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# A Case-Based Introduction to Modeling Occupational Inhalation Exposures to Chemicals

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# A Case-Based Introduction to Modeling Occupational Inhalation Exposures to Chemicals

A case-based approach that demonstrates how industrial hygienists can apply exposure modeling in daily practice.

Edited by Chris Keil, PhD, CIH



## **Table of Contents**

FOREWORD	ix
References	x
PREFACE	xi
ACKNOWLEDGMENTS	
CHAPTER 1: MODELING IN THE FRAMEWORK OF INDUSTRIAL HYGIENE PRACTICE	
The Industrial Hygienist and Exposure Assessment	
Assessing Inhalation Exposures to Chemicals	
The Role of Modeling in Exposure Assessment	
Physical-Chemical Concentration Modeling	4
Current Applications of Air Concentration Modeling for Regulatory Purposes	5
How Close Is Close Enough?	6
Advancing the Use of Models in Exposure Assessment	7
References	7
CHAPTER 2: INFORMATION GATHERING FOR AIR CONCENTRATION MODELING	9
Information About the Chemical	
Information About the Airspace	
Worker Activity Information	
The Importance of the Information-Gathering Step	
References	
CHAPTER 3: VOLATILE LIQUID SPILL	
Scenario	
Information Gathering	
Modeling Approach 1: Zero-Ventilation Model	
Interpreting the Modeled Concentration	
Modeling Approach 2: Well-Mixed Room Model	
Conclusions	
References	

CHAPTER 4: LOCAL EXHAUST VENTILATION FOR A SANDING OPERATION	27
Scenario	27
Information Gathering	27
Modeling Approach: Well-Mixed Room	
Interpreting the Modeled Concentration	
Conclusions	
References	
CHAPTER 5: VOLATILE LIQUID CONTAINER LEFT OPEN	
Scenario	
Information Gathering	
Modeling the Concentration in the Cabinet: Saturation Vapor Pressure Concentration	
Modeling Average Concentration in the Room: Zero-Ventilation Model	
Modeling the Decrease of Concentration in the Room: Well-Mixed Room Purging Model	
Best Practice for Control of Fugitive Emissions From Volatile Liquid Containers in Laboratories	
References	42
CHAPTER 6: BARREL FILLING INDOORS	43
Scenario	43
Information Gathering	43
Modeling Approach: Diffusion Model	45
Interpreting the Modeled Concentrations	47
Selecting Turbulent Diffusion Coefficients	49
References	50
CHAPTER 7: HISTORICAL EXPOSURES NEAR A TRICHLOROETHYLENE DEGREASER	51
Scenario	51
Information Gathering	51
Modeling Approach: Near-Field/Far-Field Model	53
Interpreting the Modeled Concentration	55
References	
CHAPTER 8: PRESSURIZED GAS RELEASE	59
Scenario	59
Information Gathering	59
Modeling Approach 1: Zero-Ventilation Model	61
Interpreting the Modeled Concentration – 1	62
Modeling Approach 2: Two-Box Model of a Slow Release	62
Interpreting the Modeled Concentration – 2	63
References	64

CHAPTER 9: VENTILATION REQUIREMENTS FOR A FLAVORING PROCESS	65
Scenario	65
Information Gathering	65
References	71
Appendix	72
CHAPTER 10: CLEANING WITH PRODUCT CONTAINING ACETIC ACID	75
Scenario	75
Information Gathering	
Modeling Approach 1: Well-Mixed Box With Rapid Evaporation of Acetic Acid	
Modeling Approach 2: Time-Varying Well-Mixed Box Concentration With Repeated Mass Applications and Decreasing Emission Rates	79
Modeling Approach 3: Steady-State Well-Mixed Box Concentration With Repeated Mass Applications and Decreasing Emission Rates	
Interpreting the Modeled Concentration	83
References	83
CHAPTER 11: EXPERIMENTAL DETERMINATION OF MODEL PARAMETERS	85
Case 1: Dust Emissions From Mixer Loading	85
Case 2: Ventilation Rate in a Room Without Mechanical Ventilation	87
References	89
CHAPTER 12: ORGANIC CHEMISTRY TEACHING LAB EXPOSURE AND A FIRST EXPLORATION OF MONTE CARLO MODELING	91
Scenario	
Information Gathering	91
Steady-State Well-Mixed Room Model	92
Capturing Variability in Parameters: Best Case and Worst Case	
Capturing Variability in Parameters: An Introduction to Monte Carlo Approaches	94
Applying a Monte Carlo Approach to the Chemistry Lab	96
Using Excel to Do the Monte Carlo Simulation of the Scenario	97
References	98
CHAPTER 13: FILLING A CONTAINER WITH A MIXTURE AND USING IHMOD 2.0 FOR MODELING CALCULATIONS	90
Scenario	
Using IHMOD 2.0.	
Conclusion	
References	

CHAPTER 14: OXYGEN DEFICIENCY HAZARD IN A STORAGE TANK	
Scenario	
Information Gathering	
Modeling Approach: Near-Field/Far-Field Model	
Interpreting the Modeled Outputs (Concentration and Partial Pressure)	
Conclusions	
Appendix A: Oxygen Deficiency Hazard	
Appendix B: Mass Balance Equations	
References	
CHAPTER 15: USE OF AEROSOL SOLVENTS IN AN AUTO SHOP	
Scenario	
Information Gathering	
Modeling Approach	
Interpreting the Modeled Concentrations	
An Additional Consideration for Evaporation Rates	
References	
CHAPTER 16: FURNITURE STRIPPING WITH METHYLENE CHLORIDE: INTRODUCING TH	HE ADVANCED
REACH TOOL (ART V1.5)	
Scenario	
Information Gathering	
Modeling Approach: The Advanced Reach Tool	
Using ART: A Walk-Through of Entering Inputs	
Running the Art V1.5 Model and Interpreting the Results	
Appendix A: More About ART	
Appendix B: Bayesian Module	
Appendix C: Activity 1 Configuration Screens	
References	
CHAPTER 17: RECONSTRUCTION OF A LABORATORY SPILL	
Introduction	
Background	
Initial Modeling Approaches	
Probabilistic Modeling	
Summary of Modeling Results	
Discussion	
Conclusion	
Acknowledgments	
Appendix A: Estimating the Generation Rate	
Appendix B: Estimating the Near-Field Volume and Flow Rate (β)	
References	

CHAPTER 18: UNDERSTANDING THE LIMITATIONS OF MATHEMATICAL MODELS AND PROACTIVE COMMUNICATION OF MODELING RESULTS	163
Knowing the Limitations of Mathematical Models	163
Proactive Communication of Modeling Results	164
Conclusions	168
References	169
CHAPTER 19: FEEDING MODELS USING SIMPLE AND SOME NOT-SO-SIMPLE MEANS	171
Introduction	171
Models Are Beasts That Need to Be Fed	171
Trading Conservatism for Data	172
Chamber Case Studies	173
The "Leaky" Chamber	
The Disappearing Biocide	175
Simple Stuff With Big Payouts	176
Postscript	176
References	176

# Chapter 1 Modeling in the Framework of Industrial Hygiene Practice

Chris Keil, PhD, CIH

A standard and useful definition of industrial hygiene is "the anticipation, recognition, evaluation, control, and management of hazards arising in and from the workplace." Evaluating the level of risk posed by hazards is rooted in the process of exposure assessment. In exposure assessment, the industrial hygienist characterizes exposure to an environmental agent in terms of the route, intensity, duration, and frequency of the exposure. The exposure assessment is then used to make a judgment about the acceptability of the exposure and whether the exposure needs to be controlled.

## The Industrial Hygienist and Exposure Assessment

Best practice exposure assessment will include information on the full distribution of exposures experienced by a worker or group of workers.<sup>1</sup> This "exposure profile" reflects the between-worker exposure variability exhibited within a group of similarly exposed workers. Additionally, each individual worker will have a within-worker variability of exposures from day to day and even from task to task. A group of workers that have the same general exposure profile based on similarity of jobs and tasks is called a similar exposure group (SEG).<sup>1</sup>

Once a good exposure profile has been developed for an SEG, the industrial hygienist then compares the exposure profile to a benchmark decision-making value to judge whether the exposure is acceptable, uncertain, or unacceptable. Exposures judged as acceptable should be scheduled for regular reassessment. Unacceptable exposures need to be controlled and then reassessed to assure acceptability. Sometimes the first pass through exposure characterization does not provide enough information to make a judgment of "acceptable" or "unacceptable," leading to an uncertain exposure profile. When uncertain exposure profiles arise, more information is gathered to refine the exposure characterization and move toward being able to confidently judge the acceptability of the exposure. In all these cases, the exposure assessment and decisions should be documented.

## **Assessing Inhalation Exposures to Chemicals**

As is the case for all exposure characterizations, inhalation exposures are expressed in terms of intensity and time components. The intensity of air pollutants is the concentration of the chemical that a person is breathing. To fully understand risks from an exposure, more information than just the concentration is needed. How long and how often the concentrations are inhaled are required to fully characterize an exposure profile.

Once an exposure profile is determined by air sampling, modeling, or surrogate data, it is compared to some decision criteria to judge the acceptability of the exposure. The starting point for establishing a decision criterion, or "acceptable level," is an occupational exposure limit (OEL). A number of organizations produce OELs. Table 1.1 describes some of the most common OELs. Organizations involved in developing new chemical compounds or using chemicals without an OEL often establish internal OELs for use in worker protection. An exposure assessor then establishes their own/company's "acceptable exposure" based on all available information. This acceptable exposure is often less than the regulatory limit, as many regulations may be decades old and not reflect current science regarding risks from the chemical.

Chapter 1: Modeling in IH Practice

### Table 1.1: Common Occupational Exposure Limits

Organization	Occupational Exposure Limit	Notes
Occupational Safety and Health	Permissible Exposure Limit (PEL)	Legal limits in United States.
Administration (OSHA)		Majority were established in 1970.
		Many do not reflect current scientific information and are "inadequate for ensuring protection of worker health." <sup>2</sup>
National Institute for Occupational Safety and Health (NIOSH)	Recommended Exposure Limit (REL)	Not a regulatory requirement, but a recommended guideline. Updated as new information on chemicals becomes available.
American Conference of Governmental Industrial Hygienists (ACGIH)	Threshold Limit Value (TLV®)	Guidelines based on committee review of information on the health of a substance. Many consider these OELs the most reflective of current information.
American Industrial Hygiene Association (AIHA) until 2013, Occupational Alliance for Risk Science	Workplace Environmental Exposure Level (WEEL)	Guidelines for substances that were not being addressed by other organizations.
Scientific Committee on Occupational Exposure Limits (SCOEL)	Binding Occupational Exposure Limit Value (BOELV)	European Community minimum level of protection for workers. Considers socioeconomic factors as well as technological feasibility.
European Agency for Safety and Health at Work	Indicative Occupational Exposure Limit Value (IOELV)	European Community health-based limits.
Deutsche Forschungsgemeinschaft (DFG)	Maximale Arbeitsplatz-Konzentration (MAK)	German health-based maximum worker exposure levels.

An OEL is more than just a concentration: it is almost always written to include a time frame for which the OEL concentration is acceptable. The time frame of an OEL reflects the toxicological action of the chemical. A chemical that produces health effects after long-term exposure will typically have the OEL expressed in terms of an 8-hr time-weighted average (TWA-8). Chemicals that produce effects quickly may have OELs expressed in terms of a short-term exposure limit (STEL), a ceiling limit (C), or peak concentration. These OELs also have a time frame for which the OEL concentration is acceptable. Common time frames are 15 and 10 min.

## **Characterizing Exposure**

When it comes to determining concentrations for characterizing inhalation exposure profiles, often the first thought is to make a measurement. Industrial hygiene sampling and analysis science is quite advanced and, when properly performed, can provide an excellent measurement of air concentrations for thousands of chemicals. Yet a single air sample is only one data point in developing an exposure profile. With only a few air samples, making confident statistical conclusions about the acceptability of exposure is challenging.

For example, consider four samples taken randomly across an SEG. Suppose that each of the concentrations measured is below the predetermined OEL. A data set of four samples is not a large enough sample size to use parametric statistics to draw conclusions. Parametric statistics are the inferential statistics that almost everyone learns first: t-tests, 95% confidence intervals, etc. Parametric statistics assume that the data are normally distributed or can be transformed to be normally distributed. With only four samples in our example, a normal distribution cannot be assumed, and nonparametric statistics must be used to draw statistically based inferences. With four samples all below the OEL, a nonparametric tolerance limit statement can be made. With these results, one can be:

Chapter 1: Modeling in IH Practice

- 26% confident that 75% of all similar exposures will be below the OEL
- 5% confident that 90% of all similar exposures will be below the OEL
- 1% confident that 95% of all similar exposures will be below the OEL

Refer to Mulhausen and Damiano Appendix VIII for more detail on this approach.<sup>3</sup>

As more exposure measurements are made on an SEG and assumptions about the distribution of the exposure profile can be justified, parametric statistics will be useful in judging the acceptability of exposure. But the point of this thought experiment is to illustrate that one or two samples, even when correctly made, are of only limited use in judging the acceptability of an entire exposure profile.

Certainly, there are times when a single air measurement can shed great light on the acceptability of exposure. Consider a measurement made right at the edge of a metal plating bath. Or consider a measurement made at the edge of a degreasing station. These locations could be considered "reasonable worst case" air concentrations because they are as close to the source of the pollutant as a worker is likely to get. If the TWA-8 concentration at these locations is a small fraction of the TWA-8 OEL, it could be appropriate to judge typical exposures from these processes as acceptable based on that one sample. However, these data cannot be categorized as a substitute for a full exposure assessment.

Modern sensor technology greatly improves the ability to collect measurements when these resources are available. Although the cost is dropping and accessibility is increasing, no one sensor can measure all the potential exposures in a workplace. Also, an industrial hygienist still needs to think carefully about how, where, and when to use these resources to best characterize exposure profiles.

## The Role of Modeling in Exposure Assessment

Workplaces today are complex environments. A regularly increasing number of chemical, physical, and biological agents are entering production processes. Additionally, new processes are using agents in innovative ways. The sheer number of exposure assessments required in modern workplaces can be daunting. There are limits on resources (both time and money) needed to complete exposure assessments. The AIHA exposure assessment strategy recommends 6 to 10 measurements to characterize each SEG.<sup>1</sup> Although this number of samples can

provide statistical rigor to judge the exposure profile acceptability, collecting that many measurements for all SEGs at a workplace can be a substantial undertaking. Even when resources are available to execute statistically well-designed sampling campaigns, a priori decisions are needed to develop sampling plans. Which exposures should be measured first? Which exposures could have a lower priority for assessment? Ultimately, industrial hygienists are faced with the dilemma that it is impossible to measure all exposures everywhere at all times. It has been estimated that professional judgment is used for more than 90% of all exposure judgments without any measurement data.<sup>4,5</sup>

There are also exposures of concern that cannot be measured. A new process may be proposed, or process engineers may suggest a shift to a new material in an existing process. Before changes are made, it would be helpful to know what changes in exposures could occur. Planning for an emergency response to unplanned accidental chemical releases also requires some understanding of potential exposures.

### **Past Exposures**

- Litigation
- Epidemiology
- Follow-up of accidental exposures

### **Current Exposures**

- Prioritizing sampling
- Supporting professional judgment of acceptable exposures
- Supplementing exposure profiles with small sample sizes

### **Future Exposures**

- Planning for process change
- Anticipating exposures from process disruptions
- Emergency preplanning

**Figure 1.1:** The range of application of modeling in exposure assessment.

# Chapter 3 **Volatile Liquid Spill**

Chris Keil, PhD, CIH

## Scenario

You are working in the environmental health and safety (EHS) department in a medium-sized production facility. One morning a worker calls in sick. While on the phone, the worker tells their supervisor that they think a spill of liquid that occurred the previous day gave them the severe stomach cramps they were experiencing that morning. The worker knocked over a bottle of a chemical at their workstation, then wiped the spill up with some shop rags. At the time, they noticed the strong smell of the chemical, but it did not bother them then.

The delayed nature of the symptoms makes you wonder about the connection between the exposure and the illness. A nontypical exposure occurred, and a follow-up investigation should be done. You want to arrive at an estimate of the worker's exposure from the incident. This exposure estimate will both document what occurred and provide input as to whether the worker's abdominal pain is related to the exposure. You set out to determine what concentration the worker was exposed to because of the spill described.

## **Information Gathering**

## Information About the Chemical

You check records in the EHS office and find a short report that indicates that 18 months ago a detector tube measurement was made in the room for toluene. The measurement was made during typical operating procedures. The concentration measured was 25 mg/m<sup>3</sup>.

You then go to the worker's workstation and talk to the area supervisor. It turns out that toluene is still used intermittently for parts cleaning at the station and there is always a 500-mL bottle of toluene on the table.

You give the worker a call to get more information about the incident. From that conversation, you find that the spill took place about 5 hr into their 8-hr shift. The worker estimates that the bottle was about half-full at the time it was knocked over. Most of the liquid spilled onto the work surface. The worker wiped it up with some shop rags, then set them to the side to "dry out" about 2 m from their workstation. The shop rags were dry enough to use for another purpose about 2 hr later. The worker says they noticed the smell of toluene was stronger than usual, but it was not unbearable or concerning at the time.

Some readily available information on toluene from the NIOSH Pocket Guide<sup>1</sup> and the safety data sheet provided by the toluene vendor are shown in Table 3.1. Because this case involves symptoms, information on health effects is also included.

Chapter 3: Volatile Liquid Spill

### Table 3.1: Information on Toluene

Physical Properties	Description	Colorless liquid; sweet, pungent, benzene-like odor
	Molecular weight	92.1 g/mol
Liquid density 0.87 g/m		0.87 g/mL
	Vapor pressure	21 mmHg
	Lower explosive limit	1.1% = 11,000 ppm
Release Characteristic	Volume	250 mL (half of the 500-mL container)
	Time	All the liquid evaporated within 120 min
Health Effects	Target organs	Eyes, skin, respiratory system, central nervous system, liver, kidneys
	Effects	Irritation of the eyes and nose; confusion, euphoria, dizziness, headache, dilated pupils, lacrimation, anxiety, muscle fatigue, insomnia; paresthesia, dermatitis, liver or kidney damage
Exposure Guidelines	PEL TWA-8	200 ppm = 750 mg/m <sup>3</sup>
	PEL C	300 ppm = 1,130 mg/m <sup>3</sup>
	PEL peak	500 ppm = 1,880 mg/m <sup>3</sup>
	REL TWA-8	100 ppm = 375 mg/m <sup>3</sup>
	REL STEL	150 ppm = 560 mg/m <sup>3</sup>
	TLV TWA	20 ppm = 75 mg/m <sup>3</sup>
	IDLH	500 ppm = 1,880 mg/m <sup>3</sup>

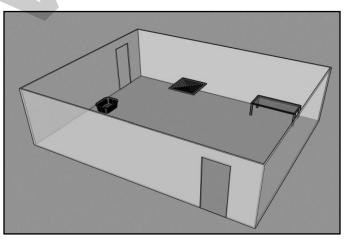
C, ceiling limit; IDLH, immediately dangerous to life or health; PEL, permissible exposure limit; REL, recommended exposure limit; STEL, short-term exposure limit; TLV, threshold limit value; TWA-8, 8-hr time-weighted average.

## Information About the Room

The room where the spill took place has dimensions of approximately 10 m  $\times$  8 m, with a 3-m ceiling. This gives a room volume of approximately 240 m<sup>3</sup>. Air is supplied through a diffuser roughly in the center of the ceiling. Information on the supply air rate is not immediately available. There is no mechanical exhaust, and air leaves the room through open doors and other gaps in the room envelope. The room layout is illustrated in Figure 3.1.

## Modeling Approach 1: Zero-Ventilation Model

Because you do not have ventilation information, you decide to start with a zero-ventilation model. Zero-ventilation models usually overestimate the



**Figure 3.1:** Room layout illustrating relative position of workbench, rag drying location (basket), and ventilation (ceiling diffuser in center).

average concentration in a room. They are quick and easy models that can help with a screening-level decision to determine whether more information and/or more advanced modeling is needed to make a better judgment about exposures.

The zero-ventilation model, Equation 3.1, assumes that the workspace is a sealed space and all of the pollutant is immediately released and mixed throughout the space. In reality, concentrations may be higher near the point

# Chapter 5 Volatile Liquid Container Left Open

Chris Keil, PhD, CIH and Kang Chen, PhD, CIE, CHMM

## Scenario

A worker opens a chemical storage cabinet after a long weekend. A wide-mouth container of a volatile liquid had been left open. There is still liquid in the container, and there is a very strong solvent odor in the cabinet. Figure 5.1 illustrates the open cabinet and jar.

The worker caps the container but then exits the room because of the intensity of the odor, leaving the cabinet open. They report the incident to the health and safety team. The team gathers to respond to the incident and quickly collects some information and data. Questions that need to be answered include the following:

- To what concentration was the worker exposed when they opened the cabinet?
- What is the concentration in the room?
- When will it be safe to enter the room again?



Figure 5.1: Container left open in cabinet (photo: Chris Keil).

## Information Gathering

## Information About the Pollutant

The chemical is identified as n-hexane. The 500-mL container was reported to be fairly full at the end of the last workweek. One team member gathers information on the chemical from the NIOSH Pocket Guide.<sup>1</sup> Table 5.1 contains information on n-hexane.

Chapter 5: Volatile Liquid Container

### Table 5.1: Information on n-Hexane

Physical Properties	Description	Colorless liquid with a gasoline-like odor
	Molecular weight	86.2
	Liquid density	0.66 g/mL
Vapor pressure 124 mmHg		124 mmHg
	Lower explosive limit	1.1% = 11,000 ppm = 38,800 mg/m <sup>3</sup>
Upper explosive limit 7.5% = 75,00		7.5% = 75,000 ppm = 264,000 mg/m <sup>3</sup>
Health Effects	Target organs	Eyes, skin, respiratory system, central nervous system, peripheral nervous system
	Effects	Irritation of the eyes and nose; nausea, headache; peripheral neuropathy: numb extremities, muscle weakness; dizziness
Exposure Guidelines PEL TWA-8 1,70		1,760 mg/m <sup>3</sup>
		176 mg/m <sup>3</sup>
		3,880 mg/m <sup>3</sup>

IDLH, immediately dangerous to life or health; PEL, permissible exposure limit; TLV, threshold limit value; TWA-8, 8-hr time-weighted average.

The cabinet has interior dimensions estimated to be  $85 \text{ cm} \times 40 \text{ cm} \times 40 \text{ cm}$ . This gives a cabinet volume of  $136,000 \text{ cm}^3$ , or  $0.136 \text{ m}^3$ .

## Information About the Room

The dimensions of the room are estimated as 20–25 ft long, 15–20 ft wide, and 8.5–10 ft high. A sketch of the room layout is shown in Figure 5.2.

Using the estimates of the room dimensions, the volume can be calculated as length  $\times$  width  $\times$  height. The room volume could be as small as 2,550 ft<sup>3</sup> (72 m<sup>3</sup>) using the low end of the dimension estimates or as large as 5,000 ft<sup>3</sup> (142 m<sup>3</sup>) using the high end. Using the average of each dimension's estimate range, the room volume would be 3,642 ft<sup>3</sup> (or 103 m<sup>3</sup>), as calculated below.

22.5 ft • 17.5 ft • 9.25 ft = 3,642 ft<sup>3</sup> • 
$$\frac{1 \text{ m}^3}{35.31 \text{ ft}^3}$$
 = 103 m<sup>3</sup>

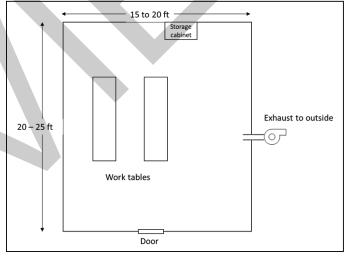


Figure 5.2: Room layout.

The team knows that because chemicals are used in the room, it is kept under negative pressure. The negative pressure is achieved by an air return on one of the walls that is exhausted outside of the building. The exhaust port to the outside is a 6-inch diameter duct. The team looks up the results from the last time the airflow through the system's fan was tested and finds that the velocity through the 6.0-inch (0.50-ft) diameter duct was measured as 591 ft/min. The volumetric airflow through the exhaust duct and thus the room can be calculated as follows:

$$Q = v \cdot A$$

(5.1)

# Chapter 9 Ventilation Requirements for a Flavoring Process

Chris Keil, PhD, CIH

## Scenario

A specialty snack food manufacturer is adding a new item to its product line. The product was developed in a test kitchen and has been approved for full-scale manufacturing. Engineers are working to develop the equipment and processes for mass production. One step of the production is to add a coating of flavoring to the small snack items. The process engineers plan to add the flavoring to the items in a heated and ventilated tumbler. The items will be loaded into the tumbler and heated to complete cooking. Then, the flavoring will be added as a slurry that is a mix of sugar, other flavors, ethanol, and water. The heated tumbler will both complete the cooking process and speed the evaporation of the liquid carrier from the slurry. The evaporation leaves the flavoring on the product. Figure 9.1 illustrates the tumbler.

The design of the tumbler draws air from the workspace through the open face of the tumbler and exhausts the air through the rear of the unit. The engineer working on the process has done some test runs, and the product is turning out well. She says that face velocity into the tumbler seems to be controlling vapor emissions into the room very well. Little or no odor of ethanol is reported near the tumbler drier. However, the engineer realizes that

because ethanol is part of the slurry, there may be a safety concern associated with the concentration of evaporated ethanol vapors in the exhaust duct. She asks members of the environmental health and safety (EHS) department if they think there might be an explosion hazard from the ethanol vapors.

Measurements of the concentration in the duct can help determine this, but some initial time spent on modeling the potential duct concentrations will help the department understand the system and what concentrations might be expected in the duct.

## **Information Gathering**

## Information About the Pollutant

Ethanol is part of the liquid mix that carries the solid flavoring. A slurry is made from 50 lbs of liquid, which is a 45% ethanol and 55% water mixture, and 20 lbs of solid flavorings. The slurry is manually poured into the operating tumbler that contains 300 lbs of food item in small pieces. The process temperature is 300°F. The tumbling action spreads the slurry, coating all the food pieces. The heat evaporates the ethanol and water into vapor, which are exhausted out of the back of the tumbler. The liquid should be entirely evaporated from the product at the end of the coating

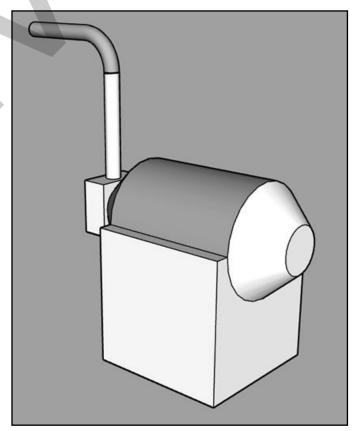


Figure 9.1: The heated, ventilated tumbler.

Chapter 9: Requirements for a Flavoring Process

process. The process engineer says that based on tests thus far, the liquid is completely evaporated after 20 min.

Table 9.1: Information on Ethano	Table	9.1:	Information	n on Ethanol
----------------------------------	-------	------	-------------	--------------

Physical Properties	Description	Clear, colorless liquid with a weak, ethereal, "wine-like" odor
	Molecular weight	46.1 g/mol
	Liquid density	0.79 g/mL
	Vapor pressure	44 mmHg
	Lower explosive limit	3.3% = 33,000 ppm
	Upper explosive limit	19% = 190,000 ppm
Room Characteristic Mass		22.5 lbs (45% of the 50 lbs of liquid in the slurry)
	Time	20 min

The initial question in this case is related to explosion hazard. The lower explosive limit (LEL) for ethanol is 3.3%, which is a gas phase volume-to-volume ratio expression of concentration. "Percent" is "parts per hundred," so 3.3% is equivalent to 33,000 ppm. Because we are working with gas volume-to-gas volume ratio concentration units, it will be useful to consider the emission rate in terms of moles and gas phase liters.

The mass and number of moles of ethanol used in the production of one batch of the product can be calculated as follows:

50 lb <sub>liquid</sub>	45 lb <sub>ethanol</sub>	453.6 g	10,206 g <sub>ethanol</sub>
batch	100 lb <sub>liquid</sub>	lb	batch
10,206 g	mol	221 mol	
batch	46.1 g	batch	

If the evaporation of ethanol over the 20-min period is constant, the emission rate can be determined by dividing the amount of ethanol used and evaporated in a batch by 20 min.

batch	510 g
20 min	min
batch	11.1 mol
20 min	min
	20 min batch

These emission rates are the emission rates if the evaporation is constant. If the evaporation rate is not constant, it is at least the average emission rate over the 20 min.

# Chapter 11 Experimental Determination of Model Parameters

Chris Keil, PhD, CIH

Obtaining inputs for modeling airborne concentrations of chemicals can be difficult for certain exposure scenarios. Using ingenuity and some "tricks of the trade" pioneered by earlier industrial hygienists, the selection of model parameters can be strengthened and improve the overall model. Two such situations will be illustrated with the cases in this chapter.

In the first case, a particle emission rate model is necessary. Models exist for liquid evaporation rates.<sup>1,2</sup> Pressurized gas releases can be modeled using the ideal gas law, as shown in Chapter 8 of this book and covered in Chapter 3 of Mathematical Models for Estimating Occupational Exposure to Chemicals, 2nd edition.<sup>3</sup> Large-scale outdoor evaporative and pressurized gas releases can be modeled with the Areal Locations of Hazardous Atmospheres (ALOHA) hazard modeling program.<sup>4</sup> Particle emissions are more difficult to characterize due to the variety of physical processes that generate them. The sanding case study of Chapter 4 presented some mass balance approaches. An approach by López Lilao et al.<sup>5</sup> presents a model to describe dustiness. But overall, particle emission rates are harder to generalize. This chapter will illustrate a simplified experimental approach to estimating particle emissions from the emptying of powder-filled bags.

In the second case, an adaptation of the well-mixed box model is used to determine ventilation rates. A variety of indoor spaces have conditions that make determining ventilation rates difficult: open windows, large doorways, out-of-reach air diffusers and returns, partial walls, etc. Although there are reported values of typical air change rates (refer to Chapter 2), there is a fairly straightforward method for getting more specific ventilation information for an indoor space if one has access to data-logging sensors.

## **Case 1: Dust Emissions From Mixer Loading**

You are asked to estimate the historical exposure of a worker to a dust as part of evidence in a lawsuit. The plaintiff claims that they suffer negative health effects from an occupational exposure 15 years prior.

The plaintiff worked in a large room where one of the operations included the filling of an unventilated mixer with 50-lb bags of powder. The plaintiff was not the mixer operator. They worked across the room from the mixing process. Powder loading created "clouds of dust," as described by the plaintiff. The mixer operator wore a respirator when loading. Although the dust was low toxicity, the plaintiff has some potentially exacerbating health conditions that are part of the complaint.

You are asked to estimate the plaintiff's exposure to the dust that is generated when he dumps the bag into the mixer. General ventilation present in the room is well documented by the company. On the other hand, information on the mass emission rate of the dust is not readily available. One way to obtain this information, if resources are available, is to experimentally simulate the process and take some measurements.

### **Information Gathering**

The plaintiff had a workstation across the room from the mixer. They would be the "far field" if a two-box model were used to calculate concentrations. Figure 11.1 illustrates the relative positions of the plaintiff's workstation to the powder loading and mixing operation.

Chapter 11: Model Parameters

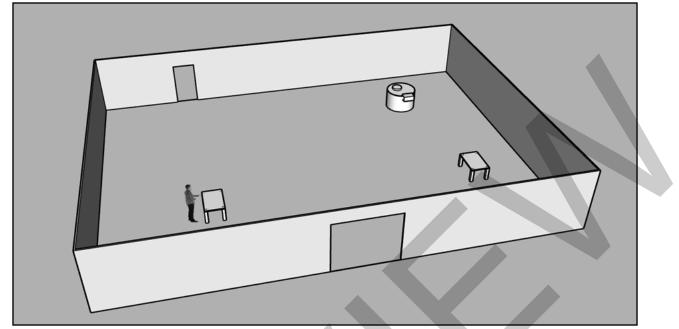


Figure 11.1: Room where exposure took place. The cylindrical-shaped mixer is to the right, and the plaintiff was across the room to the left.

Powder loading into the mixer occurred 2 or 3 times each hour. During loading, five 50-lb sacks of a dry ingredient were added to the mixer through a raised access hatch about the size of a 55-gal drum. The overall loading process took about 5 min. The plaintiff and other workers describe a faint but visible plume of dust rising from the mixer hatch during powder loading.

In talking with various workers who worked in the room, none of them mention excessive dust on horizontal surfaces even when specifically asked about it. This provides some evidence that whatever the specific size distribution of the particles, removal from the air by settling was not significant.

Bags of the powder material are still commercially available and used in industry. Attorneys will fund a simple test chamber experiment to measure the dust emission rate from emptying the sacks. Test chambers have been used to develop exposure models for several scenarios.<sup>6–9</sup>

## The Test Chamber

An 8 ft × 8 ft × 8 ft chamber is constructed (volume = 512 ft<sup>3</sup>) from readily available lumber materials. There is a 2 ft × 6 ft door for entering the chamber. An open-topped drum is positioned against the wall opposite the door. Immediately above the barrel top is a 6-inch-tall, 3-ft-wide slot (face area: 1.5 ft<sup>2</sup>). The slot is exhausted by a centrifugal fan. In line with the ductwork is a minimum efficiency reporting value (MERV) 16 air filter. MERV 16 filters remove particles down to 0.3 µm with >90% efficiency. The filter is 2 ft × 2 ft and 6 inches deep. The chamber set up is illustrated in Figure 11.2.

The fan is rated to move up to 2,300 ft<sup>3</sup>/min. When the system is assembled, the average face velocity of the slot is 1,100 ft/min. With a slot area of 1.5 ft<sup>2</sup>, this gives an in-operation volumetric flow rate of 1,650 ft<sup>3</sup>/min.

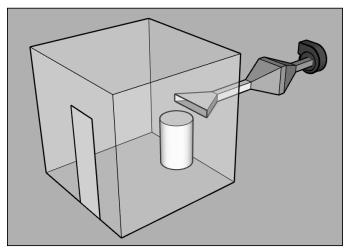


Figure 11.2: Set up of the experimental chamber.

Chapter 17: Reconstruction of a Lab Spill

Variable	Units	Statistical Model	Constant (or Mode)	Min	Мах	Comments
Frequency		Constant	1			а
Duration	min	Constant	30			b
G	mg/min	Triangular	1,330	810	1,900	С
Q	m³/min	Constant	28.3			
V	m <sup>3</sup>	Constant	85			
V <sub>N</sub>	m <sup>3</sup>	Constant	0.26			b
β	m³/min	Triangular	9.6	7.1	11.9	е
t <sub>g</sub>	min	Constant	30			f
t <sub>1</sub>	min	Constant	0			g
t <sub>2</sub>	min	Constant	0 or 30			g

Table 17.2: Variables for the "Two-Box, Constant Emission" WMR Model

All variables must be assigned either a constant or a statistical distribution, such as uniform, triangular, normal, or lognormal distribution.

a – In TEAS, the Frequency is used for repeating tasks. Here we have a single incident.

b – Set the Duration of the task or the time of interest.

c – Refer to Appendix A.

d – Based on a 1-m diameter hemisphere on the floor surrounding the spill. (Refer to Appendix B.)

e – Refer to Appendix B.

f – The t<sub>g</sub> variable indicates the time that the "source" is emitting. In this scenario, it is assumed that the spill is emitting vapor at a constant rate during the 30 min of interest.

g – In TEAS, the worker is assumed to enter the near field at time  $t_1$  and leave the near field at time  $t_2$ . For far-field concentrations, set both to 0.

The two critical variables for a two-box constant emission WMR model are the generation rate, G (mg/min), and near-field ventilation rate,  $\beta$  (m<sup>3</sup>/min). I describe how I modeled both variables in Appendices A and B. For each, I chose to use a triangular distribution. The triangular distribution—which consists of a mode (i.e., the most frequently occurring value), min, and max—is perhaps the most popular distribution used in modeling for describing the actual distribution for a variable and the variability and/or uncertainty in the estimates of the variable.

Following Burton, I used the Hummel Equation<sup>2</sup> for estimating the generation rate of a spill with a fixed surface area but added variability to several of the variables to reflect uncertainty. I also followed the recommendations of Keil and Nicas<sup>3</sup> for applying the Hummel Equation to circular spills (refer to Appendix A).

In the two-box model, the near-field volume (V<sub>N</sub>) represents a zone of high concentrations near the source. Cube, box, or cylinder shapes have been used in the literature; however, in recent years, the hemisphere seems to be the most popular near-field shape and will be used here. I set the diameter at 1 m, which seemed a reasonable width for encompassing both the spill and the upper torso of an employee kneeling nearby. To estimate the near-field flow rate  $\beta$  (m<sup>3</sup>/min), I used Burton's measured air velocity at the floor of 40 fpm but added ± 25% to account for possible day-to-day variability and measurement error. This allowed me to model  $\beta$  using a triangular distribution. The details regarding the calculation of V<sub>N</sub> and  $\beta$  are in Appendix B.

The room volume V (m<sup>3</sup>) was calculated, and the room ventilation rate Q (m<sup>3</sup>/min) was measured by Burton. The time of generation ( $t_g$ ) was set to 30 min. In TEAS, the  $t_1$  and  $t_2$  variables (Table 17.2) are used to indicate the location of the worker relative to the near field. The worker is assumed to enter the near field at time  $t_1$  and leave the near field at time  $t_2$ . This allows flexibility in describing patterns of worker exposure. To calculate near-field concentrations, set  $t_1 = 0$  and  $t_1 =$  duration. To calculate far-field concentrations, set both to zero. TEAS then assumes that the worker is in the far field for the duration of the task.

Comments:

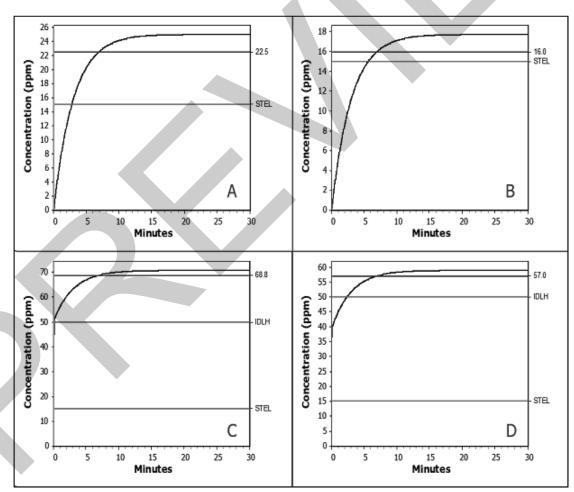
- 1. We will ignore any evaporative cooling effects, which will slightly reduce the emission rate.
- 2. A spill can also be treated as a decreasing emissions scenario, but we would need to know the mass of acetic acid that was spilled and a scenario-specific emission rate constant for acetic acid.
- 3. We are not trying to predict an "exposure profile." This was a one-time exposure scenario. We are attempting to describe the range of possible exposures experienced by the first responders to this spill.

### Simulate Random Exposures

### Test the Model

With TEAS, you can simulate the concentration curve for a single task or a series of tasks. First, test that the WMR model is predicting what you think it should by generating several single-task concentration curves. Four are shown in Figure 17.5. Charts A and B in the figure show examples of the far-field concentration curve. Charts C and D show examples of the near-field concentration curve. In each instance, TEAS generated random values for the G and  $\beta$  variables. The remaining variables were assigned the fixed values in Table 17.2. The near-and far-field concentration curves—which represent the concentration at each time, t—were calculated using Equations 15.3–15.6 from Chapter 15.

For each chart in Figure 17.5, the black and blue curves represent the concentration curve (i.e., the concentration at time t) and task average curve (i.e., the average concentration for the duration of the task). For reference,



**Figure 17.5:** Example concentration curves. Charts A and B represent far-field concentrations. Charts C and D represent near-field concentrations. IDLH, immediately dangerous to life or health; STEL, short-term exposure limit.

Chapter 18: The Limitations of Mathematical Models

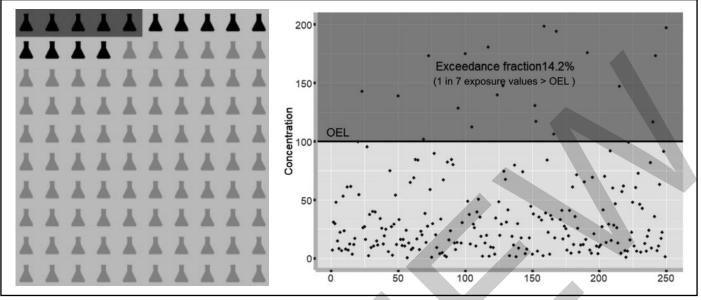


Figure 18.3: The exposure distribution plots to show the occupational exposure limit (OEL) exceedance proportion.

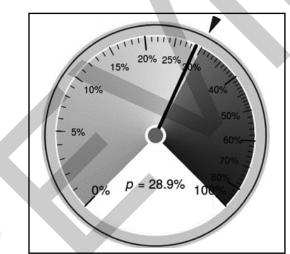
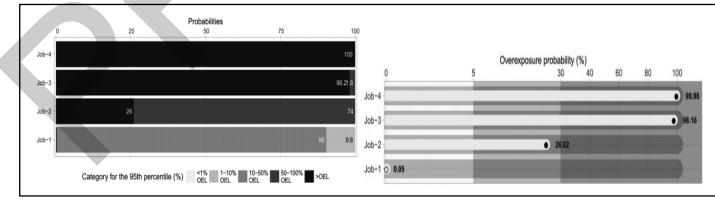
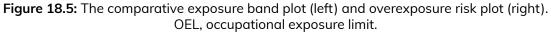


Figure 18.4: The risk gauge indicating the probability value falling into the corresponding risk category.

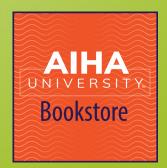




## A Case-Based Introduction to Modeling Occupational Inhalation Exposures to Chemicals

Edited by Chris Keil, PhD, CIH

This collection of case studies is written to provide an application-based "on ramp" to the mathematical modeling of inhalation exposures to chemicals. Seeing the models as integral tools for everyday exposure assessment questions will make these resources more readily accessible for industrial hygienists and other OEHS professionals as they improve the quality of their exposure judgments.



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