A GENERAL MATHEMATICAL TREATMENT OF HAZARDS TO NBC COLLECTIVE PROTECTION SYSTEMS WITH APPLICATIONS TO PARTICULAR CASES

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   This work was performed under the Naval Aircraft Combat Survivability
   Program's Task F-82-11 "Aircraft Protection/Decontamination Requirements"
Item 20 continued

>for Naval Air Operations in a CBR Environment."
PREFACE

This document presents a general mathematical development of the theory of vapor contamination hazards to nuclear, biological and chemical (NBC) collective protection systems. An important general result is derived and then illustrated by applying it to selected examples of special interest in studies of NBC defense.

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<tr>
<td>$R$</td>
<td>A fixed control volume or region, e.g., the interior of a collective protection system</td>
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<td>$V$</td>
<td>Volume in $m^3$ of $R$</td>
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<tr>
<td>$F_i(t)$</td>
<td>Instantaneous volume rate of flow in $m^3/min$ of inflow stream $i$</td>
</tr>
<tr>
<td>$F_o(t)$</td>
<td>Instantaneous volume rate of flow in $m^3/min$ of the outflow stream; see Eq. (2)</td>
</tr>
<tr>
<td>$I$</td>
<td>Number of inflow streams</td>
</tr>
<tr>
<td>$C_R(t)$</td>
<td>Instantaneous concentration in $mg/m^3$ of contaminant vapor in $R$; see Eq. (5), (9) and (11)</td>
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<tr>
<td>$Q_R(t)$</td>
<td>Instantaneous mass in $mg$ of contaminant vapor in $R$; see Eq. (1) and (4)</td>
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<tr>
<td>$E_j(t)$</td>
<td>Instantaneous stopping power or efficiency of filter/absorber unit $j$; see Eq. (3)</td>
</tr>
<tr>
<td>$C_{Aj}(t)$</td>
<td>Instantaneous concentration in $mg/m^3$ of contaminant vapor at the output of filter/absorber unit $j$</td>
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<tr>
<td>$C_i(t)$</td>
<td>Instantaneous concentration in $mg/m^3$ of contaminant vapor in inflow stream $i$</td>
</tr>
<tr>
<td>$F_{Aj}(t)$</td>
<td>Instantaneous volume rate of flow in $m^3/min$ through filter/absorber unit $j$</td>
</tr>
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<td>$J$</td>
<td>Number of filter/absorber units</td>
</tr>
<tr>
<td>$K$</td>
<td>Number of evaporating sources</td>
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<tr>
<td>$G_k(t)$</td>
<td>Instantaneous rate of evaporation in $mg/min$ of contaminant vapor source $k$ at time $t$</td>
</tr>
<tr>
<td>$C_o(t)$</td>
<td>Weighted average inflow stream contaminant vapor concentration in $mg/m^3$ (see Eq. (6.1))</td>
</tr>
<tr>
<td>$F_{Ao}(t)$</td>
<td>Total rate of flow in $m^3/min$ through the filter/absorber units; see Eq. (6.2)</td>
</tr>
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E(t) Weighted average filter/absorber stopping power or efficiency; see Eq. (6.3)

G_o(t) Total rate of evaporation in mg/min of the contaminant vapor sources in R; see Eq. (6.4)

α(t) Instantaneous fractional ventilation rate; see Eq. (8.1)

β(t) Instantaneous rate of introduction of contaminant vapor per unit volume of R in mg · min⁻¹ · m⁻³; see Eq. (8.2)

t₀ A time to which initial concentrations and dosages are referenced

D_R(t) Vapor dosage in mg-min/m³ accumulated in R from time t₀ to time t; see Eq. (10)

D_R(∞) Total vapor dosage in mg-min/m³ accumulated in R over all time; the limit of D_R(t) as t → ∞; see Eq. (13) and (15)

C_R(∞) The limit of C_R(t) as t → ∞

T A time chosen large enough that β(z) < α₀ for z ≥ T

T₁ The time at which a change in the value of α occurs

α₀ Value of α for t₀ ≤ t < T₁

α₁ Value of α for T₁ ≤ t < ∞
INTRODUCTION

Our purpose is to demonstrate a useful and interesting general result in the theory of vapor* contamination hazards to collective protection systems. The combination of the generality of the result and the simplicity of its proof may be new—at least I do not recall having seen either of them before. In any event, both the general result and its elegant proof deserve to be more widely known. It can easily be used to obtain for particular cases the following striking results.

Example 1.—Suppose that shortly before an NBC attack a collective protection shelter with no filtered air supply is imperfectly sealed so that a small but persistent flow of outside air enters the shelter. If this sealed posture of the shelter is maintained indefinitely, then the total vapor dosage inside the shelter is the same as the total vapor dosage outside the shelter. Furthermore, this result holds irrespective of:

1. The size of the shelter (provided its volume is constant)
2. The leakage flow rate (provided it is a positive constant)
3. Changes with time of the contamination vapor density in the outside air (provided it approaches zero as time passes).

Example 2.—Suppose that some liquid contaminant is inadvertently brought into a previously uncontaminated collective protection shelter that is provided with a perfectly filtered air intake and has no leaks from the outside air. Then the total vapor dosage in mg-min per cubic meter inside the shelter is equal to the total mass in mg of contaminant that eventually vaporizes divided by the shelter's volume ventilation rate in cubic meters per minute. Furthermore, this result holds irrespective of:

*For brevity, all airborne contaminant (whether vapor or aerosol) is referred to as "vapor." Similarly, "vaporizing" includes re-aerosolizing and so forth.
1. The size of the shelter (provided its volume is constant)

2. The volume ventilation flow rate (provided it is a positive constant)

3. Changes with time of the liquid contaminant's vaporization rate (provided it approaches zero as time passes).

The generalization of these particular cases, and the result which will be demonstrated in the following sections, can be stated in words as follows. Consider a collective protection shelter whose volume is fixed and whose volume ventilation rate in cubic meters per minute is kept constant. Then the total vapor dosage in mg-min per cubic meter inside the shelter is equal to the total mass of contaminant vapor in mg that is initially within or subsequently introduced into the shelter, divided by the shelter's volume ventilation rate. Furthermore, this result holds irrespective of:

1. The size of the shelter (provided its volume is constant)

2. The shelter's volume ventilation flow rate in cubic meters per minute (provided it is a positive constant)

3. Changes with time of the rate in mg per minute at which contaminant vapor is introduced into the shelter by vaporization of internal sources, by the influx of imperfectly filtered outside air, or both (provided that the total rate of introduction of contaminant vapor approaches zero as time passes)

4. The initial concentration of contaminant vapor within the shelter.

The presentation of this general result begins with a description of the even more general case in which the shelter's ventilation rate
may vary with time. Since at this level of generality we have not been able to deduce any particularly noteworthy properties of the total vapor dosage, we specialize it to the case of a constant ventilation rate. The general result is then proved for this case, and it is shown how Examples 1 and 2 are obtained as particular instances of it.
DESCRIPTION OF THE GENERAL SITUATION

Consider the region R shown in Figure 1. R could be any fixed control volume or region with a constant volume of $V \text{ m}^3$, but it usually is interpreted to be the interior of a collective protection system. Assume that any contaminant vapor in R is well-mixed so that its vapor concentration $C_R(t)$ in mg/m$^3$ is the same at all points of R. Thus, if $Q_R(t)$ is the mass in mg of the contaminant vapor in R then

$$Q_R(t) = V \cdot C_R(t). \quad (1)$$

If the contaminant vapor is not well-mixed there may be "hot spots" of higher than average concentration in R which are balanced by "cold spots" of lower than average concentration.

Suppose that R contains K pieces of solid or liquid contaminant and that piece k vaporizes at the rate $G_k(t)$ mg/min. Suppose that R is fed by I influx streams and that influx stream i has a volume flow rate of $F_i(t)$ m$^3$/min and a contaminant vapor concentration of $C_i(t)$ mg/m$^3$. Then the total rate of volume flow into R through the influx streams is

$$F_0(t) = \sum_{i=1}^{I} F_i(t), \quad (2)$$

Suppose also that R is equipped with J filter/absorber units and that unit j has a volume flow rate of $F_{Aj}(t)$ m$^3$/min and that its output stream has a contaminant vapor concentration of $C_{Aj}(t)$ mg/m$^3$. Assume that filter/absorber unit j has a stopping power or efficiency ratio

$$E_j(t) = \frac{[C_R(t) - C_{Aj}(t)]}{C_R(t)} \quad (3)$$

that is a function of time only. Assume that there is no appreciable gain or loss of volume by filtration or by contaminant vaporization, and let all flows be practically incompressible.
FIGURE 1. Flows Into and Out of Region R
Then the mass of contaminant vapor in R at time \( t \) must satisfy the mass balance equation

\[
Q_R(t+dt) = Q_R(t) + \sum_{k=1}^{K} G_k(t) \, dt + \sum_{i=1}^{I} C_i(t) \, F_i(t) \, dt
\]

\[
- \sum_{j=1}^{J} F_{A_j}(t) \left[ C_R(t) - C_{A_j}(t) \right] \, dt
\]

\[
- F_0(t) \, C_R(t) \, dt.
\]

By using equations (1), (2) and (3), equation (4) may be written as

\[
\frac{d}{dt} C_R(t) V = F_0(t) \, C_0(t) - F_{A_0}(t) \, C_R(t) \, E(t)
\]

\[
- F_0(t) \, C_R(t) + C_0(t)
\]

where we have put

\[
C_0(t) = \sum_{i=1}^{I} F_i(t) \, C_i(t) / F_0(t)
\]

\[
F_{A_0}(t) = \sum_{j=1}^{J} F_{A_j}(t)
\]

\[
E(t) = \sum_{j=1}^{J} F_{A_j}(t) \, E_j(t) / F_{A_0}(t)
\]

\[
C_0(t) = \sum_{k=1}^{K} G_k(t).
\]

Note that \( E(t) \) is dimensionless and represents a sort of weighted average filter/absorber efficiency factor, and \( C_0(t) \) is a weighted average inflow vapor concentration expressed in mg/m\(^3\). Equation (5) can be written as
\[
d\frac{dC_R(t)}{dt} = -\alpha(t) C_R(t) + \beta(t)
\]

where

\[
\alpha(t) = \frac{[F_0(t) + F_{Ao}(t) E(t)]}{V}
\]

and

\[
\beta(t) = \frac{[G_0(t) + F_0(t) C_0(t)]}{V}
\]

where \(\alpha(t)\) and \(\beta(t)\) are functions of \(t\) but do not depend explicitly on other quantities. Physically, \(\alpha(t)\) and \(\beta(t)\) are non-negative. We call \(\alpha(t)\) the instantaneous fractional ventilation rate, and \(V \cdot \alpha(t)\) the instantaneous volume ventilation rate of the region \(R\) (or of the collective protection system which it represents). Observe that \(\beta(t)\) is the instantaneous rate of introduction of contaminant vapor per unit volume of \(R\) and has the dimensions \(\text{mg} \cdot \text{min}^{-1} \cdot \text{m}^{-3}\). \(V \cdot \beta(t)\) is the instantaneous rate in \(\text{mg}/\text{min}\) at which contaminant vapor is introduced into \(R\).

Equation (7) is a linear differential equation. Its general solution is presented in many standard texts on ordinary differential equations and may be written as

\[
C_R(t) = e^{-\int_{t_0}^{t} \alpha(u) du} \left[ C_R(t_0) + \int_{t_0}^{t} \beta(z) e^{\int_{t_0}^{z} \alpha(s) ds} dz \right]
\]

where \(C_R(t)\) is the concentration in \(R\) at time \(t_0\). By definition, the dosage or cumulative \(C\)-t product in \(R\) in \(\text{mg}\cdot\text{min}/\text{m}^3\) after time \(t_0\) is

\[
D_R(t) = \int_{t_0}^{t} C_R(y) dy.
\]

At this level of generality we have not yet been able to deduce any particularly noteworthy properties of the total vapor dosage. Accordingly, we consider instead the constant ventilation rate situation.
GENERAL RESULT FOR CONSTANT VENTILATION RATES

When the ventilation rate \( \alpha \) is constant Eq. (9) reduces to

\[
C_R(t) = C_R(t_0) \exp(-\alpha(t-t_0)) + \int_{t_0}^{t} \beta(z) \exp(-\alpha(t-z)) dz
\] (11)

Our main object is to demonstrate the following general result for collective protection shelters with constant positive ventilation rates.

THEOREM: Suppose \( \alpha \) is a positive constant and \( \gamma(z) \) is such that

\[
C_R(t) \rightarrow 0.
\] (12)

Then

\[
D_R(t) = \lim_{t \to \infty} D_R(t) = \alpha^{-1} \left[ C_R(t_0) + \int_{t_0}^{\infty} \beta(y) dy \right].
\] (13)

PROOF: When \( \alpha \) is a positive constant we may solve Eq. (7) for \( C_R(y) \) and substitute the result into Eq. (10) to obtain

\[
D_R(t) = \alpha^{-1} \int_{t_0}^{t} \left[ \beta(y) dy - dC_R(y) \right]
\]

\[
= \alpha^{-1} \left[ C_R(t_0) + \int_{t_0}^{t} \beta(y) dy - C_R(t) \right].
\] (14)

But \( C_R(\infty) = 0 \) by assumption, and Eq. (13) follows immediately. QED.

Substituting from Eqs. (8.1) and (8.2) into Eq. (13) we may write

\[
D_R(\infty) = \left[ VC_R(t_0) + \int_{t_0}^{\infty} \left( G(y) + F_0(y) C_O(y) \right) dy \right] / [F_O + F_A],
\] (15)
where by the assumptions of the Theorem the denominator is a positive constant (i.e., independent of \( t \)). Observe that by Eq. (1) the first term of the numerator is the initial mass of contaminant vapor in \( R \). The second term of the numerator is the mass of contaminant vapor subsequently introduced into \( R \) by all causes. The denominator is the volume ventilation rate of \( R \). Thus the conclusion of the Theorem can be stated in words as given in the Introduction.

It can be inconvenient to verify that \( \beta(z) \) is such as to satisfy condition (12). The following Lemma is often easier to apply.

**LEMMA:** Suppose \( \alpha \) is a positive constant and

\[
\beta(\infty) = \lim_{t \to \infty} \beta(t) = 0.
\]

Then

\[
C_r(\infty) = \lim_{t \to \infty} C_r(t) = 0.
\]

**PROOF:** Given any \( \varepsilon > 0 \) fix \( T \) so large that

\[
\beta(z) < \varepsilon \alpha \text{ for } z > T.
\]

(Since by assumption \( \beta(z) \to 0 \) as \( t \to \infty \), an appropriate \( T \) can always be found). Then by breaking the integral in Eq. (11) at \( t = T \) we see that

\[
C_r(t) < \varepsilon [1 - e^{-\alpha(t-T) \alpha(z-t_0)}] + \left[ C_r(t_0) + \int_{t_0}^{T} \beta(z)e^{\alpha(z-t_0)}dz \right]e^{-\alpha(t-t_0)}.
\]

Letting \( t \to \infty \) in this last formula yields

\[
C_r(\infty) < \varepsilon.
\]

But since \( \varepsilon \) may be any positive number, we must in fact have

\[
C_r(\infty) = 0.
\]

QED
DISCUSSION

It is true that $\beta(\infty) = 0$ is not a sufficient condition for the convergence of
\[
\int_{t_0}^{t} \beta(y) \, dy
\]
to a finite limit as $t \to \infty$. However, since $\beta(y)$ is non-negative, this integral will either converge to a finite limit, or else diverge properly to $+\infty$. The latter situation corresponds to the eventual introduction as time passes of an infinite mass of contaminant vapor into $R$. Eq. (13) should be interpreted as being a relation between finite quantities when the integral on the right converges, and as asserting that when the integral diverges properly to $+\infty$ so does $D_R(t)$.

The assumption that $\alpha$ is positive is essential in both the Lemma and Theorem. When $\alpha = 0$ Eq. (11) shows that
\[
C_R(t) = C_R(t_0) + \int_{t_0}^{t} \beta(z) \, dz,
\]
and so $C_R(t)$ need not vanish even when $\beta(z)$ is identically equal to zero, which is incompatible with the conclusion of the Lemma. Substituting this expression for $C_R(t)$ into Eq. (10) yields
\[
D_R(t) = C_R(t_0)(t-t_0) + \int_{t_0}^{t} dy \int_{t_0}^{y} \beta(z) \, dz,
\]
which shows that when $\alpha = 0$ $D_R(t)$ may diverge to $\infty$ as $t \to \infty$ even when $\beta(z)$ is identically equal to zero, which is incompatible with the conclusion of the Theorem as expressed by Eq. (13).

The assumption that $\alpha$ is constant is also essential to the validity of the Theorem. For suppose that $\beta(z)$ is identically equal to zero, that $C_R(t_0) > 0$, and that $\alpha(t)$ is piecewise constant in time. Specifically, take $\beta = 0$ and let
\[
\alpha(t) = \alpha_0 \quad \text{for } t_0 < t < t_1
\]
\[
\alpha(t) = \alpha_1 \neq \alpha_0 \quad \text{for } t_1 < t < \infty.
\]
Then Eqs. (11) and (14) and the Lemma can be used to show that

\[ D_R(t) = a_0^{-1} C_R(t_0) + (a_1^{-1} - a_0^{-1}) C_R(t_0) e^{-a_0(t_1-t_0)}, \]

which is incompatible with the conclusion of the Theorem as expressed in Eq. (13) except when \( a_1 = a_0 \).

The discussion in the preceding paragraph suggests the conjecture that in the general case represented by Eqs. (9) and (10) there will be an optimal ventilation policy \( \alpha(t) \) for each schedule \( \beta(t) \) of introduction of contaminant vapor into \( R \). Determining the optimal ventilation policy \( \alpha(t) \) subject to appropriate technological constraints on the feasible ventilation rate policy may involve an application of modern control theory, the calculus of variations, or other methods. If the contaminant vapor introduction rate schedule \( \beta(t) \) is not known exactly but must instead be estimated using slow and inaccurate instruments, we conjecture that there will still be an optimal ventilation policy, although its determination may be difficult. The further development of these ideas and conjectures is beyond the scope of this document.
PARTICULAR CASES

Suppose that:

1. There is no filtration, so \( E = 0 \). (Then to satisfy the conditions of the Theorem \( P_0(y) \) must be a positive constant.)

2. The initial vapor concentration \( C_0(t_0) = 0 \).

3. There are no internal contaminant vapor sources, so \( G_0(t) = 0 \).

4. The vapor concentration \( C_0(y) \) in the influx stream is the same as in the outside air.

This situation corresponds to Example 1 in the Introduction. By Eq. (15) the total vapor dosage inside the shelter will be

\[
D_R(\infty) = \int_{t_0}^{\infty} C_0(y) \ dy,
\]

which is the same as the total vapor dosage outside the shelter, as asserted in the Introduction.

This mathematical result does, however, neglect some potentially important considerations. For example, when the shelter volume \( V \) is large and the leakage flow is slow, the vapor concentration inside the shelter may be much lower than outside, although (since we know that the total vapor dosage will be the same inside as outside) the inside vapor concentration must persist for a correspondingly longer period of time. In reality, however, some contaminant vapor is adsorbed on surfaces within the shelter and the effect of this is relatively more important the larger the shelter (because it will have a larger adsorbing surface) and the lower the vapor concentration (because adsorption will cause a proportionally larger decrease in the vapor concentration levels). Also, since the human body does neutralize
and/or eliminate contaminants at some rate, sufficiently low vapor concentrations will not accumulate and produce intoxification. In addition, it is possible for the external vapor concentration to eventually fall below the internal vapor concentration. Should this occur, shelter occupants should either abandon it or open it up and air it out (an action that increases the ventilation rate and deliberately violates its assumed constancy).

Next suppose that

1. The initial vapor concentration $C_R(t_0) = 0$.

2. The influx vapor concentration $C_o(y) = 0$.

This corresponds to Example 2 in the Introduction. By Eq. (15) the total vapor dosage inside the shelter will be

$$D_R(\infty) = \int_{t_0}^{\infty} C_o(y) \, dy / [F_0 + F_A]$$

i.e., it is the ratio of the total mass of agent that eventually vaporizes divided by the shelter's volume ventilation rate, as asserted in the Introduction.

This mathematical result does, however, neglect some potentially important considerations. For example, if the outside vapor concentration is lower than that inside, then shelter personnel should abandon the shelter or air it out (which deliberately violates the assumed constancy of the ventilation rate). Although the mathematical result holds for any size shelter, larger shelters tend to have larger volume ventilation rates. However, they also tend to have more traffic entering and leaving them and so may experience more liquid or solid contamination. It is not clear which of these effects predominates. When the evaporation rate is sufficiently slow relative to the volume ventilation rate the vapor concentration level will be low and adsorption and biological resistance can become important factors.
CONCLUSIONS

We have demonstrated a useful and interesting general result in the theory of vapor contamination hazards to collective protection systems. The combination of the generality of the result and the simplicity of its proof may be new. Whether new or not, the general result and its simple proof deserve to be more widely known. The general result for a constant ventilation rate was illustrated by showing how Examples 1 and 2 are obtained as particular cases.

We have also shown that the general result need not hold when the ventilation rate fluctuates. Thus there presumably are optimal ventilation policies or schedules, although the further development of this suggestion is beyond the scope of this document.
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