Using Variations of the Well-Mixed Room (WMR) Models to Assess Chemical Exposures

Part 1: Chamber characterization and two model assessments

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Introduction

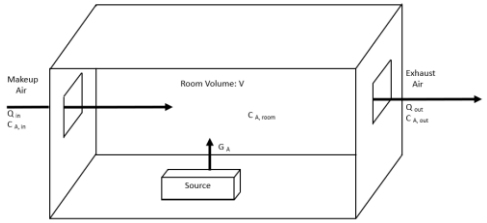
This project focuses on improving current predictive occupational inhalation exposure models by adding variables for exposure controls in order to predict exposure to various chemicals in workplace scenarios. It is a first in a series of projects with the primary goals of developing better predictive exposure models to decrease uncertainty in exposure assessments and to expand use of the models to multiple industries and workplace scenarios using aerosols.

Problem

Models for predicting inhalation exposures in occupational settings are critical for comprehensive exposure assessments. Yet most models such as the WMR model are not widely used for reasons including: a perceived lack of "validation," a lack of guidance on model use, concerns about accounting for all relevant variables, poor knowledge of model input variables, and unknown precision in estimates. Furthermore, predictive mathematical inhalation models in use are focused on only gases and vapors (not aerosols) and are lacking variables that account for exposure controls (e.g. local exhaust ventilation and recirculating air).

The Well-Mixed Room (WMR) Models

The WMR Model is used to estimate the exposure intensity of individuals working within one space (room) with an emission source. The model assumes perfect air mixing and equivalent contaminant concentrations throughout the room. Based on certain parameters, contaminant concentrations can be estimated for the whole room using a set of mass balance equations.

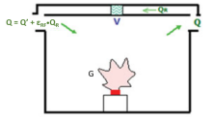


WMR: $VdC = Gdt - CQdt$

Here, Contaminant A is generated from a source. Exposures to workers in this situation are expected to be similar regardless of their location in the room. This version of the WMR Model does not consider the use of exposure controls (i.e. recirculated and filtered room air; local exhaust ventilation) nor particle dynamics. Examples of these are shown right.

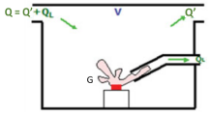
Standard WMR Model Variables		
Variable	Units	Definition
$C_{A,in}$	mg/m³	Concentration of contaminant A in the makeup air
$C_{A,out}$	mg/m³	Concentration of contaminant A in the exhaust air
$C_{A,room}$	mg/m³	Concentration of contaminant A in the room air
G_A	mg/min	Generation rate of contaminant A
Q_{in}	m³/min	Flowrate of makeup air
Q_{out}	m³/min	Flowrate of exhaust air
V	m³	Room volume

Adjusted WMR Model Variables		
Variable	Units	Definition
Q	m³/min	Flowrate of air moving through the room. $Q_{in} = Q_{out}$
Q'	m³/min	Flowrate of air entering the room
Q_L	m³/min	LEV ventilation rate
Q_R	m³/min	Room recirculation ventilation rate
ε_L	unitless; range: 0-1	Efficiency of LEV system
ε_{RF}	unitless; range: 0-1	Efficiency of recirculation system



WMR with recirculating room air:

$VdC = Gdt - C(Q' + \varepsilon_{RF} \cdot Q_R)dt$



WMR with LEV :

$VdC = (1 - \varepsilon_L)Gdt - C(Q' + Q_L)dt$

Methods

A highly-controlled exposure chamber (Fig.1) was characterized by comparing manually set air flows rates (0 – 20 m³/min) to measured air exchange rates. Acetone and toluene vapors were generated using a Harvard syringe pump and concentrations measured using photoionization detectors. Variables for engineering controls were then added to the standard WMR model then evaluated under controlled conditions in a series of chamber studies using acetone. Model inputs were controlled and measured to generating over 100 pairs of modeled and measured exposure estimates. By varying conditions (generation rate (G: 0.25 - 1 mg/min); air flow rate (Q: 1 - 12 m³/min); efficiency of collection with LEV (ε_L: 0.5 - 1.0)) in the chamber one at a time, model performance with different engineering controls across a range of conditions was evaluated. Measured and modeled exposure estimates were compared using log-linear regression.

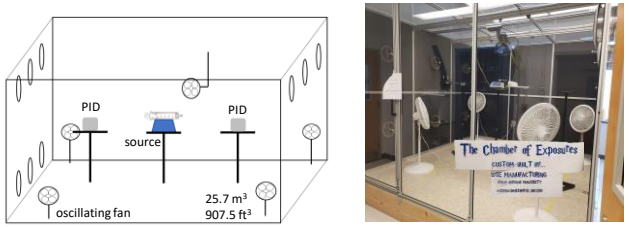


Figure 1. Schematic of the Chamber of Exposures (left) and an experiment in progress (right).

Results

Chamber characterization with the decay studies indicated that the flowmeter provides a very good approximation of the true air exchange rate the chamber is set at ($r^2 = 0.834$). Model performance for the standard WMR model was excellent, with almost perfect agreement between the modeled and measured concentrations ($r^2 = 0.992$). Percent difference values between the measure and modeled values were less than 10% (average percent difference = 6.85%). Model performance for the WMR+LEV model is limited to a handful of data points (experiments interrupted due to COVID) but preliminary results suggest positive agreement ($r^2 > 0.6$). Comparison of the modeled LEV efficiencies and those determined experimentally had an average percent difference of 12%.

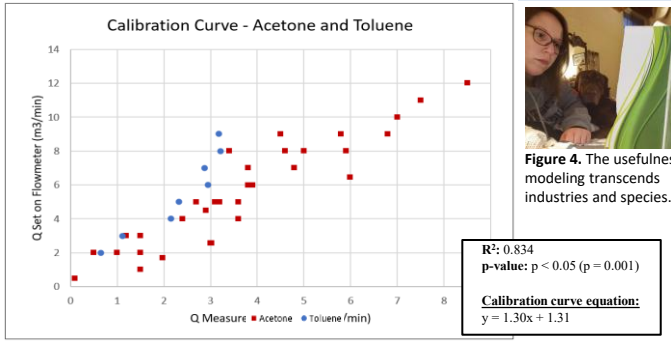


Figure 2. Exposure chamber calibration (characterization) curve comparing air flow rate set on flowmeter to the air flowrate measure from decay experiments.

Figure 4. The usefulness of modeling transcends industries and species.

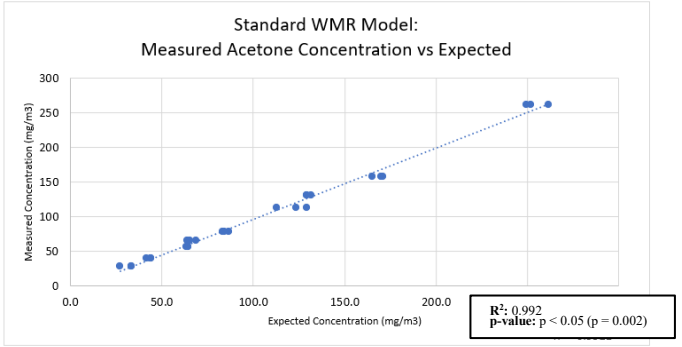


Figure 3. Standard WMR comparison of measured and expected acetone concentrations.

Application to Workplace Exposure Scenarios

Predictive models are useful in occupational exposure assessment, but their accuracy and usability in real workplace scenarios is unknown when exposure controls are incorporated. This work aims to: (1) improve currently used exposure assessment tools; (2) examine different workplace scenarios using various engineering controls; and (3) provide a decision framework for model selection. This research is the first in a series of projects intended to improve existing exposure modeling tools for predicting worker exposure to hazards. Next steps include evaluating the models for exposure to aerosols by including variables for particle dynamics (e.g. gravitational settling, impaction, and eddy and Brownian diffusion) into the models.

References and Acknowledgements

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