm</td>
<td>50 ppm</td>
</tr>
</tbody>
</table>

A 180 mm Hg approximately equals 24,000 Pa and corresponds with a medium level of volatility using Table 2.
B Selected using Table 4.
C Selected using Table 5.
D Selected using Table 6.

Table B4. Example QLEA Model Assessment

<table>
<thead>
<tr>
<th>ID</th>
<th>SEG</th>
<th>Chemical Agent</th>
<th>DR</th>
<th>HI</th>
<th>AR</th>
<th>EC</th>
<th>Inhalation Risk Factor</th>
<th>Model Final Rating</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Lacquer Finish</td>
<td>Acetone</td>
<td>5(^B)</td>
<td>2(^B)</td>
<td>2(^B)</td>
<td>10(^B)</td>
<td>200(^C)</td>
<td>3(^D)</td>
</tr>
</tbody>
</table>

A The ACGIH TLV was used in all QLEA Model Assessments. The TLV for Acetone is 500 ppm.
B Selected using Table 7.
C Calculated using Equation 17.
D Selected using Table 8.

Phase 3: Model Validation and Data Analysis

The final phase of this study involved comparison of model estimates for each SEG with corresponding measured exposure data extracted from the HHE report. Tests of significances were conducted at alpha (\(\alpha\)) = 0.05.