US ARMY EDGEWOOD CHEMICAL BIOLOGICAL CENTER
CHEMICAL BIOLOGICAL AGENT SIMULANT KNOWLEDGE (ASK) V2.0 DATABASE

William P. Ashman, Raymond E. Jablonski and Mark Harrah
US Army ECBC, SBCCOM
ATTN: AMSSB-RRT-IM
5183 Blackhawk Road
Aberdeen Proving Ground, MD 21010-5234

ABSTRACT

This paper describes the US Army's Edgewood Chemical Biological **C**enter (ECBC) computerized Agent/Simulant Knowledge (ASK) V2.0 Data Base. ASK V2.0 contains structural, physical-chemical and toxicological properties, environmental fates, and simulant applications (uses) information modules for approximately 1300 chemical biological (CB) agents, tested or proposed candidate CB simulants, and other CB related materials. Additionally, using the ASK V2.0 database's chemical agent physicochemical-toxicological property module's data retrieval and analysis user interface, an immediate agent versus simulant properties comparison can be obtained. Currently, the ASK V2.0 database utilizes MicroSoft® Windows Access, Excel, and a stand-alone Java® application. The ASK V2.0 database framework will be summarized and the current version of the data base tool will be described.

INTRODUCTION

The U.S. chemical and biological (CB) defense community requires accurate, verifiable CB agent and simulant (a material that can be substituted for the agent) information for the efficient development and acquisition of CB defense systems and equipment. Historically [1-8], under various organizational names (CRDC, CRDEC, ERDEC,etc.), the U. S. Army Edgewood Chemical Biological Center (ECBC) has served as the lead chemical stimulant/ agent knowledge organization. Currently, ECBC has an Agent / Simulant Knowledge (ASK) project to acquire, collate and verify CB agent, simulant and CB related materials data. As part of the ASK project, ECBC has developed and continues to upgrade a computerized chemical biological ASK database. ASK V2.0 is the current version. A previous paper [9] describes the initial 2001 ECBC Simulant Center V1.0 computerized database that was the foundation of the current ASK database. ASK V2.0 is a CB information repository modular system that contains standardized CB physical-chemical, toxicological, applications (use), and environmental fate and effects information. Additionally, ASK V2.0 includes a chemical agent / simulant user computer interface [10] that allows for ranking the relevance of a simulant based on physical /chemical properties of interest. The availability of this CB centralized information repository system allows for immediate data searching, analysis and retrieval, and eliminates weeks to months of effort in identifying the appropriate materials and accurate data that are needed to develop the equipment and models that enhance the Army's speed and precision. This database provides not only a platform for obtaining standard data values and for calculating, evaluating and analyzing data, but also supports identifying CB data gaps not resolved or filled by current information. ASK V2.0 contains data for approximately 1300 agent, simulant, agent

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED
01 JUL 2003	**N/A**	**-**

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
US Army Edgewood Chemical Biological Center Chemical Biological Agent Simulant Knowledge (Ask) V2.0 Database	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **US Army ECBC, SBCCOM ATTN: AMSSB-RRT-IM 5183 Blackhawk Road Aberdeen Proving Ground, MD 21010-5234**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release, distribution unlimited

13. SUPPLEMENTARY NOTES
See also ADM001523.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			
unclassified	**unclassified**	**unclassified**	**UU**	**8**	

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

precursors, by-products and toxic industrial materials. ASK V2.0 provides data used for recommending candidate simulant materials.

Currently, ASK information is only available to Department of Defense, U. S. Government Agencies, and qualified government contractors. All others requiring the ASK data base information must request access from appropriate ECBC authorities. It is planned to have the ASK database available on-line via a password protected web site.

ASK DATABASE V2.0

ASK DATABASE V2.0 DATA, SOFTWARE AND MODULES

ASK V2.0 incorporates the ECBC computerized databases (CASDC[1], the Environmental Fate and Effects Database[11], ECBCSC V1.0[9] and includes additional data acquired by literature search, simulant user discussions, and chemical agent, simulant data summaries. It contains approximately 1300 CB materials (agents, candidate or proposed simulants, agent precursors and byproducts, TIC's and TIM's). There are approximately 250 various physico-chemical, toxicological and environmental fate data fields. Additional data fields can be added as needed. ASK 2.0 contains 4 major CB database modules: (a) Physicochemical- Toxicological Properties; (b) Simulant Applications; (c) Environmental Fate and Effects; and (d) Structure. ASK V2.0 utilizes Microsoft® Office[12] (Excel, Access) software that is currently readily accessible and useable by the CB research community within the U.S. Department of Defense and other government agencies. With the exception of (c) which uses Access, all modules use Excel. ASK V2.0 includes a newly developed stand-alone user computer interface[10]Java®[13] application. This report's figures are images of the computer output from the ASK V2.0 user interface.

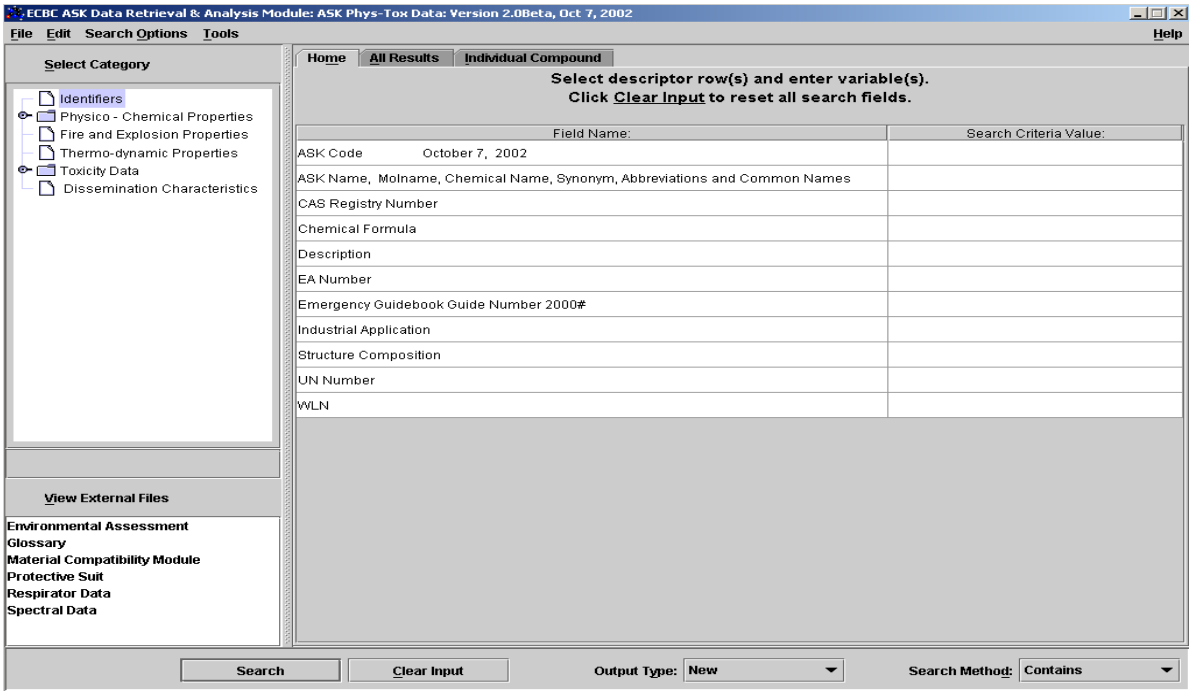

Figure 1. ASK V2.0 Physicochemical-Toxicological Module Identifier Data Fields

ASK V2.0 converts the Excel CB data module's spreadsheet to reformat the CB data for use by the user computer interface data, mining tool. The ASK V2.0 user can organize, manipulate and output (insert, reorder, sort, search, delete, review, calculate properties, print, save, etc.) the data as desired. ASK V2.0 contains various material identifiers (Figure 1) (structure, molecular name, common synonyms, the ASK database code, CAS registry number, and chemical formula, etc.). Therefore, the user can use the ASK database material identifiers as a link to obtain CB data from other ASK data modules (environmental fates, simulant application) and other data sources (internet search engines, other chemical information databases).

ASK V2.0 DATABASE PHYSICOCHEMICAL – TOXICOLOGICAL PROPERTIES MODULE

The ASK V2.0 Physicochemical – Toxicological Properties Module contains approximately 1300 CB materials (agents, candidate or proposed simulants, agent precursors and byproducts, TIC's and TIM's). There are approximately 231 various physico-chemical, toxicological data fields. The data fields (Figure 2) are categorized into Identifiers; Physico-Chemical Properties (Density / Vapor and Solubility/ Permeation subgroups); Fire and Explosion Properties; Thermo-dynamic Properties; Toxicity Data (many subgroups); and Dissemination Characteristics.

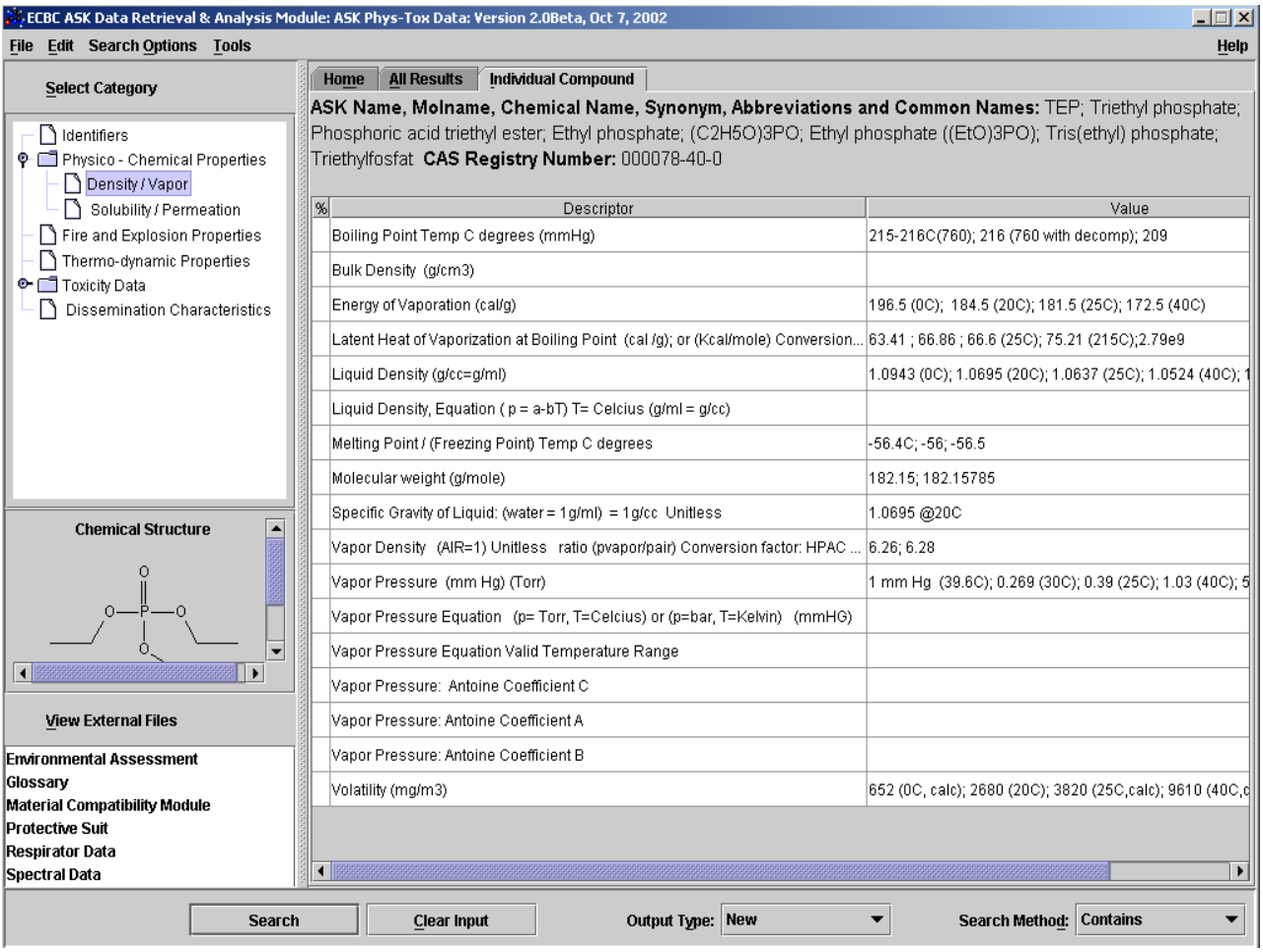

Figure 2. ASK V2.0 Physicochemical-Toxicological Properties Module Categories and Density / Vapor Subgroup Data Fields

ASK V2.0 DATABASE SIMULANT APPLICATIONS MODULE

ASK V2.0 Simulant Applications data module contains 9 data base descriptor fields (Table 1), approximately 300 materials, categorized into 14 major application areas (Table 2) for approximately 1380 actual or recommended uses. Table 3 is an example of a Simulant Applications module information Excel spreadsheet output.

Table 1. ASK V2.0 Simulant Application Module Data Fields

Column	Definition
A	ASK Code
B	Molname
C	Synonym
D	Simulant application
E	Agent simulated
F	Date
G	Industrial application
H	Comments
I	CAS Registry Number

Table 2. ASK V2.0 Simulant Application Module Master Categories

Binary (see Dissemination)
Contamination
Decontamination
Detection
Dissemination
Environment Studies
Filters (see Protection)
Mask Studies (see Protection)
Properties
Protection
Reactivity
Toxicity
Training & Trials
Vapor & Volatility

Table 3. Simulant Applications Module Information

molname	Simulant Application	Agent Simulated	Date reported or incorporated	Comments
DIETHYL ETHYLPHOSPHONATE	used GB sim in transparent materials survivability trials. Matched for methyl-phosphorus group. Ref 87	GB	11-Aug-87	
DEEP,DIMP	Decontamination Critical Strain Polymers	GB,GD,VX	88	
TEP,DMMP,DEEP	Properties Solubility,Diffusion(polym)	GB,GD,VX,HD	87	
DEEP	Detection	HD	70	
DEEP	Detection	VX	70	
DEEP	Ecotoxicity earthworms (ADE486742)	VX	96	
DICHLOROTETRAFLUOROETHANE	Protection charcoal filter tests GB	GB		
DICHLOROTETRAFLUOROETHANE	screened as GB simulant of charcoal filter tests	GB	11-Aug-87	banned ozone depleting substance.

ASK V2.0 ENVIRONMENTAL FATES AND EFFECTS MODULE

ASK V2.0 Environmental Fate and Effects Data Base[9] contains 78 materials with 41 data field descriptors . The output is in Access text paragraph format.

ASK V2.0 STRUCTURE MODULE, ASK V2.0 EXTERNAL FILES AND PHYSICAL PROPERTY CALCULATIONS

ASK V2.0 Structure Module contains the structures of approximately 1000 ASK chemical materials. ASK V2.0 has the capability to link with and access external files (Figure 2, View External Files box). These external files contain CB information (e.g Respirator data,detrection data) and can be added as needed without reformatting. Ask V2.0 can calculate for a specified temperature, vapor pressure, liquid density, and surface for selected chemical materials.

RESULTS

ASK V2.0 QUERY SEARCH STRATEGY

The ASK database can query the various modules. The ECBCSC V1.0 paper[9] describes the use of the simulant applications and environmental fate modules. This paper will emphasize the use of the newly developed user ASK V2.0 computer user interface mining tool[10] for the ASK V2.0 Physicochemical-Toxicological Module. The ASK V2.0 Data Search Example (Section 3.2) illustrates ASK V2.0 capabilities.

ASK V2.0 DATA SEARCH EXAMPLE

Problem: A project involves an outdoor experiment. The goal is to find a material that can simulate nerve agent GD's volatility, boiling point and vapor pressure. The individual performing the task does not know GD's volatility, boiling point or vapor pressure value(s) or the material (simulant) to use.

Step 1. First, access the ASK V2.0 computer user interface program; and select the ASK Physicochemical- Toxicological Module. ASK V2.0 allows incorporating more than one module and incorporating user specific data modules.

Step 2. Click the Tools command and click on the Match button. A Match module with the names of ASK chemicals available for matching will pop up. Either find the chemical name GD in the list (Click on the name to select it (highlight), or type in a chemical identifier for GD (soman). Click the OK button.

Step 3. The program then requests the user for which properties (data fields that the user wishes to match). Click on the GD desired data fields (i.e., highlighted fields- boiling point; vapor pressure; volatility). Click the OK button.

Step 4. The program will automatically search the 1300 materials in the ASK data base and identify which materials best match the GD physical properties selected. The program lists the matching ASK chemicals and gives a relative matched property ranking. For example, the compound triethyl phosphate (TEP) has a 90.6137% match while the compound diethyl malonate has a 72.7506% relative ranking. For this query, triethyl phosphate is selected and will be used to illustrate additional ASK V2.0 user interface capabilities.

Step 5. Select and Click on the row that has the compound triethylphosphate. The program will automatically bring up all the TEP data. In order to display the requested data, Click on the physicochemical properties category in the Select Category box of the user interface window. The data for TEP for the properties listed will be given. The structure of TEP is also displayed. By clicking on the other categories in the Select Category box, a specific category box will pop up, and the TEP data for those categories will be displayed.

Step 6. ASK V2.0 allows the user to calculate properties such as vapor pressure, liquid density and surface tension for various temperatures for those materials that have identified equations for those properties. Click on the Tools command and select calculate properties. A calculation window will pop up. Scroll until one finds the TEP compound and the desired property equation. Type in the desired temperature and the program automatically calculates and displays the calculated value.

Step 7. Ask V2.0 allows for immediate display of the data value reference source. Click on the cell that contains the data point and the data reference data pops up. Additionally, ASK V2.0 gives the user the option to select which data values to print, to save the data, and to review the print page prior to printing so that one can customize the print out. The data references for the properties selected are automatically printed out.

SUMMARY AND DISCUSSION

ASK DATA BASE UPGRADES (ASK V2.0)

ECBCSC V1.0[9] gives the results of the previous versions of the ASK database. This paper reports on the upgrade ASK V2.0. ASK upgrades will continue for the next several years. Included will be incorporating additional CB information and verifying data (i.e., environmental fate and effects, simulant applications, chemical and biological properties, environmental assessment data, detection data) and making the database more accessible to the CB user community. It is planned to identify, obtain and incorporate additional critical properties for current applications (i.e., spectral data for standoff detection) and to upgrade the developed ASK V2.0 online user interface. During the original ECBC simulant program, the development of a computerized biological simulant and toxin database was initiated[14] and

resulted in two biological related databases. In future ASK versions, it is planned to incorporate additional biological agent, simulant properties data.

ASK V2.0 ACCESS AND QUERY REQUESTS

When ASK V2.0 is placed on-line, ASKV2.0 information will be available to Department of Defense, U.S. Government Agencies and their qualified contractors having a need for agent simulant-related data. Until then, individuals can have their queries processed by contacting the authors. Direct inquiries can be made by phoning (410)-436-3430 or (410) 436-3566 by e-mail; william.ashman@sbccom.apgea.army.mil or ray.jablonski@sbccom.apgea.army.mil.

CONCLUSIONS

The chemical and biological defense community (i.e., battlefield management, field testing, laboratory testing, standoff detection, etc.) requires accurate, verifiable information on CB materials. The ASK V2.0 database repository and its user computer interface addresses that need. ASK V2.0 provides an updated computerized chemical biological material database that can be used to search, retrieve, calculate and analyze CB data quickly and efficiently. Planned upgrades to ASK will further enhance and address the CB community ability to meet its CB defense milestones.

ACKNOWLEDGEMENTS

The authors acknowledge the technical contributions of Phillip Coon, Dr. George Famini, Stephen Lawhorne, Kelly Cooney-Allen, Jason Lawhorne, Jennifer Miller, Wendel Shuely, Dr. Randall Wentsel, and Dr. William White for their efforts in the simulant program, in creating the earlier ASK foundation databases and in providing helpful technical advice and historical information. We would also like to acknowledge the contributions of Dr. Harold Banks, Ann Butrow, Patrice Abercrombie. Nancy Chester, Allan Mai, Kent Mai, Jan Kolakowski,and Kyong Park for their efforts in supporting the ASK projects data collection, validation and computer programming efforts.

DISCLAIMER

The findings in this report are not to be construed as an official Department of the Army position unless so designated by other authorizing documents. The use of trade names or manufacturers' names in this report does not constitute an official endorsement of any commercial products. This report may not be cited for purpose of advertisement.

REFERENCES

1. Coon, Phillip and Famini, George, *Data Base Users' Guide for the Chemical Agent Simulant Data Center (Second Edition)*, CRDEC-SP-037, U. S. Army Chemical Research Development and Engineering Center, Aberdeen Proving Ground, MD, August 1991.
2. Coon, Phillip et al, *Data Base Users' Guide for the Chemical Agent Simulant Data Center*, CRDEC-SP-88032, U. S. Army Chemical Research Development and Engineering Center, Aberdeen Proving Ground, MD, November 1988.
3. White, William E., *Simulant Program*, CRDEC-SP-88012, U. S. Army Chemical Research Development and Engineering Center, Aberdeen Proving Ground, MD, February 1988.
4. Stuempfle, A.K., and White, W.E., Lockwood, P., Lawston, I., and Chinn, K., *International*

Task Force-8 Simulants and Training Agents, Final Report, CRDEC-SP-003, U. S. Army Chemical Research Development and Engineering Center, Aberdeen Proving Ground, MD, December 1988.
5. Howard, P.H., Sage, G.W., Robinson, J.P., and Jackson, J., *Environmental Fate Assessments of Chemical Agent Simulants*, CRDC-CR-86016, U. S. Army Chemical Research and Development Center, Aberdeen Proving Ground, MD, March 1986.
6. Bennett, S.R., Bane, J.M., Benford, P.J., and Pyatt, R.L., *Environmental Hazards of Chemical Agent Simulants,* CRDC-TR-84055, U. S. Army Chemical Research and Development Center, Aberdeen Proving Ground, MD, August 1984.
7. Rhodes, J., Cowan, H.L., and Famini, G.R., *Proceedings of the Eight International Simulant Workshop,* U.S. Army Edgewood Research, Development, and Engineering Center, Aberdeen Proving Ground, MD, April 1996.
8. White, W.E., *Proceedings of the Second International Simulant Workshop,* U.S. Army Chemical Research, Development, and Engineering Center, Aberdeen Proving Ground, MD, December 1988.
9. Ashman, William and Banks, Harold, 'Edgewood Chemical Biological Center Simulant Center', *Proceedings of the 5th Joint Conference on Standoff Protection for Chemical and Biological Defense*, Williamsburg, VA, 24-28 Sept 2001
10. Harrah, Mark, ASK Database User Interface JAVA Application Program, (unpublished data) Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD 21010-5424
11. Wentsel, Randall and Lawhorne, Stephen*, Environmental Fate and Effects Data Base*, Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD 21010-5424
12. Copyright © Microsoft Office 2000 SR-1 Professional, Microsoft Corporation, One Microsoft Way, Redmond, Washington 98052-6399 U.S.A. All rights reserved.
13. Copyright © JAVA, JAVA RunTime (JRE) Environment Standard Edition, v. j2re-1_4_4_win, http://java.sun.com/j2re/, Sun Microsystems, 2002
14. Coon, Phillip (unpublished data bases), Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD 21010-5424