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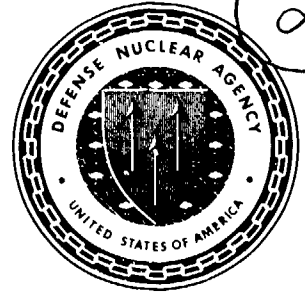
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**Chemical Weapons Process Parameters
Volume 3—Users' Guide**

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1308 Continental Drive
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Technical Report

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CONVERSION TABLE

Conversion factors for U.S. customary to metric (SI) units of measurement

| To Convert From | To | Multiply |
|--|--|------------------------------|
| angstrom | meters (m) | 1.000 000 X E-10 |
| atmosphere (normal) | kilo pascal (kPa) | 1.013 25 X E+2 |
| bar | kilo pascal (kPa) | 1.000 000 X E+2 |
| barn | meter ² (m ²) | 1.000 000 X E-28 |
| British Thermal unit (thermochemical) | joule (J) | 1.054 350 X E+3 |
| calorie (thermochemical) | joule (J) | 4.184 000 |
| cal (thermochemical)/cm ² | mega joule/m ² (MJ/m ²) | 4.184 000 X E-2 |
| curie | giga becquerel (GBq)* | 3.700 000 X E+1 |
| degree (angle) | radian (rad) | 1.745 329 X E-2 |
| degree Fahrenheit | degree kelvin (K) | $t_K = (t_F + 459.67) / 1.8$ |
| electron volt | joule (J) | 1.602 19 X E-19 |
| erg | joule (J) | 1.000 000 X E-7 |
| erg/second | watt (W) | 1.000 000 X E-7 |
| foot | meter (m) | 3.048 000 X E-1 |
| foot-pound-force | joule (J) | 1.355 818 |
| gallon (U.S. liquid) | meter ³ (m ³) | 3.785 412 X E-3 |
| inch | meter (m) | 2.540 000 X E-2 |
| jerk | joule (J) | 1.000 000 X E+9 |
| joule/kilogram (J/Kg) (radiation dose absorbed) | Gray (Gy) | 1.000 000 |
| kilotons | terajoules | 4.183 |
| kip (1000 lbf) | newton (N) | 4.448 222 X E+3 |
| kip/inch ² (ksi) | kilo pascal (kPa) | 6.894 757 X E+3 |
| ktap | newton-second/m ² (N-s/m ²) | 1.000 000 X E+2 |
| micron | meter (m) | 1.000 000 X E-6 |
| mil | meter (m) | 2.540 000 X E-5 |
| mile (International) | meter (m) | 1.609 344 X E+3 |
| ounce | kilogram (kg) | 2.834 952 X E-2 |
| pound-force (lbf avoirdupois) | newton (N) | 4.448 222 |
| pound-force inch | newton-meter (N·m) | 1.129 846 X E-1 |
| pound-force/inch | newton/meter (N/m) | 1.751 268 X E+2 |
| pound-force/foot ² | kilo pascal (kPa) | 4.788 026 X E-2 |
| pound-force/inch ² (psi) | kilo pascal (kPa) | 6.894 757 |
| pound-mass (lbm avoirdupois) | kilogram (kg) | 4.535 924 X E-1 |
| pound-mass-foot ² (moment of inertia) | kilogram-meter ² (kg·m ²) | 4.214 011 X E-2 |
| pound-mass/foot ³ | kilogram/meter ³ (kg/m ³) | 1.601 846 X E+1 |
| rad (radiation dose absorbed) | Gray (Gy)** | 1.000 000 X E-2 |
| roentgen | coulomb/kilogram (C/kg) | 2.579 760 X E-4 |
| shake | second (s) | 1.000 000 X E-8 |
| slug | kilogram (kg) | 1.459 390 X E+1 |
| torr (mm Hg, 0°C) | kilo pascal (kPa) | 1.333 22 X E-1 |

*The becquerel (Bq) is the SI unit of radioactivity; Bp = 1 event/s.

**The Gray (Gy) is the SI unit of absorbed radiation.

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SECTION 1 SCOPE

1.1 IDENTIFICATION.

The Chemical Weapons Process Parameters (CWPP) Data System has been developed to identify viable processes for the production of chemical warfare (CW) agents and other chemicals deemed to pose a risk to the objectives of the draft Convention on Chemical Weapons (CWC). CWPP also contains process information on CW precursors. CWPP assembles this information into a flexibly usable format, automated for use on a microcomputer.

CWPP has been developed to guide the user through an evaluation of the processes that lead to the production of a CW agent. This manual provides the user with a basic understanding of the Data System options and menus. Full familiarity with the capabilities of the system can best be obtained by actually using the system. A detailed discussion on utilizing the Data System for technical analysis is presented in the Chemical Weapons Process Parameters. Final Report.

1.2 PURPOSE.

The CWPP Data System is designed as a stand-alone automated system for the identification of viable chemical production processes. A methodology overview for CWPP is presented in Section 2. Additional consideration has been given to future use of the data beyond this initial effort. This may include incorporation of the data into other models. Accordingly, the data features of CWPP are designed to accommodate future portability and expandability of the system.

The automated Data System is intended for use by individuals who have a general familiarity with basic functions of the microcomputer and MS-DOS. The system has been designed so as not to require a technical or scientific background for data retrieval. However, to fully utilize the capabilities of the system, the user should have a knowledge of chemical production processes.

SECTION 2 DATA SYSTEM OVERVIEW

2.1 METHODOLOGY OVERVIEW.

The CWPP Data System was developed to provide an understanding of the processes that are necessary for chemical agent production. This understanding will provide a baseline to support analysis of technical approaches, technologies, and required R&D for verification as specified in the CWC.

The data collected for the CWPP Data System describes the process steps for the production of CW agents. The data includes the economic, technological, and chemical process conditions for the production of a CW agent or precursor chemical. In order to integrate this information into an automated system, this data has been divided into three groups.

Three groups (files) of data contain the distributed information regarding each chemical agent production process. These files are the chemical file, the process file, and the link file. The chemical file contains general information on each chemical, such as chemical name and synonyms. The process file contains information on the synthesis of each chemical. The link file contains a list of chemicals that use a particular chemical as a key feed. The specific fields of the three data files are provided in Figure 1.

2.2 DATA SYSTEM OVERVIEW.

The CWPP Data System is designed to be a user-friendly, self-teaching program. As such, this manual is written to provide: 1) the user with basic information necessary for effective use of the system, 2) information on the design and structure of data to allow for future additions of chemicals and chemical processes, and 3) sufficient technical reference information for future expansion of the system.

The Data System provides two main functions to the user. The first is the ability to recall data on the various production processes and chemicals to the screen or as printed output. Second, the user is given the opportunity to evaluate a specific production process by applying scores and weights to the ranking factors of the data to determine the relative worth of that process. A detailed discussion of these ranking factors and the rationale behind the evaluation algorithm is provided in the Chemical Weapons Process Parameters, Final Report.

CWPP is designed for use on 100% IBM-compatible microcomputers. Specific hardware requirements are presented in Section 3.1.

| Chemdb.dsf | Procedb.dsf | Linkdb.dsf |
|---|--|---|
| <ul style="list-style-type: none"> - Chemical Schedule Number - Chemical Name - Synonyms - Waste Treatment Products - Economic Availability - Military Considerations - Unproven Processes | <ul style="list-style-type: none"> - Process Step Datasheet Number - Special Name for Process Step - Key Feeds - Supplementary Feed - Reagents/Catalysts - Feed Impurities - Process Impurities - Process Step Details - Waste Handling - Technical Signature - Materials - Technical Signature - Physical - Technical Signature - Auxiliary - Technical Signature - Safety | <ul style="list-style-type: none"> - Chemical Schedule Number - Intermediate to database Chemical |

Figure 1. Database files and associated fields.

SECTION 3 DATA SYSTEM INSTALLATION

3.1 HARDWARE REQUIREMENTS.

To run the CWPP Data System, the following equipment is required:

- IBM-PC 286, 386, 486 or 100% compatible running MS-DOS 3.0 or higher.
- At least one diskette drive capable of reading a 1.2Mb 5-1/4 inch double-sided, high-density diskette (for loading of the software).
- Approximately 2 MB disk storage for CWPP program and data files.
- At least 640K total Random Access Memory (RAM) with approximately 300K available memory. Available memory may be checked by using the DOS **CHKDSK** command.

The system is developed for interactive use. Data and analysis results are produced for the user on the monitor screen but may also be produced in hardcopy if an appropriate printer is available. Provisions have been incorporated into the program to allow for printing of various data items using an Epson-compatible printer. A printer is not required for program operation.

The CWPP Data System is written for use on any IBM-PC XT or AT compatible microcomputer using MS-DOS. An EGA color monitor or better is preferred for program operation. The Data System must be loaded onto a hard drive.

3.2 STANDARD CONFIGURATION.

There is a standard configuration for CWPP. The standard configuration includes an IBM-compatible PC AT with a hard disk drive and an EGA color monitor display. Extensive testing of CWPP on alternative configurations has not been performed. An Epson 286e Dot Matrix or similar parallel printer connected to parallel printer port 1 is also standard. CWPP maintains all program, data, and temporary working files within one directory called \CWPPDS.

3.3 INSTALLING THE CWPP DATA SYSTEM.

Software for the installation of the CWPP Data System is included with the database system files on the diskettes provided. The installation process will perform the following three functions:

1. Create a directory called \CWPPDS on a disk drive specified by the user.
2. Copy all necessary system and database files into the directory \CWPPDS.
3. Create and install a batch file for executing the Data System in the root directory of the C: hard disk drive.

Before installing or using CWPP, it is important to make backup copies of the original diskettes. Do not use the original disks for installing or running CWPP. This precaution will prevent the accidental damage or erasure of the original disks/files. This will also allow the reinstallation of the Data System in its original state should this become required.

The DOS command **COPY** (or **DISKCOPY**) may be used to make backup copies of the original diskettes. The DOS command **COMP** (or **DISKCOMP**) may then be used to compare the originals with the copies. Refer to your DOS manual for further information on these commands.

In order to properly install CWPP, the user is prompted to enter the letter of the hard drive on which the system is to be installed. Normally, this will be C:. For more information about drive specifications, consult the MS-DOS user's manual.

To perform the installation process, perform the following steps:

1. Insert "Disk 1" into the A: drive
2. Exit or quit all programs and go to a DOS prompt
3. Type **A:** <Enter>
4. Type **INSTALL** <Enter>
5. Enter the drive on which to install the program (see Figure 2)
6. Insert additional diskettes as prompted

**Input drive where CWPP Data System should be installed
followed by a colon, e.g., C:**

Figure 2. Prompt from the install program and sample response.

3.4 RUNNING THE CWPP DATA SYSTEM.

Upon successful completion of the installation procedure, the file, CWPP.EXE, will reside in the root directory of the C: drive. When executed, this file will run the CWPP Data System. To execute the file from the root directory, enter the following command at the DOS prompt:

CWPP <Enter>

Should there be a problem in executing the Data System, check to make sure that the root directory is the current directory. Also, review the hardware requirements specified in Section 3.1 to ensure hardware compatibility. If the program still does not execute, reinstall the program by repeating steps 1 through 6 of Section 3.3.

3.5 PROCESSING TIME.

Processing time for utilizing the various options of CWPP varies depending upon the operation and the speed of the computer system which is being used. Generally, all operations are performed swiftly. There may be some minor delays on accessing a specific piece of chemical or process data depending on the machine.

SECTION 4 DATA SYSTEM PROGRAM OVERVIEW

4.1 PROGRAM FLOW.

The program maintains all possible process chains for the production of specific chemicals based upon precursor and feedstock information within the database. The analyst may select each of the process chains, one at a time, for evaluation. At certain steps in the process chain, the analyst may decide the best alternative is to purchase rather than produce a precursor.

A series of menus allow the user to enter choices of factor values to rate each component of a process chain. The factors are assigned numerical values by the user on a lowest-to-highest scale of 0 to 10, 10 being the best possible score. Relative weights of the factors have values between 0 and 1.0. For a detailed discussion behind the theory of entering these values, and what each factor/weight represents, refer to the Chemical Weapons Process Parameters, Final Report.

After all factors have been entered, a summary computation is performed to evaluate the current chain. Each set of factors may be saved under a user-defined filename for future reference.

The intent of this Data System is to guide the analyst through an analysis of the chemical production process, thereby determining the best approach for producing a chemical. An alternative use of the system is to query the database based on a set of user-defined search criteria. The user may search any single or multiple fields in either the chemical or process data file using a key word(s). All matches are then displayed to the analyst for review.

4.2 PROGRAM RESTRICTIONS.

CWPP is designed to allow the user to perform an analysis of the chemical production process. The algorithm which performs the actual scoring calculation is hard-wired into the system. Using a different algorithm would require program modifications.

The Data System has been designed to allow for integration into other databases. Having the data in an ASCII text file format allows for great flexibility in integrating the data into another system. However, such integration has not been attempted during the CWPP Project.

4.3 USING THE MENU SYSTEM.

All menus and submenus work similarly. To move between menu/submenu options and select options:

- Pressing <Up>, <Down>, <Right>, or <Left> arrow keys moves the cursor between options.
- Options are highlighted as the cursor is moved.
- Pressing <Enter> will select the highlighted option.

Selecting an option will either execute that option or display another set of options to further define the operation.

The <Esc> key may be pressed to back up to the previous menu while within most menus.

Figure 3 is a flow diagram which depicts the menu and submenu options.

4.4 THE HELP SYSTEM.

A key element of the user-friendliness of the CWPP Data System is the on-screen help feature. Using the help feature offers the user immediate advice regarding how to perform various actions allowed under the system.

At any point within the CWPP Data System, the user can press the Help key, <F1>, to get instant assistance. Pressing the <Esc> key will leave the help system.

4.5 DATA FORMAT.

The data within CWPP has been characterized within a "template" concept. Within this template, information on the production of CW agents is categorized by the economic, technological, and chemical process conditions under which a chemical may be produced.

Information within the Data System falls under two broad categories. First, for each chemical there is a general data page which provides information on the chemical itself. Second, each chemical has one or more information sets which provide data on the production process of that chemical.

The data collected under these two categories are accessed through the automated CWPP Data System as free format ASCII text files. The data fields which depict these categories are separated within the ASCII text files by a special delimiter. A special delimiter is also used to separate data between individual chemicals.

For a detailed discussion of the template concept, refer to the Chemical Weapons Process Parameters, Final Report.

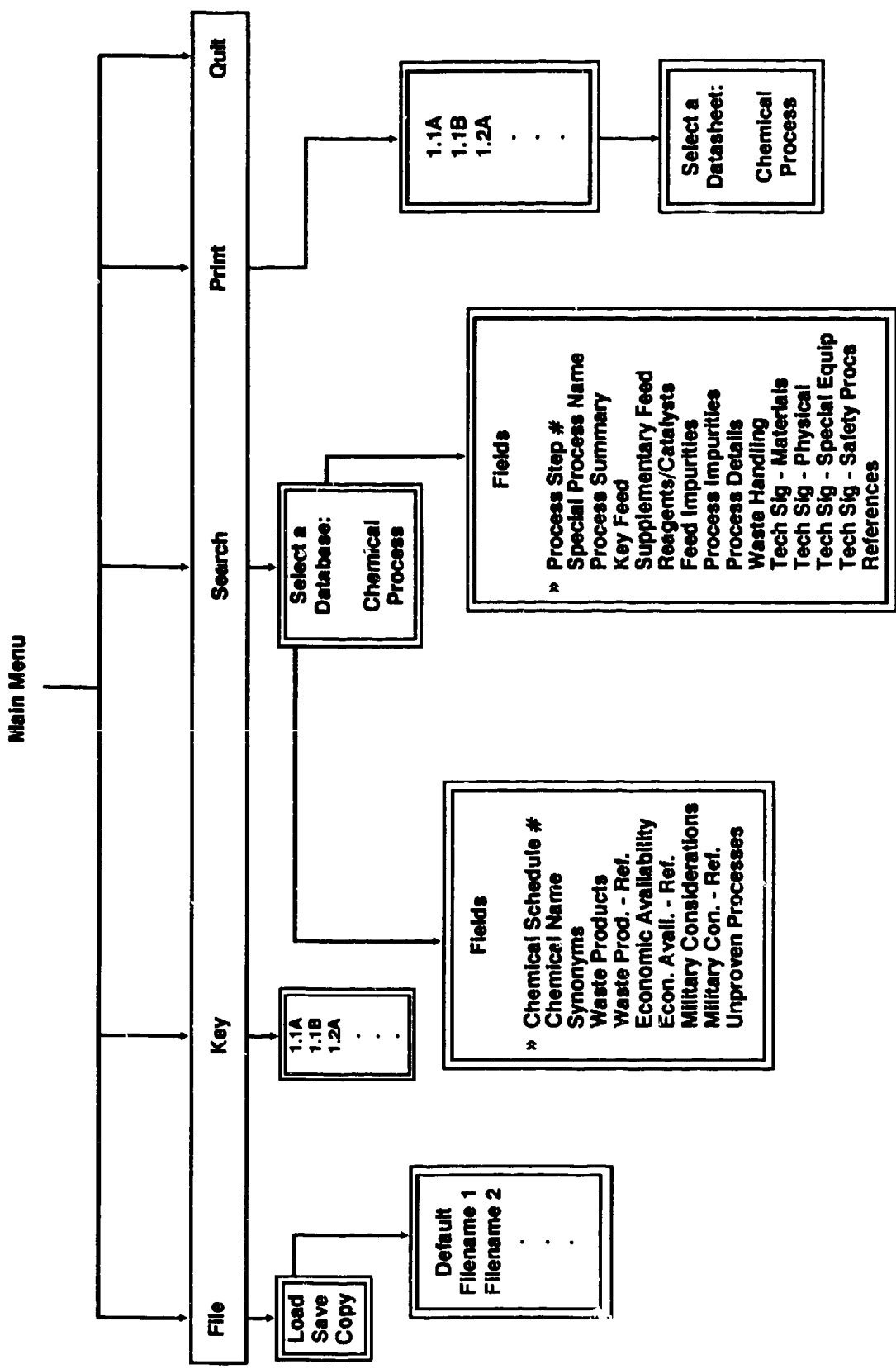


Figure 3. Flow diagram of program menus and submenus.

SECTION 5 THE MAIN MENU

The CWPP Data System Main Menu allows the user to select from five options:

- 1) **[File]** - allows the user to load the scores developed during a previous analysis. This option also allows the user to save the analysis under a user-specified filename (see Section 6).
- 2) **[Score]** - allows the user to select a chemical for analysis. The user may use the default scores or develop a unique set to perform the analysis. Under this option, the user may also review data sheets related to a specific chemical or process (see Section 7).
- 3) **[Search]** - gives the user the option to search the database of chemicals or processes based on user-specific search criteria (see Section 8).
- 4) **[Print]** - presents the user with a variety of options to obtain hard copies of analyses or data within the CWPP database (see Section 9).
- 5) **[Quit]** - terminates the program and exits to DOS (see Section 10).

Each of these options may be selected by using the **<Left>** and **<Right>** arrow keys to highlight the appropriate option and then pressing **<Enter>**. The pertinent submenus allowing for further definition of the particular menu option will then be displayed.

SECTION 6 FILE SUBMENU

Selection of the **[File]** option from the Main Menu will display a submenu that allows the user to **[Load]**, **[Save]**, or **[Copy]** scores developed during an analysis (see Figure 4).



Figure 4. The main menu.

6.1 LOAD OPTION.

The **[Load]** option of the **[File]** Submenu allows the user to retrieve the results saved from a prior analysis (see Figure 5).



Figure 5. File submenu.

Selection of the **[Load]** option will display a menu of available files (see Figure 6).

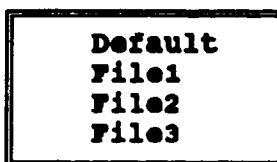


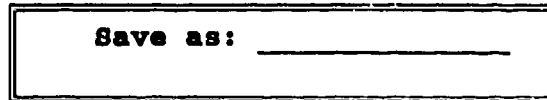
Figure 6. Menu of available files to load.

To choose a file, move the highlight bar to the desired file and hit **<Enter>**. A special file called **DEFAULT** contains the defaults for the chemical of interest. This default information is automatically loaded when a chemical is selected for analysis, but can be reloaded should the need arise to replace changes made to the scores with the default values.

6.2 SAVE OPTION.

The **[Save]** option of the **[File]** Submenu allows the user to save the scores developed during the latest analysis.

If the **[Save]** option is selected, the user will be asked to supply a filename under which to save the information (see Figure 7).



A rectangular dialog box with a double-line border. Inside, the text "Save as:" is followed by a horizontal line for text entry.

Figure 7. Prompt for entering filename.

If the filename already exists, the user will be asked whether to overwrite the information contained in it (see Figure 8).



A rectangular dialog box with a double-line border. Inside, the text "File exists. Overwrite? Y/N:" is followed by a horizontal line for text entry.

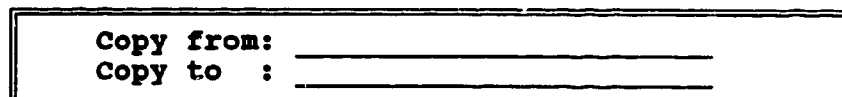
Figure 8. Prompt to overwrite during save option.

Choosing to overwrite the file will save the new information under that filename. If the user chooses not to overwrite, the program will again ask for a different filename to save under.

6.3 COPY OPTION.

The **[Copy]** option of the **[File]** Submenu allows the user to copy one file of scores to a file with a different name.

If the user selects the **[Copy]** option, the program will ask for the name of the file to copy (see Figure 9).



A rectangular dialog box with a double-line border. Inside, the text "Copy from:" is followed by a horizontal line, and "Copy to :" is followed by another horizontal line.

Figure 9. Prompt to copy a file.

It will also ask the user for the name of a file to which the information will be copied. If the filename already exists, the user will be asked if the user wants to overwrite the information contained in it (see Figure 10).

File exists. Overwrite? Y/N: _____

Figure 10. Prompt to overwrite during copy option.

Choosing to overwrite the file will copy the new information to that filename. If the user chooses not to overwrite, the program will again ask the user for a filename under which to copy the information.

SECTION 7 SCORE SUBMENU

7.1 CHAIN DESCRIPTION.

A "chain" in the CWPP Data System consists of a sequence of chemicals and processes such that every chemical in the chain has a corresponding process. The CWPP Data System uses the Schedule code numbers Schedule chemicals in the Chemical Weapons Process Parameters database to construct all possible combinations of chemicals and the proven processes that produce them for all Schedule 1, 2, or 3 chemicals. Each chain is a unique combination of those chemicals and processes. All possible chains for Schedule 1, 2, and 3 chemicals have been provided on the installation disk as individual files. These files are automatically copied during the installation process.

To begin scoring, select a chemical from the <Score> submenu. Schedule 1, 2, and 3 chemicals are presented in a scrolling text window with the chemical schedule numbers to the left with the corresponding chemical name on the right. The user browses through the submenu by pressing the <Up> or <Down> keys. Pressing <F2> will display a list of synonyms for the chemical. As an example, the display of the information for Sarin is shown in Figure 11.

The <F3> and <F4> keys allow the user access to the database information on the chemical and its processes. Pressing <F3> displays a menu containing a list of chemical information headings (see Figure 12). Moving the highlight bar to the appropriate heading and pressing <Enter> displays the selected information in a window (see Figure 13). Pressing <Esc> returns to the chemical information menu and allows the user to examine additional information in the database or to press <Esc> and return to the <Score> menu. Pressing <F4> displays a menu containing a list of process numbers (see Figure 14). Moving the highlight bar to the desired number and pressing <Enter> displays a list of information headings (see Figure 15). Moving the highlight bar to the appropriate heading and pressing <Enter> displays the selected information (see Figure 16). Pressing <Esc> returns to the process information menu and allows the user to examine additional information in the database or to press <Esc> and return to the <Score> submenu.

When the chemical of interest is highlighted in the <Score> submenu, select the chemical for analysis by pressing <Enter>. Figure 17 presents a sample listing of chemicals as presented to the CWPP Data System user.

File Score Search Print Quit F1 for help

| | |
|-------|---|
| 1.10 | |
| 1.11 | |
| 1.12A | |
| 1.12B | |
| 1.13 | |
| 1.1A | O-ISOPROPYL METHYLPHOSPHONOFUORIDATE [107-44-8] |
| 1.1B | |
| 1.2A | |
| 1.3A | |
| 1.4A | |
| 1.4B | |
| 1.4C | Sarin |
| 1.4D | GB |
| 1.4E | |
| 1.4G | |

Figure 11. Schedule number, chemical name, and synonyms.

File Score Search Print Quit F1 for help

| |
|-------------------------|
| 1.10 |
| Chemical Information |
| Chemical Schedule # |
| Chemical Name |
| Synonyms |
| Waste Products |
| Waste Prod. - Ref. |
| Economic Availability |
| Military Considerations |
| Military Con. - Ref. |
| Unproven Processes |

Figure 12. Selecting chemical information for review with F3 key.

File Score Search Print Quit F1 for help

1.10

Chemical Information

1.1A

(U)** [1.1A] is of no commercial or research interest outside of very small scale use in permitted CW defensive activities. Any party seeking militarily significant quantities will have no option other than covert production.

The USEPA databases give no indication that it is produced, imported or consumed in the US.

Figure 13. Selected chemical information displayed on screen.

File Score Search Print Quit F1 for help

1.10

1.1A.1

1.1A.2

1.1A.3

1.1A.4

1.4A

1.4B

1.4C

1.4D

1.4E

1.4G

Figure 14. A list of process numbers.

File Score Search Print Quit F1 for help

1.10

Process Information

Process Step #

Special Process Name

Process Summary

Key Feed

Supplementary Feed

Reagents/Catalysts

Feed Impurities

Process Impurities

Process Details

Waste Handling

Tech Sig - Materials

Tech Sig - Physical

Tech Sig - Special Equip

Tech Sig - Safety Procs

References

Figure 15. A menu of process information heads.

File Score Search Print Quit F1 for help

1.10

Process Information

1.1A.1

(U) Fluorination ame

Supplementary Feed

Reagents/Catalysts

Feed Impurities

Process Impurities

Process Details

Waste Handling

Tech Sig - Materials

Tech Sig - Physical

Tech Sig - Special Equip

Tech Sig - Safety Procs

References

Figure 16. Display of selected process information.

File Score Search Print Quit

| | |
|-------------|--|
| 1.10 | |
| 1.11 | |
| 1.12A | |
| 1.12B | |
| 1.13 | |
| 1.1A | O-ISOPROPYL METHYLPHOSPHONOFUORIDATE [107-44-8] |
| 1.1B | |
| 1.2A | |
| 1.3A | |
| 1.4A | |
| 1.4B | |
| 1.4C | |
| 1.4D | |
| 1.4E | |
| 1.4G | |

Figure 17. Press enter to select a chemical for scoring.

When a chemical has been selected, a chain of chemicals and processes is displayed. A separate window allows the user to scroll through a list of names for the chemical codes and processes (see Figure 18).

File Score Search Print Quit F1 for Help

| | |
|-------------------------------------|--|
| Current chain: | |
| [1.1A] | {1.1A.2}[2.1A][5.40][5.2]{2.1A.3}[2.1B] |
| [3.11] | {5.40.1}{5.2.1}{2.1B.2}[3.8A]{3.11.1}[3.9][3.10] |
| [3.8A.1] | {3.6}{3.9.1}{3.10.1}[3.9]{3.6.1}{3.9.1} |
| CHEMICAL & PROCESS NAMES | |
| 3.9 | SULFUR MONOCHLORIDE, S2C12 [10025-67-9] |
| 3.9.1 | Direct process (monochlorination of sulfur) |
| 3.6 | PHOSPHORUS TRICHLORIDE [7719-12-2] |
| 3.6.1 | Phosphorus halogenation |
| 3.10 | SULFUR DICHLORIDE [10545-99-0] |
| 3.10.1 | Sulfur dichloride formation |
| 3.9 | SULFUR MONOCHLORIDE, S2C12 [10025-67-9] |
| 3.9.1 | Direct process (monochlorination of sulfur) |

Figure 18. Reviewing a chain for scoring.

Upon pressing <Enter> the user is prompted to select the chain for scoring, or to view the next chain. Answering <N> presents an alternative chain. Pressing <Y> will allow the user to score the current chain. (see Figure 19)

```

File      Score      Search      Print      Quit      F1 for Help
-----
Current chain:  [1.1A]{1.1A.2}[2.1A][5.40][5.2]{2.1A.3}[2.1B]
                  [3.11]{5.40.1}{5.2.1}{2.1B.2}[3.8A]{3.11.1}
                  [3.9][3.10]{3.8A.1}[3.6]{3.9.1}{3.10.1}[3.9]
                  {3.6.1}{3.9.1}

Select current chain? (y or n): y
  
```

Figure 19. Selecting a chain for scoring.

7.2 ANALYSIS FOR RANKING PROCESSES.

The main function of the CWPP Data System is to aid in the analysis of the acquisition of Schedule 1, 2, or 3 chemicals, and the production capabilities of countries or groups suspected of producing or acquiring chemical weapons.

7.2.1 Assigning Factor Scores.

The factor scores are assigned as the user browses through the information pertinent to each factor. For individual steps in a chain, or single or multiple process step data sheets, the user will enter factor values between 0 and 10, with a score of 10 denoting the most desirable or least difficult and 0 denoting useless or impossible (see Figure 20).

```

File      Score      Search      Print      Quit      F1 for Help
-----
                                  3.9.1
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
c Process Step Difficulty           : 8_
d Availability of Civilian Tech     : 8_
e Equipment Uniqueness              : 6_
f Commercial Availability            : 7_
g Environmental Signature            : 8_
gp Byproducts and Waste Treatment   : 8_
  
```

Figure 20. Scoring a process.

At any time during the scoring of a process, the user may press the <F3> or <F4> keys to access information on the process or its resultant chemical. Pressing <F3> displays a menu containing a list of chemical information headings (see Figure 21). Moving the highlight bar to the appropriate heading and pressing <Enter> displays the selected information in a window (see Figure 22). Pressing <Esc> returns to the chemical information menu and allows the user to examine additional information in the database or to press <Esc> and return to the <Score> menu. Pressing <F4> displays a menu containing a list of process numbers (see Figure 23). Moving the highlight bar to the appropriate heading and pressing <Enter> displays the selected information (see Figure 24). Pressing <Esc> returns to the process information menu and allows the user to examine additional information in the database or to press <Esc> and return to the <Score> submenu.

Using the <F3> and <F4> keys the user can view any database information of significance in deciding the value for a particular factor. Once all factor values for any step in the chain have been entered, the user is presented with the resultant score and the option to buy or produce the chemical in question (see Figure 25).

File Score Search Print Quit F1 for help

```

      3.9.1
      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
  Chemical Information    Ity                : 8_
                        lian Tech        : 8_
                                          : 6_
                                          : 7_
                                          : 8_
                        e treatment : 8_
  Waste Products
  Waste Prod. - Ref.
  Economic Availability
  Econ. Avail. - Ref.
  Military Consideratins
  Military Con. - Ref.
  Unproven Processes
    
```

Figure 21. A menu of chemical Information.

```

      3.9.1
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXX
Chemical Information      Ity      : 8_
(U) [3.9] is hydrolyzed by water at room temperature at a
moderate rate, rapidly at higher temperatures. In the vapor
state, slow hydrolysis gives a mixture of HCl, sulfur dioxide,
and hydrogen sulfide. In solution, the latter two compounds
react further to polythionic acids and elemental sulfur.
Various reducing agents and some metallic oxides and sulfides
react to give elemental sulfur.
    
```

Figure 22. Displaying chemical information during scoring.

```

      3.9.1
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXX
Process Information      Ity      : 8_
Process Step #      lian Tech      : 8_
Special Process Name      : 6_
Process Summary      ity      : 7_
Key Feed      ture      : 8_
Supplementary Feed      e treatment : 8_

Reagents/Catalysts

Feed Impurities
Process Impurities
Process Details
Waste Handling
Tech Sig - Materials
Tech Sig - Physical
Tech Sig - Special Equip
Tech Sig - Safety Procs
References
    
```

Figure 23. A menu of process information.


```
3.9.1
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXX
Process Information          Ity          : 8_
3.9.1
(U) Iron filings, iodine or a trace of ferric chloride.

Supplementary Feed
Reagents/Catalysts
Feed Impurities
Process Impurities
Process Details
Waste Handling
Tech Sig - Materials
Tech Sig - Physical
Tech Sig - Special Equip
Tech Sig - Safety Procs
References
```

Figure 24. Displaying process information during scoring.

```
SCORES-- BUY 0.01, PRODUCE 0.07
Scores indicate PRODUCE decision
Press <Y> for PRODUCE <N> for BUY
>>Y
```

Figure 25. Decision to buy or produce.

Based upon the scores for the likelihood of production and for the purchase of the chemical, the user decides whether production or purchase is more likely. The scores are presented in a text window with the default decision, which is based upon calculations using the numerical scores and a factor z (a consistent bias between 0.1 and 9, applied to the technical side of the comparison), which is assigned a value along with the weights. The default's decision may be changed by typing the appropriate key, either <Y> or <N>.

Once all intermediate steps in the chain have been scored, the user is presented with the score sheet for the end chemical, the one selected when <Score> was first chosen. Scores for the end chemical, typically a Schedule 1 or 2 chemical, are slightly different from those in the intermediate steps in that one also evaluates the military

considerations and technical sophistication of integrating all the individual reaction process steps in addition to all of the previously evaluated factors. Upon consideration of the data, the user enters final scores and the entire chain is evaluated, with the final score indicating the relative likelihood of production.

When the chemical of interest is highlighted, select the chemical for analysis by pressing <Enter>.

7.2.2 Calculating Rankings.

Chains may be ranked according to the likelihood of production, determined by the scores calculated using the weights entered during analyses. Determining the rank of a chain may be done by simply comparing the final scores, obtained by printing out the results of the analyses.

Once a chain has been fully scored, and the analyses results are displayed on the screen, the user is given the opportunity to print out these results. Results printed out will be for the current chain only. It is recommended to print out each analysis during the evaluation process.

SECTION 8 THE SEARCH MENU

The **<Search>** option in the Main Menu gives the user the ability to retrieve the Schedule numbers of chemicals or processes containing specific information. The user will select the fields in which to search and the string to be found, and the computer will respond with a list of Schedule numbers or processes that contain the specified data.

The first choice the user must make is whether information should come from the chemical or process database. This choice is made from the first **<Search>** Submenu (see Figure 26). The chemical database contains all the information about the chemical while the process database contains the information about the procedures used to produce the chemical.

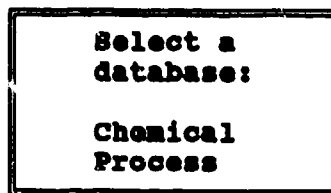


Figure 26. SEARCH submenu #1.

Once the choice of the database to be searched has been made, the user will be presented with the next Submenu to choose the fields in which the program is to look for the information (see Figures 27, 28). This Submenu contains the names of all the fields in the selected database. The user selects the fields by using the **<Up>** and **<Down>** arrow keys to move the highlight bar overtop of a field name, and then by using the **<Space Bar>** to toggle the field between selected and not selected. Selected fields will be indicated by a '*' next to the field name. Pressing **<F2>** will accept the user's field choice and prompt for the search string.

```
Fields
>> Chemical Schedule #
    Chemical Name
    Synonyms
    Waste Products
    Waste Prod. - Ref.
    Economic Availability
    Econ. Avail. - Ref.
    Military Considerations
    Military Con. - Ref.
    Unproven Processes
```

Figure 27. Field submenu for chemical database.

```
Fields
>> Process Step #
    Special Process Name
    Process Summary
    Key Feed
    Supplementary Feed
    Reagents/Catalysts
    Feed Impurities
    Process Impurities
    Process Details
    Waste Handling
    Tech Sig - Materials
    Tech Sig - Physical
    Tech Sig - Special Equip
    Tech Sig - Safety Procs
    References
```

Figure 28. Field submenu for process database.

After the user has chosen the fields to be searched, a window opens and prompts for the string for which to search (see Figure 29). The user may now enter a string of up to 35 characters which will be searched for in the fields previously specified. Pressing <Enter> will accept the string and execute the search.

```
Enter string (max 35 chars) for:
Key Feeds
Kodak_____
```

Figure 29. Prompt for search string.

Upon completion of the search, a window will open with the results of the search (see Figure 30). The information the search returns is the schedule number and name of any chemicals that are found to contain the search strings. The user will be able to browse through this list using the <Up> and <Down> arrow keys. A status bar at the top of the window will inform the user of the total number of finds and the one which is currently displayed. An unsuccessful search will produce the message "None Found".

```
RESULTS
Total: 32          Current: 1
>> 2.10
    2.4
    3.11
    3.2
    3.4
    3.5
    3.6
```

Figure 30. Result of search on chemical database.

If the user has completed a search of the chemical database, selecting the chemical of interest and pressing <F3> displays a menu containing a list of chemical information headings (see Figure 31). Moving the highlight bar to the appropriate heading and pressing <Enter> displays the selected information (see Figure 32). Pressing <Esc> returns to the chemical information menu and allows the user to examine additional information in the database or to press <Esc> and return to the <Search> menu. If the user has completed a search of the process database, selecting the process of interest and pressing <F4> displays a menu containing a list of process information headings (see Figure 33). Moving the highlight bar to the appropriate heading and pressing <Enter> displays the selected information (see Figure 34). Pressing <Enter> returns to the process information menu and allows the user to examine additional information in the database or to press <Esc> and return to the <Search> menu.

The user can return to the Main Menu by pressing <Esc>.

Select a

as

Chemical Information

Chemical Schedule #

Chemical Name

Synonyms

Waste Products

Waste Prod. - Ref.

Economic Availability

Econ. Avail. - Ref.

Military Considerations

Military Con. - Ref.

Unproven Processes

Enter string (max 35 chars) for:
Economic Avail.

Kodak _____

~~RESULTS~~

Total: 32 Current: 1

>>2.10

2.4

3.11

3.2

3.4

3.5

3.6

Figure 31. A menu of chemical information after a search.

Select a

as

Chemical Information

Enter string (max 35 chars) for:

2.10

Producers in the US: Morton-Thiokol, Rhone-Poulenc (Alcolac) (a 1990 directory gives only Alcolac). Other distributors and possible producers in recent years: Cardinal Chemical, Crucible Chemical, Dow, Phillips Chemical, Witco, M&T Chemicals, American Piorganics, ICN Biomedicals, Kodak, Serva Biochemicals, Sigma Chemical; with up to 50 industrial processors and 100 consumers. Among the USEPA databases, [2.10] appears in the original TSCA Inventory database with three producers, Witco producing 0.01-1 million lb and Ora and Alcolac with 0.1-1 million each, and one importer with no volume in 1977; in the Update, with Alcolac, Morton and Phillips producing CBI amounts; and in the Penta Consumption database, with 36 CBI listings and 20 specified products (mostly polymers and all but one listed by a single company in California).

Figure 32. Displaying the results of a search on chemical information.

Select a

Process Information

Process Step #

Special Process Name

Process Summary

Key Feed

Supplementary Feed

Reagents/Catalysts

Feed Impurities

Process Impurities

Process Details

Waste Handling

Tech Sig - Materials

Tech Sig - Physical

Tech Sig - Special Equip

Tech Sig - Safety Procs

References

Enter string (max 35 chars) for:
Process Details

Vacuum _____

~~RESULTS~~

Total: 14 Current: 1

>>1.2A.1

1.4A.1

1.4A.3

1.4A.6

1.4A.7

1.6A.1

1.6B.1

Figure 33. A menu of process information after a search.

| | |
|---|----------------------------------|
| Select a | |
| as | |
| Process Information | Enter string (max 35 chars) for: |
| | 1.2A.1 |
| <p>(U) Add [2.2A] to a stirred reactor, followed by a carrier solvent, chlorobenzene. The use of a carrier solvent in this reaction is not strictly necessary, but it makes it easier to control the slurry formed when the solid materials are added. It also helps to remove the toxic product from the solids present. To the solution, add two moles of solid [5.23] and one mole of ethanol. It may be necessary to have a better cooling medium than just water, since the reaction is highly exothermic and the temperature should be maintained at a maximum of 40 C.</p> <p>The product contains sodium chloride as a solid by-product of the reaction and [5.23] which was added to convert the liberated HCl to [3.2]. The solids are removed by filtration in a closed vacuum system in order to separate them from the highly toxic liquid product. The final product may be obtained by</p> | |

Figure 34. Displaying the results of a search on process information.

SECTION 9 PRINT

The **[Print]** option enables the user to acquire a hardcopy of a specific chemical or process datasheet. Once this option has been selected from the Main Menu, a submenu appears (see Figure 35) enabling the user to select a key chemical for which to print a datasheet. This submenu consists of two separate windows. The first is a scrolling window that contains the chemical Schedule numbers from which the user may choose. The second window contains the chemical name of the currently highlighted Schedule number. The **<Up>** and **<Down>** arrow keys move the highlight bar, and **<Enter>** selects the highlighted chemical.

File **Score** **Search** **Print** **Quit F1 for help**

| |
|--|
| 1.10 1.11 1.12A 1.12B 1.13 1.1A 1.1B 1.2A 1.3A 1.4A 1.4B 1.4C 1.4D 1.4E 1.4G |
| BIS (2-CHLOROETHYL) SULFIDE [505-60-2] |

Figure 35. Key selection submenu for print.

After a key has been selected, the Key Selection Submenu disappears, and a window opens reminding the user of the key and chemical name that was selected. The user is prompted for which datasheet chemical or process to print for that key (see Figure 36). If **[Chemical]** is selected, the chemical datasheet is printed and the user is returned to the Main Menu. If **[Process]** is selected, and only one process exists for the selected key, the process datasheet is printed and the user is returned to the Main Menu.

File **Score** **Search** **Print** **Quit F1 for help**

| |
|--|
| Selected Key: 1.4A Name: BIS(2-CHLOROETHYL)SULFIDE [505-60-2] |
| Select a Datasheet: Chemical Process |

Figure 36. Sample datasheet type selection.

If more than one process datasheet exists for the key, a window appears (see Figure 37) with a list of process numbers and their associated process names. The user is then asked to enter the number of the process to be printed. Once this choice is made, the process datasheet is printed, and the user is returned to the Main Menu.

| |
|---|
| Select Key: 1.4A Name: BIS(2-CHLOROETHYL)SULFIDE [505-60-2] |
| Process associated with selected key: 1.4A.1 Geyman (Victor Meyer-Clarke) Process 1.4A.2 Allied (Guthrie) Process. "60 C Process" 1.4A.3 Levinstein Process. "30 C Process" 1.4A.4 French Cattelain/British H3 Process 1.4A.5 South African (DESA) Process 1.4A.6 HT Process 1.4A.7 HQ (variant of [1.4A.9]) 1.4A.8 HBD. HCD 1.4A.9 US thiodiglycol process Enter # (1-9) of process to print: ___ |

Figure 37. Sample process number selection.

SECTION 10 QUIT

To exit the program from other submenus, the user must first press <Esc> a number of times to return to the Main Menu. Pressing <Esc> too many times will not have any negative effects on program operation.

Selection of the [Quit] option from the Main Menu allows termination of the program. If changes to the scores were implemented in the current analysis, the user will be asked to save these changes before quitting (see Figure 38).

```
Scores not saved.  
Save now? Y/N: _
```

Figure 38. Prompt to save current analysis.

Answering <N> will terminate the program and return to DOS. If the answer is <Y>, the user will be asked for a filename under which to store the information (see Figure 39).

```
Save as: _____
```

Figure 39. Prompt for entering filename to save.

Choosing the name of an existing file will result in the program asking if the existing file should be overwritten (see Figure 40).

```
File exists. Overwrite? Y/N: _
```

Figure 40. Prompt to overwrite existing file.

If the answer is <N>, the program will again ask for a filename. Answering <Y> will save the scoring under the chosen filename, exit the run, and return the user to DOS.

APPENDIX A

HANDLING OF MIXED PUBLIC, CONFIDENTIAL, AND CLASSIFIED DATA IN ANALYSES AND IN REPORTS FROM THE SYSTEM

The diskettes provided with the original CWPP Data System contain only unclassified data. As such, it may be distributed via floppy diskette or over non-secure telephone lines. The system may be run on non-secure computers. Any printed output from the original CWPP Data System may be printed on non-secure printers using unclassified printer ribbons.

Use of CWPP information must be compatible with the purpose for which the data is maintained. Paper waste products should be disposed of properly and all output products and storage media be labelled, protected, and handled appropriately.

APPENDIX B

ERROR MESSAGES

The CWPP Data System is designed to be user-friendly during program execution. The program continually checks for proper input. Messages prompting the user for input will appear as required by the program. Some common errors are described below.

Power failure

- Should the operation of the CWPP Data System be interrupted for any reason, such as power loss, any changes entered since the last time the scoring data was saved will be lost. Therefore, it is recommended to save changes frequently during input.

Program does not start properly

- Due to hardware problems such as hard disk failure, the program may not start or execute properly. Consult your computer's user manual for instructions on correcting the hardware problem. The program may then be reinstalled from the backup diskettes if necessary.
 - Certain MS-DOS and CWPP error messages may be encountered during installation or execution of the program. These messages, their causes, and how to correct them are listed below. Refer to the MS-DOS reference and user's manual for further assistance.

General Failure error reading drive X: Abort, Retry, Ignore?

- This is a device error. It usually means the MS-DOS could not read the data from the disk properly. This is often due to an unusable or unformatted disk or because the diskette is not inserted properly in the drive.
 - Try reinserting the diskette in the drive and closing the drive door. Press **R** for retry. You may need to obtain a new diskette.

Disk error reading(/writing) drive X:

- This is a device error. It usually means the diskette or hard disk you are attempting to access is defective or unusable.
 - Try another floppy diskette. If the problem is with the hard disk, consult your computer's user manual.

File not found

- MS-DOS could not find the file specified, or an attempt was made to rename a file with a name already present in the directory.
 - Check to see that you entered the filename correctly or try a different filename.

Insufficient disk space

- The specified disk is full and does not contain enough space or memory to perform the specified operation.
 - If the operation specifies using a floppy diskette, insert another formatted diskette and try the operation again. Another option is to delete unnecessary files from the hard drive or floppy diskette and try again.

Invalid drive or filename

- An invalid drive or filename was entered.
 - Try the command again with a valid drive name or filename. Refer to the MS-DOS user's manual for further guidance.

APPENDIX C

REFERENCED DOCUMENTS AND NOTES

Chemical Weapons Process Parameters, Final Report, Volume 1, October 1991.

MS-DOS Reference Manuals – The Users' Guide and Technical Reference Manual are referred to in this document as MS-DOS Reference Manuals. MS-DOS is the trademark of Microsoft Corporation. Exact manual titles and contents may vary depending on the document vendor or supplier of the particular copy of the operating system on a specific computer.

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August 1, 2001

MEMORANDUM TO DEFENSE TECHNICAL INFORMATION CENTER
ATTN: OCQ/MR LARRY DOWNING

SUBJECT: DOCUMENT CHANGES

The Defense Threat Reduction Agency Security Office reviewed the following documents in accordance with the Deputy Secretary of Defense Memorandum entitled, "Department of Defense Initiatives on Persian Gulf War Veterans' Illnesses" dated 22 March 1995, and determined that the documents were unclassified and cleared for public release:

DNA-TR-93-84, AD-B244408, Acoustic Resonance Spectroscopy in CW Verification Tooele Field Trial (August 1992).
DNA-TR-93-129-V1, AD-B192045, Global Proliferation – Dynamics, Acquisition Strategies and Responses, Volume 1 – Overview.
DNA-TR-93-129-V2, AD-B192046, Global Proliferation – Dynamics, Acquisition Strategies and Responses, Volume 2 – Nuclear Proliferation.
DNA-TR-91-216, AD-B163637, Harmonizing the Chemical Weapons Convention with the United States Constitution.
DNA-TR-92-180, AD-B175230, Evaluation of the Concept of a List for the BWC.
DNA-TR-92-61, AD-B167663, Basic State Party Functions and Skills Under CWC.
DNA-TR-92-66, AD-B167357, Domestic Reporting Requirements for Chemical Industry.
DNA-TR-91-213, AD-B163260, Analysis of the Interactions Between Treaties.
DNA-TR-93-70, AD-B177262, Chemical Weapons Convention Inspections of Private Facilities Application of United States Environmental and Safety Laws.
DNA-TR-92-182, AD-B173450, Commercial Products from Demilitarization Operations.
DNA-TR-91-217-V3, AD-B169350, Chemical Weapons Process Parameters, Volume 3 – Users' Guide.
DNA-TR-92-116-SUP, AD-B175292, Technical Ramifications of Inclusion of Toxins in the Chemical Weapons Convention (CWC), Supplement.
DNA-TR-92-128, AD-B175452, Task 1 Report Target Vapor Identification and Database Development.
DNA-TR-92-196, AD-B174940, Task 2 Report Algorithm Development and Performance Analysis.
DNA-TR-93-68, AD-B178109, CW Detection Instrument R&D Design Evaluation.

Enclosed is a copy of the referenced memorandum. If you have any questions, please call me at 703-325-1034.

Ardith Jarrett
ARDITH JARRETT
Chief, Technical Resource Center