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U.S. ARMY CHEMICAL AND BIOLOGICAL DEFENSE COMMAND

ERDEC-TR-108

**SIMULANT SELECTION AND ENVIRONMENTAL ASSESSMENT
FOR OPEN-AIR TESTING**

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RESEARCH AND TECHNOLOGY DIRECTORATE

March 1994

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Aberdeen Proving Ground, MD 21010-5423

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE 1994 March	3. REPORT TYPE AND DATES COVERED Final, 92 Jun - 92 Jun	
4. TITLE AND SUBTITLE Simulant Selection and Environmental Assessment for Open-Air Testing			5. FUNDING NUMBERS PR-10162622A553	
6. AUTHOR(S) Duncan, Donald P., LTC, OD; Famini, George R.; Wentsel, Randall S.; and Mann, Teresa M.				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) DIR, ERDEC,* ATTN: SCBRD-RTC, APG, MD 21010-5423			8. PERFORMING ORGANIZATION REPORT NUMBER ERDEC-TR-108	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)			10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES *When this study was conducted, ERDEC was known as the U.S. Army Chemical Research, Development and Engineering Center (CRDEC), and the authors were assigned to the Research Directorate.				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) Scientists and engineers involved in chemical defense assessment in material design often need to perform open-air testing with chemical agent simulants. Before using any simulant in outdoor tests, it is necessary to compile relevant data on the likely environmental consequence of using the chosen simulant in a particular configuration and identify that no expendable environmental impact is likely to occur. Simulant selection and environmental impact assessment are highly specialized areas for which knowledge of past activities and current data are particularly necessary. Accordingly, CRDEC has invested considerable effort to develop basic research data pertinent to simulant selection and environmental assessment and catalog it in easily accessible data bases (CRDEC Chemical Agent Simulant Data Center; Environmental Fate & Effects). The purpose of this report is to help ensure that all who need to have simulants for open-air testing, and prepare the accompanying environmental assessment documentation, know about the CRDEC simulant data support facilities and understand how they can be used. The report is designed to be read in conjunction with Army Environmental Compliance Regulations (e.g., CRDEC-SP-039).				
14. SUBJECT TERMS Chemical agent simulants Open-air testing Environmental			15. NUMBER OF PAGES 55	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT UL	

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PREFACE

The work described in this report was authorized under Project No. 10162622A553, CB Defense/General Investigation. This work was started and completed in June 1992.

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SIMULANT SELECTION AND ENVIRONMENTAL ASSESSMENT FOR OPEN-AIR TESTING

1. INTRODUCTION

Scientists and engineers involved in applied research or development programs related to chemical defense assessment or materiel design often need to perform open-air testing with chemical agent simulants. Before conducting open-air testing activities with simulants, a systematic examination of possible and probable environmental consequences was prepared, and the results documented according to applicable federal, state, and local regulations.^{1,2}

In fulfilling the above mentioned responsibilities, these mission-oriented scientists and engineers select the most appropriate simulant for the particular application at hand. They also compile relevant quantitative data on the likely environmental consequences of using the chosen simulant in a particular application scenario and certify (through the Environmental Assessment (EA) documentation process) that no unfavorable environmental impact is likely to occur.

Simulant selection and environmental impact assessment are highly specialized areas for which knowledge of past activities and current data is particularly necessary. Accordingly, the Research Directorate at the U.S. Army Chemical Research, Development and Engineering Center (CRDEC)* has invested considerable effort over the past 8 to 10 years in developing basic research data pertinent to simulant selection and environmental assessment. In addition, this data has been catalogued in easily accessible databases to make the basic research knowledge as available as possible to support specific developmental activities.

In particular, the Chemical Agent Simulant Data Center (CASDC)^{3,4,5} contains extensive data on the physical and chemical properties of chemical agent simulants. A short summary of the CASDC database is given in Appendix A. This database currently contains information on 694 simulant compounds. The Chemometric and Biometric Modeling Branch,** Physics Division, periodically updates the scientific data in CASDC. The database can be accessed*** via the initial menu (Option 2) in the CRDEC Database Management System (Appendix B).

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An extensive database covering the environmental fate and hazards associated with chemical agent simulants is also available. This database is known as the Chemical Fate and Effects (CF&E) database⁶⁻¹⁴ when it is referred to as a component of the Simulant Program and otherwise as the Environmental Fate and Effects (EF&E) database. A short history* of the CF&E database for chemical agent simulants is given in Appendix C. Currently, information exists for 68 chemicals. The scientific data is continuously updated by the Environmental Toxicology Branch,* Toxicology Division. This database can also be accessed via the initial menu (Option 1) in the CRDEC Database Management System.**

The extensive database support facilities described above are of maximum value to overall Army development efforts only when routinely and systematically used by applied researchers and development project managers, who expect to become involved in open-air testing with chemical agent simulants. The purpose of this paper is to help ensure that the existence of such support facilities is widely understood by those who have to choose simulants for open-air testing and who must prepare the required environmental assessment documentation. To this end, the paper "walks through" how the databases can be used to help select a proper simulant and then illustrates via example the nature of the judgement calls that are made in analyzing environmental impact. As such, the paper is intended to be read in conjunction with the overview of Army environmental compliance regulations described in an earlier publication.¹

The following section contains the illustrative material showing how the two databases can be used for complimentary analysis. The last section contains conclusions and recommendations for further work.

2. SIMULANT SELECTION AND ENVIRONMENTAL ASSESSMENT

This section discusses the way in which the CASDC and the CF&E database can be used together to help choose an appropriate simulant for a particular application and subsequently screen it for potential environmental impact. The examples follow the methodology used in a document entitled "Significance of Expected Environmental Protection Trends for Continued Use of GB, GD, and VX Simulants" (unpublished data, March 1994).

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For the purposes of this report, we will assume that the chemical agent to be simulated is GB. Using CASDC, it is possible to produce a list of compounds that have been used to simulate GB. Such a list is shown in Table 1.

Table 1. GB Simulants

Name	CRDEC No.	CAS Registry No.
Diethyl Ethylphosphonate	002	78-38-6
1-Bromobutane	007	109-65-9
Diisopropylmethyl-phosphonate	108	1445-75-6
Dimethylmethylphosphonate	116	756-79-6
Dimethylpposphonate	119	868-85-9
Methylacetoacetate	180	105-45-3
1,2,3-Trichloropropane	221	96-18-4
Diethyl Methylphosphonate	251	683-08-9
Ethyl-2-Hydroxypropionate	252	97-64-3
2,4-Hexadienyl Acetate	264	-----
Chlorobenzene	608	108-90-7

Deciding which simulant is a "best match" to the actual agent can be determined using the "ratio distance" method described by R. Crosier.¹⁵ Using this method, the various properties associated with the simulant (denoted S_i) are combined with the corresponding properties of the actual agent (denoted A_i) according to the following formula.

$$\text{antilog} \sum_{i=1}^N \left[\log \left(\frac{S_i}{A_i} \right) \right]^2$$

Different kinds of experiments, however, may require a tighter match to certain properties than others. For example, experiments emphasizing droplet evaporation and vapor dissemination might require close matches on volatility and density, whereas experiments dealing with decontamination and contact issues might put a premium on surface tension and

density.^{5,15,17} Such sensitivity studies and hierarchial clustering techniques have been reported in a previously published report.¹⁶

To illustrate the kind of sensitivity studies that may be required, we assume that the key properties needed for matching simulant to agent are as follows:

- surface tension, normal boiling point, vapor pressure, density, volatility, and molecular weight
- volatility and density only
- surface tension and density only

Knowing the specific values versus the actual agent values for the above combination of properties is necessary to apply the ratio distance formula. These values, which can be extracted from the CASDC database, are listed in Table 2.

The results of applying the ratio distance metric to the values shown in Table 2 are displayed in Table 3. As can be seen from Table 3, the simulants that "best match" the actual agent vary depending upon which sets of properties are deemed most important to match. For example, the top three matches considering surface tension and density only (decontamination or contact studies) are the compounds CRDEC No. 002, 251, and 108. For experiments in which volatility and density are relatively more important, (droplet evaporation and vapor dissemination studies) the top three matches are CRDEC No. 119, 221, and 252. These results graphically illustrate the importance of thoroughly understanding the properties that are most important to simulate in a particular experimental configuration. Once this is done, the data in the CASDC database, together with the ratio distance calculation, can be used to determine a "rank ordered" list of simulants to be considered for use.

We turn now to the use of the CF&E database to associate environmental impact data with the simulants that appear on the rank ordered list from the above mentioned steps.

For example, suppose we were interested in simulants for the surface tension and density properties (decontamination and contact studies). Of the simulants displayed in Table 2, only the following three are currently in the CF&E database:

- CRDEC No. 108, CAS #1445-75-6, Diisopropylmethylphosphonate (DIMP)
- CRDEC No. 116, CAS #756-79-6, Dimethylmethylphosphonate (DMMP)
- CRDEC No. 119, 868-85-9, Dimethylphosphonate (DMHP)

Table 2. GB Simulant Properties

CRDEC No.	Surface Tension	Normal Boiling Point	Vapor Pressure	Density	Volatility	Molecular Weight
002	28.68 @ 20 °C	198 @ 760 mm Hg	0.3814 @ 25 °C	1.03 @ 20 °C	3407 @ 25 °C	166.158
007	25.46 @ 20 °C	19 @ 760 mm Hg	40 @ 25 °C	1.27 @ 25 °C	295000 @ 25 °C	137.02
108	28.78 @ 20 °C	190 @ 760 mm Hg	0.274 @ 25 °C	0.976 @ 25 °C	2654 @ 25 °C	180.186
116	36.8 @ 20 °C	173 @ 760 mm Hg	0.613 @ 25 °C	1.16 @ 25 °C	4900 @ 20 °C	124.077
119	37.6 @ 20 °C	171 @ 760 mm Hg	4.52 @ 25 °C	1.2 @ 25 °C	26500 @ 20 °C	110.05
180	36.1 @ 20 °C	172 @ 760 mm Hg	1.58 @ 25 °C	1.07 @ 25 °C	9900 @ 20 °C	116.118
221	37.8 @ 20 °C	158 @ 760 mm Hg	3.53 @ 25 °C	1.39 @ 20 °C	28000 @ 20 °C	147.432
251	30.24 @ 20 °C	194 @ 760 mm Hg	0.159 @ 20 °C	1.04 @ 30 °C	1323 @ 20 °C	152.131
252	29.9 @ 25 °C	154 @ 760 mm Hg	1.9 @ 20 °C	1.03 @ 25 °C	123000 @ 20 °C	118.134
264	--	--	--	--	--	140.184
608	33.56 @ 20 °C	132 @ 760 mm Hg	10.0 @ 22.2 °C	1.11 @ 20 °C	61084 @ 22.2 °C	112.56
GB	26.5 @ 20 °C	157.7 @ 760 mm Hg	2.1 @ 20 °C	1.095 @ 20 °C	16199.4 @ 20 °C	140.1
	25.9 @ 25 °C		2.9 @ 25 °C	1.089 @ 25 °C	22063.1 @ 25 °C	

Table 3. Sensitivity Analysis on Ratio Distances for GB Simulants

All Six Properties		Volatility and Density Only		Surface Tension and Density Only	
CRDEC No.	Distance	CRDEC No.	Distance	CRDEC No.	Distance
119	1.92	119	1.23	002	1.10
221	2.06	221	1.82	251	1.15
180	2.92	252	1.90	108	1.16
608	6.50	180	2.23	007	1.17
252	7.71	608	3.25	252	1.17
116	8.97	116	4.51	608	1.27
002	16.03	002	6.48	180	1.36
108	24.27	608	8.34	116	1.40
251	36.83	251	12.25	119	1.44
007	70.54	007	13.43	221	1.53

The information contained in the CF&E database on each of these compounds is shown in Appendix D.

In judging the acceptability of using the above simulants for open-air testing, same assumptions have to be made. We assume in this paper that documented evidence of mutagenicity, reproductive effects, tumorigenicity, human exposure criteria, and ecotoxicity would signal a potential user that difficulties in securing the appropriate EA approval lie ahead.

For example, consider the first compound listed above - DIMP. As can be seen from examining the information in Appendix D, DIMP is not listed in the Toxic Substance Conservation Act (TSCA) inventory, as a hazardous waste under Resource Conservation Recovery Act (RCRA), or as a hazardous substance under Comprehensive Environmental Response, Compensation, and Liabilities Act (CERCLA) or Federal Water Pollution Control Act (FWPCA). Diisopropylmethylphosphonate has been found to be nonmutagenic when administered to mice, rats, and dogs. In experiments with rats, no teratogenic effects or dose-related reproduction responses occurred. No information about tumorigenicity exists in the database. No threshold limit values for human exposure criteria have been found. From the above data, any opponent to a publicly advertised EA notice clearly would have considerable difficulty in blocking proposed open-air testing based on documented evidence of mammalian toxicity.

From the standpoint of ecotoxicity, there is evidence that DIMP can cause gross (transient) phytotoxicity response to tall fescue and short-needle pine. Diisopropylmethylphosphonate also can burn the leaf tips of Black Valentine beans and Whitchita Wheat at aqueous concentration of 10-40 ppm. In addition, LD50 values of 1500 $\mu\text{g/g}$ have been established for the soil/earthworm assay. Thus, depending on the "scale" of the experiment that a researcher/developer might be planning and the relative "sensitivity" of the local community, there exists some grounds for anticipating a possible delay in obtaining EA approval. Examination of the environmental fate data also contributes to this concern, because DIMP biodegradation in soil and water is quite slow and bioconcentration in some plants has been demonstrated.

We next consider DMMP. Dimethylmethylphosphonate is listed in the TSCA inventory but is not listed as a hazardous waste under RCRA or as a hazardous substance under CERCLA or FWPCA. In the absence of metabolic activation, DMMP produced no mutagenic effects to bacteria (*salmonella*) in Ames tests but was mutagenic to mouse lymphoma cells. There is also evidence that DMMP reduces sperm counts, sperm mobility, and fertility for male rats. The National Toxicology Program (NTP) is currently testing DMMP for carcinogenic activity. Dimethylmethylphosphonate is not listed in NTP's latest Annual Report on carcinogens; however,

data will probably support an NTP classification of "reasonably anticipated to be a carcinogen" - sufficient evidence in animals and inadequate data in humans. No threshold limit values have been established for DMMP, although, DMMP is known to cause irritation to the eyes, skin, and respiratory tract. Also, the Surgeon General has approved the use of thickened DMMP for use in field decontamination vulnerability tests. From the above, it is clear that enough data on unfavorable effects for non-humans exists to sustain concerns that might be raised by an EA opponent. Some evidence also exists for ecotoxicity-bluegills and fathead minnows. At the least, a potential, researcher/developer should anticipate delays in obtaining EA approval for open-air testing with DMMP although "scope and scale" would also figure significantly into the analysis.

The last compound we consider is DMHP. The TSCA inventory lists DMHP, but it is neither listed as a hazardous material by DOT, nor as a hazardous waste under RCRA, or as a hazardous substance under CERCLA or FWPCA. No information about mutagenicity or reproductive effects is available in the CF&E database. The NTP is testing DMHP for carcinogenicity. No threshold limit values for human exposure to DMHP have been established. Other than the fact that phosphonates will undergo photolytic reactions with sunlight to produce orthophosphonates, which in turn can serve as a sole phosphorous source to aquatic plants, no issues exist with regard to ecotoxicity. Based on the above, obtaining EA approval to conduct open-air testing with DMHP should be relatively straightforward.

The above discussions illustrate that unlike the "algorithmic nature" of trying to match properties of an agent to a simulant, deciding whether a particular simulant will easily pass through the EA process is highly judgmental. The information contained in the CF&E database is essential for producing evidence of potential mammalian or ecotoxicity and for demonstrating that the researcher/developer proposing an open-air test with simulants has followed the "prudent man" rule by consulting available data sources, which can be presumed to be current and scientifically accurate. However, judgments and interpretations that may be site specific, as well as dependent upon proposed scope and scale of the experiment, still have to be rendered. In cases where the researcher/developer is uncertain about the nature of the decision that can be supported by the available data, consultation with the Environmental Quality Office is essential. It may also be advisable to ask for "expert judgment" after a thorough and systematic preliminary analysis using the CASDC and the CF&E databases, as well as the EQO file of previous EAs, has been performed.

3. CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER WORK

In this paper, the two key U.S. Army Chemical Research, Development and Engineering Center (CRDEC) databases that have been examined are Chemical Agent Simulant Data Center (CASDC) and the Chemical Fate and Effects (CF&E). These databases have been developed over the last 8 to 10 years that made possible the systematic use of basic research data to select appropriate simulants and screen them for environmental impact. Our focus has been on illustrating how these two databases, which are accessible via the CRDEC Database Management System, can be used by an applied research/development project manager who must choose an appropriate simulant for open-air testing and in conjunction with the Environmental Quality Office (EQO) gain timely approval for use of the simulant by following the Environmental Assessment documentation process.

To illustrate the problem of simulant choice, we chose a particular agent (GB), accessed via CASDC the set of all compounds that had been used to simulate GB, and then produced a set of "rank ordered" lists by applying R. Crosier's "ratio distance" metric (unpublished data, March 1994). We then accessed the CF&E database to discover what kinds of information are available to support "findings of no significant impact statements" or "otherwise" in the required Environmental Assessment (EA) documentation for open-air testing with the various simulants. Of the eleven simulant compounds in the CASDC, only three were also cross-referenced in the CF&E database. Examination of the data for these three simulants revealed that two simulants would be questionable (one highly so) for use in open-air testing; whereas, one simulant would probably be appropriate under most experimental situations. Relatively more than was the case with simulant selection (via the ratio distance metric), substantial context-dependent judgment is required to interpret the implications of the data that is available for the potential environmental impact of open-air testing with simulants. Recourse to "expert judgment" may often be advisable after preliminary analysis, using the above databases and the EQO's file of previous EA documents, has been completed. To assist in this access to "experts", CRDEC has recently formed a Simulant Use Committee (Appendix E). This committee should provide the beginnings of what may become a much more automated set of "expert system" capabilities build around the CASDC and CF&E databases.

With this long-term (and difficult) goal in mind, there are several areas where additional research work appears to be warranted.

The first deals with the addition of a "ratio distance" calculational element to the CASDC. Currently, it is possible to use the database screening features in CASDC to list various

subsets of the 694 compounds in the database and their associated properties. It would be convenient to be able to then apply a "ratio distance" calculation to the chosen list of simulants for a particular agent and a particular set of properties that are thought to be most appropriate to the experiment being considered. Such a capability would provide a useful "first pass" at a "rank-ordered" list and make any subsequent interactions with the Simulant User Committee more productive. Refinements on this idea could in time lean to an "expert system" program that would combine data in CASDC together with a knowledge base of rules provided by simulant experts and provide an on-line "simulant choice service" to applied researchers or development project managers. Such a capability would be even more helpful if it could also access the data in CF&E together with a knowledge base of rules about potential environmental impact. This latter capability is likely to be extremely difficult (if at all possible) as considerable variability in applications and the context-dependent nature of judgements that have to be made in the environmental acceptability area.

A second area for further work deals with the incorporation of the EQO's past files of EA documents into CASDC. These EA documents offer "precedent" information that can be helpful to a developer contemplating using certain simulants for open-air testing. These documents currently exist in "hard copy" form in the EQO. It would be of considerable value if the key precedent data in each could be extracted and added to the simulant records in CASDC. In this way, a developer could identify at the time of simulant analysis whether an EA had been filed before, and if so, who the appropriate point of contact for further information might be.

The last area deals with closing data gaps between compounds in CASDC and those in CF&E. There are about ten times as many compounds in CASDC as in CF&E. Given the expense required to conduct extensive experiments or environmental fate and effects for simulants, it is unlikely that this gap will be closed in the near future. Current efforts with finite resources will continue to follow prioritization schemes such as those described in⁸ as well as respond to requirements from multiple Government customers. Conceivably, software packages are now becoming available to estimate toxicity values when certain chemical properties of the simulant are known and could be of considerable help in closing the data gap between CASDC and CF&E, as well as responding to "new threats". The TOPKAT system (conversation with H. Salem, R. Wentzel, and N. Chester, CRDEC, June 1992) under development by the Toxicology Division is an example of this emerging set of capabilities as is the software produced by COMPUDRUG.¹⁸ These new capabilities should be given added emphasis in future work activities supporting the Simulant Program.

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APPENDIX A

CRDEC'S SIMULANT PROGRAM



**CHEMICAL
RESEARCH,
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ENGINEERING
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CRDEC'S SIMULANT PROGRAM

March 1992

The cost and risk associated with the extensive use of chemical or biological warfare agents for developing and testing military equipment has led to an aggressive application of simulants. Simulants are chemicals or chemical substances that mimic one or more properties of chemical or biological agents. Different simulants are often used, depending on the application, because it is not possible to select a compound as a simulant where all properties are exactly the same as the agent.

The Simulant Program was created to consolidate simulant information and data, develop a systematic approach to selecting simulants, and to establish CRDEC as a focal point for simulant technology. A major goal of the program was to collect and collate data in a systematic and retrievable form so that subsequent workers can benefit from previous research. By including the rationale for simulant selection, subsequent users should be able to continue the line of reasoning or change for their specific application. The availability of this information should minimize the perfunctory adoption of a simulant for the wrong purpose. For documentation on CRDEC's simulant program, refer to CRDEC-SP-88012, *Simulant Program*, February 1988.

As a way of identifying simulant needs and assisting engineers and scientists to identify those needs, the simulant program sponsors an annual workshop dealing solely with simulant-related issues. Having just completed its sixth year, the International Simulant Workshop is held the first week of March; the seventh workshop will be held 2-4 March 1993. The proceedings from previous years are documented in CRDEC-SP-002, *Proceedings of the Second International Simulant Workshop*, December 1988, CRDEC-SP-011, *Proceedings of the Third*

International Simulant Workshop, November 1989, and CRDEC-SP-025, *Proceedings of the Fourth International Simulant Workshop*, July 1990. The proceedings of the Fifth and Sixth International Workshop are currently in publication. If you desire additional information on our simulants program or the workshop, please contact George R. Famini at (410) 671-2670 or DSN 584-2670.

CRDEC's Simulant Data Center serves as a repository for simulant information that can be easily retrieved through computer searches. Because it is part of the Data Management Office system, the data base is accessible, via CRDEC's *Workplace Automation System*, to those with authorized userid and password. The data base contains numerical data on chemical and physical properties and textual information on the use and application of simulants. All of the compounds frequently used as simulants are included as well as others that were previously considered. Today there are 750 compounds in the data base, and we expect this number to continue to increase as new information becomes available.

Detailed information on the Simulant Data Center is available in the *Data Base Users' Guide for the Chemical Agent Simulant Data Center (Second Edition)*, CRDEC-SP-037. This guide contains discussions of all the data items, procedures for conducting searches, and qualifying information. Further information can be obtained from the Simulant Data Center Manager, Phillip A. Coon, (410) 671-3248 or DSN 584-3248.



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THE CRDEC SIMULANT PROGRAM

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INTRODUCTION

Because of the emphasis on environmental, security and health issues, chemical and biological agent simulants have become very widely used in the development and testing of chemical defense equipment and procedures. In fact, in many cases, only testing involving simulants can be done. This includes outdoor testing, testing at a non-surety laboratory (such as a university) are two examples. Although the use of simulants date back some thirty years, much of the results, selection criteria, etc. remains fragmented and unknown to most DoD simulant users.

In an effort to rectify this problem, the U.S. Army Chemical Research, Development and Engineering Center developed a simulant program, responsible for the accumulation and dissemination of simulant related information. Now in it's eighth year, the program provides physical and chemical property data on prospective simulants, as well as recommendations on which simulants might be appropriate for a given experiment.

The Simulant Program was begun in an effort to address four aspects of testing and experimentation with simulants: a) acting as a central repository for simulant related information, b) measurement of important physical and chemical properties, c) development of physical and chemical property estimation routines, and d) assist the end item developer in the selecting the appropriate simulant for his/her application.

The Simulant Program is divided into three general areas of concentration; databasing and modeling, environmental and toxicological properties, and physical and chemical properties. Each of these areas focuses on a specific area where deficiencies have been identified regarding information on simulants.

DATABASING

In order for the Simulant Program to be effective in disseminating information in a timely and efficient manner, it was necessary to compile as much data pertinent to the use of chemical simulants and preserve it in a computerized database. In this way, information regarding simulants can be readily retrieved. To date, the Simulant Program manages two databases, the Chemical Agent Simulant Data Center (CASDC) and the Chemical Fate and Effects Database (CFED).

The CASDC project was begun when it was realized that, although there was a lot of physical, chemical, toxicological, and application data on chemical agent simulants, the data was located in many different places. As such, selecting the most appropriate was often "hit or

miss", depending on the particular source a scientist happened to find. With the greater constraints on agent testing, and the complete moratorium on outdoor testing of agents, it was vital that as much information regarding simulants was available to as many people as possible.

The CASDC resides on a DEC Vax 11/785 running the VMS operating system. The MACCX-II software for Molecular Design, LTD is used to manage the database. MACCS-II is specifically designed for chemical databases and provides a graphical interface, structure visualization, and a "point and click" menu system. MACCS-II permits, not recall of all stored information on a particular data record, but also complex searching involving any of the data fields. Specific numbers can be searched for (for example a compound that boiled at exactly 200C), or ranges can be searched (all compounds can be identified if they boil between 190-210 C). In addition, sequential searching is also possible, where the "hit list" from one search is the input list for the next search. This allows for searching on multiple properties.

The CASDC is principally used to store and search for physical and chemical property data on chemical simulants. In addition, some information on each simulant has been included on the particular application, toxicity, and whether it was actually used or just recommended or screened for simulant use. The CASDC currently contains property data on over 700 compounds that have been used, or considered for use as simulants. Table 1 lists the specific properties that is available in the CASDC.

The CASDC is commonly used in one of two manners. A user who knows which simulant he/she wishes to utilize in a given experiment may search for the specific compound, and extract the physical and chemical properties on that compound. Alternately, a user may come to the CASDC without any idea of what simulant to use. In this case, the most important physical or chemical properties will be identified (usually with help from Simulant Program scientists).

A second database maintained by the Simulant Program is the Chemical Fate and Effects Database (CFED). The CFED contains fate and effects information and related properties on (currently) 68 chemical species, including the most commonly used outdoor simulants. The CFED also resides on the same VAX as the CASDC, but because the need for chemical structure and graphics was less compared to the textual requirements, is programmed under RBase.

The CFED

MODELING

Modeling has become an important aspect of the simulants program in two basic areas: 1) development of prediction or estimation models for a variety of physical, chemical, biological and thermodynamic properties, and 2) use of molecular modeling and computational chemistry in simulation and simulant selection. Both areas have had a significant and direct impact on the Simulant Program, and both continue to play important roles in the selection of simulants.

The estimation and prediction of properties has provided valuable information when

screening potential new simulants. While it is impossible to measure appropriate properties for large numbers of chemical compounds, it usually only takes a few minutes to use many of the estimation methods currently available. Although there are a great deal of routines available in the literature, because of the unique nature of the compounds of interest to CRDEC, most of the estimation methods had to be reparameterized or completely redone.

The growth of molecular modeling and computational chemistry has surfaced as an important aspect of the Simulant Program. Computational chemistry programs are capable of computing or estimating a variety of physical and chemical properties (described more in depth in a subsequent paragraph). Molecular modeling capabilities at CRDEC allow one to compute a number of properties, and permit direct comparisons between the computed properties of the simulant and the computed properties of the agent.

ENVIRONMENTAL

With increasingly more stringent requirements being placed on the use of chemical agent simulants, awareness as to identifying "environmentally safe" simulants has dramatically increased over the past several years. Because outdoor testing is necessary, and in many cases cannot be adequately modeled by chamber or laboratory test, making sure there is an adequate list of approvable outdoor simulants is a major thrust within the Simulant Program.

The environmental area has been actively involved in using existing state-of-the-art techniques for measuring the toxicity and environmental damage of simulants. In addition, research is underway to develop new methodologies that are faster and cheaper than existing tests, but still provide sufficient information for detailed analysis and determination of the environmental hazard.

Because of the changing requirements, many simulants in use outdoors today may be banned from use in the very near future (1-3 years). It is, therefore, paramount that those suspect simulants be identified, and that research is begun to find adequate replacements for those simulants.

PHYSICAL AND CHEMICAL PROPERTIES

The proper selection of a chemical (and a biological) agent simulant is an adequate match of appropriate physical and chemical properties. Without this proper match, an entire experiment or test could be invalidated and the results meaningless. Knowing the physical and chemical properties of the agents and the simulants, then, is a vital aspect of the simulant selection procedure, and provides the foundation for the CASDC, good simulant selection criteria and methods, etc.

For this reason, the Simulant Program has an active program to measure a variety of physical and chemical properties of chemical agent simulants. Although, in principle, the

physical properties group could be asked to measure any property of a simulant, the most commonly asked for properties are vapor pressure and liquid density. - 1/5 COS-7. T_e Lex

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APPENDIX B
CRDEC DATABASE MANAGEMENT SYSTEM

CRDEC Data Base Management System

1. Fate & Effects Data Base
2. Simulants Data Center (MACCS)
3. ILO Chemical & Physical Properties (MACCS)
4. ILO Toxicity Screening Data Base
5. EPA Safety Data Sheets
6. Chemical/Physical Properties Data Base
7. Chemical Hazard Response Information System (CHRIS)
8. Registry of Toxic Effects of Chemical Substances (RTECS)
9. Materials Properties and Compatibilities Data Base (PLASTEC)
10. Analytical Methods for Agents and Simulants
11. Fine Chemicals Directory (MACCS)
12. Set a new password
13. Send comments or questions to the system manager
14. Exit

Enter the number corresponding to your choice:

APPENDIX C

ENVIRONMENTAL FATE AND EFFECTS DATABASE

Recent emphasis of environmental issues concerning simulants was initiated in a study led by Capt. Bennett in 1984. This effort reviewed uses of simulants and they selected 25 chemicals where summary data sheets were prepared for each chemical. These data sheets listed physical and chemical parameters as well as toxicological and environmental data. In 1985 TA3-I was started and I went to Mr. Stuempfle with a program to address data gaps in environmental data for simulants. Initial efforts concerned environmental fate assessments conducted by Howard et al., 1986 and environmental hazard ranking of chemical agent simulants by Reinbold et al., 1986, 1987. These efforts provided the information required to plan and prioritize research efforts in the environmental fate and effects area.

In 1986 - 1987 the Environmental Fate and Effects Database was developed. Initially it was a combination of the Bennett report and the Howard report. Mr. Lawhorne directed the application of the user friendly system and made it available under the Data Management Office system. The database has continued to expand from the initial 25 chemicals to 65 chemicals in 1992. Every year the database is edited with new information on existing chemicals added and additional data sheets on new chemicals developed. The format of the database and the referenced information have made this database very useful to DoD users.

Contract research efforts were initiated in FY85 and 86. Pacific Northwest Laboratory (PNL) was selected to conduct studies on DFP and DIMP. The data generated are indicated on Figure 1. Syracuse Research Corp. (Howard et al.) generated environmental fate assessments. The Corps of Engineers Construction Engineering Research Laboratory (CERL) conducted research on hazard ranking and environmental risk on simulants. Under TA3-I research was also conducted to determine the transport and microbial toxicity of C-8 in soil columns. In FY87 and 88, PNL continued to conduct research on selected simulants CEES and BIS. CERL assessed potential ecological impacts from simulant use through a survey of simulant use at US Army installations. Inhouse laboratory research was initiated to screen simulants for their toxicity to plants and earthworms. Dr. White and I identified additional simulants and in FY88 the major Directorates were asked for input. Research was initiated on the transport of simulants in soil in FY89 and 90. Studies continued on screening simulants for terrestrial toxicity and PNL conducted research on DEM and MS. In FY91 and 92, PNL focused on environmental fate issues of MS in soil. Inhouse research concerned identification of the toxic component of the PCAS/CADS training mixtures. Research was initiated to address aquatic toxicity data gaps using Daphnia magna and the Microtox system.

ENVIRONMENTAL FATE AND EFFECTS DATABASE

**CHEMICAL RESEARCH, DEVELOPMENT
AND ENGINEERING CENTER**

**DR. R. WENTSEL
ENVIRONMENTAL TOXICOLOGY BRANCH**

OF CHEMICALS ACCESSIBLE ON E-MAIL THROUGH 2-DMO

COMPOUNDS IN THE FATE & EFFECTS DATABASE

<u>CAS NO.</u>	<u>NAME</u>
1336-21-6	Ammonium Hydroxide
505-60-2	Bis (2-chloroethyl) sulfide
126-63-6	Bis (2-ethylhexyl) 2-ethylhexyl phosphonate
3658-48-8	Bis (2-ethylhexyl) phosphonate
122-62-3	Bis (2-ethylhexyl) sebacate
109-79-5	n-Butyl mercaptan
26264-06-2	Calcium dodecylbenzene sulfonate
7778-54-3	Calcium hypochlorite
1305-78-8	Calcium oxide
	Chlorinated lime
2698-41-1	O-chlorobenzylidene malononitrille
693-07-2	2-Chloroethyl ethyl sulfide
77-92-9	Citric acid (anhydrous)
	DIESEL FUELS
	DS-2
117-81-7	Di (2-ethylhexyl) phthalate
257-07-8	Dibenz (b,f)(1,4) oxazepine
141-28-6	Diethyl adipate
762-04-9	Diethyl hydrogen phosphonate
105-53-3	Diethyl malonate
121-75-5	Diethyl mercaptosuccinate, O,O-dimethyl phosphorodithioate
311-45-5	Diethyl p-nitrophenyl phosphate
56-38-2	Diethyl p-nitrophenyl thiophosphate
84-66-2	Diethyl phthalate
2050-20-6	Diethyl pimelate
110-40-7	Diethyl sebacate
123-25-1	Diethyl succinate
111-40-0	Diethylenetriamine
55-91-4	Diisopropyl fluorophosphate
1445-75-6	Diisopropyl methylphosphonate
627-93-0	Dimethyl adipate
868-85-9	Dimethyl hydrogen phosphonate
756-79-6	Dimethyl methylphosphonate
67-68-5	Dimethyl sulfoxide
34590-94-8	Dipropylene glycol monomethyl ether
64-17-5	Ethanol
105-39-5	Ethyl chloroacetate
109-86-4	Ethylene glycol monomethyl ether
50782-69-9	O-ethyl S-(2-diisopropylaminoethyl) methylphosphonothiolate
	Improved Chemical-Biological Agent Decontaminant
123-92-2	Isoamyl Acetate
67-63-0	Isopropanol
107-44-8	Isopropyl methylphosphonofluoridate
789-6-6	Methyl Phosphonic Acid
119-36-8	Methyl salicylate

127-18-4	Perchloroethylene
108-95-2	Phenol
96-64-0	Pinacolyl methylphosphonofluoridate
110-89-4	Piperidine
25322-68-3	Polyethylene glycol 200
27306-79-2	Polyoxyethylenated tetradecyl alcohol
763-18-69	Silicon Dioxide
497-19-8	Sodium Carbonate
7681-52-9	Sodium Hypochlorite
127-52-6	Sodium benzenesulfonchloramine
1310-73-2	Sodium hydroxide
7758-29-4	Sodium tripolyphosphate
2551-62-4	Sulfur hexafluoride
	Supertropical bleach
134-63-677	Titanium Oxide
126-73-8	Tributyl phosphate
122-52-1	Triethyl Phosphite
78-40-0	Triethyl phosphate
512-56-1	Trimethyl phosphate
7646-85-7	Zinc Chloride

TYPE OF DATA

CAS REGISTRY NO.

FORMULA

SYNONYMS

PROPERTIES

BOILING POINT

FLASH POINT

MW

SOLUBILITY IN WATER

VAPOR PRESSURE

KOW

HENRY'S CONSTANT

INDUSTRIAL APPLICATIONS

ENVIRONMENTAL LAWS AND REGS:

TSCA

DOT

CERCLA

RCRA

TOXICOLOGY:

MAMMALIAN

ECOLOGICAL

CHEMICAL REACTIVITY

ENVIRONMENTAL FATE

AQUATIC: PHOTOLYSIS
HYDROLYSIS
BIODEGRADATION
VOLATILIZATION
SORPTION
OXIDATION/REDACTION

TERRESTRIAL

ATMOSPHERIC

FATE SECTIONS ON:

BIOCONCENTRATION

SOIL ADSORPTION

VOLATILIZATION FROM WATER/SOIL

WATER CONCENTRATION

SEDIMENT/SOIL CONCENTRATION

BIODEGRADATION

ABIOTIC DEGRADATION

REFERENCES

APPENDIX D

DATA FROM THE ENVIRONMENTAL FATE AND EFFECTS DATABASE

1445-75-6 Diisopropyl methylphosphonate C7H17O3P

SYNONYMS

DIISOPROPYL METHANEPHOSFONATE
 DIISOPROPYL METHYLPHOSFONATE
 DIMP
 METHANEPHOSPHONIC ACID, DIISOPROPYL ESTER
 PHOSPHONIC ACID, DIISOPROPYL METHYL ESTER
 PHOSPHONIC ACID, METHYL-, BIS (1-METHYLETHYL) ESTER
 PHOSPHONIC ACID, METHYL-, DIISOPROPYL ESTER

Chemical and Physical Properties

Boiling point extrapolated	190.000 ^C	0.000
Boiling point extrapolated	174.000 ^C	0.000
Boiling point extrapolated	211.000 ^C	0.000
Flash point	71.000 ^C	0.000
Molecular weight	180.190	0.000
Solubility (water)	1.500 g/l	25.000 ^C
Specific gravity	0.976	0.000
Vapor pressure	0.170 mm Hg	25.000 ^C
Vapor pressure	0.090 mm Hg	25.000 ^C
Vapor pressure	0.220 mm Hg	25.000 ^C
Volatility	165000.000 mg/m3	25.000 ^C

DESCRIPTION

DIMP belongs to a group of compounds known as organophosphates.

MILITARY APPLICATIONS

DIMP has spectral characteristics similar to those of the G-agents; therefore, it is used in simulations involving general remote detection.

INDUSTRIAL APPLICATIONS

DIMP has no known industrial application.

ENVIRONMENTAL LAWS AND REGULATIONS

DIMP is not listed in the TSCA inventory. DOT classified the compound as a combustible liquid (49 CFR 3173.115(b)); it should be handled as described in 49 CFR 172.101. DIMP is not listed as a hazardous waste

under the RCRA or as a hazardous substance under the CERCLA or the FWPCA.

TOXICITY

Mutagenicity: DIMP was non-mutagenic when administered to mice, rats, and dogs. (109)

Reproductive Effects: When rats were given DIMP at dietary levels of 100-3000 ppm, (109) no teratogenic effects or dose-related reproduction responses occurred.

Tumorigenicity: No information found.

Ecotoxicity: DIMP burned the leaf tips of Black Valentine beans and Whitchita Wheat at aqueous concentrations of 10-40 ppm. In greenhouse herbicidal screening tests at Ft. Detrick, DIMP spray applications at 0.1 and 1 pound per acre resulted in no injurious effects to rice, morning glory, beans, oats, and soybeans (Reference 66, pg E-4).

Cross phytotoxicity responses to both tall fescue and short-needle pine have been determined for DIMP. Severe damage occurred in both plant species at foliar mass loadings of 1 to 40 ug DIMP/cm². Tall fescue was found to be more susceptible to DIMP damage than the short-needle pine. Severely defoliated plants exhibited new growth within 21 days indicating a transient impact. In vitro studies performed indicate that photosynthesis is affected, but not dark respiration. Further studies show DIMP to inhibit photosystem II. Conditional LD50 values calculated for the soil/earthworm assay were 1500 ug/g. (322)

Human Exposure Criteria: Presently, no TLV-TWA values have been found for DIMP.

Route	Species	Dose	Effects/Remarks (Ref)
Oral	Duck	1490 mg/kg	LD50 (45)
	Bird	1000 mg/kg	LD50 (45)
	Mammal	503 mg/kg	LD50 (45)
	Cattle (calves)	750 mg/kg	LD50 (45)
Inhalation	Mice	577 mg/m ³ (43 min) average	0/10 died within 14 days after exposure. No toxic signs (325)
Percutaneous	Rabbit	>200 mm ³ /kg undiluted	No irritation at the site of application (325)
Eye	Rabbit	0.25 mm ³ /eye undiluted	Inflammation, mild to severe, neg. 24 hours; lacrimation, edema - slight, neg. 24 - 48 hrs. (325)

REACTIVITY

Alkali and Alkaline Earth Metals: An exothermic reaction may occur upon mixing DIMP with alkali and alkaline earth metals.

Azo Compounds: Azo compounds may react with DIMP to produce hazardous conditions.

Caustics: Under alkaline conditions, the hydrolysis of DIMP yields isopropyl alcohol and metal salt of methylphosphonic acid.

Epoxides: The reaction between DIMP and epoxides may produce hazardous conditions.

Mineral Acids: Excessive strong mineral acids can cause DIMP to decompose and primarily yield alcohol and methylphosphonic acid. (110)

Organic Peroxides: There is very little available information on the reaction between DIMP and organic peroxides. The reaction may produce hazardous conditions.

Oxidizing Agents: The exhaustive oxidation of DIMP can yield toxic and corrosive fumes of oxides of phosphorus, sulfur, nitrogen, and heat.

Oxidizing Mineral Acids: Excessive oxidizing acids can decompose DIMP to yield heat and toxic fumes of nitrogen oxides, sulfur oxides and phosphorus oxides.

Reducing Agents: For information on the reducing agents, see alkali and alkaline earth metals above.

Water Reactives: The water reactive materials may react with DIMP to produce highly unstable mixtures, heat and toxic and/or flammable gases.

ENVIRONMENTAL FATE AND EFFECTS

ENVIRONMENTAL FATE/EXPOSURE SUMMARY: Diisopropyl methylphosphonate (DIMP) is a by-product of GB nerve gas production. The military use of DIMP is as a G-agent simulant. No industrial or consumer uses of DIMP were found in the literature. DIMP biodegrades in the soil but at a very slow rate. Biodegradation in water is extremely slow also. Photolysis (both direct and indirect) and hydrolysis are insignificant removal mechanisms for DIMP. DIMP does volatilize slowly from soil but is not expected to volatilize much from water. Atmospheric half-life is estimated to be 3.0 days based on hydroxyl radical oxidation. Sorption to soil may occur to some extent but DIMP will migrate extensively in groundwater. Bioconcentration in animals has not been demonstrated; however, bioconcentration in some plants has.

ARTIFICIAL SOURCES: DIMP may be released to the environment as emissions or in wastewater during the production of GB nerve gas of which it is a by-product (152). It may also be released or spilled during its transport, storage or use as a G-agent simulant (118)

TERRESTRIAL FATE: DIMP is mobile in soil as evidenced by its groundwater migration at the Rocky Mountain Arsenal (152,153). O'Donovan and Woodward (154) also demonstrated that DIMP is mobile under simulated irrigation conditions. DIMP, in spite of its relatively high water solubility and low vapor pressure evaporates from soils (119). Evaporation losses were 19% from a soil biometer flask (119), < 5% from dry soil and 18% from moist soil in 10.4 days (154). DIMP applied in irrigation water is ultimately distributed throughout the soil profile, thus demonstrating that DIMP moves with irrigation water. A hydrolysis half-life for DIMP in groundwater has been estimated at 687 years (66), indicating that hydrolysis in soils will be an insignificant removal mechanism.

AQUATIC FATE: Biodegradation of DIMP in natural waters was not observed after a twelve week incubation period (119). Hydrolysis and photolysis are insignificant removal mechanisms (119). DIMP did not bioconcentrate in either ducks or quail (155) or in bluegills (156).

ATMOSPHERIC FATE: DIMP in the atmosphere is estimated to have a half-life of 3.0 days based on oxidation by hydroxyl radicals (126). Its high water solubility would also suggest that washout of DIMP will be an important process.

BIODEGRADATION: In aqueous media, DIMP did not biodegrade after incubation for 12 weeks in natural water or for 6 weeks with acclimated soil organisms (119). Additionally, no biodegradation was observed when DIMP was supplemented with other carbon sources such as glucose, yeast extract, glycerol, and succinate. In soil, however, DIMP was biodegraded. Soil which had been inoculated with acclimated soil mineralized DIMP at a faster rate than unacclimated soil. However, biodegradation rates were slow: the unacclimated soil would have required more than 3 years and the acclimated soil more than one year to mineralize 50% of the DIMP. These rates were at 25 C; at 10 C, DIMP biodegradation in soil almost completely stopped (119).

ABIOTIC DEGRADATION: DIMP hydrolysis half-lives at 10 C, extrapolated from hydrolysis rates at 95, 70, and 80 C (66), were calculated to be 530 years (119) and 687 years (66). Extrapolation was to 10 C since this was considered to be a more representative temperature of groundwater in a temperate climate (66). Photolysis was also found to be an insignificant removal mechanism for DIMP (119). DIMP, in both distilled and Rocky Mountain Arsenal water, did not photolyze when exposed to light (>290 nm) for 232 hours (9.7 days) (119). In the atmosphere, DIMP is estimated to have a half-life of 3.0 days due to oxidation by hydroxyl radicals (126).

BIOCONCENTRATION: DIMP did not bioconcentrate in the adipose of either ducks or quail (155) or in bluegill fish (156). Slight bioconcentration did occur, however, in sugar beet, carrot, wheat and bean plants grown both hydroponically and in soil (154). In general, the leaves of the plants had the highest bioconcentration factor relative to the hydroponic medium or the soil. Wheat leaves (soil grown) were found to have a bioconcentration factor of 11.0, the highest of the plants listed above. DIMP applied to corn leaves did not translocate but when applied to sugarbeet leaves, absorbed and translocated to all parts of the plant (except to new leaves) after 72 hours (24). Repeated applications of irrigation water, which is contaminated with DIMP may result in absorption, translocation and bioconcentration of DIMP in plant tissue (24).

SOIL ADSORPTION/MOBILITY: DIMP is mobile in soil and groundwater as evidenced by its detection in groundwater outside the boundaries of the Rocky Mountain Arsenal (152,153). Some adsorption of DIMP to soil may occur, however (119). Spanggard et al. (119), found that after 32 days of operation, 87% of the added DIMP remained in the medium of a soil percolator. They speculated that the reduction of DIMP concentration may have been due to adsorption since no further decrease in DIMP concentration occurred after an additional 18 weeks of operation.

VOLATILIZATION FROM WATER/SOIL: O'Donovan and Woodward (154) studied the volatilization of radioactive DIMP (20 ppm) from dry and moist soil. DIMP was mixed with soil in columns 4 inches deep and air directed across the surfaces. After approximately 250 hours (10.4 days) of treatment, the dry soil retained over 95% of the initial radioactivity while the moist soil retained 78%. In batch soil biodegradation tests performed by Spanggard et al. (119), 19% of the total ¹⁴C-DIMP volatilized from a soil biometer flask during 24 weeks incubation. When applied to corn and sugarbeet leaves, 96-97% of the DIMP volatilized, respectively (24).

WATER CONCENTRATIONS: In 1974, DIMP concentrations as high as 44 ppm were detected in groundwater near one of the Rocky Mountain Arsenal waste disposal ponds (152). Groundwater concentrations ranged from this high concentration down to the detection limit of 0.0005 ppm (152). Groundwater from Pit 4 of the Rocky Mountain Arsenal contained 1.10 ppm DIMP while North Bog surface water contained from 0.26 to 0.27 ppm DIMP (119). DIMP concentrations in one of the waste storage ponds (Basin F) at the Rocky Mountain Arsenal was found to be 11.3 ppm (157). One document issued in 1982 (158), however, reports that the compound dimethyl methylphosphonate (DMMP) may have been incorrectly identified as DIMP. Thus, some previous monitoring data for DIMP may be incorrect.

EFFLUENTS CONCENTRATIONS: DIMP concentrations in brine effluent from GB nerve agent disposal ranged from 9 to 31 ng/g (159).

SEDIMENT/SOIL CONCENTRATION: Soil collected at the Rocky Mountain Arsenal for biodegradation studies contained from 1.0 to 2.9 ppm DIMP and soil from Pit 4 contained 7.10 ppm DIMP (119).

PROBABLE ROUTES OF HUMAN EXPOSURES: The most probable route of human exposure to DIMP is from contaminated groundwater.

756-79-6 Dimethyl methylphosphonate

(CH3O)2P(O)CH3

SYNONYMS

DIMETHOXYMETHYLPHOSPHINE OXIDE

DIMETHYL METHANE-PHOSPHONATE

DIMETHYL METHYLPHOSPHONATE

DMMP

METHANEPHOSPHONIC ACID, DIMETHYL ESTER

PHOSPHONIC ACID, METHYL-, DIMETHYL ESTER

Chemical and Physical Properties

Boiling point	181.000 °C	0.000
Density	1.155 g/cm3	25.000 °C
Density	1.145 g/cm3	20.000 °C
Flash point (closed cup)	104.400 °C	0.000
Flash point Pensky-Martins	93.300 °C	0.000
Flash point (closed cup)	43.000 °C	0.000
Flash point (closed cup)	105.000 °C	0.000
Melting point	-50.000 °C	0.000
Molecular weight	124.090	0.000
Specific gravity	1.145	20.000 °C
Vapor pressure	0.870 mm Hg	25.000 °C
Vapor pressure	0.610 mm Hg	25.000 °C
Vapor pressure	1.000 mm Hg	30.000 °C
Vapor specific gravity	4.300	0.000
Viscosity	1.810 cs	25.000 °C
Volatility	4100.000 mgm3	0.000
Volatility	4074.000 mgm3	25.000 °C

DESCRIPTION

DMMP belongs to a group of stable organophosphorus esters known as the dialkyl alkylphosphonates. It is classified as a diester of methylphosphonic acid.

MILITARY APPLICATIONS

The volatility of DMMP is similar to that of many non-persistent G-agents. Because of this, DMMP has been used to study vulnerabilities of military vehicles, shelters, protective masks, and filters, freon decontamination, chemical unit and team decontamination capabilities, and aircraft spray tank dissemination. DMMP is used commonly with thickeners and dyes.

INDUSTRIAL APPLICATIONS

In industry, DMMP is used as a flame retardant additive and viscosity depressant in resins (e.g., unsaturated polyesters and epoxies). It is used in heavy metal extraction, and solvent separation. The compound is also used as a preignition additive for gasoline, as an antifoam agent, plasticizer and stabilizer, textile conditioner and antistatic agent, and as an additive in solvents and low temperature hydraulic fluids (79).

ENVIRONMENTAL LAWS AND REGULATIONS

DMMP is listed in the TSCA inventory (45). DOT regulations classify the compound as a combustible liquid in 49 CFR 173.115(b); handling guidelines are found in the hazardous materials table (49 CFR 172.101). DMMP is not listed as a hazardous waste under the RCRA, nor as a hazardous substance under the CERCLA or the FWPCA.

TOXICITY

Mutagenicity: In absence of metabolic activation, DMMP produced no mutagenic effects to bacteria (*Salmonella*) in Ames tests (78), but was mutagenic to mouse lymphoma cells (with and without metabolic activation) (79).

Reproductive Effects: (162). DMMP reduced sperm counts, sperm mobility, and fertility of male rats. With increasing doses of DMMP, the number of pregnancies decreased, the mean litter size decreased, and the percent of resorptions increased.

Tumorigenicity: The National Toxicology Program (45) is currently testing DMMP for carcinogenic activity.

Ecotoxicity: TLm (96 hr.): 51 mg/l for bluegills (*Lepomis macrochirus*); 38-68 mg/l for fathead minnows (*Pimephales promelas*) (Dugway Proving Ground, unpublished data).

Human Exposure Criteria: Presently, no TLV-TWA values have been established for DMMP. The compound causes irritation of the eyes, skin, and respiratory tract. An organophosphorous compound, DMMP apparently has little or no effect on cholinesterase levels (US Naval Surface Weapons Center, 1982 Draft Report) (162). The Army Surgeon General has approved thickened DMMP for use in field decontamination vulnerability tests as described in reference 163.

Carcinogenesis: Sufficient evidence exists to indicate that DMMP causes cancer of the kidney in male rats. There is no evidence of carcinogenic activity in female rats or female mice. The study of carcinogenic activity in male mice was inadequate because of decreased survival rates. DMMP is not listed in NTP's latest Annual Report on Carcinogens, however data will probably support an NTP classification of "reasonably anticipated to be a carcinogen." This is equivalent to an IARC classification of 2B (sufficient evidence in animals and inadequate data in humans) (272).

Route	Species	Dose	Toxic Effects (Ref)
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Oral	Rat	150 mg/kg (in corn oil)	LD50 (326)
	Rat	>4640 mg/kg	LD50 (79)
Percutaneous	Rabbit	>4640 mg/kg	LD50 (79)
Eye	Rabbit		Nonirritant (79)
Skin	Rabbit	4 hr. exposure	Mild Irritant (79)

REACTIVITY

Alkali and Alkaline Earth Metals: When DMMP is mixed with these metals, an exothermic reaction may occur.

Azo Compounds: DMMP may react with azo compounds to produce hazardous conditions. However, little information is available on these conditions.

Caustics: DMMP is slowly hydrolyzed under alkaline conditions to produce an alkali salt of methylphosphonic acid and methyl alcohol (23).

Non-oxidizing Mineral Acids: The non-oxidizing mineral acids can hydrolyze DMMP to highly flammable methyl alcohol (flash point 11 C) and methylphosphonic acid, a fairly strong acid (first ionization constant (pk1) 2.3 at 20 - 25 C (48)).

Organic Peroxides: Mixing DMMP with organic peroxides may create hazardous conditions; however, little information is available.

Oxidizing Agents: Exhaustive oxidation of DMMP can yield toxic and corrosive fumes of oxides of phosphorus and other toxic compounds.

Oxidizing Mineral Acids: Excess oxidizing mineral acids can decompose DMMP to yield toxic fumes such as nitrogen oxides, sulfur oxides, and phosphorus oxides.

Reducing Agents: In general, dialkyl alkylphosphonates are resistant to reducing agents. Materials such as sodium or aluminum amalgam have little effect. Stronger reducing agents do react, but information is scant. An exothermic reaction may occur, especially if the DMMP contains some water.

Water Reactives: DMMP can react with water reactive materials to yield heat along with toxic and/or flammable gases.

ENVIRONMENTAL FATE AND EFFECTS

ENVIRONMENTAL FATE/EXPOSURE SUMMARY-ENVS: Between 0.2 and 2 million pounds of DMMP are manufactured annually in the United States. It is used as a flame retardant and as a viscosity depressant in polyester and epoxy resins. A military use of DMMP is as a simulant for non-persistent G-agents. It is not known how much DMMP enters the environment, but it may be released during its manufacture and use.

DMMP will hydrolyze to the half ester and methanol with an estimated half-life of 13.2 years at 21 C. Half-lives in muddy water range from 7-210 days, depending on the initial DMMP concentration and the temperature. DMMP half-lives in soil range from 0.2-60 days with an average half-life of 12.4 days. No information was found on volatilization rates, photolysis, or biodegradation.

ARTIFICIAL SOURCES-ARTS: A total of 200,000 to 2 million pounds of DMMP were manufactured in 1977 by Mobil Oil Corporation and Stauffer Chemical Company (121). These two companies continue to be the sole producers of DMMP in the United States(192). DMMP is used as a flame retardant, as an intermediate in the manufacture of several other flame retardants (e.g., Fryol 76, Antiblaze 19), and as a viscosity depressant in polyester and epoxy resins (166). In the latter use, DMMP may be used as both a viscosity depressant and flame retardant in the manufacture of bathtubs and shower stalls (166). A military use of DMMP is as a simulant of non-persistent G-agents (118).

TERRESTRIAL FATE: DMMP will hydrolyze in moist soils. Although no information was found, hydrolysis rates in moist soil will probably be similar to those in water. In environmental chamber studies, DMMP at initial concentrations in soil from 100-1000 ug/g had half-lives from 0.2 - 60 days (167). The average half-life was 12.4 days. Temperatures ranged from 10-40 C, wind speed from 0-4 mph, and the soil moisture content from 1-5%. The transport of degradation process responsible for the loss of DMMP was not determined.

AQUATIC FATE: DMMP in water will hydrolyze to form the half ester and methanol (168). Hydrolysis half-lives, extrapolated from data at higher temperatures (80, 90, and 98 C)(122) and unspecified pH, are estimated to be 13.2 years at 20 C and 43.3 years at 10 C. In a study performed by the U. S. Army (167), DMMP half-lives in muddy water ranged from 7-210 days. The 7 day and 210 day half-lives corresponded to initial DMMP concentrations of 500 and 1000 ug/g and temperatures of 40 and 10 C, respectively. The removal mechanism for DMMP, however, was not specified. Removal may have been due to one or more mechanisms such as volatilization, adsorption, hydrolysis, biodegradation, and photolysis.

ATMOSPHERIC FATE: The atmospheric half-life for DMMP is estimated to be 1.6 months (171).

ABIOTIC DEGRADATION: DMMP will hydrolyze to the half ester and methanol (168). Half-lives for DMMP are calculated to be 13.2 years and 43.3 years at 20 C and 10 C, respectively. These two half-lives were calculated from kinetic data collected at 98, 90, and 80 C (122). The corresponding rate constants ($k \times 10^{-6} \text{sec}^{-1}$) for these three temperatures were 1.92, 1.15, and 0.50. Activation energy was 19.7 kcal/mole and the log A factor was 5.87. The pH, however, was unspecified. No information was found on DMMP photolysis. Information is, however, available on a similar compound, diisopropyl methylphosphonate (DIMP). DIMP, in both distilled and Rock Mountain Arsenal water, did not photolyze when exposed to light ($>250 \text{ nm}$) for 232 hours (9.7 days) (119). Thus, photolysis of DMMP may also be insignificant.

BIOCONCENTRATION: The high water solubility of DMMP suggest that it will not bioconcentrate in aquatic organisms.

SOIL ADSORPTION/MOBILITY: The high water solubility of DMMP suggests

that it will not sorb to soils or sediments. Therefore, DMMP would be expected to leach through soil and possibly enter groundwater.

VOLATILIZATION FROM WATER/SOIL: The low vapor pressure (0.61 mm Hg at 25 C) (118) and high water solubility of DMMP suggests that it will not readily volatilize from water or soils. However, DMMP has been detected in the air near a liquid waste pond at concentrations as high as 109,000 ng/m³ (187).

ATMOSPHERIC CONCENTRATIONS: DMMP ambient air concentrations at three different locations near the edge of a hazardous liquid lagoon were 109,000, 10,600, and 2450 ng/m³ (187). Concentrations at two sites approximately one mile from this lagoon were 31 and 20 ng/m³.

PROBABLE ROUTES OF HUMAN EXPOSURES: Human exposure to DMMP probably will occur primarily in occupational settings. Specifically, exposure may occur at DMMP production sites and where DMMP is used as a flame retardant and as a viscosity depressant in polyester and epoxy resins.

868-85-9 Dimethyl hydrogen phosphonate

(CH3O)2P(O)H

SYNONYMS

DIMETHOXYPHOSPHINE OXIDE
DIMETHYL HYDROGEN PHOSPHITE
DIMETHYL HYDROGEN PHOSPHONATE
DIMETHYL PHOSPHITE
DIMETHYL PHOSPHOROUS ACID
DMHP
PHOSPHONIC ACID, DIMETHYL ESTER
PHOSPHOROUS ACID, DIMETHYL ESTER

Chemical and Physical Properties

Boiling point	171.000 °C	0.000
Boiling point	72.500 °C	25.000 °C
Flash point closed cup	95.000 °C	0.000
Melting point	29.000 °C	0.000
Molecular weight	110.000	0.000
Octanol/H2O part. coef.	0.490	0.000
Solubility (water)	490000.000 mg/l	0.000
Specific gravity	1.200	25.000 °C
Vapor pressure	1.500 mm Hg	20.000 °C
Viscosity	1.060 centisto	25.000 °C
Volatility	19200.000 mg/m3	20.000 °C

DESCRIPTION

DMHP is the chemically neutral dimethyl ester of phosphorous acid.

MILITARY APPLICATIONS

DMHP is a simulant used in studying the spectroscopic behavior and ionic reactions of the chemical agent VX.

INDUSTRIAL APPLICATIONS

DMHP is routinely used in industry as a lubricant additive and as an adhesive. (26)

ENVIRONMENTAL LAWS AND REGULATIONS

DMHP is listed in the TSCA inventory. (45) The compound is not listed as a hazardous material by DOT, as a hazardous waste under the RCRA.

or as a hazardous substance under the CERCLA or the FWPCA.

TOXICITY

Mutagenicity: No information found.

Reproductive Effects: No information found.

Tumorigenicity: As of January 1983, (45) DMHP is being tested by the National Toxicology Program for carcinogenicity.

Ecotoxicity: Phosphonates will undergo photolytic reactions with sunlight to produce orthophosphates. The orthophosphates can serve as a sole phosphorus source to aquatic plants. (23)

Human Exposure Criteria: Presently, no TLV-TWA values have been established for DMHP.

Route	Species	Dose	Toxic Effects (Ref)
Oral	Rat	4250 mg/kg	LD50 (45)
Eye	Rabbit	20 mg/24 hrs.	Severe Irritation (45)
Skin	Rabbit	500 mg/24 hrs.	Moderate Irritation (45)

REACTIVITY

Alkali and Alkaline Earth Metals: These metals may replace the phosphorus-bonded hydrogen on DMHP to yield hydrogen gas (highly flammable and explosive) and the metal derivative of the diester. (48)

Azo Compounds: Little information was available according to reference 26; however, it is possible that reactions between azo compounds and DMHP may produce hazardous conditions.

Caustics: Under alkaline conditions, DMHP undergoes hydrolysis to yield methyl alcohol (see mineral acids below) and the corresponding salt of phosphonic acid. Also, some heat may be produced.

Epoxides: Mixing these materials with DMHP may produce hazardous conditions.

Mineral Acids: DMHP may be hydrolyzed by strong mineral acids to yield methyl alcohol (highly hazardous, flash point: 11 C) and phosphonic (phosphorous) acid.

Organic Peroxides: Reaction between these peroxides and DMHP may create hazardous conditions.

Oxidizing Agents: Along with heat, exhaustive oxidation of DMHP may yield toxic and corrosive fumes containing oxides of phosphorus, sulfur, and nitrogen.

Oxidizing Mineral Acids: The reaction between DMHP and oxidizing acids

may yield heat and toxic fumes containing oxides of nitrogen, phosphorus and/or sulfur.

Reducing Agents: See Alkali and Alkaline Earth Metals above.

Water Reactives: In addition to toxic and/or flammable gas such as hydrogen, (48) DMHP may react with these materials to produce heat.

ENVIRONMENTAL FATE AND EFFECTS

ENVIRONMENTAL FATE/EXPOSURE SUMMARY: Dimethyl hydrogen phosphonate is produced in significant quantities and is used as a flame retardant and chemical intermediate, and in lubricant additives and adhesives. It is not known how much is released into the environment. In soil, DMHP will probably hydrolyze and leach into groundwater (where it will completely hydrolyze); it will not volatilize significantly. In water, DMHP will hydrolyze but will not evaporate readily nor sorb to sediments or biota. It is not known if DMHP biodegrades, although it may photodegrade since diethyl hydrogen phosphonate appears to be photosensitive. The fate of DMHP in air is not known, although photolysis may occur.

ARTIFICIAL SOURCES: DMHP is used as a flame retardant in textiles (161) and as a chemical intermediate, lubricant additive, and in adhesives (69). It is used by the military as a simulant for the spectroscopic behavior and ionic reactions of the chemical agent VX (161).

TERRESTRIAL FATE: DMHP will hydrolyze in moist soils. Although no half-life can be estimated for the soil matrix, the hydrolysis should be at least as fast as in water. DMHP will leach extensively, possibly reaching groundwater where it should hydrolyze completely since its hydrolysis half-life appears to be one to two weeks (122).

AQUATIC FATE: DMHP released to water will hydrolyze with a half-life of 10 days at 25 C and 19 days at 20 C (122). Basic conditions speed the hydrolysis (132). The ethyl homologue of DMHP has been reported to photolyze (134) indicating that DMHP may also photolyze; however, no rates can be estimated for either compound (134). DMHP will not sorb to sediments or biota and little or no volatilization will occur.

ATMOSPHERIC FATE: One study reports that DMHP will photolyze in moist air; however, no environmentally significant rates can be estimated from their data (134).

ABIOTIC DEGRADATION: DMHP will hydrolyze in water (pH unspecified) with a half-life of 10 days at 25 C and 19 days at 20 C (122). This is based on kinetic data obtained at higher temperatures (50-90 C) to determine an activation energy (E) of 22 (Kcal/mole) and a preexponential coefficient (A) of $1.26 \times 10^{+10}$ where $K=A \exp(-E/RT)$. Hydrolysis appears to be faster in base, although reports conflict as to how much faster hydrolysis will be. A French study (133) presented data for base hydrolysis that predicted a half-life on the order of several days would be expected for DMHP under environmental conditions (pH 7, see Reference 120) while another study (132) presented data that predicted a half-life of 93 min. under environmental conditions. A homologue of DMHP has been reported to photolyze indicating the DMHP may also, although no rates were determined (134).

BIOCONCENTRATION: The low octanol/water partition coefficient suggests that DMHP will not bioconcentrate in aquatic organisms.

SOIL ADSORPTION/MOBILITY: The low octanol/water partition coefficient suggests that DMHP will not sorb to soils or sediments and, therefore, would be expected to leach through soil, possibly reaching groundwater if complete hydrolysis did not occur first.

VOLATILIZATION FROM WATER/SOIL: The vapor pressure (1.5 mm Hg at 20 C), ability to hydrogen bond, and the high water solubility suggests that DMHP will not volatilize from water or soils readily.

PROBABLE ROUTES OF HUMAN EXPOSURE: Primary human exposure appears to be from its use as a flame retardant in textiles.

APPENDIX E
SIMULANT ADVISORY COMMITTEE

SIMULANT ADVISORY COMMITTEE

- Expedited by CDE-PAT
- Purpose
 - Provide a Better Conduit for Simulant Related Information
 - Get Other ARMY Organizations Involved
 - Identify Future Requirements for WA-03
- Provide Guidance to Simulant Users
 - As Early in the Process as Possible
 - Information the Developer can Use
- Fits Well into the Goals of the Simulant Program
- Kickoff Meeting Set for 2 March

SIMULANT ADVISORY COMMITTEE COMPOSITION

- Permanent

- 3 CRDEC (G. Famini, A. Brozena, P. Coon)
- 1 AMSAA (F. Liu)
- 1 DPG (P. Harvey)
- 1 USAF (J. MacDougal)

- Ad Hoc

- 1 MRDC/OTSG (G. Berezuk)
- 1 NRDEC (D. Rivin)
- 4 CRDEC (T. Mann, R. Wentsel, C. Whalley)
- 1 TECOM (C. Chan)
- 1 DPG (L. Condie)
- 1 MTL (A. Wilde)
- 1 NSWC
- 1 AEHA
- 2 USAF, Brooks AFB, Eglin AFB

