EDGEWOOD
RESEARCH, DEVELOPMENT & ENGINEERING CENTER
U.S. ARMY CHEMICAL AND BIOLOGICAL DEFENSE COMMAND

ERDEC-TR-354

CHEMICAL-MATERIAL DATA BASES:

CHEMICAL DEFENSE MATERIAL DATA BASE

Wendel J. Shuely

RESEARCH AND TECHNOLOGY DIRECTORATE

April 1997

Approved for public release; distribution is unlimited.

19970721 037

Aberdeen Proving Ground, MD 21010-5423

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.

DEPARTMENT OF THE ARMY
U.S. Army Edgewood Research, Development and Engineering Center
Aberdeen Proving Ground, Maryland 21010-5423

ERRATUM SHEET

30 October 1997

REPORT NO.	ERDEC-TR-354
TITLE	CHEMICAL-MATERIAL DATA BASES: CHEMICAL DEFENSE MATERIAL DATA BASE
AUTHORS	Wendel J. Shuely
DATE	April 1997
CLASSIFICATION	UNCLASSIFIED

Please remove the front cover from copies of ERDEC-TR-354 sent to you earlier in 1997 and attach the enclosed replacement cover. Previously printed covers were inadvertently printed with the incorrect activity name and logo.

Sandra J. Johnson
SANDRA J. JOHNSON
Chief, Technical Releases Office

19970721057
AD-A327593

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	3. REPORT TYPE AND DATES COVERED
	1997 April	Final, 95 Apr - 95 Jul

4. TITLE AND SUBTITLE
Chemical-Material Data Bases: Chemical Defense Material Data Base

5. FUNDING NUMBERS
PR-1O262622A553

6. AUTHOR(S)
Shuely, Wendel J.

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
DIR, ERDEC, ATTN: SCBRD-RTC, APG, MD 21010-5423

8. PERFORMING ORGANIZATION REPORT NUMBER
ERDEC-TR-354

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

An overview of the Chemical Defense Material Data Base (CDMD) is provided and includes a survey of the data base's current capabilities and contents. Emphasis is placed on comparing the current CDMD with previously released ones and on the anticipated capabilities of future releases. The CDMD's background and evolution are surveyed, and current system configurations are listed. The data base's contents are documented by record count functions applied to the occurrence frequency of materials, chemicals, and test properties. The plans for future system enhancements are described. Finally, a typical search example is followed via computer monitor screen views.

14. SUBJECT TERMS		15. NUMBER OF PAGES
CDMD	Material data base	38
Chemical resistance	Chemical material compatibility	16. PRICE CODE
Chemical protection	Chemical Defense Material Data Base	

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

Blank

PREFACE

The work described in this report was authorized under Project No. 1O262622A553, CB Defense/General Investigation. This work was started in April 1995 and completed in July 1995.

The use of either trade or manufacturers' names in this report does not constitute an official endorsement of any commercial products. This report may not be cited for purposes of advertisement.

This report has been approved for public release. Registered users should request additional copies from the Defense Technical Information Center; unregistered users should direct such requests to the National Technical Information Service.

Acknowledgments

The author acknowledges Joseph D. Williams, U.S. Army Edgewood Research, Development and Engineering Center (ERDEC), and Fran Crimmins, Chemical-Biological Information Analysis Center (CBIAC), for obtaining historical records. The author also acknowledges S. Jones, CBIAC, for answering queries related to this overview. The discussions with S. Lawhorne, U.S. Army Chemical and Biological Defense Command, and J. McNeely, Battelle Edgewood Office, and the manuscript review by D. Fielder and V. McHugh (ERDEC) are appreciated.

Blank

CONTENTS

1. INTRODUCTION 7

2. BACKGROUND 7

3. EVOLUTION OF THE DATA BASE 8

4. SYSTEM CONFIGURATIONS 8

5. DATA BASE CONTENT INVENTORY 9

6. FUTURE ENHANCEMENT PLANS 9

6.1 Data Management 9
6.2 Data Base Technology 10
6.3 Materials Science 10
6.4 Integration of Testing and Data Base 11

7. ACCESS TO THE CDMD 11

8. DATA BASE QUERY EXAMPLE 12

9. SUMMARY 12

APPENDIX - EXCERPTS FROM BULLETIN ON THE CHEMICAL DEFENSE MATERIALS DATA BASE (CDMD) 33

BIBLIOGRAPHY: MATERIALS SELECTION FOR CHEMICAL RESISTANCE . . 37

BIBLIOGRAPHY: CHEMICAL DEFENSE MATERIALS DATA BASE 38

FIGURES

1	Organizational Structure of the CDMD Within the DTIC Hierarchy	15
2	Material Problems Dominate Queries to the CBIAC on Chemical Defense Topics	15
3	Data Management Methodology Rationale for Development of a Chemical-Material Compatibility Data Base	15
4	Materials Science Methodology Rationale for Development of a Chemical-Material Compatibility Data Base	16
5	Evolution of Chemical-Material Data Base: PC Version	16
6	Integration of Data Bases Contributed by Chemical Defense Laboratories	17
7	ERDEC Upgrades to the Chemical Defense Materials Data Base: 1989-1995	18
8	Configurations of Chemical-Material Data Base	18
9	Chemical-Material Data Base: Mainframe Configuration	19
10	Chemical-Material Data Base: Configuration Required to Operate a PC Version (Minimum)	19
11	Record Count of Data in the CDMD (Version 4.1 1995)	19
12	Contents of the Chemical-Material Data Base	20
13	Chemicals in the CDMD	20
14	Frequency of Materials in the CDMD by Composition Class, Physical State, and Functional Class	21
15	Ranking of the Frequency of Occurrence of Property Data	21
16	CDMD Future Based on the Data Management Plan	22
17	Potential Improvements Based on Data Base Technology	22
18	Systematic Strategy for a Materials Science Approach to Enhancing the Capabilities of a Materials Data Base	23
19	Material Science Based Enhancements to a Chemical-Material Compatibility Data Base	23
20	Direct Test-to-Data Base	24
21	Computerized Format Modules for Documentation of Liquid Effect on Material Properties	25
22	Standard Test Methods (STM) Modified for Chemical-Material Compatibility Testing and Documented with Computerized Test Report Formats	26
23	CDMD Access, Availability, and Current Users	26
24	Access Methods	27
25	CDMD Navigation from the Main Menu	28
26	Data Tables Menu	29
27	Material Selection Form	29
28	<F2> Choice Menu for the Material Form	30
29	Chemical Selection Form	30
30	Test Descriptions Display	31
31	Test Data Display T Option	31
32a	Test Data -- Summary Display	32
32b	Test Data -- Summary Display (Continued)	32

CHEMICAL-MATERIAL DATA BASES:

CHEMICAL DEFENSE MATERIAL DATA BASE

1. INTRODUCTION

This review of the Chemical Defense Material Data Base (CDMD) provides an overview of its current capabilities and contents, emphasizing a comparison with previous releases with additional emphasis on the anticipated capabilities of future releases. The review has been divided into the following:

- background and evolution (Sections 2 and 3)
- current system configurations (Section 4)
- data base content inventory (Section 5)
- future enhancement plans (Section 6)
- access to the CDMD (Section 7)
- data base query example (Section 8)

2. BACKGROUND

The relative position of the CDMD in the Defense Technical Information Center (DTIC) can be shown by referring to an hierarchial outline (Figure 1). DTIC has recently decentralized by sponsoring over 20 topical Information Analysis Centers (IACs). One of these is the Chemical Biological Defense IAC (CBIAC), which is located at the U.S. Army Edgewood Research, Development and Engineering Center (ERDEC), MD. From a functional viewpoint, an IAC might contain bibliographic and/or numerical data bases. The CDMD is one of the numerical data bases CBIAC maintains. The CBIAC has access to other numerical data bases developed by ERDEC (e.g., physical property, simulant, and toxicological data bases).

One method of estimating the relative import of chemical-material compatibility data is to compare the fraction of materials related queries to all other types of chemical defense queries sent to the CBIAC. Although the NBCCS/Materials category is only one of about 15 categories, material data base questions represent over one-fifth of the inquiries and, in general, require more staff time per inquiry (Figure 2).

Several changes in the rationale for developing later versions of the data base are summarized in Figure 3. The chemical-materials data base was to remain a numerical rather than bibliographic data base; although, references to source documents were retained. Absolute values of the test properties were recorded whenever possible, unlike most commercial data bases that contain only relative values or ratios of final to initial values. Classification judgements were removed; these judgements assigned terms such as "good" or "poor" to specific ranges of property value loss. Increased standardization was either implemented or planned such that the relational capabilities of the data base could be employed. With respect to materials science and test development for the data base (Figure 4), an emphasis was placed on equilibrium properties for single chemical-polymer pairs at single standardized time-temperature conditions to increase the probability

of developing relational rankings of material resistance. Strategies for broadening the search parameters by widening or relaxing search parameter ranges were formulated to allow the option of obtaining higher risk, relational rankings of materials.

Further background information on the CDMD is provided in the Bibliographies and Appendix. The Appendix contains excerpts from a copy of the bulletin on the Chemical Defense Materials Data Base. A bibliography on Material Selection for Chemical Resistance contains only reports available for distribution to the public. The second bibliography, Chemical Defense Materials Data Base, contains publications with limited distribution.

3. EVOLUTION OF THE DATA BASE

The early evolution of the chemical material data base can be seen by tracking the personal computer (PC) RBase versions (Figure 5). Note that Versions 2 and 3 are similar in content; however, Version 3 was also transferred to a dBase4 version in 1989-90, specifically for international distribution. This transfer was only possible by obtaining one-time release approvals for each of the source documents referenced in the data base. The latest CDMD RBase version is labelled as a nominal Version 4 but is only used internally by the CBIAC staff as an interim buffer for uploading and downloading data into the CDMD on the VAX system.

The latest version of the CDMD resulted from an integration of four DoD data bases (Figure 6). These source data bases were as follows:

- PLASTEC Chemical Biological Data Base from Picatinny Arsenal
- USAF chemical defense materials data base
- Materials Technology Laboratory Army Laboratory Information System (ALISS) structure
- Natick Laboratory hardcopy test forms 833 and 1045 for textile properties

Several examples of the upgrades to the CDMD can be provided (Figure 7), to include, the transition to the VAX; the incorporation of changes based on customer feedback; the simplification of the structure; the increase in search speed; the improvement in report formatting; the addition of new data sets; and the installation of complementary chemical resistance data bases for commercial chemicals with relevance to chemical defense.

4. SYSTEM CONFIGURATIONS

The combinations of computer hardware, operating system, and data base system change incrementally at a fairly steady rate. The current and upcoming system configurations can be surveyed by noting the listings in Figure 8. The stand alone mainframe or minicomputer is the official, supported version of the CDMD. This is a VAX computer with the VMS operating system and Relational Data Base (RDB) software system [Digital Equipment Corporation (DEC), Manard, MA]. A microVAX is employed by a data base contractor to upgrade, then upload new system capabilities; therefore, this configuration might be considered an alternate implementation. The CDMD is currently being installed on a workstation based network for a directorate of U.S. Army Research

Laboratories (ARL); this is a Silicon Graphics workstation with a UNIX operating system and Oracle data base software. The PC based CDMD system employs MS-DOS and RBase data base software; however, a migration is being considered to a PC with Windows and Access data base software in the future.

The system configuration details for the CDMD are shown in Figure 9, and the minimum system configuration for the PC version is shown in Figure 10.

5. DATA BASE CONTENT INVENTORY

The most straightforward method of monitoring the increase in the data base contents is to employ the inherent "records count" functions. This current survey is limited to the output of these various data base self-inventory operations. The most general overview of the current contents is provided in Figure 11. This figure shows over 1100 material compositions that have been tested, 175 chemicals that have been used in material exposure tests, and 76 properties that have been measured. Overall, the CDMD (Version 4.1 in 1995), contains about 20,000 test property values. Figure 12 documents the changes in the contents since 1989. The columns list the contents at 1989, 1995, and the increase between 1989 and 1995, respectively. The number of chemicals has increased several times, and the number of specific material compositions has increased from 655 to over 1100 representing a 1.65X increase. In 1989, these 655 materials were from 184 general classes. The number of different types of tests increased by 1.25X. The overall number of measurements increased from 9500 to about 20,000 or a factor of about 2X. The documents increased from 785 to over 1000 for a factor of about 1.3X.

Figure 13 lists the breakout of the number of chemicals in various categories. Note that the agent/decontaminant sequence represents exposure of the same material by agent and decontaminant. The frequency of materials tested grouped by either functional class (coating, adhesive) or by physical state (elastomer, plastic) is listed in Figure 14. A comparison of the most frequently recorded test properties is contained in Figure 15. This comparison shows the current and 1991 rankings to be identical, with the exception of corrosion rate for metals, which was replaced at third-most-frequent by indentation hardness in 1995.

6. FUTURE ENHANCEMENT PLANS

6.1 Data Management.

The plans for the CDMD enhancements can be grouped into data management, data base technology, materials science, and integration with materials testing. The current data management plan includes (Figure 16) the following:

- maintaining continued access through the CBIAC
- considering the addition of different levels of security and access for different sets of users
- continuing the addition of test data as reports are published
- continuing to publish hard copy compilations of the data base contents as databooks

• modifying the record definitions to comply with commercial standards, such as ASTM E49 on Computerization of Material and Chemical Property Data

6.2 Data Base Technology.

Several additions to the system depend on cost/performance trends in data base technology. These potential improvements include (Figure 17) incremental improvements to retrieval and reporting systems; addition of graphical user interfaces (GUI) and graphical outputs; addition of the source documents as text images; production of CD ROM with tables, graphics, and source document text images; and restructuring the relational data base search strategy to employ the data lists and data links already inherent in the current design (conversation with S. Lawhorne, CBDCOM, July 1995).

6.3 Materials Science.

The materials science enhancements revolve around converting the chemical-materials data base from a simple data retrieval system into an information system. This approach targets developing built-in capabilities that will allow the relational features of the data base to be employed to support ranking and selection of materials for various chemical resistance scenarios. These data base capabilities can be grouped into several levels (Figure 18). The simplest additional feature is programmed self-inventory to alert the user to the occurrence or nonoccurrence of data for the material compositions, test types, or chemicals of interest. Performed periodically, these "record count" tally functions would give the system manager and users feedback on the trends in data addition to the data base. This type of capability is being added currently.

Another group of enhancements has been titled Programmed Self-Critique. In this case, the contents and new input would be scanned for nonsensical or illogical deviations from expected values for each record and then flag records with deviations from test standards. The identification of the exact composition of tested materials is provided at several levels of precision in the source text documents and these need to be classified as to the level. An automated scanning of the record fields for self-consistency and test standard conformance should result in the automatic labeling of the deviant field with either a pre-composed or customized warning/disclaimer to the user.

Programmed self-evaluation of the relational capabilities of the overall data base contents includes automated analyses that provide prompted guidance on search value ranges and/or data densities, etc., that yield that most ranked materials in a data base query. Elements would include updated determination and plotting of the frequency distribution of test parameter values. For example, a user might compose a query to encompass a number of ranges of several variables. Temperature might quite naturally be selected as a 5 ° range encompassing 23-27 °C. The user might then leave with 3 data base 'hits' ranking the 3 materials. A query range of 3 ° between 28-30 °C might have yielded 10 hits of ranked materials, but there is no way for the user to know this. The self-evaluation capability would then recommend values and ranges of test parameters to allow various favorable search results, such as high precision of test property results or maximum number of ranked materials.

A periodic programmed self-evaluation of the entire data base contents should systematically increment search parameter value ranges and plot the number and type of relations recorded for material compositional variables (difficult) and numerical test

parameters (easy). Heuristic trends in material compatibility could also be determined, statistically analyzed, and updated when relevant new data was input. In the final stage, programmed search strategies could be implemented, to include various material benchmarking methods for chemical resistance, material ranking schemes, and material selection algorithms.

Another set of material science bases enhancements to any chemical-material compatibility data base is based on correction of deficiencies (Figure 19). One reason that few or no data base search hits are obtained to rank materials for selection is that identical or equivalent material test data were cataloged under different material tradenames or nomenclature. The most automated solution is the purchase and installation of a commercial computer trade name data file to link to the material nomenclature files. The remainder of the unlinked equivalent material compositions would need to be discovered through a tedious, expert review.

The current data base structure mixes material composition types. For example, physical state, above or below the glass transition temperature (i.e., elastomers versus thermosets), is mixed with functional use types (such as sealants) and material form types (such a coatings). All of these can also be an elastomer. Conversion of the structure to harmonize with ASTM E49 guidelines for material data bases might correct most of these mixed material type classifications.

Many test methods generate several properties each and the test and property nomenclature are similar or identical. Also, in performing 'record count' functions on the data base, several properties derived from the identical data set are tallied and the distinction between tests and properties is again lost.

6.4 Integration of Testing and Data Base.

The integration of material testing with the materials data base has been reviewed (see Bibliographies), therefore, only a brief survey is provided here. The traditional method of data cataloging from hardcopy reports involved the method with high cost and long delays as shown in Figure 20 (right side). The method proposed and implemented involves developing common data records for the computerized test report and the data base (see Figure 20, left side). Currently, the transfer media is diskettes (or could be other electronic storage form). To implement this integration, the computerized format modules shown in Figure 21 have been developed, based on ASTM E49 guidelines. The standard test methods for which the ASTM E49 computerized test reports have been initiated are listed in Figure 22 and are in various stages of completion.

7. ACCESS TO THE CDMD

Access to the CDMD is provided through the CBIAC. Current eligibility is limited to the category, U.S. Government and Contractors, although some data subsets might have the category, U.S. DoD and Contractors (Figure 23). There were over 400 users registered for direct dial-in access. Most occasional CDMD users obtain data by submitting an inquiry, in which case, CBIAC staff use the data base to produce hardcopy reports that are mailed/faxed to the requestors (Figure 24).

One access issue is the downloading of a version in the category "Approved for public release, distribution is unlimited." International collaborators would have access to this category version. A variety of candidate strategies could be formulated for creating such a version and each would have advantages and disadvantages in terms of cost, time delays, and fraction of the data base converted.

8. DATA BASE QUERY EXAMPLE

A detailed example on a typical CDMD search can be found in the User's Manual. A brief example is explained in this section. The dial-in users access to the various data base files from the "Main Menu" is shown in Figure 25. One has access to the contents of the various "Nomenclature and Description" files. Most queries contain the following three elements: a material composition, a chemical, and a test type with associated time-temperature exposure conditions. The "Query" results in test property data for the selected material-chemical-test. The first computer monitor screen lists the three files one can "Search for Data By..." (Figure 26). The next monitor screen shows the "Material Selection Form" in Figure 27. The common code name PEEK (poly ether ether ketone) has been entered in the example. The next screen (Figure 28) shows the capability of the system for providing a "Choice Menu" when requested for the "Material Form" entry. The next screen (Figure 29) depicts the "Chemical Selection Form" with the entry "ds2" keyed in for the example (DS2: Decontaminating Solution 2). The "Test Parameter Form" screen has had "Flexibility" keyed in for the "Property Code." Because "Flexibility" is not a well known standard test, a "Test Description" display screen can be requested, as shown in Figure 30. The test "Data Display" screen (Figure 31) reports the test result and any important exposure conditions. Note that in this example, the "Average Value" record is blank because flexibility testing yields a PASS or FAIL at a specific thickness. A "Summary Display" for the "Test Data" is shown in the next two screens (Figure 32) to complete the example.

9. SUMMARY

Chemical-material compatibility data is one of the most frequently requested types of information within the chemical defense community. The Chemical Defense Material Data Base has constantly evolved from 1987 to date. The trend in this evolution is toward an absolute numerical data base with structure and fields that increase the capabilities as a true relational data base. The hardware and software requirements are modest and several widely available systems can be used. The contents of cataloged data has more than doubled in the last 5 years; however, most large, homogenous data sets have now been entered. The plans for future enhancements have been divided into four areas, which are those areas based on data management, data base technology, materials science, and integration with testing. Slow progress can be forecast for the data management improvements, whereas other areas will await further investment for additional progress.

The access to the data base is currently adequate for U.S. Government and contractor staff. Open literature access is complicated by the regulatory approvals from authors that is required to release limited distribution data. Release of an intact data base

can be prevented by the inability to locate or otherwise obtain a single author's approval. These regulations designed for single hard copy reports have not been reconsidered with respect to modern compilations of report data into computer data bases.

A typical example of a query search has shown the data base to be moderately easy to use and somewhat "self-teaching."

Blank

Defense Technical Information Center (DTIC)

Information Analysis Centers (IACs, >20)

Chemical and Biological Defense IAC, at ERDEC (CBIAC)

Bibliographic Data Bases

Numerical Data Bases

Chemical Defense Materials Data Base (CDMD)

Figure 1. Organizational Structure of the CDMD within the DTIC Hierarchy

1/5th of the queries to the CBIAC concern Materials/NBCCS although Materials/NBCCS represents only 1/15th of the topic categories

Figure 2. Material Problems Dominate Queries to the CBIAC on Chemical Defense Topics

- Numerical Data (Not Bibliographic)
- Absolute Values (Not Relative/Ratio)
- No Classification Judgements (i.e., Good, Poor)
- Increased Standardization to Support Search, Compare, Sort, and Rank Strategies

Figure 3. Data Management Methodology Rationale for Development of a Chemical-Material Compatibility Data Base

- To prevent data obsolescence due to changes in chemical formulations, exposure times, and temperature profiles, emphasis was placed upon:

  1) equilibrium properties instead of transient properties
  2) single chemical-polymer pairs
  3) single exposure time-temperature conditions

- To increase the probability of obtaining successful relational searches to rank materials, strategies for widening the search parameter ranges were formatted.

Figure 4. Materials Science Methodology Rationale for Development of a Chemical-Material Compatibility Data Base

Version	Period	Features/Distribution
1.0 (RBase)	1987	USAF
2.0 (RBase)	1989	USAF
3.0 (DBase 4)	1989	One Time Release Approval for International Distribution
4.0 (RBase)	1995	CBIAC Inhouse Buffer System for Uploading/ Downloading Data to the Mainframe

Figure 5. Evolution of Chemical-Material Data Base: PC Version

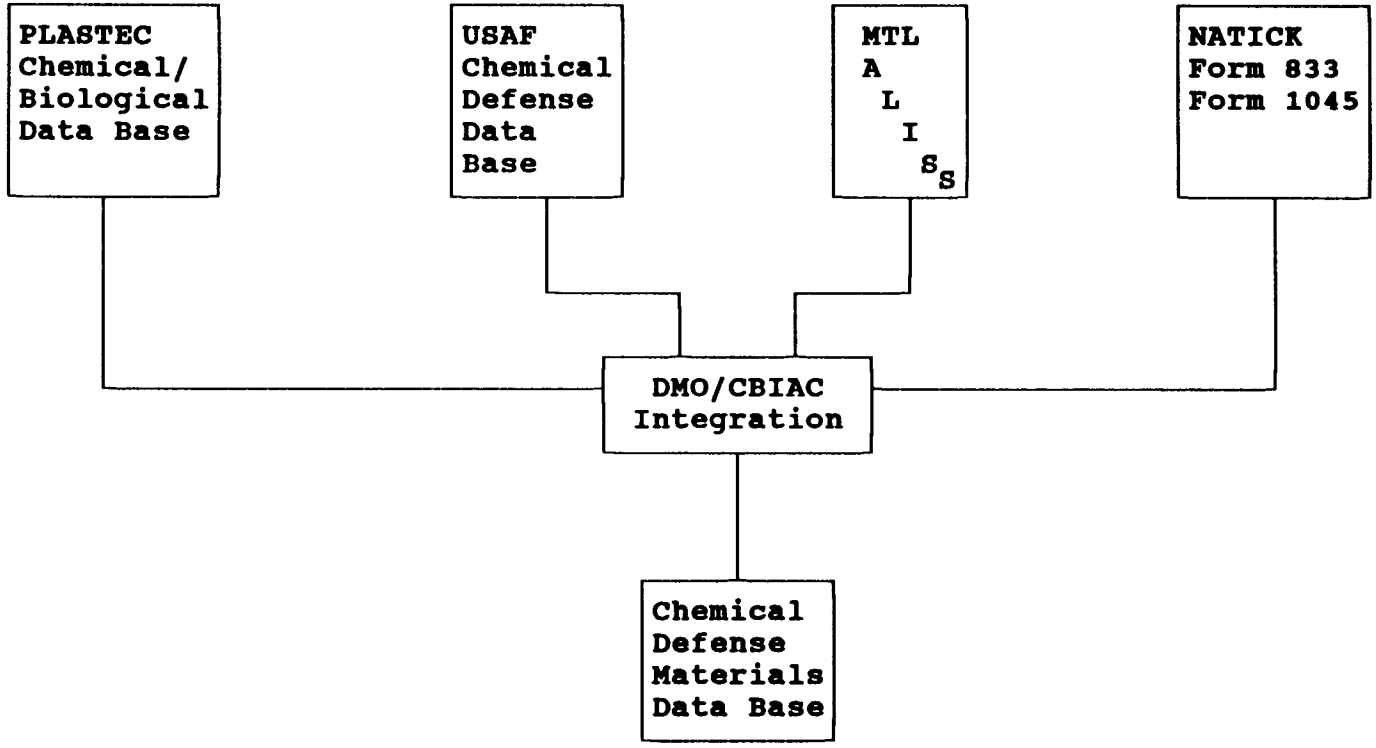

Figure 6. Integration of Data Bases Contributed by Chemical Defense Laboratories

- Transitioned data base from microcomputer to ERDEC VAX
- Incorporated changes bases on user feedback
- Simplified data base structure
- Improved data retrieval and reporting capabilities
- Gathered and catalogued additional data sets
- Installed a commercial chemical resistance data base

Figure 7. ERDEC Upgrades to the Chemical Defense Materials Data Base: 1989-1995

Computer Type	Operating System/ Computer/ Data Base System	Organization
Mainframe	VAX/VMS/RDB	ERDEC/CBIAC (Official, Supported Version)
Minicomputer	MicroVAX/VMS/RDB	Upload System Upgrades
Workstation	SGI/UNIX/Oracle	ARL/SLAD (incomplete)
(PC) Personal Computer	PC/DOS/RBase PC/MS-LAN/WIN/Access and/or CD-ROM	CBIAC Inhouse; Candidate Migration Path

Figure 8. Configurations of Chemical-Material Data Base

Computer	DEC	VAX	Model 11/780
Operating System	DEC	VMS	Version 6.0
Data Base System	DEC	RDB	Version 4.x
Screen Interface	Vermont Views		Version 4.0

Figure 9. Chemical-Material Data Base: Mainframe Configuration

Hardware:	IBM Compatible PC 386+ RAM: 1 MB Hard disk: 20 MB	
Operating System:	MS>DOS	Version >3.1
Data Base System:	RBase Version	($ 400. est, US)
	Candidate Migration Path:	Microsoft Windows Access Data Base

Figure 10. Chemical-Material Data Base: Configuration Required to Operate a PC Version (Minimum)

1,106	Materials
175	Chemicals
76	Properties
19,861	Data Points

Figure 11. Record Count of Data in the CDMD (Version 4.1 1995)

Period:	1989	1995	1989-95 Increase
Chemicals (C):	40 est	175	4.4x
Materials (M):			
Specific:	655	1100	1.65x
Classes:	184	Unk (>184)	----------
Tests (T):	60	76	1.25x
Properties (C-M-T):	9,500	20,000	2x
Documents:	785	1018	1.3x

Figure 12. Contents of the Chemical-Material Data Base

34	AGENT
22	AGENT/DECONTAMINANT, IN SEQUENCE
34	DECONTAMINANT
71	INDUSTRIAL
14	SIMULANT
175	TOTAL

Figure 13. Chemicals in the CDMD

56	ADHESIVE/SEALANT
102	COATING
34	COMPOSITE FIBER FILLED MATRIX
203	ELASTOMER
14	COMPOSITE LAMINATES
180	METAL
488	PLASTIC
3	POL (Petroleum Oil Lubricants)
15	TEXTILE
11	WOOD

Figure 14. Frequency of Materials in the CDMD by Composition Class, Physical State, and Functional Class

	1995	1991
●	Weight Change	Weight Change
●	Tensile: Strength, Elongation, Modulus	Tensile Strength
●	Indentation Hardness	Corrosion Rate Indentation Hardness

Figure 15. Ranking of the Frequency of Occurrence of Property Data

- Continued Access via CBIAC
- Potential for Developing Additional Levels of Security and Access
- Continued Addition and Maintenance of Test Data by the CBIAC
- Continued Updates of CDMD Databook
- Further Compliance with Commercial Practices, Specifications, and Standards (e.g., ASTM E49 Computerization of Material and Chemical Property Data)

Figure 16. CDMD Future Based on the Data Management Plan

- Further Improvements to Retrieval and Reporting Systems
- Potential Development of Graphical User Interfaces and Graphical Outputs
- Potential Integration of Complete Source Documents as Imaged Text as an On-line Capability
- Potential Development of CD ROM Containing Complete Data Base Tables and Graphics Documented by Imaged Text of Source Documents

Figure 17. Potential Improvements Based on Data Base Technology

- Programmed Self-Inventory to Document the Contents
  - -- Occurrence/Nonoccurrence of Property Data on Materials/Chemicals
  - -- Output/Plot Contents Trends as a Function of Time
- Programmed Self-Critique
  - -- Flag Deviations from Standard Test Exposure/Control Parameters
  - -- Classify the Precision of the Material Specimen Documentation
  - -- Add Standardized or Customized Disclaimers and Warnings
- Programmed Self-Evaluation of Relational Capabilities
  - -- Determine the Frequency Distribution of Test Parameters
  - -- Recommend Ranges of Test Parameters for Searches
  - -- Analysis of Relations Formed versus Search Parameter Range
  - -- Automated Heuristic Analysis for Correlations
- Programmed Global Search Strategies for Materials
  - -- Benchmarking by Comparing Current versus Candidate
  - -- Automated Ranking of Materials to Avoid: Deselection
  - -- Automated Selection of Candidates for Confirmatory Testing

Figure 18. Systematic Strategy for a Materials Science Approach to Enhancing the Capabilities of a Materials Data Base

- Provide a commercial Trade-Name data base data dictionary files to cross-reference tested materials to identical/related materials.
- Program alternate/optional material composition classification schemes to provide alternates to mixed categories of composition class, physical state, functional class, and form.
- Program a record conversion to ASTM E49 standards.
- Clarify nomenclature between test name and property name and single test methods that produce several properties with similar names.

Figure 19. Material Science Based Enhancements to a Chemical-Material Compatibility Data Base

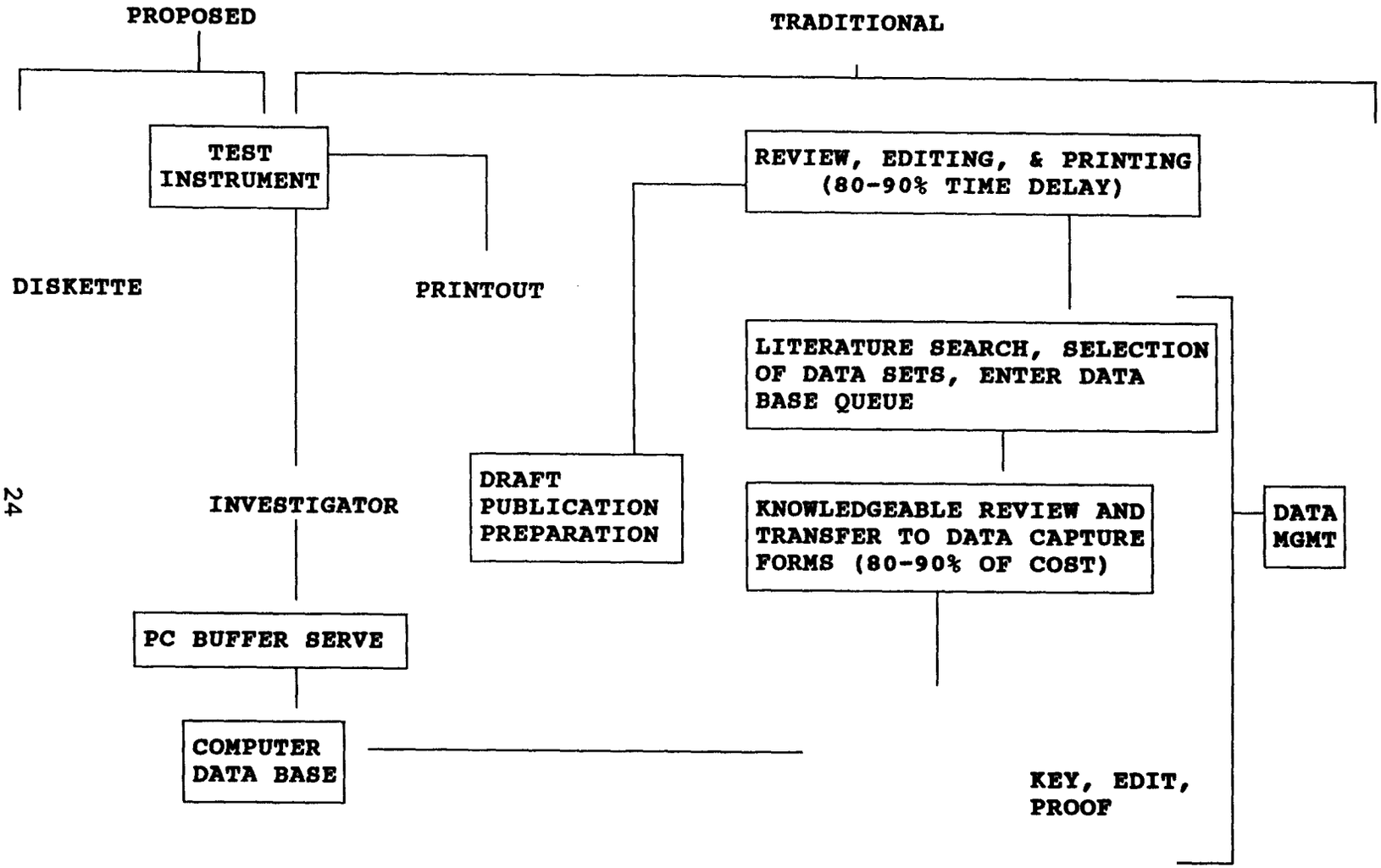

Figure 20. Direct Test-to-Data Base

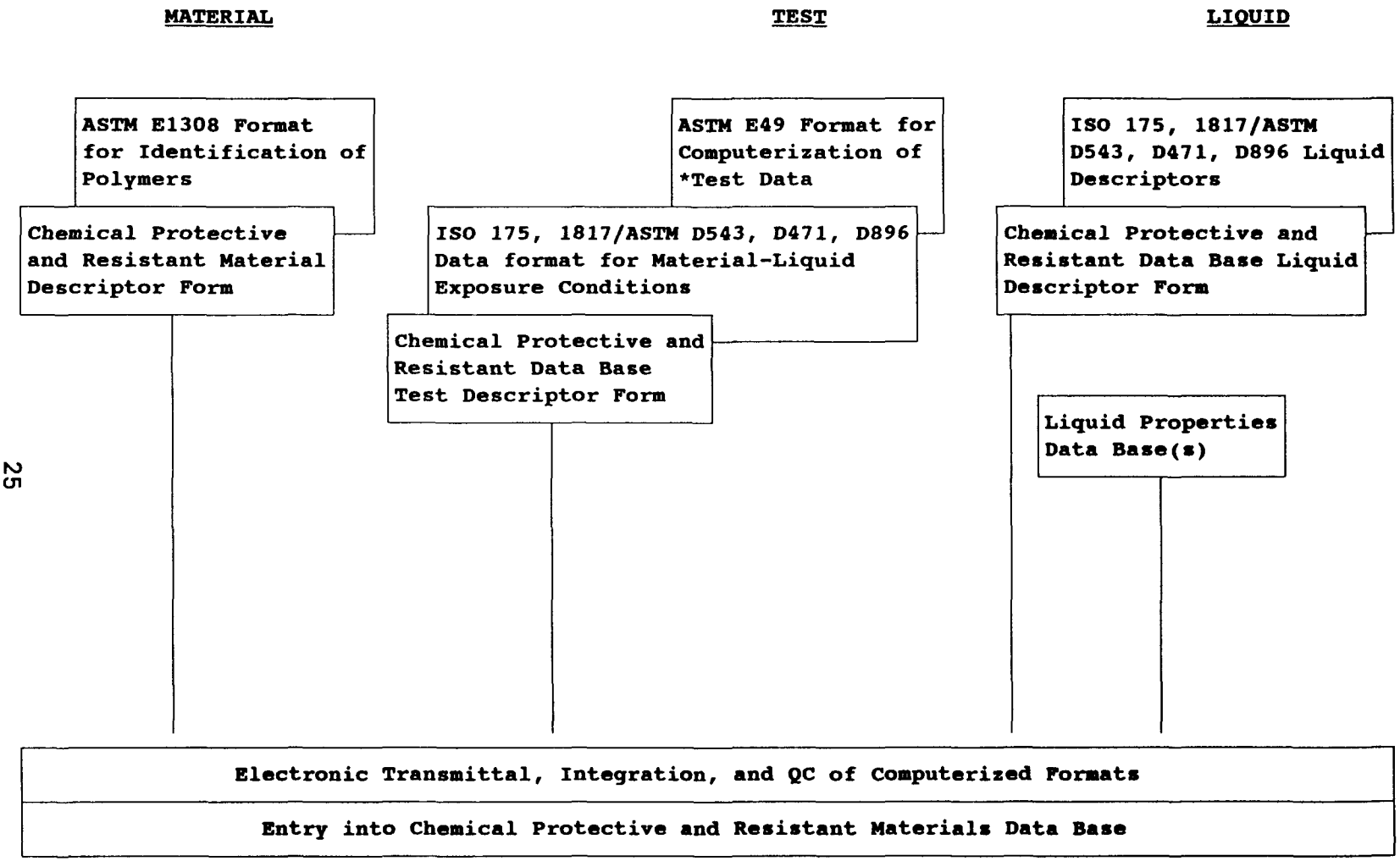

Figure 21. Computerized Format Modules for Documentation of Liquid Effect on Material Properties

STM	TITLE
D 3132	POLYMER SOLUBILITY SCREENING
D 471	SORPTION & DESORPTION (ELASTOMERS) EQUILIBRIUM SOLUBILITY DESORPTION DIFFUSION COEFFICIENT FRACTION EXTRACTED
D 543	SORPTION & DESORPTION (THERMOPLASTICS) SAME PARAMETERS AS FOR D 471
D 471	CHEMICAL EXPOSURE (ELASTOMERS)
D 543	CHEMICAL EXPOSURE (THERMOPLASTICS)
D 412	TENSILE PROPERTIES (ELASTOMERS)
D 638	TENSILE PROPERTIES (THERMOPLASTICS)

Figure 22. Standard Test Methods (STM) Modified for Chemical-Material Compatibility Testing and Documented with Computerized Test Report Formats

- Access -- Provided/Monitored by CBIAC COTR
- Availability -- Currently Limited to U.S. Government and its Contractors
- Users: Direct Dial-In (1995)

U.S. DoD	163
U.S. DoD Contractors	264
Total	427

- Users: Inquiry and Referral Service
  Over 20% of inquiries to the CBIAC

Figure 23. CDMD Access, Availability, and Current Users

- Through Manager, Inquiry and Referral Service
  (410) 676-9030; (410) 676-9703 fx
  email: joness@battelle.org
  mail: Battelle Edgewood OPS/CBIAC
  2113 Emmorton Park Rd, Suite 200
  Edgewood, MD 21014-1037

  8 hours maximum per query.

- Direct: Dial-in by registering and obtaining a system password.

Figure 24. Access Methods

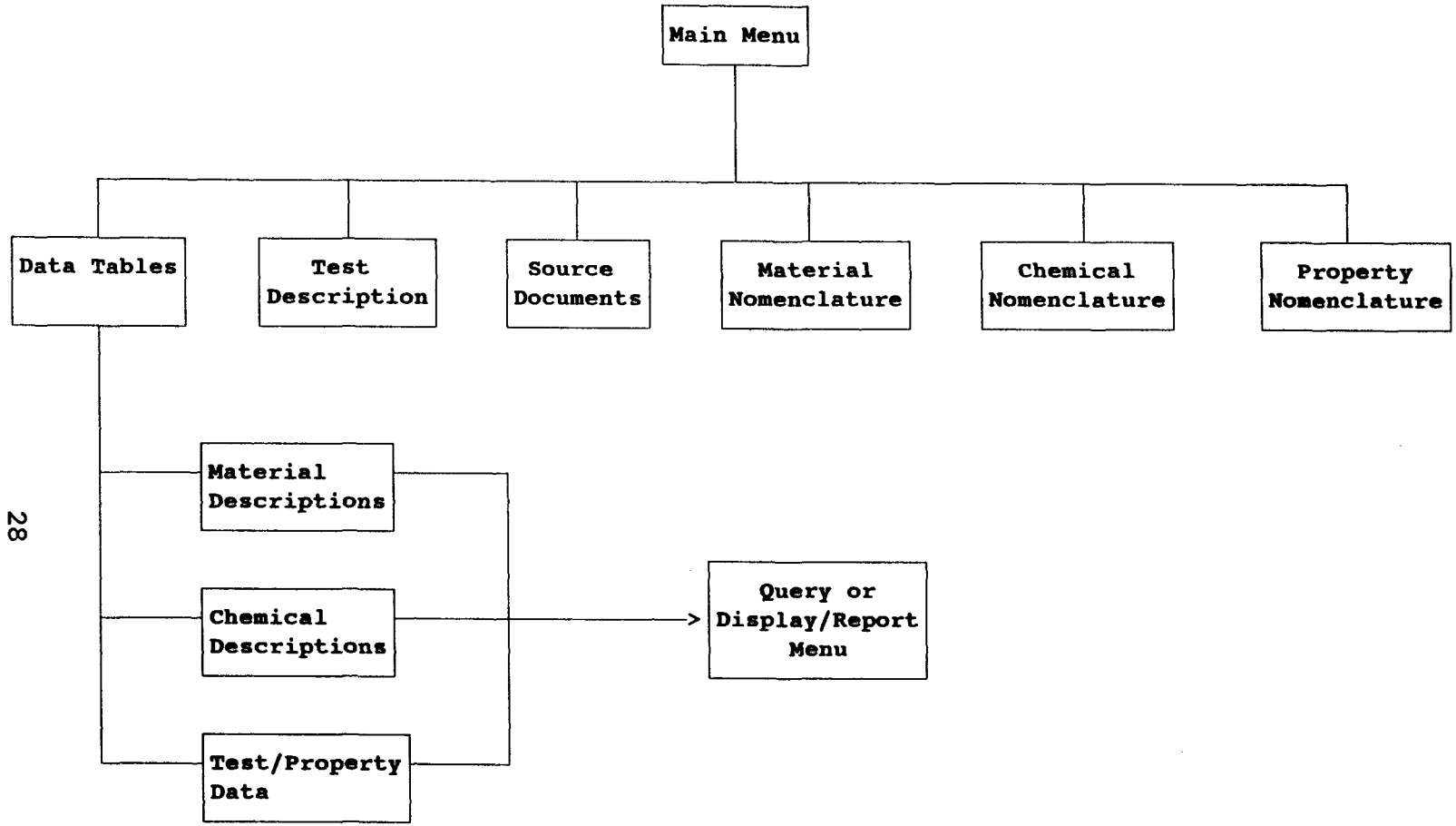

Figure 25. CDMD Navigation from the Main Menu

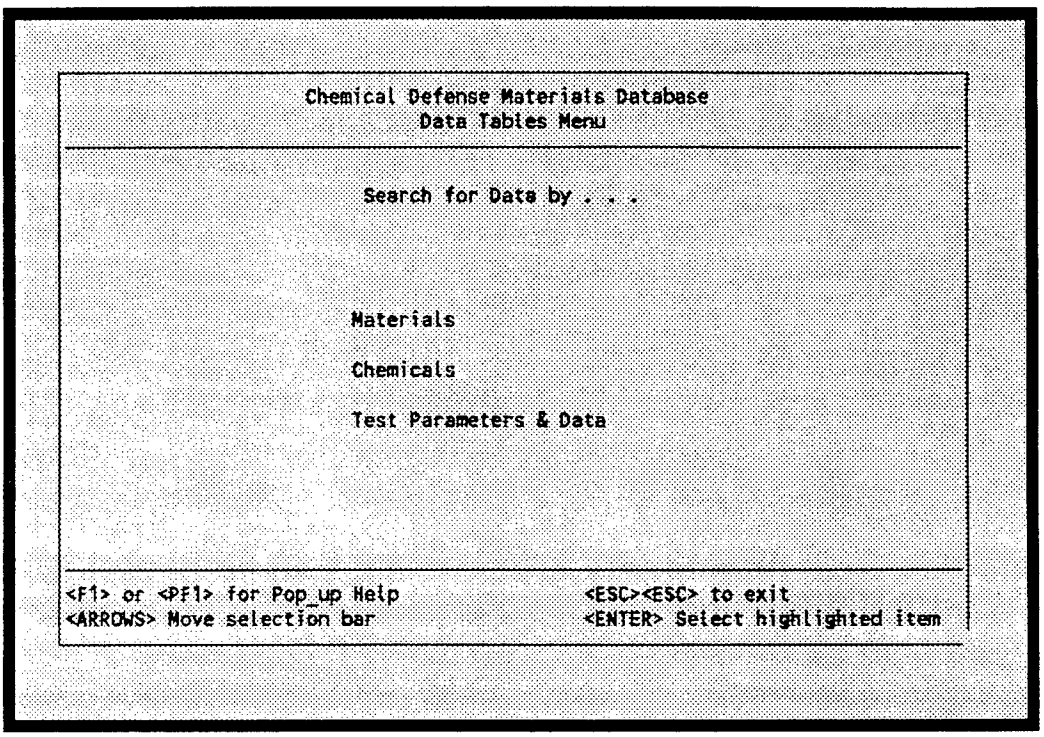

Figure 26. Data Tables Menu

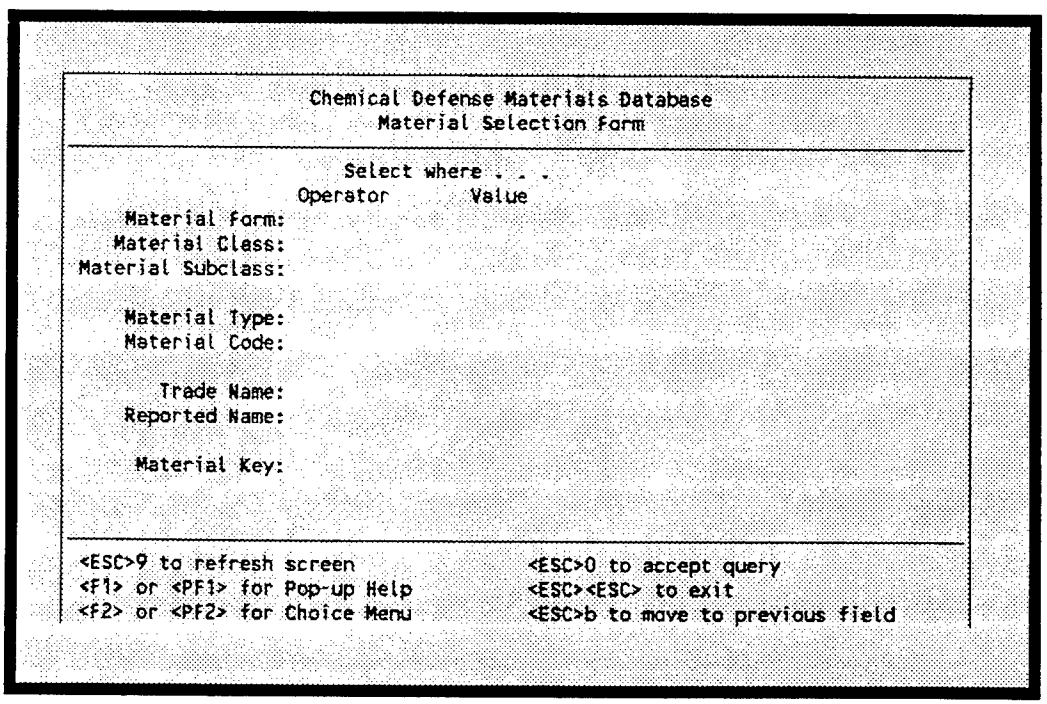

Figure 27. Material Selection Form

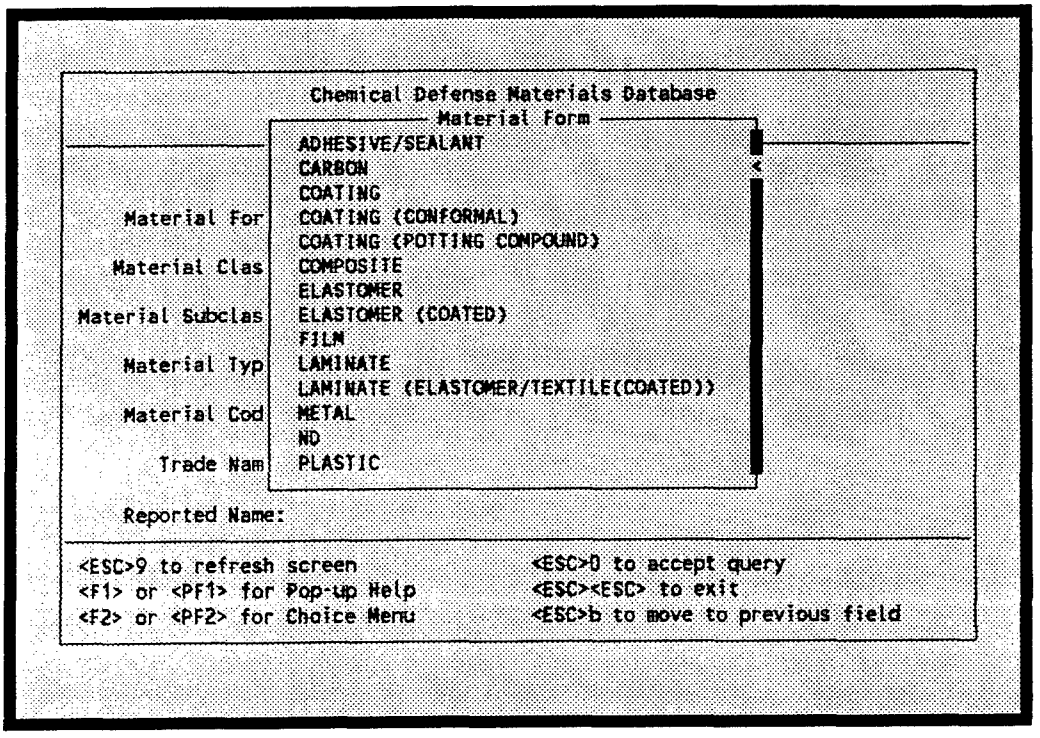

Figure 28. <F2> Choice Menu for the Material Form

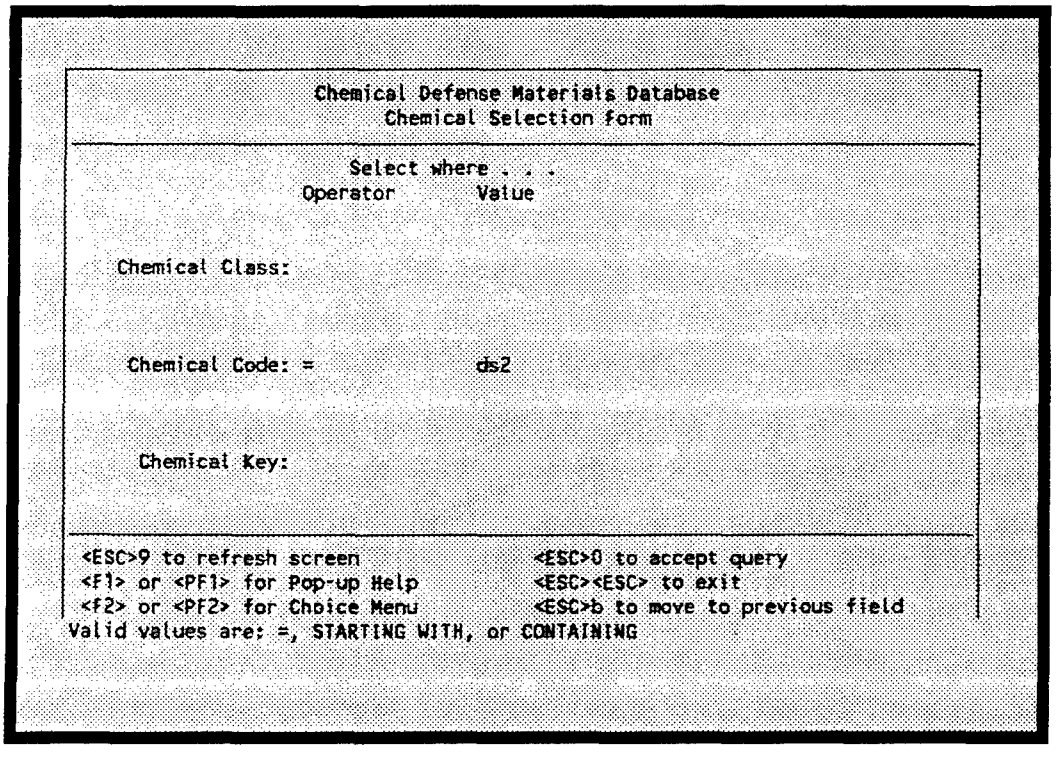

Figure 29. Chemical Selection Form

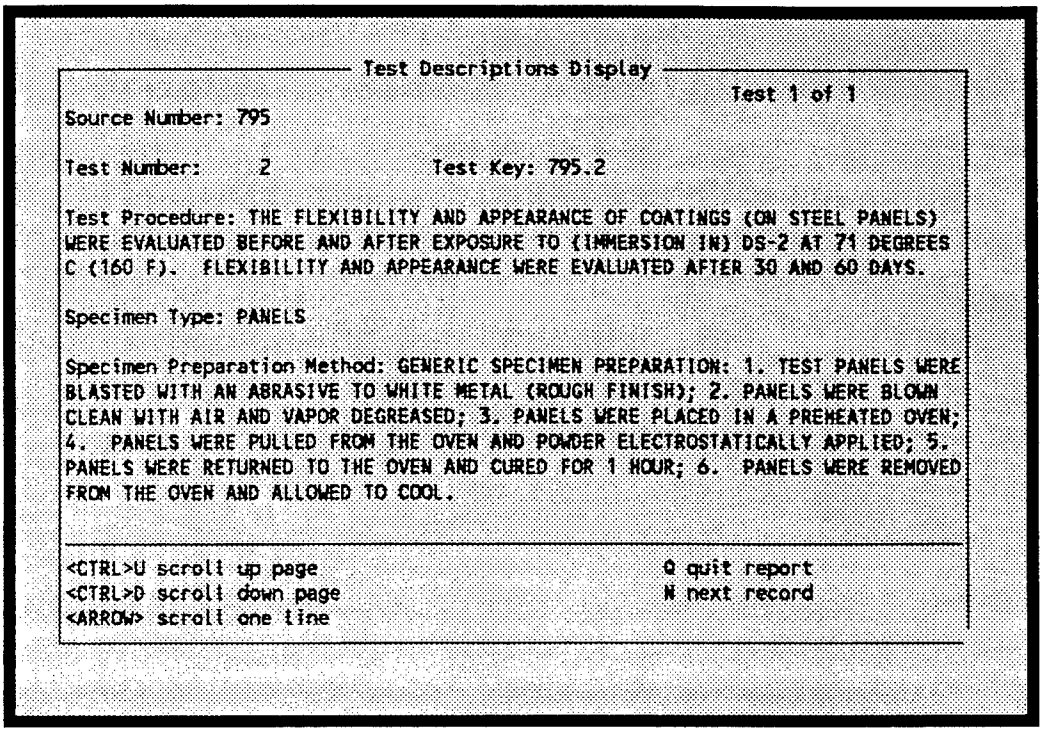

Figure 30. Test Descriptions Display

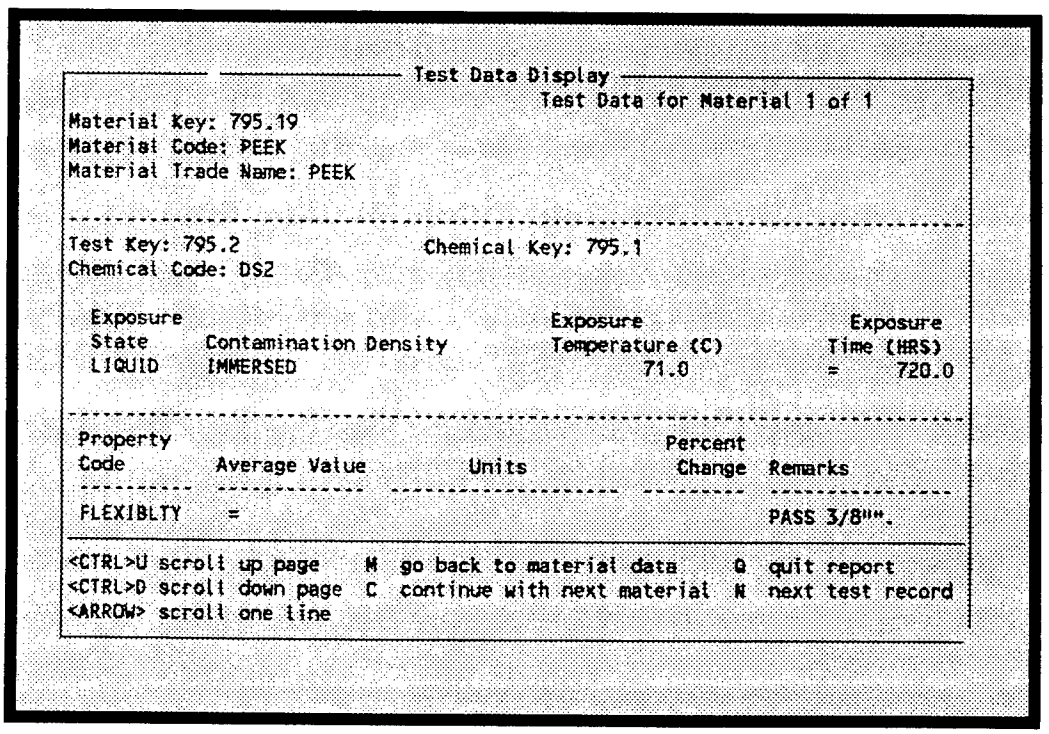

Figure 31. Test Data Display T Option

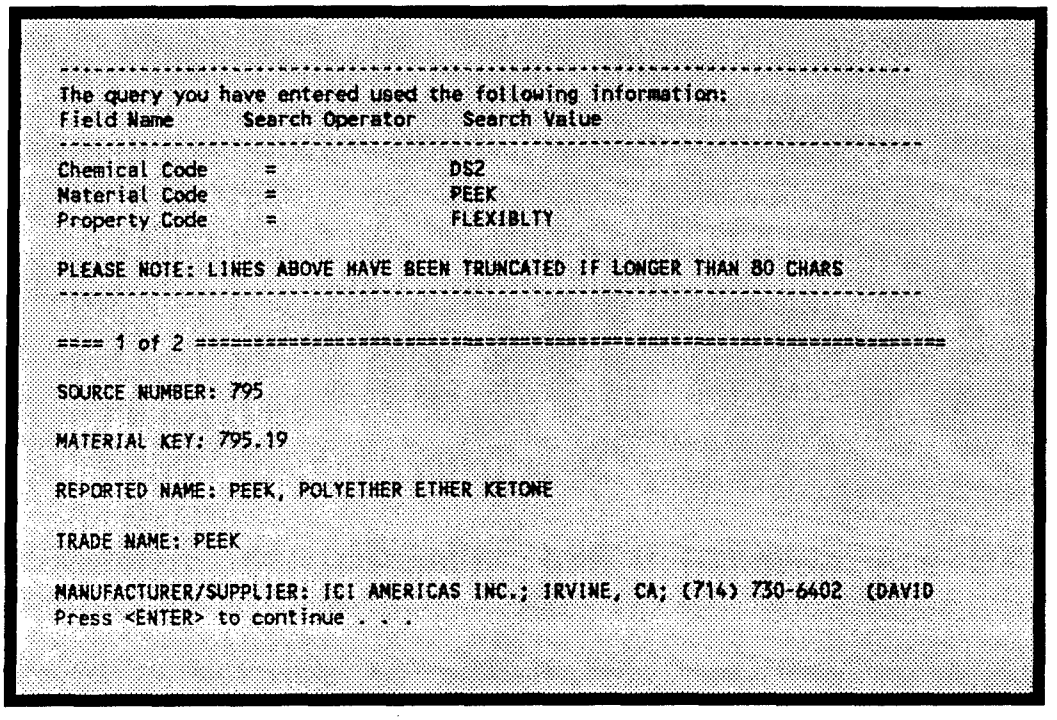

Figure 32a. Test Data -- Summary Display

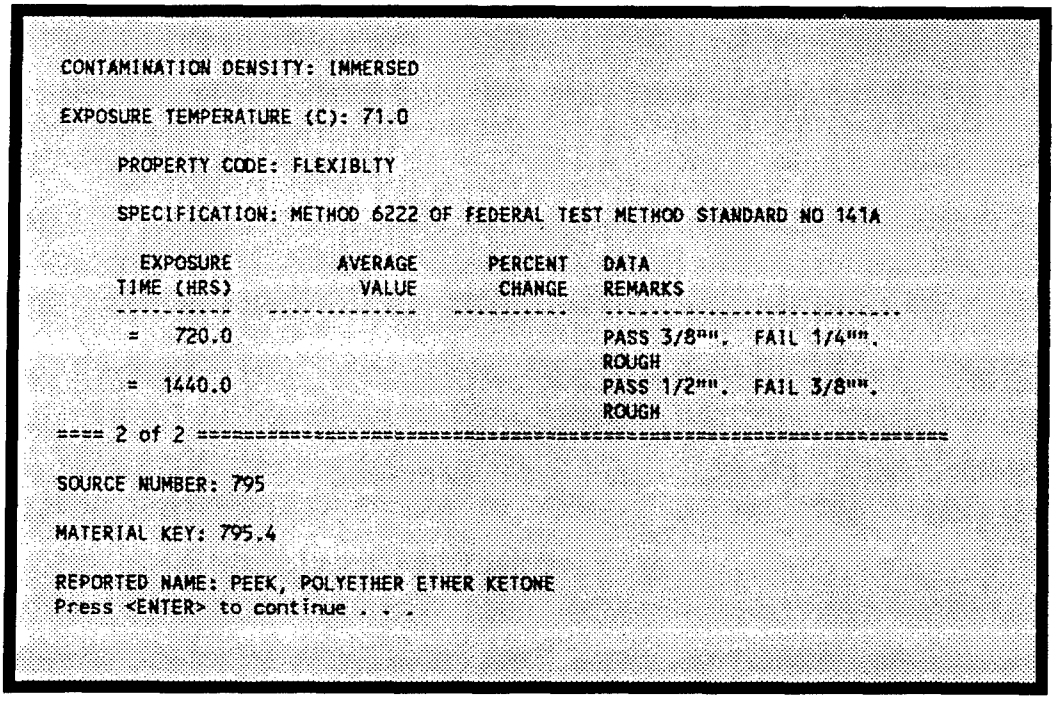

Figure 32b. Test Data -- Summary Display (Continued)

APPENDIX

EXCERPTS FROM BULLETIN ON THE CHEMICAL DEFENSE MATERIALS DATA BASE (CDMD)

FORWARD

Operation Desert Storm underscored the reality of U.S. Forces facing an adversary equipped to wage chemical warfare. Our preparedness is vital to discouraging the use if chemical warfare in any future conflicts. Our "Defense-Based Deterrence" philosophy dictates that our forces must be, and be perceived to be, able to perform their mission in any battlefield environment. In attaining this position, our equipment must be able to perform its mission before, during and after chemical agent and decontaminant exposure with little degradation. To achieve the level of hardness and decontaminability required, it is imperative that designers and developers of military hardware make material selections which address resistance to contaminated battlefield. The Chemical Defense Materials Data Base (CDMD) has been designed and structured to begin to address this need.

This data base is an expanded and greatly enhance version of the former U.S. Air Force materials data base developed in the mid-eighties. The CDMD now resides on a Digital Equipment Corporation (DEC®) VAX® computer maintained by CRDEC. The transition to a mainframe computer has enhanced both the functionality of the data base as well as its accessibility. The transition has also enabled the CDMD users to gain access to additional chemical/biological (CB) data bases through the Chemical/Biological Information System (CBIS).

DATA BASE STRUCTURE AND CONTENT

The CDMD is comprised of the following eight record types (a record is simply a structure used for storing and manipulating a group of related information elements or "fields" in a computerized data base):

1. Test Parameters and Data
2. Material Descriptions
3. Test Descriptions
4. Chemical Descriptions
5. Sources
6. Material Nomenclature
7. Chemical Nomenclature
8. Property Nomenclature

The Test Parameters and Data records contain the data detailing the effects of chemical warfare agents and decontaminants upon specific properties (e.g. physical, mechanical, electrical, optical) of materials. This information is the focus of the data base.

Changes in properties of materials are reported as a function of the time of exposure to contaminants or decontaminants. Test parameters such as exposure state, concentration, and temperature as also reported in this record.

The Material, Chemical, and Test Description records contain complete descriptions of the materials, chemicals, and test methods used in a test program.

The source records contain information identifying the report from which data was extracted. For the most part, these sources are Department of Defense (DoD) technical reports for which the Source records contain the report title, authors, performing organizations, publication data, keywords, abstract, etc.

The Nomenclature records contain synonyms, acronyms, codes and/or alternate names used to identify chemicals, materials, and material properties. These records help standardize the data base and aid in searching for information.

USING THE DATA BASE

Anyone who has used materials data bases knows that mastering the terminology can be the source of a great deal of frustration. But, using the CDMD is simple and straightforward. You do not need to be an experience or expert computer user to use the system effectively.

The CDMD employs a Query-by-Example (QBE) system for information retrieval. The QBE system is a menu-driven system but is more flexible and powerful than most menu-driven applications. Queries are formulated by entering search criteria on a form.

Searching the data base is simplified even further by allowing users to select search criteria from many pop-up menus like the one display below.

Thus, users do not need to have extensive knowledge of materials or CB nomenclature to use the system effectively. The system also includes on-line help which can be called up at any time while running the program.

ACCESSING THE DATA BASE

You do not need sophisticated or expensive hardware and software to access the CDMD. Best of all, there is no charge for using the system. The only costs you will incur are phone charges. The DoD CBIS and the CDMD are accessible via either commercial phone lines or the DoD internet system. You will need to use or emulate a DEC terminal (VT100). If you are using a personal computer and the commercial phone system, you will need a communications software package (e.g., XTALK®, PROCOMM®, SMARTERM®, etc.) in order to emulate the DEC terminal. If you are using internet, you can use the program telnet to emulate the DEC terminal.

ACCESS POLICY

The majority of the information in the Chemical Defense Materials Data Base (CDMD) *is limited to U.S. Department of Defense (DoD) agencies and their contractors and is considered to be export-controlled technical data* that can only be distributed to U.S. Government agencies and "qualified" U.S. contractors (per DoD Directive 5230.25, Withholding of Unclassified Technical Data from Public Disclosure).

Therefore, **access to the CDMD is limited to U.S. DoD agencies and "qualified" U.S. DoD contractors having a need for information related to Chemical Warfare or Chemical and Biological Defense (CW/CBD).**

CONTRACTOR QUALIFICATION

DoD contractors can apply for qualification by writing or calling the Defense Logistics Services Center (DLSC) using the address or phone numbers provided below:

Commander
Defense Logistics Services Center
ATTN: DLSC-FEB
Federal Center
Battle Creek, MI 49017-3084

Commercial: (616) 961-4358
DSN: 932-4358
Toll Free Number: 1-800-352-3572

REGISTRATION

To apply for access to the data base, request an application form by writing or calling the CBIAC using the address or phone number provided below:

CBIAC
ATTN: CDMD Registration
2113 Emmorton Park Road, Suite 200
Edgewood, Maryland 21040-1004
Commercial: (410) 676-9030

Blank

BIBLIOGRAPHY

MATERIALS SELECTION FOR CHEMICAL RESISTANCE

Shuely, Wendel J., and McNeely, James J., Material Selection Guide Derived from a Material-Chemical Comparability Database: Feasibility Based on Database and Predictive Model Evaluation, CRDEC-TR-397, U.S. Army Chemical Research, Development and Engineering Center, Aberdeen Proving Ground, MD, September 1992, UNCLASSIFIED Report (AD A266 058).

Shuely, Wendel J., "Integration of Test Methodology, Material Database, and Material Selection/Deselection Strategies for a Chemical-Material Compatibility System" in Proceedings of the Fourth International Symposium on the Computerization and Use of Materials Property Data, NIST/ASTM, Gaithersburg, MD, October 1993, UNCLASSIFIED Report.

Shuely, Wendel J., "Test Methodology for Development of Corrosion Resistant Polymeric Materials: Predictive and Experimental Methods for Chemical Resistance Screening" in Proceedings of the 12th Biennial Symposium on Managing Corrosion with Plastics, Volume XI, Chapter 19, pp 19-1 to 19-17, November 1993, UNCLASSIFIED Report.

Shuely, Wendel J., and Ince, B.S., "Thermogravimetric Method for Measurements of Equilibrium and Transport Properties Relevant to Chemical-Polymer Compatibility Evaluation" in Proceedings of the 22nd Conference of NATAS, pp 254-259, September 1993, UNCLASSIFIED Report.

Shuely, Wendel J., "Predictive Methodology for Evaluating the Interaction of Polymeric Materials with Chemicals Based on Computer-Stored Phase Diagrams," in Proceedings of the 1993 ERDEC Scientific Conference on Chemical Defense Research, 16-19 November 1993, CRDEC-SP-024, U.S. Army Chemical Research, Development and Engineering Center, Aberdeen Proving Ground, MD, August 1994, UNCLASSIFIED Report (AD A288 753).

Shuely, Wendel J., "Experimental Methodology for Evaluating Polymer-Chemical Interaction Based on a Polymer Solubility Determination" in Proceedings of the 1993 ERDEC Scientific Conference on Chemical Defense Research, 16-19 November 1993, CRDEC-SP-024, U.S. Army Chemical Research, Development and Engineering Center, Aberdeen Proving Ground, MD, August 1994, UNCLASSIFIED Report (AD A288 753).

Shuely, Wendel J., "Test Methodology for Chemical Resistance of Materials" in Proceedings of the Symposium on NBC Contamination Survivability, C. Braungart and L. D'Elicio, Eds., ARL-CR-189, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, October 1994, UNCLASSIFIED Report.

Shuely, Wendel J., "Computerized Polymer Solubility Phase Diagrams and Prediction of Polymer-Liquid Interaction," in American Chemical Society Papers, COMP 95, April 1995.

BIBLIOGRAPHY

CHEMICAL DEFENSE MATERIALS DATA BASE

McNeely, J.J.; Zamejc, E.R.; Johanns, K.J.; et al; "Development of a Chemical Defense Data Base"; Battelle Columbus Division; BCD-663-87-01; UNCLASSIFIED; U.S. Air Force ASD/XRP; AFWAL-TR-87-4053; Contract No. F33615-83-C-0132, July 1987.

McNeely, J.J.; Zamejc, E.R.; et al; "Advanced Development of the USAF Materials Data Base"; Battelle Columbus Division; UNCLASSIFIED; U.S. Air Force AFWAL/MLSA; AFWAL-TR-89-4006; Contract No. DLA 900-86-C-2045 Mod P00014 (CBIAC Task 10); March 1989.

McNeely, J.J.; McClure, J.E.; Johanns, K.J.; "Development of a Chemical Warfare Materials Compatibility Database"; Battelle Edgewood Operations; U.S. Army Chemical Research, Development and Engineering Center; Contract No. DLA 900-86-C-2045 Mod P000120, CLIN 0002EX (CBIAC Task 169); May 1990.

Kaufman, M.; Jones, S.; and McNeely, J.; Chemical Defense Materials Databook, ARL-TN-45, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, April 1995, UNCLASSIFIED Report.

CBIAC. The Chemical Defense Materials Database User's Guide Version 4.1. May 1994.

CBIAC. The Chemical Defense Materials Database Cataloguer's Guide Version 4.1. May 1994.

DEPARTMENT OF THE ARMY
CDR USACBDCOM
ATTN AMSCB CIR M
5232 FLEMING ROAD
APG MD 21010-5423

OFFICIAL BUSINESS

STANDARD B