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Vaporized Hydrogen Peroxide
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Abstract

The SARS-CoV-2 virus has put a strain on the supply and distribution of N95 masks, with some hospitals electing to reuse masks after disinfection. Currently, vaporized hydrogen peroxide (VHP) mask disinfection systems are being deployed at multiple locations throughout the United States, for example in shipping containers and in small rooms. Such enclosures will be of a different size, have different surface materials and have varying air change rates; all these parameters will impact the VHP dose that the masks receive. This paper describes a spreadsheet tool to estimate the VHP concentration in air of such a room. The tool employs a single-zone mass balance analysis that accounts for room size, VHP losses to surfaces and air change rate. This tool is intended to support VHP disinfection efforts by providing estimates of VHP concentrations in the room being employed, but it does not describe or provide guidance on VHP disinfection applications.

Introduction

The SARS-CoV-2 virus has put a strain on the supply and distribution of personal protection equipment, including N95 masks (Chaudhuri 2020, Nierenberg 2020). One approach to help alleviate this shortage is to disinfect and reuse masks. The disinfection process must be effective against the target organism, not damage the mask or impact the fit, and be safe for the wearer after disinfection (3M 2020). A wide range of physical or chemical processes have been proposed for disinfecting masks, including ultraviolet irradiation, hydrogen peroxide (liquid, vapor and plasma), microwaves, moist heat, ionization radiation and ethylene oxide (3M 2020, Centers for Disease Control and Prevention 2020).

Vaporized hydrogen peroxide (VHP) has been used in hospitals to disinfect medical equipment and rooms (Rutala et al. 2008, Otter et al. 2009, Canadian Agency for Drugs and Technologies in Health 2014, Rutala and Weber 2015). In addition, VHP has been recently demonstrated to eliminate aerosolized bacteriophages used as proxies for SARS-CoV-2 (e.g., T1, T7, and *Pseudomonas phage phi-6*) in masks (Kenney et al. 2020).

As of April 2, 2020, Battelle Memorial Institute is deploying VHP disinfectant systems (Figure 1, approved by FDA on March 29, 2020 (Hinton 2020)) in shipping containers across the United States to treat up to 80 000 N95 masks per day (Hale 2020, Ostriker 2020). In addition to shipping container systems, some hospitals are setting up disinfection systems in small rooms (Medicine 2020). As SARS-CoV-2 continues to spread, more small rooms within hospitals or other locations may increasingly be used for disinfecting masks. Such rooms will be of a different size, have different surface materials and have varying air change rates; all these parameters will impact the effective VHP dose that the masks receive. Materials such as carpet have been shown to reduce indoor VHP concentrations by up to an order of magnitude (Corsi et al. 2005). Failure to account for surface losses in these rooms may inhibit effective N95 mask disinfection.



Figure 1: Battelle Memorial Institute VHP masks decontamination system. Photo used with permission (John Clay email 4/6/2020).

Room VHP concentrations have been reported to be in the range of 0.14 to 8 g m⁻³ (Battelle 2016, Centers for Disease Control and Prevention 2020). Note that these room concentrations used to disinfect masks using VHP may exceed NIOSH relative exposure limits (0.0014 g m⁻³) (Akers and Agalloco 2013, NIOSH 2020). Given the strong dependence of room or enclosure VHP concentrations on room size, surface materials and air change rates, those applying this approach need to estimate these concentrations when pursuing VHP disinfection of masks.

This paper describes a spreadsheet tool to estimate the VHP concentration in air of a room being used to disinfect masks that employs a single-zone mass balance analysis. This tool is intended to support VHP disinfection efforts by providing estimates of VHP concentrations in the chamber being employed, but it does not describe or provide guidance on VHP disinfection applications. Nor does it address safety considerations in using VHP for disinfection of masks (Akers and Agalloco 2013), including migration of vaporized hydrogen peroxide into adjacent rooms. Other important considerations include effective VHP dose, disinfection times, and air mixing in the room to ensure all masks are subject to similar VHP concentrations. These issues need to be addressed in consultation with facility management staff and with safety and occupational health personnel prior to using VHP to disinfect masks.

Method

This paper describes a spreadsheet tool that allows a user to estimate the VHP concentration in air of a room being used to disinfect masks. The tool accounts for room size, surface losses and air change rate using a mass balance approach. It can also be used to estimate the mass of disinfectant deposited on the masks. The tool employs a single zone analysis in which the VHP concentration is characterized by a single value throughout the room. The mass balance equations on which the tool is based are provided in the appendix. The tool can be downloaded from <https://www.nist.gov/el/energy-and-environment-division-73200/nist-multizone-modeling/software-tools/VHP-disinfection>.

Recent efforts to disinfect masks with VHP have employed a four-phase process: **Conditioning**, **Gassing**, **Dwell**, and **Aeration** (Battelle 2016, Kenney et al. 2020). The first phase, Conditioning, is the period during which the chamber is brought to the desired temperature and relative humidity and does not involve VHP injection, so it is not covered by this tool. During both the Gassing and Dwell phases VHP is injected into the room, with the former involving increased VHP flow to achieve the target concentration more rapidly. Gassing phase emissions sources and flow rates may be greater than those during Dwell phases. The Aeration phase is used to vent the chamber after the disinfection process has ended.

The tool allows the user to enter different durations, emission source strength, and flow rate for the **Gassing**, **Dwell** and **Aeration** phases. To use this tool, input data are entered into the green cells shown in Figure 2.

For the (1) **Gassing** and (2) **Dwell** phases:

- Enter the phase **Duration** (h).
- Enter the **Mechanical flow** into the room (m³ h⁻¹). This flow should not include any recirculating flow in closed-loop systems. The calculated **Air change rate** (h⁻¹) for each phase is the sum of the

Infiltration rate (h^{-1}) and **Mechanical ventilation** multiplied by the **Room volume**. If the **Mechanical Flow** is unknown, adjust the **Mechanical Flow** and **Infiltration rate** values until a realistic **Air change rate** value for the phase is displayed. See the **Infiltration Rate** discussion below for more details.

Inputs

1) Gassing Phase	
Duration, h	0.33
Mechanical Flow, $\text{m}^3 \text{h}^{-1}$	1.00
Total Air change rate, λ , h^{-1}	0.17
a) In Room Source	
Emission source in room E, g h^{-1}	120
b) Injection Source	
Concentration in injected air, C_{inj} , g m^{-3}	0
Flow rate of injected air, Q_{inj} , $\text{m}^3 \text{h}^{-1}$	0

Masks	
Diameter, m	0.15
Number	100

Room	
Length, m	2
Width, m	3
Height, m	2.5
Initial Concentration, $C_{initial}$, g m^{-3}	0
Infiltration rate, λ , h^{-1}	0.1

2) Dwell Phase	
Duration, h	2.50
Mechanical Flow, $\text{m}^3 \text{h}^{-1}$	1.00
Total Air change rate, λ , h^{-1}	0.17
a) In Room Source	
Emission source in room E, g h^{-1}	80
b) Injection Source	
Concentration in injected air, C_{inj} , g m^{-3}	0
Flow rate of injected air, Q_{inj} , $\text{m}^3 \text{h}^{-1}$	0

3) Aeration Phase	
Duration, h	0.50
Mechanical Flow, $\text{m}^3 \text{h}^{-1}$	200.0
Total Air change rate, λ , h^{-1}	13.43

Surfaces	Surface adsorption		Deposition Velocity,	
	area, A , m^2	Surface material	V_d , cm h^{-1}	$V_d * A / V$, h^{-1}
Walls	25	Concrete w/Sealer	600	10.0
Ceiling	6	Concrete	800	3.2
Floor	6	VCT	75	0.3
Masks	3.5	Paper/HVAC Duct	600	1.4
Other Surfaces with Large Areas	0.0	-	0	0.0

Figure 2: The input screen of the disinfection tool.

VHP can either be released directly inside the room using a VHP generator or injected into the room using a generator located outside the room. Emission rates for the release process not being used should be input as zero. Set the VHP source strength for **Gassing** and **Dwell** phases as follows:

- **Emission source in the room.** If the VHP source is in the room, enter the emission rate (g h^{-1}). Use this option if the generation system is externally located but operates on a “closed loop cycle.” Previous mask disinfection research used in-room VHP sources emitting at a rate of 120 g h^{-1} to 960 g h^{-1} (Battelle 2016, Centers for Disease Control and Prevention 2020, Kenney et al. 2020).
 - Enter the **Emission source in room** (g h^{-1})
 - Enter zero for the **Concentration in injected air** (g m^{-3})
 - Enter zero for the **Flow rate of injected air** (g m^{-3})
- **Generated outside the room.** If the VHP source is external to the room, enter the injection rate to the room (g m^{-3}). This option is provided for completeness. No known mask disinfection systems have been implemented in this manner to the knowledge of the author.
 - Enter zero for the **Emission source in the room** (g h^{-1})
 - Enter the **Concentration in injected air** (g m^{-3})
 - Enter the **Flow rate of injected air** ($\text{m}^3 \text{ h}^{-1}$).

For the (3) **Aeration** phase:

- Enter the phase **Duration** (h).
- Enter the **Mechanical flow** into the room ($\text{m}^3 \text{ h}^{-1}$). See the **Infiltration Rate** discussion below for more details about the **Air change rate**.

Mask and room properties are entered on the right side of the input screen.

- **Masks. Diameter** of mask (m), assuming it is circular. This value is used to calculate the total surface area of the mask including both sides. Enter the **Number** of masks being disinfected inside the room.
- **Dimensions.** Length, width and height of the room (m)
- **Initial Concentration in room.** Initial VHP concentration in the room (g m^{-3}). In most cases this value will be zero.
- Estimate the **Infiltration rate** for the room (h^{-1}). The infiltration rate is the rate at which air enters the room when the disinfection system is not running and the room is isolated from the building ventilating systems (i.e., supply, return and exhaust vents are sealed). Rarely is the infiltration rate zero. Very airtight rooms may have infiltration rates as low as 0.1 h^{-1} . More typical rooms may have infiltration rates from about 0.3 h^{-1} to 0.5 h^{-1} or even higher (Persily et al. 2009). These values are estimates for use in these calculations; the user should consider the specific room in their application in consultation with engineering, facility and safety staff in estimating or measuring this parameter. In general, a higher estimated infiltration rate will be more conservative as it will lead to lower calculated VHP concentrations. It will also lead to shorter estimated times before the room concentration returns to background levels during the aeration phase, which need to be considered in planning disinfection efforts.
- Enter the **Surface materials** and the **Deposition velocities** (cm h^{-1}) for each material.

Work by Corsi et al. (2005) determined hydrogen peroxide deposition velocities using a Bioquell Clarus-C generator operated in closed-loop mode using 50 % H_2O_2 producing a VHP chamber concentration of 1 g m^{-3} . Test were done on 23 different building materials using 50 L chambers at room temperature with an air change rate of 2.4 h^{-1} . These data are presented in Figure 3.

To account for deposition processes, the user should determine the surface materials that best represent the walls, ceiling, floor and any other materials of substantial surface area in the room. Once the appropriate materials are identified, determine the deposition velocity from Figure 3. In Figure 3, VCT is vinyl composite tile, MDF is medium density fiberboard and GWB is gypsum wall board. Once the appropriate materials are selected, determine the approximate deposition velocity from Figure 3. The deposition velocities characterize how fast the VHP is removed by the various surfaces.

In ideal cases, there is nothing in the disinfection room for VHP to deposit to other than the walls, ceiling, floor, masks and mask racks. If there is a large surface area of another material in the room, that area can be accounted for in the last surface input. The total exposed area of these surfaces should be entered (m²) and a deposition velocity best representing the surfaces should be selected from Figure 3 for the large surface.

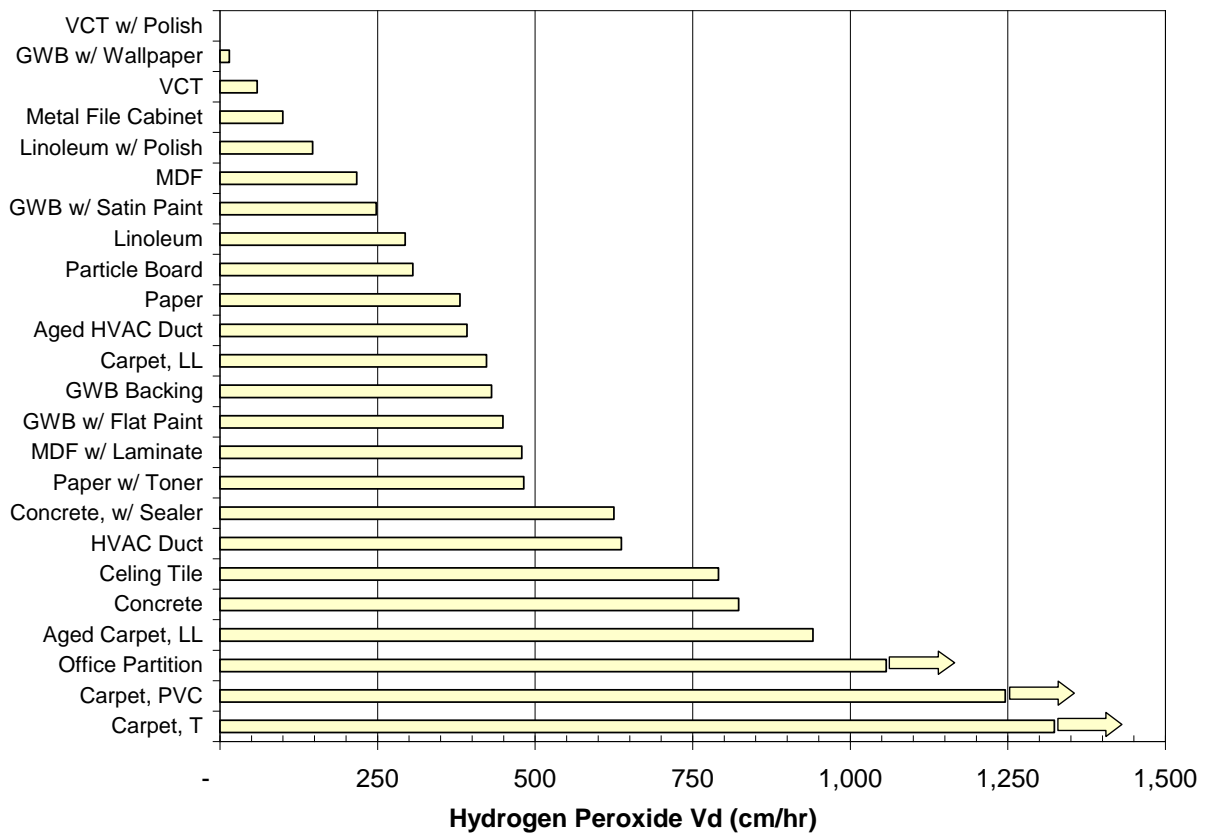


Figure 3: Steady-state hydrogen peroxide deposition velocities over all experiments (arrows indicate values greater than the bar length shown). Reproduced from Corsi et al. (2008). Values with arrows indicate minimum deposition velocity values due to VHP concentrations below detection limits for these materials.

The model will automatically update the results as soon as any cells are entered. The worksheet has two tabs (shipping container and general room). The calculations in each tab are identical and either tab can be modified.

Results

The model has both tabular and graphical output. The table in Figure 4 summarizes the results. The first line shows the maximum predicted room airborne VHP concentration when surface losses are accounted for, and the second line shows the maximum concentration without surface losses. The third line shows how much lower the peak concentration will be when losses due to surfaces are accounted for compared to the case without losses. The fourth line shows the VHP dose that the masks are estimated to experience (the integration of concentration multiplied over time). The fifth line predicts what percent of the injected mass will be deposited onto the masks. The last line predicts what percent of the injected mass will be deposited onto the room surfaces.

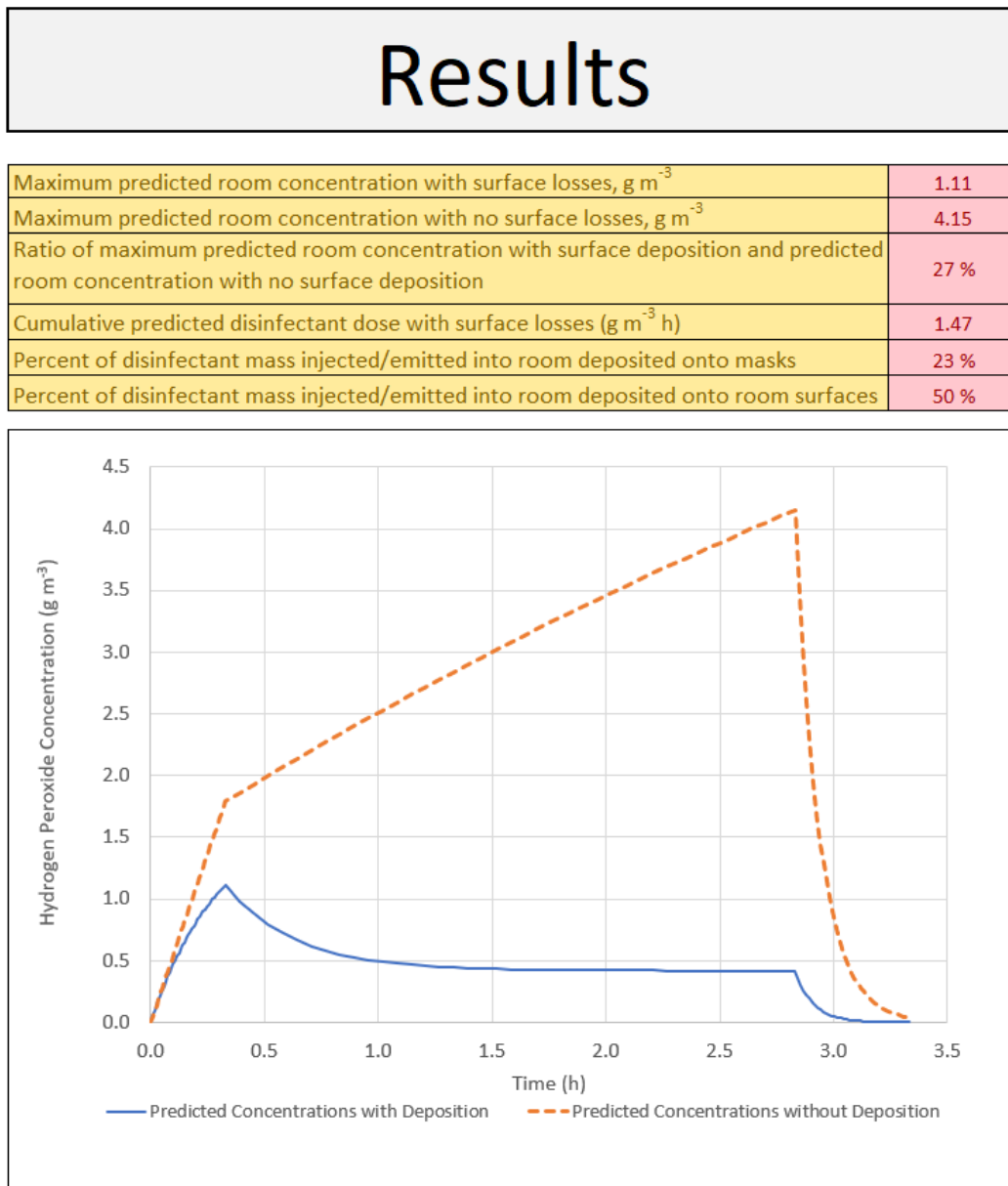


Figure 4: Results of model. Graph shows room airborne VHP concentration predictions with and without surfaces losses accounted for.

Figure 4 shows the room airborne VHP concentration predictions for conditions where the losses to room surfaces are accounted for (solid blue) and are not accounted for (dashed orange). The difference in these lines for this case demonstrates the role that room surfaces have in impacting the disinfectant dose to the masks.

The second table in the results section (not shown in Figure 4) describes parameter values. The calculated **Total airflow** values ($\text{m}^3 \text{h}^{-1}$) for each phase includes the **Mechanical Flow**, the **Flow rate for the injection system**, and **Infiltration air**. The **Total loss rate** for each phase accounts for losses to surfaces and total airflow.

Summary

This tool can be used to estimate the concentration of hydrogen peroxide disinfectant in a mask disinfectant room utilizing Vaporized Hydrogen Peroxide (VHP) to help plan an effective VHP disinfection application by predicting the concentration of the disinfectant received by masks. The model predicts that rooms with lower surface-to-volume ratios, lower air change rates, fewer masks and surface materials with lower hydrogen peroxide deposition velocities (Figure 3) will result in higher steady state VHP concentrations.

This tool does not describe or provide guidance on VHP disinfection applications, including safety issues that should be addressed in consultation with facility management staff and with safety and occupational health personnel prior to using VHP to disinfect masks.

Disclaimer

Certain commercial equipment, instruments, or materials are identified in this paper in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

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Appendix

Single-zone mass balance equation for a room accounting for ventilation, source and deposition:

$$\frac{dC}{dt} = \frac{Q_{inj}}{V} \cdot C_{inj} - \lambda \cdot C + \frac{E}{V} - V_{d1} \cdot \frac{A_1 \cdot C}{V} - V_{d2} \cdot \frac{A_2 \cdot C}{V} - V_{d3} \cdot \frac{A_3 \cdot C}{V} - V_{d4} \cdot \frac{A_4 \cdot C}{V} \quad (1)$$

Where:

C	Chamber concentration, g m^{-3}
t	Time, h
λ	air change rate, h^{-1}
C_{inj}	Injected Concentration, g m^{-3}
Q_{inj}	Injected flow rate, $\text{m}^3 \text{h}^{-1}$
E	Emission rate, g h^{-1}
V	Room volume, m^3
$V_{d,i}$	Deposition velocity for material i, m h^{-1}
A_i	Area of material i, m^2

The analytical solution for the concentration in the room air is:

$$C = C_0 \cdot \exp(-k \cdot t) + \frac{Q_{inj} \cdot C_{inj} + E}{kV} (1 - \exp(-k \cdot t)) \quad (2)$$

Where

C_0	Initial room concentration (typically zero), g m^{-3}
k	Total loss rate, h^{-1}

$$k = \lambda + \frac{Q_{inj}}{V} + V_{d1} \cdot \frac{A_1}{V} + V_{d2} \cdot \frac{A_2}{V} + V_{d3} \cdot \frac{A_3}{V} + V_{d4} \cdot \frac{A_4}{V} + V_{d5} \cdot \frac{A_5}{V} \quad (3)$$

The analytical solution was applied to each phase with the initial room concentration for each phase being determined by the last room concentration of the previous phase.

Assuming the disinfection dose can be calculated by multiplying the airborne concentration by time, the dose can be determined by:

$$D = \int_0^t C dt = \left(\frac{C_0}{k} \cdot (1 - \exp(-k \cdot t)) \right) + \frac{Q_{inj} \cdot C_{inj} + E}{kV} \left(t + \frac{1}{k} (1 - \exp(-k \cdot t)) \right) \quad (5)$$

Where:

D	Dose, $\text{g m}^{-3} \text{h}^{-1}$
-----	---------------------------------------

To compare to calculations without accounting for deposition the solution for the concentration in the room air is:

$$C = C_0 \cdot \exp(-\lambda \cdot t) + \left(\frac{Q_{inj} \cdot C_{inj} + E}{\lambda V} \right) (1 - \exp(-\lambda \cdot t)) \quad (4)$$

In addition, the disinfectant mass deposited on each material can be determined by:

$$M_i = \int_0^t V_{di} \cdot A_i \cdot C dt = V_{di} \cdot A_i \left(\frac{C_0}{k} \cdot (1 - \exp(-k \cdot t)) + \frac{Q_{inj} \cdot C_{inj} + E}{kV} \left(t + \frac{1}{k} (1 - \exp(-k \cdot t)) \right) \right) \quad (5)$$

Where:

M_i Disinfectant mass on material i, g

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