# Decommissioning of Toxic Chemicals in Vehicle Interiors Using Hot Air

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Decontamination of Toxic Chemicals in Vehicle Interiors Using Hot Air

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Abstract

A computer model is presented which describes the desorption of liquid chemicals of intermediate volatility from vehicle interiors. The initial contamination level may be derived by measurement of the concentration of the desorbing chemical vapor as a function of time. The model has been applied to both alkyd and polyurethane painted vehicles and used to determine the residual contamination remaining in vehicles after decontamination with hot air.

Introduction

Chemical spills are not uncommon in modern society where large volumes of industrial chemicals are transported by rail or by road. Considerable effort is expended to clean up spills from accidents and to decontaminate transport vehicles, individuals and the surrounding terrain. We have previously
described studies detailing the removal of chemical contamination from vehicle exteriors by natural weathering with sun and wind \cite{1}. However it is unlikely that such processes would be effective in the enclosed interiors of vehicles into which contamination has been either spilled or transferred from contaminated people.

Personnel carrying out decontamination frequently must wear protective clothing and respirators or self contained breathing apparatus as protection against toxic vapors. This protective equipment imposes a severe physiological burden on workers due to heat stress and limits the effective operating time for an individual. The problem is exacerbated in warm climates where the time which can be spent in protective clothing while undertaking physical work is greatly reduced. Any process which helps in the removal and reduction of contamination will reduce the requirement for decontamination and also will reduce the time during which workers must wear protective clothing. Removal of contamination from vehicle interiors will reduce the hazard to emergency personnel. It is difficult to devise a treatment process for chemical neutralization that will destroy chemicals absorbed into organic materials. However, physical processes are well suited for the decontamination of vehicles and equipment that contain a wide variety of materials ranging from metals to glass and paints to polymers. The former may be highly resistant to chemical penetration while many of the latter are highly absorbent.

Recent emphasis in removing chemicals has been on physical processes that do not involve aggressive chemicals and are relatively benign to equipment. In particular, procedures involving steam and hot air have been identified \cite{2} as of potential utility. Higher temperatures will accelerate removal of contamination from surfaces by evaporation and from the bulk material through desorption. The only limitation is the thermal stability of the materials. Altmann \cite{3} has shown that the temperature of hot air should not exceed 150 °C if deterioration of thermoplastics is to be avoided. For example, decontamination processes for natural and butyl rubbers may be limited to 130–150 °C, the temperature above which their thermal stability is compromised.

The diffusion of a chemical from a surface has been demonstrated to reveal a number of interesting characteristics. The kinetics are not always strictly linear; indeed, the level of the chemical seems to play a role in defining its release at low levels and for particular simulant types. The release mechanism seems to have a dependency on the surface type from which the chemical is desorbing. These facts coupled with the experimental complexi-
ties associated with monitoring the release and subsequent diffusion of chemical vapor must be considered if a single model is to be developed to describe observations.

We have recently described such a model that describes the desorption of a liquid chemical from vehicle exteriors [1]. This model has enjoyed considerable success in its application to accounting for simulant levels observed as a function of time and released from a variety of surface types. In the present study we show that the model also can be used to describe the release of chemicals of intermediate volatility from vehicle interiors. As a consequence, the initial contamination level may be derived by measurement of the concentration of the desorbing chemical vapor as a function of time.

The model is of general application to both alkyd and polyurethane-coated vehicles. We have used it to determine the residual contamination of two chemical simulants, methyl salicylate (MS) and dimethyl methylphosphonate (DMMP), remaining in vehicle interiors after their decontamination with hot air. The efficacy of hot air as a practical process for removing chemical contamination is also demonstrated.

Modeling Studies

There are essentially two distinct approaches to the development of a model to describe the response of a system:

1. a mechanistic approach and
2. an empirical approach.

If the basic science underlying the system whose response is to be described is both well understood and not too complex, a mechanistic approach tends to be favored. It will yield a model with gross properties as reflected in the data and may admit the analysis of conjectures in regard to the system being studied.

On the other hand, complex systems for which accurate calculations may be performed may be best developed using an empirical approach. The distinction between the two approaches is that one is driven by an exploratory motivation (the mechanistic approach) and the other by a data fitting approach (the empirical approach). That is, one characterizes mechanisms, and the other characterizes data.

We have developed an empirical approach to the analysis of simulant desorption data because of the intrinsic complexity of chemical desorption pro-
cesses resulting from the wide variety of surfaces and materials present in vehicle interiors. While it is possible to develop a mechanistic model of the desorption of a simulant from a simple flat painted surface, such an approach is impractical for complex systems such as vehicles that include a wide variety of materials and surfaces.

Previous studies have shown that the evaporation of MS from alkyd painted plates followed first-order kinetics and that approximately 20% of the simulant is absorbed strongly by the surface. The absorbed simulant will desorb more slowly creating a prolonged vapor hazard. However, the evaporation of MS from polyurethane paint could not be described adequately by the first-order model; the data reflected predominantly a zero-order kinetic evaporative loss profile. While painted surfaces form a large part of the interiors of Army Landrovers, they are by no means the dominant surface. Large areas of vinyl and canvas also exist which will have different rates and possibly different mechanisms of simulant evaporation and desorption.

Our preliminary efforts to model mechanistically the desorption data [1] from vehicles were unsuccessful due to the complexity of the systems. However the empirical analysis approach proved to be most valuable. Although an empirical model must be based upon data, it will be, if it is to be successful, based upon both the gross features of the data and the micro features of the data. The gross features of the data are the qualitative features that we notice recurring as we glance through plots of replicated responses or glean from discussing the observations with experimenters. The micro features of data reflect variations from experiment to experiment and may encapsulate data aspects, which, if not absorbed into the model, may compromise the capacity of the model to describe the data’s gross features.

Gross features of the data include such traits as turning points (maxima and minima), asymptotes, flatness of peaks, behavior at short times, inflexions and linearizing transformations. Micro features of the data are largely evident through their interference with the consistency of the gross features and in areas in the data susceptible to system error.

Our investigation of desorption studies has revealed the following gross features:

1. an approximately exponential response phase followed by asymptotic leveling,
2. a consistent small deviation from a simple exponential response, and
3. a micro feature that implies that early observations may be susceptible to data collection error.
Assembling these into a simple empirical model has yielded the following function which we have found to be able to:

1. describe consistently the simulant desorption data, and
2. highlight experimental problems (e.g., contamination) which will thus draw attention to data sets that are not fully consistent with the model proposed.

\[
y = P_1(1 - e^{-P_2(t-P_4)P_3})
\]  

(1)

where \( y \) is the expected cumulative dosage. For this function we see that

- \( P_1 \) is the asymptotic level of desorption data,
- \( P_2 \) is an estimate of the desorption rate constant,
- \( P_3 \) is a measure of the degree of adherence to linear kinetics, and
- \( P_4 \) is an offset parameter which serves to accommodate uncertainties in the actual sample time particularly associated with early observations.

**Model Parameters**

If used systematically in a data fitting sense eq 1 has been found to yield constant and sensible estimates for its parameters. The model describes the desorption of moderate levels of contaminant which do not reach saturated vapor levels. It will not apply for very small or very large values of surface contamination. Furthermore, if we require, calculates and their errors can be accurately determined. In this section of the report we outline a standard approach to model fitting.

**The Asymptotic Value: \( P_1 \)**

A major aim of the investigation has been to estimate the model parameter \( P_1 \), which is experimentally related to the asymptotic value of the cumulative dosage of vapor released by the vehicle, and to calibrate \( P_1 \) as an indicator of initial exposure to simulant. The latter addresses the question of "given a profile of simulant desorption through time can we, by fitting eq 1 to this profile, infer the initial exposure of the surface from which the simulant desorbed". This issue was addressed in an earlier report [1]. Flattening of the response will be evident from the horizontal tendency of the data when plotted in either linear or semi-logarithmic mode. Indications of problems in this regard are evident from a final estimate of \( P_1 \) that is much larger than the
final datum value, an inaccurate estimate (error in excess of 20%) and slow convergence to the final fit.

The Time Offset: $P_4$

Although only a micro feature of the data, the capacity of $P_4$ to (a) improve the fit and (b) compromise the fitting procedure is quite dramatic. The time offset dominates the first unit (1 h or so) of eq 1, though if it is not carefully set or controlled it may drift to a value larger than the time point coinciding with the first observation and cause a numerical error.

The Desorption Rate Constant: $P_2$

For the moment, neglecting $P_4$ and setting $P_3$ equal to 1, we see that $P_2$ defines the rate of rise of eq 1.

\[
\text{Writing } y = \ln(1 - y/P_1) \quad (2)
\]

we find that

\[
y = -P_2 t + \log(1/P_1) \quad (3)
\]

Thus we see, using observations after three units or so, that initial estimates for $P_2$ can be obtained from the slope of the semi-logarithmic plot given by eqs 2 and 3. The rate of rise of eq 1 is defined by $P_2$. Its value seems ordinarily to adjust to around 0.1/h for MS and 0.2/h for DMMP. The most sensitive domain of $y$ to $P_2$ is from 1 h to 3-4 h. Whilst improved estimates of $P_2$ will be achieved using the inverse observation form of data weighting, this is not recommended as we are usually motivated primarily to explain the higher observations (i.e., asymptotic values) and secondarily to explain the overall response. In any case, there are rarely any problems with the estimation of $P_2$.

The Deviation from Linear Desorption: $P_3$

Our earlier investigations have shown that under certain conditions and at certain stages during the desorption process, the kinetics of desorption become nonlinear. The purpose of $P_3$ is to facilitate that trait in the model. Differentiating and rearranging eq 1, we find that

\[
y = -P_2 y [t' y^{-1} P_3 (1 - P_1/y)] \quad (4)
\]

where $t' = t - P_4$

which reduces to a first order linear differential equation if $P_3 = 1$. If $P_3$
encurses to a boundary then usually we find that contamination or some other problem exists in the data. Otherwise, based on response measurements in its dominant range (4–15h), $P_3$ is usually consistently and sensibly estimated.

Sensitivity Analysis

In our discussion above on the model parameters, we alluded to the “dominant ranges”. In particular we suggested that the most sensitive, or dominant ranges of the response function eq 1 to $P_2$ and $P_3$ were 1 h to 3–4 h and 4 h to 15 h, respectively. For any response function $y$ with parameter $\theta$,

$$\theta_i = \frac{\theta_i}{\theta_0} \quad y^* = \frac{y}{y_0}$$

$$\tilde{\theta}^* = (\theta_1^*, \theta_2^*, \ldots, \theta_n^*)$$

$$dy^* = \frac{\partial y^*}{\partial \theta_1^*} d\theta_1^* + \frac{\partial y^*}{\partial \theta_2^*} d\theta_2^* + \ldots + \frac{\partial y^*}{\partial \theta_n^*} d\theta_n^*$$

$$(5)$$

where

$$d\tilde{\theta}^* = (d\theta_1^*, d\theta_2^*, \ldots, d\theta_n^*)$$

and

$$\tilde{S} = \begin{pmatrix} \frac{\partial y^*}{\partial \theta_1^*}, & \frac{\partial y^*}{\partial \theta_2^*}, & \ldots, & \frac{\partial y^*}{\partial \theta_n^*} \end{pmatrix}$$

is the dynamic sensitivity of $y$ to $\tilde{\theta}$ which can be calculated by post-multiplying both sides of eq 5 by the identity matrix $I$ with dimension $n \times n$. Then we have

$$dy^* I = \tilde{S} d\tilde{\theta}^* I$$

$$dy^* = \tilde{S} d\tilde{\theta}^*$$

and post-multiplying by the inverse gives

$$\tilde{S} = dy^*(d\tilde{\theta}^*)^{-1}$$

where each element in $\tilde{S}$ is given by:

$$S_i = \frac{dy^*}{\partial \theta_i^*} = \frac{dy/dy_0}{d\theta_i/\theta_{i0}} = \frac{d \ln y^*}{d \ln \theta_i^*}$$
The dynamic sensitivity is of considerable importance for two reasons:
1. it helps to isolate parameters in \( y \) which may be difficult to estimate and
2. it helps to ensure that the distribution of observations with time is appropriate to allow accurate estimation of all the model's (response) parameters.

In Figure 1 we present a plot of the sensitivity \( S \) for each of the parameters in eq 1 and the following observations can be made:

1. The dominant range of \( P_4 \) is that associated with the earliest values of \( y \) (i.e., \( t \leq 1 \) h).
2. The dominant range of \( P_2 \) is from 1 h to 3–4 h.
3. The dominant range of \( P_3 \) is from 4 h to 15 h.
4. The dominant range of \( P_1 \) is for time values beyond 15 h.
5. The early time range is dominantly influenced by two parameters \( P_3 \) and \( P_4 \), however because \( P_3 \) also dominates a later response region its resolution in association with the observations there will permit the resolution of \( P_4 \) in the early response range.
6. Because of the unique time ranges in which each of the parameters has a major effect on the response, accepting (5), an adequate sampling strategy out to 48 h should characterize the response, and hence provide an adequate set of observations for the identification of each parameter. Our current sampling strategy includes observations at the following time points: 1(1)8, 10(2)24, 27(3)36, 40(4)48, where \( m(n)p \) means advancing from \( m \) h to \( p \) h in steps of \( n \) h.

Experimental

Desorption Chamber

The chamber in which the studies were carried out was constructed of stainless steel and was thermally insulated and temperature controlled. Total volume of the chamber was 93 m\(^3\). Mechanical circulation of the air inside the chamber ensured rapid mixing of desorbing vapor.

Our toxic chemical simulants, DMMP and MS, were chosen because of their intermediate volatilities. They are commonly used as simulants for other toxic industrial and military chemicals for this reason.

Analysis

The MS vapor concentrations were monitored by sampling into propylene glycol in sequential sampler bubblers. The sequential samplers each held 12 bubblers containing 5 mL propylene glycol as the absorbing medium and were programmed to sample the chamber over a 48-h time span. The bubbler contents were analyzed subsequently for MS by UV spectroscopy. Similarly, DMMP was sampled into diethyl phthalate in sequential sampler bubblers. Bubbler contents were analyzed for DMMP by gas chromatography using a flame photometric detector.

Vehicles

The vehicles chosen were Army Landrovers complete with canvas canopies. The vehicles were coated with two paint systems; in-service Matt Olive Drab Alkyd paint or Low Gloss Olive Drab Aliphatic Polyurethane paint (PUP) to GPC-P 154/3 [4]. The vehicle interiors essentially consisted of painted metal on the floors and dashboard, canvas in the canopy and vinyl seat covers.
For calibration purposes, known quantities of liquid simulant were applied as 5-μL droplets from a syringe to the various interior surfaces of the vehicle. For the hot air decontamination studies, liquid simulants were sprayed on to the interior surfaces in known quantities from a syringe.

The contaminated vehicle was driven into the sealed chamber which was temperature controlled at 25 ± 1 °C. Simulant desorbing inside the vehicle was monitored by collection for later analysis in four sets of sequential samplers arranged at head height in the driving and passenger positions. In the studies on decontamination with hot air, the contaminated vehicles were allowed to stand for 30 minutes to permit simulant to soak into materials and to mimic more closely a real situation. They were then decontaminated with hot air at 130 °C for either 30 or 60 minutes. Appropriate hot air at a flow rate of 50 L/min was supplied from a Karcher FB 60 E Hot Air Generator and blown into the rear compartment through two flexible ducts. The vehicles were placed in the chamber immediately once decontamination was complete. Analysis of all data about the desorption of simulants from inside the vehicles was carried out using CONSAM which is the interactive version of the SAAM modeling program and allows the user to develop mathematical models to fit experimental data [4].

Results and Discussion

Previous studies have shown that the evaporation of MS from alkyd painted surfaces follows first-order kinetics and that the evaporation of MS from polyurethane paint shows a zero-order kinetic loss profile. That simple first-order kinetics do not describe the evaporation of simulants from both alkyd and polyurethane vehicles is evident from considerations of the nature of change of the surface area of the simulant as it evaporates. It is likely that the nature of simulant kinetics will be initially zero order. Then, as the simulant evaporates to a stage where its surface area is reducing linearly, the kinetics will be first-order, and finally nonlinear. Other absorbent materials present inside vehicles, such as canvas and vinyl, may complicate the kinetics of simulant desorption. Chemical contamination can remain, held by capillary action in cracks and crevices even when the major part of the vehicle surface is contaminant-free. Regardless of the nature of the surface, outward diffusion of contamination vapor is accelerated by the increased temperatures resulting from decontamination.
There is no way of determining the various phases of desorption and it was more useful to explore an empirical rather than a mechanistic approach as the desorption profile may span several regions of applicability of a mechanism. Furthermore, we are more concerned with the accuracy of a prediction and the estimation of the residual contamination than with desorption mechanisms. We therefore attempted some empirical experimentation with the model developed for vehicle exteriors which was potentially flexible enough to absorb the key kinetic features alluded to above and to explain the data for both types of vehicles.

Modeling of Simulant Desorption from Vehicles Interiors

Evaporation of MS simulant from the painted external surfaces of the vehicles has been shown previously to be first-order for ALKYD vehicles and zero-order for PUP-painted vehicles. The interiors of both vehicles have considerable surface areas of canvas and vinyl which may desorb with first-order kinetics and tend to mask the behavior of the polyurethane paint. Furthermore, the constitution and gloss level of the painted surface has a consider-
able influence on the desorption and evaporation kinetics. However this may well be masked by the large proportion of other absorbent materials.

Simulant was applied to the vehicle interior surfaces as described in the Experimental section and the cumulative desorption of simulant into the vehicle was measured. Figures 2 and 3 summarize the fits of the above model to a series of studies relating to three levels of DMMP and MS simulant contamination density, respectively, for each of the two types of vehicles. Each plot is the mean of four replicates. The vehicles were not subject to decontamination in this series and vapor sampling started immediately after contamination.

The fitted plots were produced from the experimental data using CONSAM and the developed empirical model, eq 1. The data were used to define the model and to relate initial contamination levels to parameters derived from the model. The derived parameters and associated standard deviations are given in Table 1 for DMMP and in Table 2 for MS.

Of particular interest is the fact that $P_3 \approx 1$ for MS on both vehicles, implying that MS desorption is linear. In contrast, $P_3 \approx 0.5$ for DMMP, implying that desorption departs considerably from linearity.

With the initial conditions (initial simulant contamination level) known for each experiment, the estimated $P_1$ for studies in which neither $P_2$ nor
Table 1: Derived model parameters for DMMP desorption from vehicle interiors.

<table>
<thead>
<tr>
<th>Veh.</th>
<th>DM</th>
<th>$P_1$</th>
<th>$P_2$</th>
<th>$P_3$</th>
<th>$P_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pc</td>
<td>858</td>
<td>28.7 ± 4.0</td>
<td>0.179 ± 0.022</td>
<td>0.430 ± 0.026</td>
<td>0.894 ± 0.004</td>
</tr>
<tr>
<td>Pc</td>
<td>481</td>
<td>11.0 ± 0.3</td>
<td>0.220 ± 0.005</td>
<td>0.586 ± 0.018</td>
<td>0.844 ± 0.040</td>
</tr>
<tr>
<td>Pd</td>
<td>309</td>
<td>7.2 ± 0.6</td>
<td>0.296 ± 0.021</td>
<td>0.383 ± 0.022</td>
<td>0.932 ± 0.020</td>
</tr>
<tr>
<td>Ad</td>
<td>858</td>
<td>27.0 ± 4.1</td>
<td>0.118 ± 0.016</td>
<td>0.452 ± 0.018</td>
<td>0.895 ± 0.028</td>
</tr>
<tr>
<td>Ad</td>
<td>550</td>
<td>13.0 ± 0.6</td>
<td>0.235 ± 0.008</td>
<td>0.490 ± 0.018</td>
<td>0.954 ± 0.017</td>
</tr>
<tr>
<td>Ad</td>
<td>309</td>
<td>8.0 ± 0.6</td>
<td>0.154 ± 0.007</td>
<td>0.591 ± 0.037</td>
<td>0.795 ± 0.099</td>
</tr>
</tbody>
</table>

*aVehicle type.  bDimethyl methylphosphonate in milligrams.  cPUP.  dALKYD.

Table 2: Derived model parameters for MS desorption from vehicle interiors.

<table>
<thead>
<tr>
<th>Veh.</th>
<th>MS</th>
<th>$P_1$</th>
<th>$P_2$</th>
<th>$P_3$</th>
<th>$P_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pc</td>
<td>880</td>
<td>12.0 ± 0.1</td>
<td>0.106 ± 0.003</td>
<td>0.902 ± 0.015</td>
<td>0.558 ± 0.006</td>
</tr>
<tr>
<td>Pc</td>
<td>598</td>
<td>5.6 ± 0.04</td>
<td>0.114 ± 0.007</td>
<td>0.958 ± 0.003</td>
<td>0.851 ± 0.102</td>
</tr>
<tr>
<td>Pc</td>
<td>422</td>
<td>4.1 ± 0.02</td>
<td>0.106 ± 0.007</td>
<td>1.055 ± 0.028</td>
<td>0.591 ± 0.105</td>
</tr>
<tr>
<td>Ad</td>
<td>880</td>
<td>11.1 ± 0.11</td>
<td>0.137 ± 0.006</td>
<td>0.817 ± 0.022</td>
<td>0.633 ± 0.084</td>
</tr>
<tr>
<td>Ad</td>
<td>598</td>
<td>7.9 ± 0.03</td>
<td>0.113 ± 0.005</td>
<td>0.961 ± 0.017</td>
<td>0.692 ± 0.067</td>
</tr>
<tr>
<td>Ad</td>
<td>422</td>
<td>3.5 ± 0.01</td>
<td>0.084 ± 0.007</td>
<td>1.150 ± 0.030</td>
<td>0.410 ± 0.119</td>
</tr>
</tbody>
</table>

*aVehicle type.  bMethyl salicylate in milligrams.  cPUP.  dALKYD.

$P_3$ was constrained was regressed on simulant dosage, depicted in Figure 4. Within the region under study, $P_1$ is related to the initial contamination level as follows:

$$P_1 = 38.0(\text{IC}) - 5.0$$ for DMMP

and $$P_1 = 17.0(\text{IC}) - 3.0$$ for MS

where $\text{IC}$ is the initial contamination level in grams.

The desorption rate constant, $P_2$, has a value of around 0.1/h for MS and 0.2/h for DMMP. This constant may be influenced by several physical properties of the simulants. In general terms, surface tension will affect the spread-
Figure 4: Plot of $P_1$ vs initial contamination level of simulants [A] DMMP and [B] MS for ALKYD and PUP vehicles using unconstrained values of $P_1$.

Table 3: Values of parameter $P_2$ and physical properties of simulants.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>DMMP</th>
<th>MS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_2$/h</td>
<td>0.2</td>
<td>0.1</td>
</tr>
<tr>
<td>Surface tension (dyne/cm)</td>
<td>35.9</td>
<td>38.8</td>
</tr>
<tr>
<td>Vapor Pressure at 25 °C (torr)</td>
<td>0.613</td>
<td>0.165</td>
</tr>
<tr>
<td>Solubility parameter</td>
<td>10.6</td>
<td>10.6</td>
</tr>
</tbody>
</table>

ing of simulant over the surface and the penetration into cracks and crevices. Vapor pressure will affect the evaporation of the simulant from the surface. The solubility of the simulants in the various organic materials of the vehicles will affect their diffusion into and out of the bulk materials. Molecular size and specific interactions between simulant and materials will influence the rate of desorption from the surfaces.

We have detailed some relevant physical properties of the simulants in Table 3, above. The lower surface tension and higher vapor pressure of DMMP compared to MS result in increased spreading and evaporation rates and are reflected in the values of $P_2$. The solubility parameters for DMMP and MS are the same, implying that the simulants are equally absorbed by the organic
Figure 5: Desorption of MS from vehicle interiors [A] PUP, [B] ALKYD after hot air decontamination for 30 or 60 minutes - experimental data and CONSAM Fit for various levels of initial contamination. The unbroken line is the CONSAM fit.

materials in the vehicles. Dimethyl methylphosphonate is a smaller molecule than MS and will therefore diffuse out of absorbent materials more rapidly. Specific interaction between MS and polymeric materials, possibly due to hydrogen bonding, will also reduce the relative rate of desorption of MS. Such complexity governing the desorption of organic liquids from complex systems mitigates against the utility of a mechanistic approach to desorption and reinforces the benefits of the empirical data analysis approach.

Desorption of Simulants from Contaminated Vehicles after Decontamination with Hot Air

Total cumulative dosages of MS desorbing from PUP and ALKYD vehicle interiors after decontamination with hot air for 30 minutes are shown in Figure 5. Similarly dosages of DMMP desorbing from the vehicle interiors after decontamination are displayed in Figure 6. The fitted plots were produced from the developed empirical model using CONSAM. Levels of residual sim-
Figure 6: Desorption of DMMP from vehicle interiors [A] PUP, [B] ALKYD after hot air decontamination for 60 minutes - experimental data and CONSAM fit for various levels of initial contamination. The unbroken line is the CONSAM fit.

Table 4: Derived values of parameter $P_1$ and calculated values of residual MS simulant after hot air decontamination.

<table>
<thead>
<tr>
<th>Vehicle</th>
<th>Simulant Level (g)</th>
<th>Decontamin. Time (mins)</th>
<th>$P_1$</th>
<th>Residual MS (mg)</th>
<th>Decontamin. Effic. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PUP</td>
<td>1.14</td>
<td>60</td>
<td>ND</td>
<td>ND</td>
<td>100</td>
</tr>
<tr>
<td>ALKYD</td>
<td>1.09</td>
<td>60</td>
<td>ND</td>
<td>ND</td>
<td>100</td>
</tr>
<tr>
<td>PUP</td>
<td>2.38</td>
<td>60</td>
<td>0.95</td>
<td>250</td>
<td>90</td>
</tr>
<tr>
<td>ALKYD</td>
<td>2.24</td>
<td>60</td>
<td>5.8</td>
<td>540</td>
<td>77</td>
</tr>
<tr>
<td>PUP</td>
<td>1.10</td>
<td>30</td>
<td>3.7</td>
<td>410</td>
<td>63</td>
</tr>
<tr>
<td>ALKYD</td>
<td>1.10</td>
<td>30</td>
<td>3.9</td>
<td>430</td>
<td>60</td>
</tr>
<tr>
<td>PUP</td>
<td>2.20</td>
<td>30</td>
<td>6.8</td>
<td>600</td>
<td>73</td>
</tr>
<tr>
<td>ALKYD</td>
<td>2.24</td>
<td>30</td>
<td>9.0</td>
<td>730</td>
<td>67</td>
</tr>
</tbody>
</table>
Table 5: Derived values of parameter $P_1$ and calculated values of residual DMMP simulant after hot air decontamination.

<table>
<thead>
<tr>
<th>Vehicle</th>
<th>Simulant Level (g)</th>
<th>Decontamin. Time (mins)</th>
<th>$P_1$</th>
<th>Residual DMMP (mg)</th>
<th>Decontamin. Effic. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PUP</td>
<td>1.19</td>
<td>60</td>
<td>3.90</td>
<td>247</td>
<td>79</td>
</tr>
<tr>
<td>ALKYD</td>
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<td>4.93</td>
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<td>78</td>
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<tr>
<td>PUP</td>
<td>2.07</td>
<td>60</td>
<td>8.62</td>
<td>372</td>
<td>82</td>
</tr>
<tr>
<td>ALKYD</td>
<td>2.39</td>
<td>60</td>
<td>6.52</td>
<td>316</td>
<td>87</td>
</tr>
<tr>
<td>PUP</td>
<td>4.63</td>
<td>60</td>
<td>14.4</td>
<td>526</td>
<td>89</td>
</tr>
</tbody>
</table>

In these tables we also present the efficiency of hot air decontamination. It is evident that treatment with hot air at 130 °C for periods around 60 minutes is an effective way to reduce contamination. There is little evidence of any difference in performance between the polyurethane and alkyd painted vehicles. This is due to the large area of canvas and vinyl which are common to the test vehicles and which mask differences between the two coatings. Vehicles in which the interiors are mainly painted metal may decontaminate at different rates dependant on the paint properties. Methyl salicylate is more readily decontaminated than DMMP even though the volatility of the latter is higher. This may be attributable to the greater interaction and solubility of DMMP in the paints, canvas and vinyl seat material.

Commercial transport vehicles are coated with a variety of paint types and have a range of interiors fittings and materials. These interiors are likely to be chemical absorptive and similar to the alkyd coated vehicle in our study. As a consequence, hot air decontamination may be considered effective for a wide range of commercial vehicles. Decontamination efficiency will depend on the interaction of contamination with the materials as well as the volatility of the chemical involved. For chemicals with a volatility less than or equal to that of MS, decontamination with hot air at 130 °C for 60 minutes is an effective process. The model we have described is flexible enough to include such variations.
Notation

DMMP  dimethyl methylphosphonate
MS  methyl salicylate
$P_1$  the asymptotic level of desorption data
$P_2$  an estimate of the desorption rate constant
$P_3$  a measure of the degree of adherence to linear kinetics
$P_4$  an offset parameter which serves to accommodate uncertainties in the
actual sample time particularly associated with early observations
$S$  dynamic sensitivity of $y$ to a given parameter
$t$  time from start
$\theta$  a generic parameter
$y$  cumulative dose of toxic chemical

References

contamination from vehicles by exposure to sun and wind. *J. Hazardous

national Symp. Protection Against Chemical Warfare Agents*. The Swedish

vate Communication.

drab, lustreless, two pack. GPC-P-154/3.