

18 May 2011

MEMORANDUM FOR Chemical, Biological, Radiological and Nuclear Defense Test and Evaluation Executive, Office of the Deputy Under Secretary of the Army, Taylor Building, Suite 8070, 2530 Crystal Drive, Arlington, VA 22202

SUBJECT: Test and Evaluation Capabilities and Methodologies Integrated Product Team (TECMIPT) Recommendation for the Test Operating Procedure (TOP) 08-2-196, Simulant Selection for Laboratory, Chamber and Field Testing

1. The Collective Protection (CP) Commodity Area Process Action Team (CAPAT) has completed their review of the subject Test Operating Procedure in accordance with the DUSA-TE Instructions to the TECMIPT, the Standards and Development Plan, and the TECMIPT Standard Operating Procedure (SOP). All signatory members of the CAPAT have provided their concurrence to this TOP, with the exception of the Joint Program Executive Office for Chemical Biological Defense (JPEO-CBD).
2. The decision of the JPEO-CBD to not sign the concurrence sheet was not based on the details of the TOP. Their decision was based on the appropriateness of the information to be documented as a TOP.
3. Based on the concurrence of the CAPAT, I recommend this TOP be accepted as a Test and Evaluation Standard.



CARL M. EISSNER
TECMIPT Chair

TECMIPT Test Operations Procedures (TTOP) 8-2-196, Simulant Selection for Laboratory, Chamber and Field Testing

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CAPAT Review & Concurrence: May 2011

Test and Evaluation Capabilities and Methodologies Integrated Process Team (TECMIPT) Participants:



NIST



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REFERENCES:

(a) *Chemical and Biological Defense Program (CBDP) Test and Evaluation (T&E) Standards Development Plan*, dated 19 July 2010.

(b) *Memorandum of Understanding (MOU) Among the Department of National Defence of Canada the Secretary of State for Defense of the United Kingdom of Great Britain and Northern Ireland and the Secretary of Defense on Behalf of the Department of Defense of the United State of America concerning the Research, Development and Acquisition of Chemical, Biological and Radiological Defense Materiel*, dated June 2000. Amendment One, dated August 2006.

COLPRO CAPAT recommends approval of Test Operations Procedure (TOP) 8-2-196 Simulant Selection for Laboratory, Chamber, and Field Testing. If an organization non-concurs, a dissenting position paper will be attached.

CONCURRENCE SHEET	
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REPORT DOCUMENTATION PAGE

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15. SUBJECT TERMS Decision analysis and evaluation model; Data Analysis Team; DAT; physicochemical; simulant assessment; usability; weights; measure; goal; chemical warfare threat; collective protection; ColPro; subject matter expert; SME; agent-simulant relationship; ASR; simulant score assessment; simulant selection.						
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US ARMY DEVELOPMENTAL TEST COMMAND
TEST OPERATIONS PROCEDURE

*Test Operations Procedure 08-2-196
DTIC AD No.

25 April 2011

SIMULANT SELECTION FOR LABORATORY, CHAMBER, AND FIELD TESTING

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1. SCOPE.

a. This Test Operations Procedure (TOP) provides the standard method for preparation, planning, conduct, and reporting of the simulant selection process for use in testing components and systems. The method identifies chemicals to simulate chemical warfare threats during testing of components and systems in realistic and operationally relevant scenarios.

b. This procedure tailors simulant selection to the needs of specific tests in any commodity area where testing with chemical simulants is required.

c. Simulant selection progresses through the following phases:

(1) Framing the Problem and Defining Threat Requirements. The Program Manager (PM)/customer will identify and outline the relevant primary physical and chemical properties for compounds that will be sought during a review of scientific literature for new candidate simulants.

(2) Identifying and Screening Potential Simulants. Personnel will collect simulant data on significant physical properties. This may be accomplished by canvassing databases for candidate simulants. Searches should be conducted using defined ranges of properties (e.g., boiling point ranges and toxicity level ranges).

(3) Selecting Simulants. Personnel will input physicochemical and usability data into the decision analysis and evaluation model (paragraph 4.1.4) to select the candidate simulants whose properties best match the significant properties of the agents to be simulated. Usability data addresses practical considerations regarding the actual use of the simulants, such as detectability and material compatibility.

(4) Verifying Simulant Physicochemical Properties. Personnel will verify and document the quality of the physical property data for the model-selected simulants before any laboratory validation testing begins (paragraph 4.4).

(5) Establishing Agent-Simulant Relationships (ASRs) and Conducting Usability Testing. Personnel will validate the effectiveness and usability of the selected simulants through laboratory testing. Once the simulant has been selected, verified, and documented, it will be used to simulate the agent of interest for the specific program; however, this testing is outside the scope of this TOP and will not be discussed.

d. The test procedures described in this document should be referenced and/or incorporated into a detailed test plan (DTP) or similar document for each test in which simulant selection is used. These procedures may be modified in the DTP to accommodate specific testing requirements. Alterations, however, should be made only after a full consideration of how the changes may affect the reliability and validity of the resulting data. Any alterations, along with a description of the desired effect, and consequent changes in the assessment process must be fully described in the DTP.

(1) The simulant selection procedures described in this TOP are limited to selecting simulants for chemical warfare threats. Some or most of the procedures described in this TOP may not be applicable for selecting simulants for biological warfare agents (BWAs).

(2) If the decision analysis and evaluation model is found to be sensitive to small changes in the weights, then the decision analysis and evaluation model must be revised. A small change in the measure or goal weight (paragraph 4.1.4) may affect the ranking of the candidate simulants.

(3) The quality of the results from this selection process will depend on the accuracy of the desirable physical properties to be simulated, as identified and provided by the testing program, and on the quality and experience of the selection team. The availability of funding and resources for research will also impact the result of this process for selecting a simulant suitable for a specific program. The ASR and validation process is not described in this TOP.

2. FACILITIES AND INSTRUMENTATION.

No special facilities required.

2.1 Resources.

Physicochemical property data can be obtained from the literature and from commercial chemical and physical properties databases. Simulant selection teams will require access to both sources to search for candidate simulants. Previous simulant selection processes include:

- a. US Army Dugway Proving Ground (DPG) Fiscal Year 2006 Annual Report for Simulant Selection for Protective Equipment, Document Number WDTC-XX-09-084¹.
- b. DPG Fiscal Year 2007 Annual Report for Simulant Selection for Protective Equipment Testing, Document Number WDTC-XX-09-083².
- c. DPG Draft Final Test Report for Joint Expeditionary Collective Protection (JECP) Simulant Selection, Document Number WDTC-TR-09-070³.

2.2 Databases.

Previous simulant selection processes have used the following resources:

*Superscript numbers correspond to Appendix C, References.

Database

Agent Simulant Knowledgebase
(ASK)

Features

1. Developed by US Army Edgewood Chemical and Biological Center (ECBC).
2. Contains physicochemical properties of legacy simulants.
3. Contains physicochemical properties of agents.
4. Free to use from the Chemical, Biological, Radiological and Nuclear Defense Information Analysis Center (CBRNIAC).

Beilstein

1. One of the world's largest organic chemical databases.
2. Contains more than 10 million organic compounds.
3. Contains physicochemical properties of compounds and references to source literature.
4. Lists several different values for each physicochemical property of a particular compound with literature references. These values will need to be reconciled and verified for each candidate simulant selected.
5. Available through paid subscription.

SciFinder

1. Contains physicochemical properties of commonly used organic and inorganic compounds including references to source literature.
2. If a physicochemical property for a particular compound is not available from the literature, SciFinder will provide a predicted value.
3. Provides vendor and price information for each compound in the database.
4. Available only through paid subscription.

Knovel

1. Database of scientific literature.
2. Provides references to sources that may contain physicochemical properties unavailable in other databases.
3. Available only through a paid subscription.

Database

Design Institute for Physical Properties (DIPPR)

Features

1. Small database containing verified and validated physicochemical data.
2. All property values shown for each listed compound have been experimentally validated.
3. Available only through paid subscription to a database service such as Knovel.

Material Safety Data Sheet (MSDS)

1. Available from any vendor of the chemical.
2. MSDSs may vary slightly from vendor to vendor for the same compound.

National Institute of Standards and Technology (NIST) Chemistry WebBook

1. Database maintained by NIST containing the physicochemical properties of compounds.
2. Available for free at:
<http://webbook.nist.gov>.

3. REQUIRED TEST CONDITIONS.

3.1 Preparations for the Simulant Selection Process.

3.1.1 Resources.

a. Simulant Selection Team. A group encompassing subject-matter experts (SMEs); individuals experienced in field, chamber, and/or laboratory testing; individuals experienced with model development and database searches; and other applicable groups. The simulant selection team will meet regularly to review (and redefine as appropriate) project scope, schedule, search criteria, and documentation progress.

(1) Some of the SMEs must have extensive experience in chemical testing. Some of these SMEs must be experts in specific types of chemical testing, such as testing of filters, swatches, laboratory, chamber, field testing, or testing in other areas where simulants will be used. It is advisable to include a human-use expert as part of the selection team. Individuals who have experience with model development, database searches, and the properties of likely candidate simulant compounds should also be included.

(2) Environmental specialists and health and safety experts must also be part of the SME group that will determine the final selection of candidate simulants.

(3) The PM will determine the responsibilities of the SMEs before the simulant selection process. The PM will consider the relative importance of the opinions of each of the SMEs based on area of expertise. For example, an environmental expert's recommendation will weigh heavily in any decision about simulants selected for field trials; however, in decisions about simulants for use in a laboratory setting, that opinion may be of less importance.

b. Decision Analysis Team (DAT). An optional group, appointed by the PM, responsible for arbitrating the process, running the decision analysis software, and recording results and decision rationales. These responsibilities can also be fulfilled by the simulant selection team.

c. Simulant Assessment Panel. A group encompassing the simulant selection team and additional technical experts with chemical knowledge and experience that will be responsible for assessing each candidate simulant found by the simulant selection team.

d. Database Resources.

(1) Database software and licenses must be obtained by the test facility in conjunction with the program funding the simulant selection project. Acquiring specific database software and software licenses may take weeks to months, depending on the availability of the software and its compatibility with the available hardware.

(2) The majority of chemical/compound database software must meet the Department of Defense (DoD), or service net worthiness requirements, before approval for use and installation on government computers.

(3) Once access to the database and its software has been acquired, members of the simulant selection team will be trained on its use and capabilities. The test facility, in conjunction with the program funding the simulant selection project, will be responsible for training the simulant selection team to use the database software.

e. Laboratory. If necessary, facilities and personnel should be obtained to perform measurements of missing candidate simulant properties in accordance with (IAW) Standing Operating Procedures (SOPs) that are reviewed by the simulant selection team and the quality assurance (QA) plan of the facility where the work will be performed (paragraph 4.3.2).

3.1.2 Test Directive.

a. Before beginning the simulant selection process, the simulant selection team must be provided with a directive that details the specific test scenario.

b. The following are some scenario elements that could be specified in the directive:

(1) Commodity area (i.e., collective protection ((ColPro)), individual protection ((IP)), decontamination ((decon)), and contamination avoidance).

(2) Testing venue (i.e., field, chamber, or laboratory).

(3) Threat (i.e., type of agent ((liquid, vapor, or aerosol))).

(4) Component (i.e., swatch and filter) or whole system testing.

(5) Concept of operation (i.e., entry/exit, rest and relaxation ((R2)), and command and control ((C2)).

c. Combinations of attributes described in paragraph 3.1.2.b will constitute a testing scenario.

3.2 Documentation.

a. All decisions made by the simulant selection team, the DAT, and the simulant assessment panel during the simulant selection process must be documented and traceable. The documentation will support verification and validation (V&V) of the simulant selection process outcome.

b. The documented information will include:

(1) The rationale for selecting the physical properties of the agent that will be simulated by the candidate simulants.

(2) The rationale for selecting SMEs.

(3) The rationale for selecting a specific database as a resource.

(4) The rationale for using specific software for model development and assessment.

(5) The rationale for selecting the screening criteria.

(6) The rationale for selecting the search criteria.

(7) The rationale for selecting a candidate simulant for a specific chemical warfare threat.

3.3 QA/Quality Control (QC).

a. The property data gathered for the candidate simulant must be verified by the simulant selection team. Only a chemical that has verified data can be ranked as a candidate simulant.

b. A combination or any one of the following four methods may be used to verify the candidate simulant data:

(1) Literature/Database Verification. The candidate simulant data will be corroborated with information from scientific journals and databases. To verify a value, the simulant selection team will find another source (accepted by the simulant selection team) that reports a similar value. The selection team will determine an acceptable range of similarity and an acceptable range of temperatures (such as temperature ranges used in the parameter searches) for each property.

(2) SME Verification. The candidate simulant data will be reviewed and verified by the SMEs who are most familiar with the compound of interest. This verification is based on the experience of the SMEs and depends on SME consensus. This method is more subjective than the other methods and should be used with caution.

(3) Modeling. A predicted modeled value and bounds on modeling error will be used to verify a value (if modeling prediction is possible). The value will be considered verified if it falls within the range predicted by the model. If a candidate simulant is ranked high after verifying the data through modeling, then the simulants may be chosen for laboratory verification. Modeling techniques may include numerical methods (e.g., molecular modeling), calculation, and estimation; however, not all models are of the same quality and caution should be used.

(4) Laboratory Verification. During the selection process, if a high-ranked candidate simulant has unverified or modeled values, then laboratory experiments may be conducted for verification at the discretion of the simulant selection team. The decision of whether to conduct laboratory trials will depend on the ranking of the candidate simulant, with preference for higher ranked candidates.

4. TEST PROCEDURES.

a. The simulant selection process will consist of five phases, starting from the point at which the need for a simulant is identified and ending with selection and validation of the best simulant (Figure 1). The five phases are described in paragraphs 4.1 through 4.5.

b. Only four of the phases are covered in this TOP. Establishing ASRs and conducting usability testing/validation procedures are outside the scope of this TOP and will not be described.

4.1 Phase 1: Framing the Problem.

a. Correctly framing the problem is essential for a successful selection of simulant(s). Incorrectly framing the problem will permit the selection process to identify simulant that does not represent the key properties of an agent. For example, if liquid viscosity is given a high weight in the selection of a simulant for an infrared (IR) detector trial, the selected simulant will likely be a poor representative of the agent and may not be detected by the IR camera.

b. To frame the problem, the characteristics and properties must be identified of the agent needing a simulant (paragraph 4.1.1). Other considerations that impact the selection of the best simulant must also be identified (paragraph 4.1.1). The properties of interest (paragraph 4.1.2) and other evaluation factors (paragraph 4.1.3) will then be used to develop a decision analysis and evaluation model (paragraph 4.1.4).

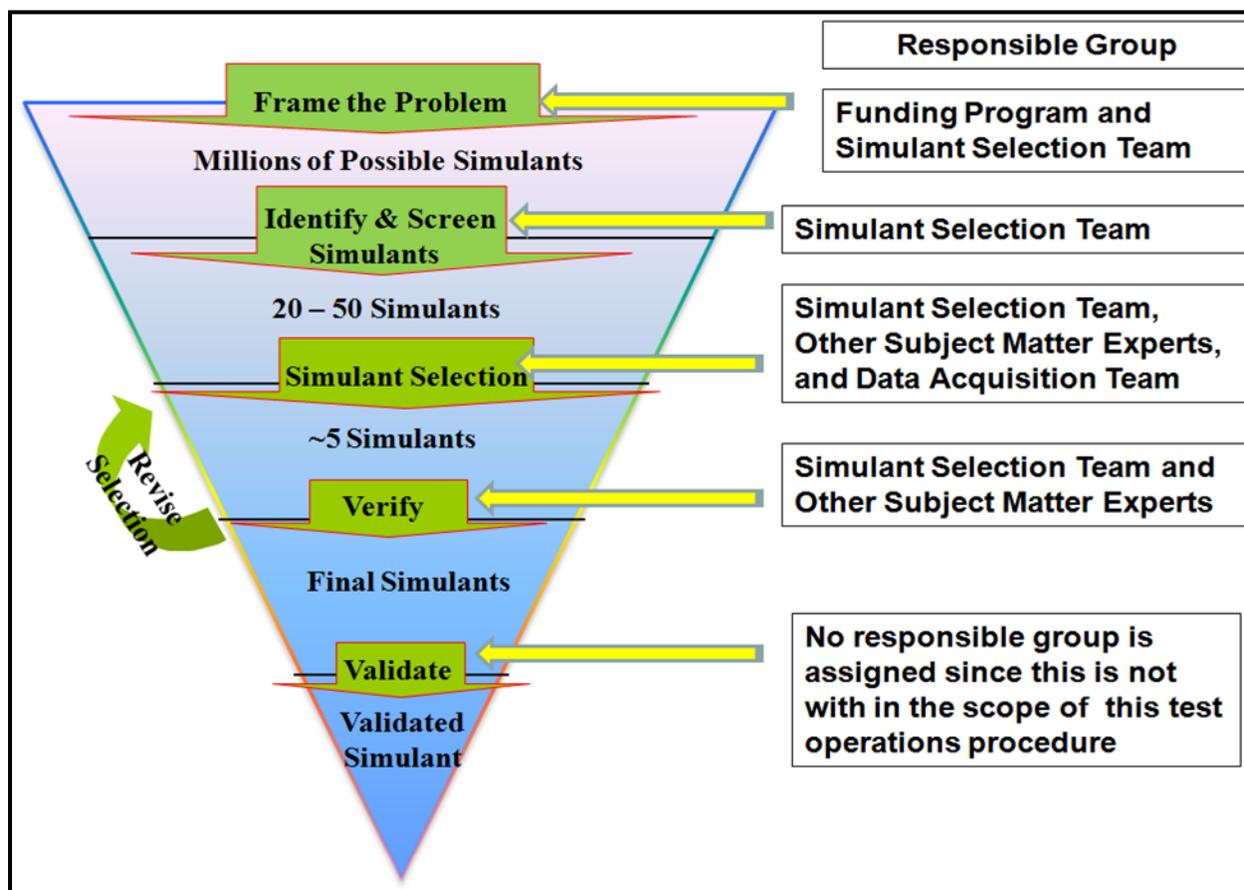


Figure 1. The five phases of the simulant selection process.

c. The properties of interest (paragraph 4.1.2) will be used to select suitable tools and databases from which the candidate simulants will be chosen. There are many chemical databases available that have different emphasis, strengths, and weaknesses. The simulant selection team will need to select a set of resources likely to give useful results. These databases can contain millions of potential simulants.

4.1.1 Phase 1A: Threat Requirements and Definitions.

In the first phase, the application for which simulants are required will be defined by five attributes:

a. **Capability Area.** The capability area is the most basic attribute of the application. It is the chemical biological (CB) defense commodity testing area(s) for which the user needs a simulant. Capability areas include protection, detection, and decontamination. Capability areas may contain sub-capability areas. For instance, sub-capability areas of detection include standoff detection and point detection; sub-capability areas of protection include IP and ColPro.

b. Scenarios. After the capability area is defined, the more specific scenario(s) of interest is determined and described. For example, a possible scenario might include an aerosol, vapor, or liquid challenge on a semi-permeable or impermeable material or filter. The scenario should be described in as much detail as possible, which will allow all participants (e.g., tester, analyst, and manager) to understand how the simulant is to be used. The scenarios will be based on the program objectives for which the simulants are being selected.

c. Agents of Interest. Next, the agents of interest are identified along with their physical and chemical properties. Agents of interest are compounds that might be considered a threat in the scenario under consideration.

d. Agent State. Testers must consider the physical state (aerosol, vapor, liquid, particulate, etc.) in which the agent would most likely be found in the given scenario. Possible dissemination methods should be taken into account, as they will further define the characteristics of the threat (such as concentration levels) and affect what state the agent might be in. For example, an agent that would normally be found as a liquid at a scenario's ambient temperature may become an aerosol or vapor threat when sprayed. The physical state of the threat is defined by requirements documentation (e.g., the operational requirements document or capabilities production document) and by input from stakeholders that have an interest in the outcome of testing.

e. Specific Test Application. The specific test application refers to the type and location of the specific test to be conducted. Considerations include whether the simulant is needed for indoor (i.e., chamber or laboratory) or outdoor testing, the specific location, and the purpose of the testing. Also, the application will include a description of the specific test methods being considered, such as swatch, filter, or man-in-simulant testing. These factors will have a significant effect on which simulants are feasible candidates.

4.1.2 Phase 1B: Properties of Interest.

a. The information generated in Phase 1A (paragraph 4.1.1) will be used to identify the agent characteristics or properties that must be simulated and other important factors that impact the choice of the best simulant for a particular application.

b. In Phase 1B, the properties of interest will be determined, and other evaluation factors will be identified. This information will lead to the development of the decision analysis and evaluation model (paragraph 4.1.4), which will account for all relevant properties/factors.

(1) To determine which agent properties must be matched, testers will first cultivate a good understanding of key interactions (chemical, physical, etc.) between the agent and the type of system being tested. The properties that govern the key interactions between the agent and the system are the properties that testers seek to match in searching for a simulant.

(a) For permeation testing of swatch materials, key interactions include the reaction between the agent and the test material, the speed that agent diffuses through the material, agent

vapor pressure, agent heat of vaporization, and the particle size distribution of the challenge aerosol.

(b) The properties that govern key interactions differ for each test method. A good simulant in one test setting could be a poor simulant in another.

(2) An extensive list of potential properties of interest and a rationale for including each property in the simulant search will be generated by the simulant selection team that will identify the most important set of physicochemical properties based on the attributes defined in paragraph 4.1.1. The following are examples of properties for swatch permeation testing: heat of vaporization, molecular dipole, vapor pressure, liquid density, surface tension, and viscosity (paragraph 4.1.4).

4.1.3 Phase 1C: Evaluation Factors.

a. Physicochemical properties are some of the important factors to consider when choosing a simulant. Usability factors, such as safety, environmental impact, flammability, shock sensitivity, explosive hazard, and stability of the simulant must also be considered. Although the properties of a compound might very closely replicate the properties of the agent of interest, difficulty in obtaining, transporting, or disposing of the simulant could still preclude its selection. Some usability criteria should be included when screening potential simulants.

b. The following list of usability factors may serve as a starting point to determine the simulant evaluation factors for a particular test application:

- (1) Medical/safety/human interaction.
- (2) Environmental impact.
- (3) Detection (analytical/referee).
- (4) Application/dissemination.
- (5) Stability.
- (6) Cost and availability.
- (7) Disposal/transport.
- (8) Storage.
- (9) Material compatibility.
- (10) Apparent presence in background.

c. To determine other evaluation factors, input from users, the testing community, and SMEs may be required. SMEs can provide information on the capabilities of the simulants under consideration, while user representatives and testers help to determine which factors are the most important to the particular testing application.

d. All evaluation factors will be reviewed by the simulant assessment panel to identify which are the most relevant, independent, and discriminating for selecting simulants. These factors will become part of the decision analysis and evaluation model, described in paragraph 4.1.4.

4.1.4 Phase 1D: Model Development.

a. A decision analysis and evaluation model will be developed as part of the simulant selection process. This model must be based on the established methods such as linear models and sensitivity analysis. The simulant selection team (based on sponsor concurrence) may elect to choose a separate DAT or act as the DAT, if the team has suitable qualifications, to monitor the process and run the decision analysis software.

b. The decision analysis and evaluation model will consist of a set of evaluation criteria, which will be derived from the physicochemical properties and usability factors identified in Phases 1B and 1C (paragraphs 4.1.2 and 4.1.3). The criteria must be relevant to the situation being addressed and be independent from one another. The criteria must also allow for discrimination between simulants.

c. The decision analysis and evaluation model can be structured in the form of a hierarchy (Figure 2). The higher-level divisions are categories of relevant physicochemical and usability properties. Each of the higher-level divisions contains physicochemical or usability measures. The evaluation measure quantifies the usability criteria of the candidate simulant as well as the physicochemical criteria similarity of the candidate simulant to the agent of interest (paragraph 4.3.3.1).

(1) The simulant selection team will choose the appropriate software for model development and assessment. Logical Decisions[®] for Windows[™] (LDW), which has been used in previous simulant selection programs, or other commercial off-the-shelf (COTS) software with similar capabilities can be used for this purpose. Figure 2 shows an LDW graphic of the model hierarchy used to choose mustard (HD) permeation simulants. Figure 3 shows an LDW graphic of the physicochemical and usability measures of HD (the width of a column for a property represents the weight assigned to that property).

(2) Alternatively, a spreadsheet could accomplish the same work by implementing the simple calculations that constitute the model. Tables 1 and 2 present the spreadsheet used to select battlefield contaminants (BFCs).

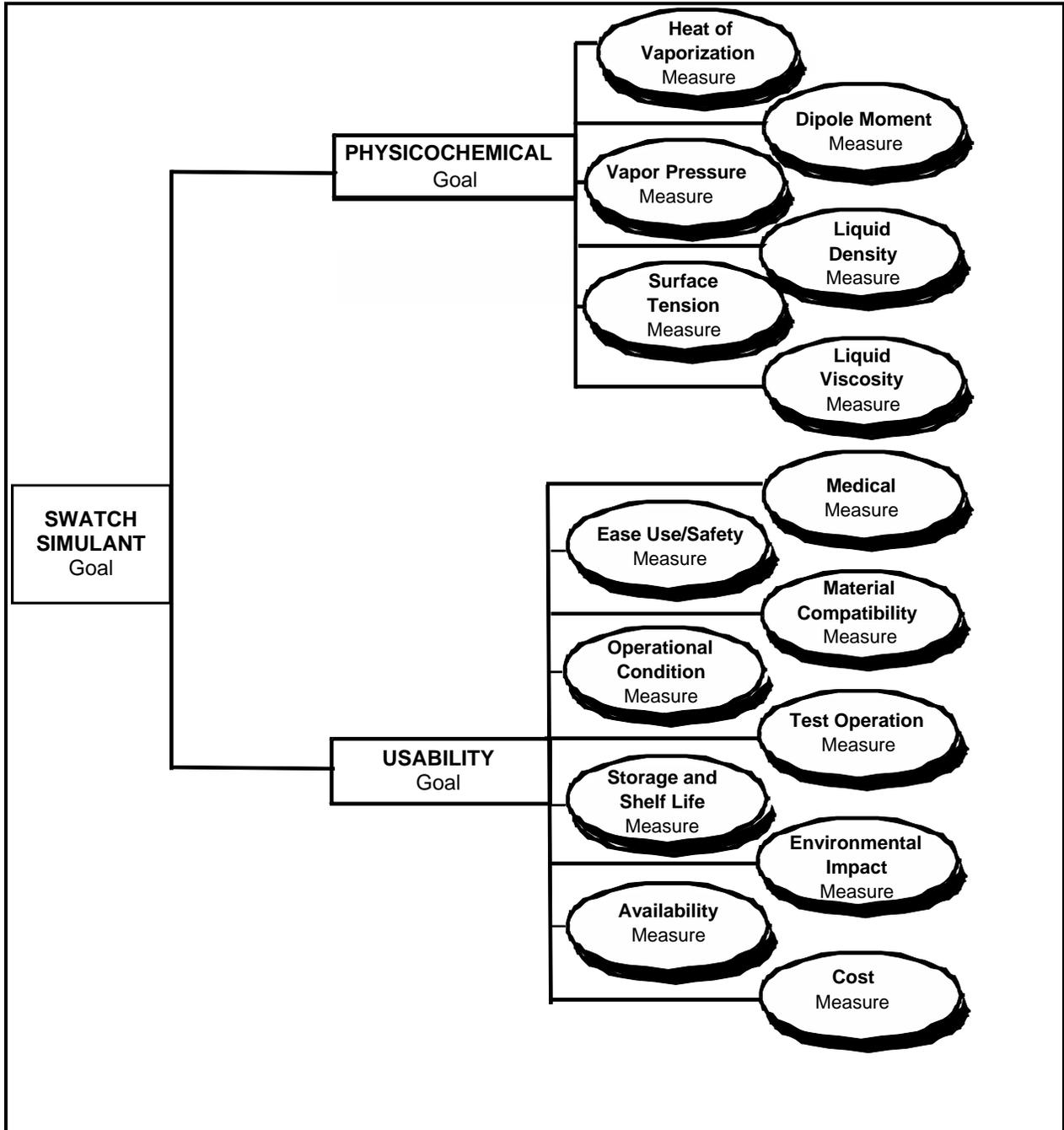
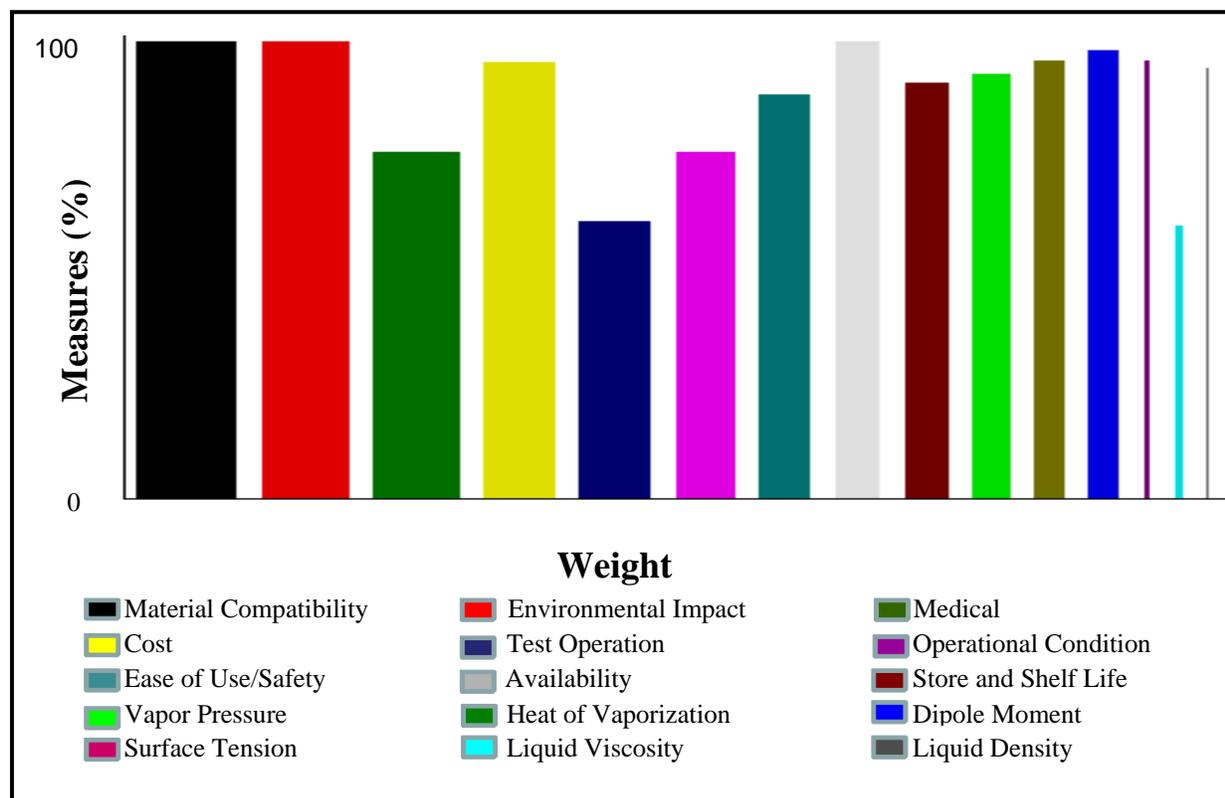


Figure 2. Sample decision analysis and evaluation model hierarchy for HD.



Note 1: The width of a column for a property represents the weight assigned to that property. The numerical values of measure represent the percentage value of the properties. A value of 100 means that the criterion for the specific property has been fully met, whereas 0 means that the criterion is not met.

Note 2: Additional information is provided in the DPG Final Test Report for JECF BFC Selection Process, Document Number WDTC-TR-09-028⁴

Figure 3. Sample physicochemical and usability measures.

d. The measures in a decision analysis and evaluation model will be a mix of quantitative (e.g., physicochemical properties, and cost) and qualitative (e.g., environmental impact) factors. For the purpose of this TOP, two types of measures are used.

(1) The usability measures determine how useable a simulant is in a particular application (field, chamber, or laboratory). With the exception of cost, most of the usability measures are qualitative measures.

(2) The physicochemical measures include the physical and chemical properties of the candidate simulants. Most of the physicochemical measures are quantitative measures.

TABLE 1. CALCULATION OF OVERALL SCORES FROM PROPERTY SCORES FOR
SELECTED BATTLEFIELD CONTAMINANTS.

BATTLEFIELD CONTAMINANT	TYPE/ CATEGORY	PREVALENCE SCORE	LIKELIHOOD SCORE	DURATION SCORE	NATIONAL FIRE PROTECTION ASSOCIATION (NFPA) HEALTH SCORE	CHEMICAL PROPERTIES SCORE	OVERALL SCORE
Acetic acid	Acids	10	0	10	0	12	32
Acids (caustic, hydrochloric)	Acids	0	0	0	0	9	9
Peracetic acid	Acids	10	10	0	0	13.5	33.5
Red fuming nitric acid	Acids	0	0	0	0	13.5	13.5
Sulfuric (battery) acid	Acids	10	0	0	0	9	19
Contact cement	Adhesives	0	0	0	5	0	5
Glue stick	Adhesives	0	0	0	10	0	10
Tack adhesive putty	Adhesives	0	0	10	10	0	20
Amines	Bases	0	0	10	0	9	19
Ammonium hydroxide	Bases	0	0	10	0	9	19
Bases (alkalis)	Bases	10	10	10	0	9	39
Morpholine	Bases	10	10	10	0	13.5	43.5
Potassium hydroxide	Bases	0	0	10	0	9	19
Sodium hydroxide	Bases	0	0	0	0	9	9
Animal waste	Biological waste	10	0	20	5	0	35
Blood	Biological waste	0	10	0	5	0	15
Body fluids	Biological waste	0	10	0	5	0	15

TABLE 2. DECISION ANALYSIS AND EVALUATION MODEL WEIGHTS FOR SWATCH, CHAMBER, AND FIELD TESTING, AS USED FOR COLPRO, SOMAN (GD), AND HD SIMULANT SELECTION

FACTOR	SWATCH WEIGHT	CHAMBER WEIGHT	FIELD WEIGHT
Physicochemical – heat of vaporization	22	16	4
Physicochemical – molecular dipole	22	16	4
Physicochemical – vapor pressure	24	19	5
Physicochemical – surface tension	0	0	0
Physicochemical – viscosity	6	4	1
Physicochemical – molar volume	8	6	1
Medical	2	3	14
Ease of use/safety	0	0	14
Material compatibility	1	4	7
Storage and shelf life	6	14	16
Environmental impact	3	6	6
Availability	2	4	10
Sum	100	100	100

e. Definitions and threshold levels will be developed for each measure. For example, the simulant selection team could define a level of toxicity that would render all candidate simulants above that level too toxic for use. These definitions are important for ensuring that all participants conducting the assessment will evaluate the candidate simulants in the same way.

f. The final step in model development is determining weights for the goals and measures, based on their relative importance to the specific test application. Then the weights will be used in Equations 1 and 2 to assess the candidate simulants. To determine the weights, 100 points will be distributed amongst each level of the model hierarchy, using various elicitation techniques. The particular weighting technique that is used will depend on each application.

Equation 1

$$g_j = \sum_{i=1}^k \frac{w_i m_i}{100}$$

Where:

- g = the score for each goal out of 100.
- w_i = the weight for each measure, a portion of the 100 total points.
- m_i = each measure which is between 0 and 100.
- k = the total number of measures in the jth goal.
- i = counting variable for measures.
- j = counting variable for goals.

Equation 2

$$S = \sum_{j=1}^n \frac{W_j g_j}{100}$$

Where:

- S = the overall simulant score out of 100.
- W = the weight for each goal, a portion of the 100 total points for goals.
- g = the score for each goal out of 100.
- n = total number of goals.
- j = the counting variable for goals.

g. Model development is an iterative process. Initial weights will be derived by the simulant selection team, and refined by the SMEs. The model may not be complete until Phase 3 of the simulant selection process (paragraph 4.3). However, the initial model will guide the search for candidate simulants by placing emphasis on the most important properties.

h. Sample models, including weights and measure definitions and performance scales are shown in Tables 2 and 3.

4.2 Phase 2: Potential Simulants Identification and Screening.

Databases can contain millions of potential simulants. This phase reduces the database to a manageable list of 20 to 50 simulants per agent to be considered during a selection meeting with the simulant selection team. The targeted list is produced by screening the database (paragraph 4.2.1) to eliminate thousands to millions of compounds with less desirable characteristics. After the list of compounds in the database has been reduced to a manageable number, the database will be searched (paragraph 4.2.2) for compounds that match the relevant physicochemical properties of the agent.

4.2.1 Phase 2A: Apply Screening Criteria.

a. Screening Criteria

(1) The screening can be based on any number of criteria for which a minimum threshold must be met. For example, for field testing, simulants will have to be approved for outdoor dissemination, unless there is an existing approval. Sample screening criteria are provided as Table 4.

(2) The screening criteria will be determined individually for each application. The screening criteria can be related to any relevant factor (e.g., properties, safety) for which a minimum threshold can be identified; if a simulant does not meet the minimum threshold, then it is removed from consideration.

b. Basic screening criteria should be applied to the database searches first. Screening the compounds in the databases can greatly improve the quality of the list because the vast majority of compounds can be eliminated. For example, most chemical agents are liquids at 25 °C and 1 atmosphere (atm). Therefore, it is often appropriate to accept only simulants that are liquids at such conditions by screening for compounds with sufficiently high boiling points.

TABLE 3. EXAMPLE OF SCALES FOR SWATCH, CHAMBER, AND FIELD TESTING AS USED FOR GD AND HD SIMULANT SELECTION

FACTOR	DEFINITION	SWATCH PERFORMANCE SCALE	SWATCH RATIONALE	CHAMBER PERFORMANCE SCALE	CHAMBER RATIONALE	FIELD PERFORMANCE SCALE	FIELD RATIONALE
Physicochemical – Surface tension	The surface tension of the simulant that should mimic the agent of interest.	ASK relevance score.	Surface tension should be measured at 25 °C; measurements between 20 and 30 °C are acceptable.	ASK relevance score.	Surface tension should be measured at 25 °C; measurements between 20 and 30 °C are acceptable.	ASK relevance score.	Surface tension should be measured at 25 °C; measurements between 20 and 30 °C are acceptable.
Physicochemical – viscosity	The dynamic viscosity of the simulant that should mimic the agent of interest.	ASK relevance score.	Viscosity should be measured at 25 °C; measurements between 20 and 30 °C are acceptable.	ASK relevance score.	Viscosity should be measured at 25 °C; measurements between 20 and 30 °C are acceptable.	ASK relevance score.	Viscosity should be measured at 25 °C; measurements between 20 and 30 °C are acceptable.
Medical	The potential for adverse health effects presented by the simulant under the conditions of the test; primarily based on health rating (HR) – an accepted summary of toxicity, on a convenient 0 to 4 scale. This work is an estimate; the final decision comes from the Human Use Committee.	100 – No health effects, minimal safety equipment required: HR 0 75: HR 1 50: HR 2 25: HR 3 0: Significant health effects if exposed; requires use of full protective suit/mask: HR 4.	Low weighting because swatch teams often use full safety equipment.	100 – No health effects, minimal safety equipment required: HR 0 75: HR 1 50: HR 2 25: HR 3 0: Significant health effects if exposed; requires use of full protective suit/mask: HR 4.	Higher weighting because chamber teams often use full safety equipment, but the decontamination team does not.	100 – No health effects: HR 0 75: minimal safety equipment required: HR 0 50: HR 1 25: HR 2 0: HR 3 or 4.	Field workers are exposed and prefer a simulant that does not require them to wear safety equipment.

TABLE 4. SAMPLE SCREENING CRITERIA

CRITERIA	COMMENTS	STAGE
Physical properties	Only consider compounds that pass the physical property screening.	Beilstein/ ASK
COTS	Only COTS compounds will be considered. Compounds will not be synthesized for this test.	SciFinder
Organic	Compounds must have at least one carbon atom.	Beilstein/ ASK
Melting point	Compounds must be liquid at temperature of testing – melt below 0 °C.	Beilstein/ ASK
Boiling point	Compounds must be liquid at temperature of testing – boil above 60 °C at or below 760 torr of pressure. Already applied.	Beilstein/ ASK
No stench	Reject any compound that is predicted to have a stench: reject any compound with the elements: selenium or tellurium, because such compounds will have a stench if their vapor pressure is high enough to meet the vapor pressure criterion. Also reject compounds that have a stench on the MSDS. NOTE: Do not reject sulfides because they resemble part of persistent nerve agent (VX), and because sulfides match detection properties of agent in flame photometric detectors (FPD).	Beilstein/ ASK
Chemical Abstracts Service (CAS) number	Compound must have a CAS number, as a key to find information about the compound.	Beilstein/ ASK
Single product	Simulant should not be a mixture. Mixture properties are hard to predict, even if all component properties are fully known. Also, composition changes during use.	Beilstein/ ASK
Safety	There will be NO radioactive elements! Reject compounds with a 1-letter or 2-letter agent designation.	Beilstein/ ASK
Detectability	This particular program requires real-time detection down to miosis levels. The miosis level of VX is very low, so simulant have to be detected to extremely low levels; therefore, use MINICAMS [®] with FPD detector (simulant must contain phosphorus or sulfur). A nitrogen-containing simulant is acceptable for swatch or chamber testing and is acceptable for field testing.	Beilstein/ ASK
Stability and reactivity	Reject organometallic compounds, e.g., those containing Boron, Arsenic, or Bismuth. Reject thiols, disulfides, boranes, acids, partial esters that have a free acidic proton, acid anhydrides, aldehydes, phenols, silicon halides, acyl halides, sulfonyl halides, isocyanates, isothiocyanates, chloroformates, nitro compounds, nitrates, orthoformates, phosphites, sulfates, sulfonates, and silicates. NOTE: These functional groups make a compound hygroscopic, reactive, or unstable. In addition, some compounds containing these groups produce toxic or corrosive products in the presence of air, water, or light. Reject some compounds by reading the MSDS for hygroscopic properties.	Beilstein/ ASK

TABLE 4. CONTINUED

CRITERIA	COMMENTS	STAGE
Functional group	Identify the major functional group of each simulant, e.g., ester. Only consider the best few compounds with each functional group for the simulant selection. The number of simulant containing each group to be considered depends on the scope of the simulant selection. In addition, consider more compounds that have more favorable functional groups.	SME review
Availability	Simulants shall be in stock from a reliable vendor. Try Sigma-Aldrich, then Fisher Scientific, Alfa Aesar, and Mallinckrodt Baker. Other vendors may be appropriate.	Vendor data
Cost	Less than \$100 per gram is the cost threshold for swatch testing. For the most promising compounds, get a quote for a 55-gallon drum. (During the selection process lower cost thresholds are used for chamber test and for field testing.)	Vendor data
Initial scores	Once all data have been gathered for each compound, sort the compounds by preliminary average physicochemical scores and only consider the higher-scoring compounds.	SME review
SME review	Reject any compound deemed unsuitable by a SME; document the reason. In particular, alkenes, alkynes, ethers, bromine compounds, and iodine compounds tend to have unfavorable chemical properties but may still be appropriate. Protic compounds like alcohols, primary amines, or secondary amines do not mimic agent. Any compounds in these categories should be reviewed by the SMEs.	SME review

4.2.2 Phase 2B: Search Criteria Application.

a. After appropriate screening criteria have been applied, the most important properties (as determined by the decision analysis and evaluation model) will be used to generate the search criteria. Search criteria should be established for no more than five parameters, thus focusing the search on the most important criteria. The use of more than five parameters is likely to result in search criteria that are too restrictive.

(1) The databases are unlikely to have data available for all the desired parameters for every compound. Therefore, using too many search parameters may eliminate desirable candidate simulants because of missing information in the databases.

(2) A one-parameter search is also not recommended. The results from a one-parameter search will include many compounds that have poor matches for properties other than that included in the search. A wide multi-parameter search will almost always give more refined results than a narrow one-parameter search (Figure 4).

b. Some of the most important properties may be unavailable in a database. If the data are unavailable, the team should find a surrogate property that could be used to conduct the search. The surrogate property should be closely related to unavailable property data. This will require a revision to the decision analysis and evaluation model. For example, the heat of

adsorption on activated charcoal is an important factor affecting the performance of a simulant for filter testing. Values for this property are rarely available in literature, so the heat of evaporation should be used as a surrogate.

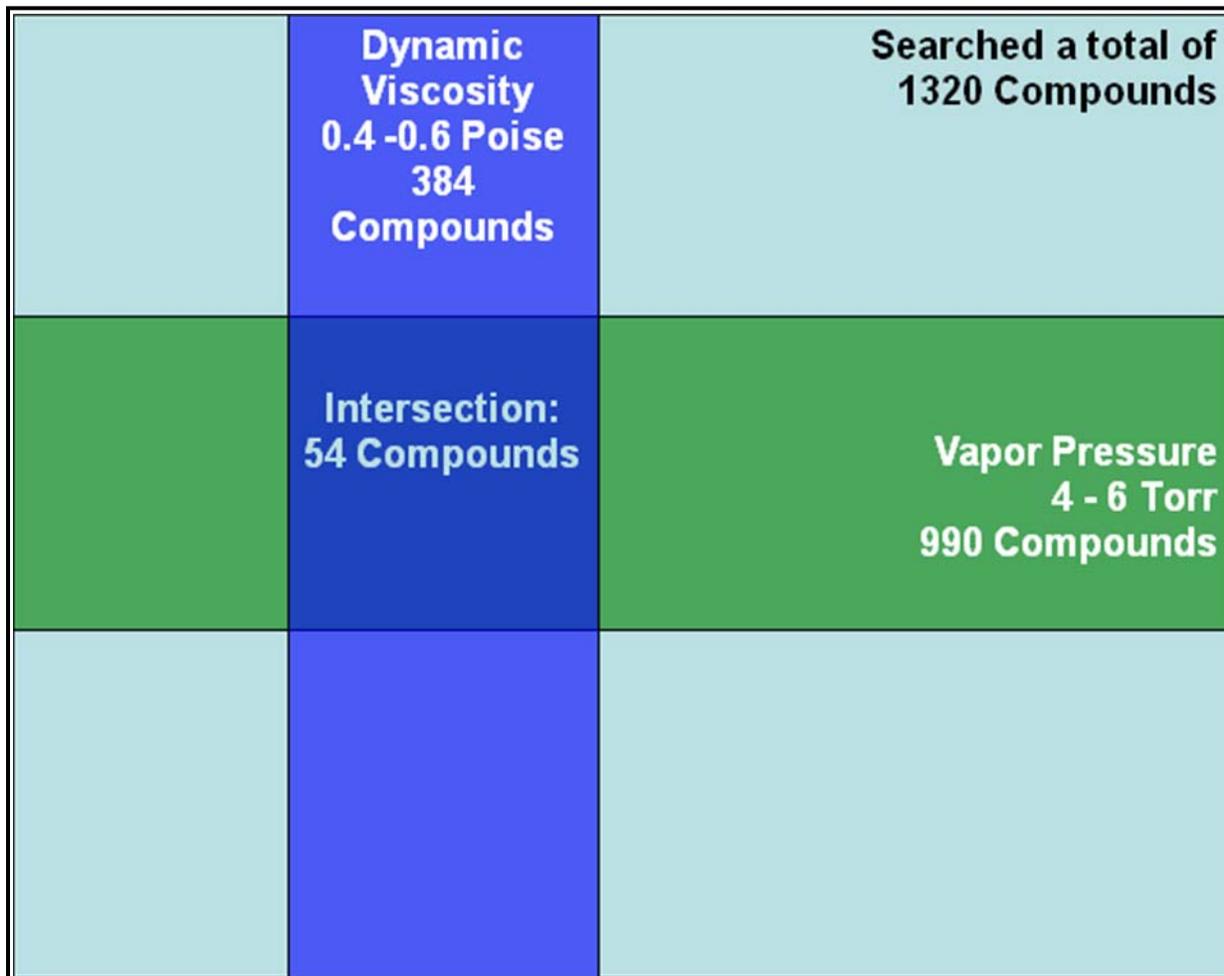


Figure 4. Example of a multi-parameter search showing the intersection between two single-parameter searches.

c. For quantitative measures, a range of values near the agent property will be searched. The importance of the property and the frequency of occurrence of property values in the database will influence the extent of this range.

(1) This range must be narrow – no more than ± 10 percent for the most important properties. For less important properties, a wider range may be acceptable. A range of ± 50 percent or more would allow more potential candidates, while still eliminating a significant number of those with the most undesirable properties. A narrow range will admit only candidate simulants that are very close to the agent's properties.

(2) These ranges can be adjusted to obtain an appropriately sized list of candidate simulants. The search becomes less selective by increasing the range, yielding more candidate simulants. These ranges will be determined and approved by the simulant selection team.

(3) Many important physical properties are temperature-dependent. Agent and simulant data are ideally measured at a standard temperature. A temperature of 25 °C is a typical temperature for Army test operations and is also a standard scientific experimentation temperature. Physicochemical data values may be accepted across a range of temperatures to allow more data (and thus a wider selection of simulants) to be considered. For example, data measured at 24 °C could be acceptable if there are no data at 25 °C. The range of acceptable temperatures can be wider for parameters that are insensitive to temperature.

d. Several resources, such as legacy simulant databases, previous test reports, etc., should be reviewed to determine which simulants have been used in the past for the agents and applications of interest. Expert knowledge of any additional compounds with potential to act as simulants should also be included. Information available through databases and published literature should be reviewed to identify all compounds that could be used as simulants for the agents under consideration.

e. After applying the search criteria, the number of candidate simulants should be reduced from millions to about 100 candidates per agent. A unique identifying number, other than the CAS number, should be chosen for each candidate simulant. Several CAS numbers may be coupled to identify a single compound. These additional CAS numbers often identify mixtures containing the desired candidate as a component.

4.3 Phase 3: Simulant Selection.

4.3.1 Phase 3A: Final Screening of Candidate Simulants.

a. The initial list of potential simulants will be screened to exclude simulants that do not meet certain minimum thresholds. This screening will reduce the number of potential simulants that require data gathering and detailed evaluation. Screening also helps to score the candidate simulants with the decision analysis and evaluation model.

b. Final screening may reveal an inadequacy in the process by which the candidate simulants were identified. This inadequacy would be indicated by the presence of a large number of undesirable compounds that could easily have been screened out. Another database search may be needed if it is found that updated search criteria should be applied.

c. Candidate simulants should be screened for usability (toxicity, shelf life, and material compatibility). For example, screening for usability; the simulant selection team may eliminate any compound that costs over \$50 per gram because it is too expensive for the intended use.

d. Additional and more constraining screening criteria may be applied to further reduce the number of candidate simulants.

(1) Subsequent screening iterations would involve applying more restrictive or additional threshold requirements to the list of simulants until an appropriate number of candidate simulants is reached.

(2) Simulants should not be eliminated at this stage just because some information on their properties (as compared with the thresholds) is unknown. These candidates (if otherwise promising) should continue into the next phase, during which data will be collected. At that time, if the data show that the simulant does not meet one or more of the screening criteria, it can then be eliminated from consideration.

4.3.2 Phase 3B: Simulant Data Collection.

a. Data will be collected on all remaining candidate simulants. The selection of data types to collect must correlate with the measures in the decision analysis and evaluation model. For example, if toxicity is one of the measures being assessed, toxicity data for each of the candidate simulants must be obtained.

(1) Values from different sources for a particular simulant property may conflict. Conflicting values should be verified by another literature/database source, by SMEs, or by modeling. As a last resort (if other verification methods are not possible), the test facility, in conjunction with the funding program, will verify conflicting values by laboratory measurement. If there is no reliable way to verify a value, the corresponding simulant may need to be removed from the list of candidate simulants.

(2) Also, there may be incomplete data for many or most of the simulant candidates.

(a) Any missing data will be collected for all remaining candidate simulants (paragraph 4.3.1) before meeting with the Simulant Selection Team.

(b) If the missing data are not available from other sources, then they may be predicted by modeling. If modeling is not possible and the data are otherwise unobtainable, the candidate may need to be removed from the list. If the SMEs believe the compound has special promise as a simulant, they may measure properties via laboratory testing to supply missing data.

(3) The data for parameters not used in the database searches will be collected to address all of the measures in the decision analysis and evaluation model.

b. Data may also be obtained through a literature search or laboratory measurement.

(1) An extensive literature search should be conducted as the first part of simulant data collection. Personnel may search such sources as databases, published reports, and any open source data that can be located (paragraph 2.2).

(a) Searches should focus on scientific journal articles rather than standard textbooks. Data availability, credibility, and gaps should be documented for each candidate simulant.

(b) The ultimate goal of the search is to find data from original sources such as actual test measurement data.

(c) With a simulant list of 200, this process could take months. The simulant selection team must decide when it has sufficient information to proceed.

(2) After the literature search, laboratory measurements can be used to generate any data still missing for each candidate simulant.

(a) Laboratory measurement may be needed to ensure fair assessment of each potential simulant.

(b) Laboratory measurement may include properties measurement and any other tests for which the capabilities and funding are available (e.g., toxicity testing). All possible precautions should be taken to ensure that as much information as possible is available for each of the potential simulants.

c. The credibility of the data source must also be considered. Any data for which the experimental details cannot be located (and is therefore unverifiable) should not be considered of equal quality to the data for which measurements can be verified. Each simulant selection team should consider, based on time and funding availability, whether it has the capability to verify the data points that are suspect. The simulant assessment panel will eliminate candidate simulants with unverifiable data.

d. After the data for the candidate simulants have been collected, any simulant with missing physicochemical data should either be dropped or included with a value for that property of zero. Where data are not available, SMEs may provide estimates based on their knowledge of the chemicals by extrapolation based on similar chemicals or through modeling. These techniques should be used only when absolutely necessary. Simulants with missing values recorded as zero will score lower overall than if all their data were available. Therefore, simulants with missing values will be less likely to be chosen than simulants with all values known.

e. The simulant selection team should use several sources to supplement its knowledge of the usability factors. For example, the NFPA diamond system may be consulted for health, flammability, and instability hazard ratings. The NFPA diamond system is used to label all chemical containers and transport vehicles. Each hazard is assigned a 0 to 4 rating, with 4 being most hazardous. Hazard ratings are obtained from the manufacturers' MSDSs and may vary depending on the manufacturer.

f. The following information must be documented for each simulant: type of data located, assessment of credibility of the data source, and data not found. The ultimate goal is to find information/data from original sources, such as actual test measurement data.

4.3.3 Phase 3C: Candidate Simulants Evaluation and Analysis.

a. After the candidate simulants have been screened, identified, and researched, the simulants will be scored using the decision analysis and evaluation models. The results will then be assessed by the simulant assessment panel.

b. A simulant assessment panel comprising the simulant selection team and technical experts with chemical knowledge and experience must convene to perform the assessment. The panel will be provided with the data collected for each candidate simulant. The assessment can be facilitated by the DAT, which would be responsible for running the decision analysis software and recording the results and/or rationale.

4.3.3.1 Scoring the Evaluation Measures.

a. Each candidate simulant will be scored individually for each of the evaluation measures, which were determined in paragraph 4.1.4. Two methods will be used to score the candidate simulants.

(1) Scoring the Usability Measures.

(a) A performance scale will be developed by the simulant assessment panel for each usability measure. The performance scales are used to evaluate how well a simulant performs relative to a specific measure. Performance scales are either continuous range (e.g., numeric range) or discrete levels (e.g., high/medium/low). The scales can also be described in natural (e.g., minutes) or constructed units. An example list of scales can be found in Table 3.

(b) Values of 100 and 0 will be assigned to the upper and lower ends of the performance scale, respectively, and intermediate values will then be derived. This will essentially translate dissimilar information into common units and allow for the comparison of scores across different measures. Two examples of performance scales are shown in Figures 5 and 6. The environmental impact scale (Figure 5) is an example of a constructed scale using labels. The cost scale (Figure 6) is a continuous scale.

<p><u>Environmental Impact Scale:</u></p> <ul style="list-style-type: none">• 100 – Expect no impact on environment• 50 – Expect some impact• 25 – Expect considerable impact• 0 – Expect severe impact, cannot be released, or does not degrade

Figure 5. Sample environmental impact scale.

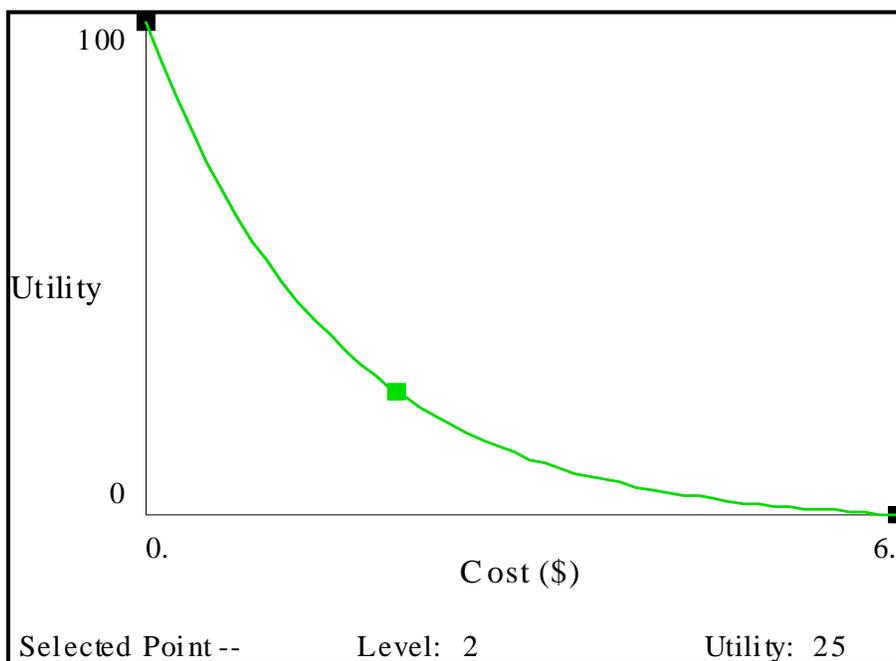


Figure 6. Usability curve for cost measure.

(c) Using the performance scale, each of the measures for each candidate simulant will be scored by the simulant assessment panel. These scores will provide the overall scores for each of the simulants.

(2) Scoring the Physicochemical Measures.

(a) Physicochemical measures are calculated using Equation 3. These measures will be used in the decision analysis and evaluation model.

Equation 3

$$r = 100 \left| \frac{x_s - x_a}{x_a} \right|$$

Where:

r = physicochemical measures.

xs = simulant property value.

xa = agent property value.

(b) Despite persistent verification, if an error is found in a simulant measure, then the value will be researched and the score will be recalculated. This score will be used in the decision analysis and evaluation model, improving the accuracy of the simulant scores.

(c) Tables 5 and 6 are examples of the scoring sheet. Comments will be documented to justify subjective ratings that were based solely on the expert knowledge of the SMEs.

4.3.3.2 Simulant Score Assessment.

a. After scoring the measures for the individual simulant has been completed, an overall score will be generated for each simulant using the model described in paragraph 4.1.4 (Equations 1 and 2).

b. The simulant assessment panel will rank candidate simulants according to score, with higher scores indicating better agreement with usability criteria (which an agent cannot do because it is expensive and highly toxic).

c. For example, Figure 7 shows the results of a GD simulant selection process for swatch testing. Each simulant must be evaluated for each application. These scores, depending on the hierarchy of the decision analysis and evaluation model, could be combined into an overall score. The bars to the right of the score show how much each measure contributed to the overall score. The higher weighted measures appear on the left. Table 7 is also another example of an evaluation result.

4.3.3.3 Candidate Simulants Assessment and Selection.

a. Sensitivity analysis is useful for determining the effects of changing the weights of the measures/goals. Sensitivity analysis tests whether a small change in the weights can create a large change in the ranking of the simulants. A sensitivity analysis must be conducted to evaluate the degree that score changes affect the simulant rankings.

b. Further analysis will then be performed to develop recommendations. The simulant assessment panel will contribute their insight about each chemical, such as possible issues with simulant properties that may not have been discovered during the simulant selection process. The SMEs may also be aware of current uses of the compound, indicating that it will be a useful simulant. The simulant assessment panel must provide a rationale for the selection of each candidate simulant.

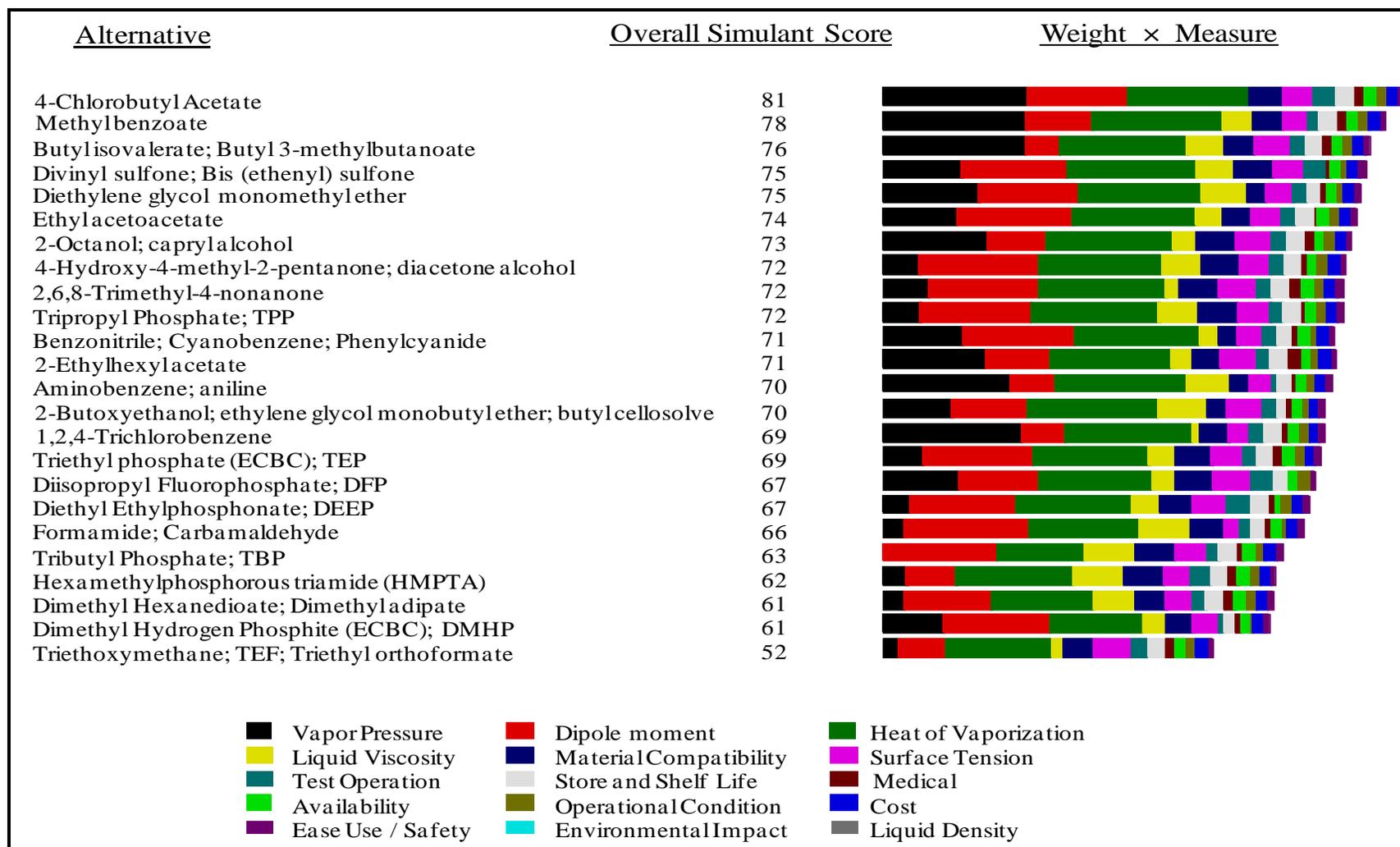
c. This phase will verify that the model is providing useful results. The analysis by the simulant scoring panel will provide a short list of high-quality candidate simulants with a documented rationale for their selection.

TABLE 5. SCORE SHEET FOR SELECTED SIMULANTS FOR PERMEATION TESTING

CHEMICAL	CAS NUMBER	MEDICAL	ENVIRONMENTAL IMPACT		EASE OF USE/ SAFETY	COST (\$/g)	AVAILABILITY
Divinyl sulfone; bis(ethenyl)sulfone	000077-77-0	3	100	25	0	4.33	100
Ethyl acetoacetate	000141-97-9	2	100	100	2	0.13	100
Ethyl dichloroacetate	000535-15-9	2	100	50	2	0.86	100
Ethyl-2- hydroxypropionate	000097-64-3	1	100	90	3	0.03	100
Formamide; carbamaldehyde	000075-12-7	2	100	75	1	0.01	100
Hexamethylphosphorous triamide	001608-26-0	1	100	75	3	4.74	100
Methyl benzoate	000093-58-3	1	100	100	2	9.74	100
Methyl salicylate	000119-36-8	1	100	100	1	0.08	100
Phenyl acetate	000122-79-2	1	100	100	2	0.09	100
P-thioxane	015980-15-1	1	100	75	3	2.82	100
Quinoline	000091-22-5	2	100	25	3	0.22	100
Tributyl phosphate	000126-73-8	2	75	25	1	0.15	100
Triethoxymethane	000122-51-0	1	100	75	3	0.12	100
Triethyl phosphate	000078-40-0	1	100	85	1	0.01	100
Tripropyl phosphate	000513-08-6	2	75	50	1	3.17	100

TABLE 6. SCORING SHEET FOR SELECTED BATTLEFIELD CONTAMINANTS (BFCS)

BATTLEFIELD CONTAMINANT/ COMPOUND	STATE AT 25 °C AND 1 ATM, AS NORMALLY USED	PREVALENCE ON BATTLEFIELD (HIGH, MEDIUM, OR LOW)	PREVALENCE SCORE	LIKELIHOOD OF EXPOSURE (HIGH, MEDIUM, OR LOW)	LIKELIHOOD SCORE	DURATION OF JECP MATERIAL CONTACT (MINUTES, HOURS, OR DAYS)	DURATION SCORE	NFPA HEALTH SCORE	CHEMICAL PROPERTIES	CHEMICAL PROPERTIES SCORE
Camouflage Face Paints (Stick Desert, Loam)	Paste	Medium	50	Low	0	Hours	50	50	Not Available	0
Composite Fiber	Solid	High	100	High	100	Hours	50	50	Inhalation hazard if burned.	0
Fire Extinguisher Compounds	Foam	Medium	50	Low	0	Minutes	0	50	See aqueous fire fighting foam (AFFF) and carbon dioxide (CO ₂)	0
Static Guard	Liquid	Medium	50	Low	0	Minutes	0	100	Combustible, irritant	10



NOTE: The bars to the right of the overall simulant score show how much each physicochemical weight and measure contributed to the overall score. The higher weighted measures appear first (reading left to right).

Figure 7. GD swatch evaluation results.

TABLE 7. BFC EVALUATION RESULT

BFC/COMPOUND	TYPE/CATEGORY	OVERALL SCORE
Diesel (fuel, exhaust, vapor)	Petroleum, oils, lubricants (vapors, exhaust)	74.5
Water (seawater, soapy water)	Other	73
Wasp spray (diazinon, pyrethums, petroleum distillates, and propellant)	Insecticides, herbicides, repellants	70
N,N-diethyl-meta-toluamide (DEET, insect repellent)	Insecticides, herbicides, repellants	69.5
Benzene	Petroleum, oils, lubricants (liquid, vapors)	69.5
Disinfectants	Cleaners, disinfectants, sterilizers, degreaser	68
Burning (cardboard, cloth, plastics, rubber, wood)	Smoke	65
Burning Fuels (diesel, gas, kerosene, jet propellant fuel, type 8 ((JP-8)), oil)	Smoke	65
Alcohols	Solvents, strippers, alcohols	59.5
Ozone	Natural/synthetic gas	59
Composite fiber	Other	55
Smoke (red, yellow, green, violet, white, tobacco)	Smoke	55
Bleach and chlorine (concentrated chlorine bleach is medical), (sodium hypochlorite)	Cleaners, disinfectants, sterilizers, degreaser	54.5
Coffee	Food and drink	54.5
Jet (fuel, exhaust, vapor)	Petroleum, oils, lubricants (liquid, vapors, exhaust)	54.5
JP-8 fuel	Petroleum, oils, lubricants (liquid, exhaust)	54.5
Spectracide mole stop repellent	Insecticides, herbicides, repellants	50

4.4 Phase 4: Verify Simulants.

a. The recommended candidate simulants must be verified. Every value used for the selection should be re-examined to be sure that it agrees with other literature sources. A good place to start this reexamination is by checking the references provided by the databases.

b. Phase 4 is a QC step to ensure that the candidate simulant from Phase 3 (paragraph 4.3) will be useful in testing.

c. If it is found that erroneous values were used in the simulant selection process, the model will be rerun with the correct values. The new scores will be generated by following the procedure in paragraphs 4.3.3.2 and 4.3.3.3. Then the revised list of simulants will be verified. It is possible that several iterations of these steps may be required.

d. Once the candidate simulants are verified, the simulant usability testing and ASR validation should follow.

4.5 Simulant Usability and ASR Validation.

a. Simulant usability and ASR validation provides empirical data to build a mathematical relationship between the performance of the test items against simulant to the performance of the test item against agent.

b. Usability Trials. Many of the candidate simulants may require new methodology. Although the simulants will be screened for issues that may make their use difficult, it is important to perform usability testing with each. It is often appropriate to combine usability testing with methodology work. Unforeseen difficulties will be readily apparent during methodology testing. Possible usability issues include issues pertaining to:

- (1) Decontamination.
- (2) Detection (analytical/referee).
- (3) Safety.
- (4) Stability.
- (5) Shelf life/storage.
- (6) Material incompatibility.
- (7) Availability.

c. ASR Trials. After the recommended simulant(s) are identified, the ASRs will be performed through comparative side-by-side testing of the agent to the recommended simulant. This testing is done to verify that the simulant will behave as expected. The ASR tests should

attempt to mirror the conditions that the agent will be exposed to during the testing application for which it was selected.

- d. This phase of the simulant selection process is outside the scope of this TOP.

5. DATA REQUIRED.

- a. Rank and order of the selected simulants.
- b. Weights for the decision analysis and evaluation model.
- c. Goals and measures used in the decision analysis and evaluation model:
 - (1) Usability measures.
 - (2) Usability measures.
- d. For each simulant:
 - (1) Physicochemical data (e.g., dipole moment).
 - (2) Usability data (e.g., cost).
- e. Rationale for selecting each candidate simulant.

6. PRESENTATION OF DATA.

The Simulant Selection Team will prepare a technical report to document the results of the 5-phase simulant selection process, with the exception of the simulant usability and ASR validation report. The simulant usability and ASR validation phase of the simulant selection process is outside the scope of this TOP.

APPENDIX A. GLOSSARY.

<u>Term</u>	<u>Definition</u>
Decision Analysis and Evaluation Model	A mathematical model used to evaluate the candidate simulants. The linear weighting of the measures used to assess the quality of a simulant is the model.
Data Analysis Team (DAT)	An optional team that is dedicated to running decision analysis software.
Goals	Objectives for the simulant that consists of measures of each criteria.
Measures	Quantifies the usability criteria of the candidate simulant as well as the physicochemical criteria similarity of the candidate simulant to the agent of interest.
Net worthiness	A certificate of net worthiness is required for software that is to be installed on government computers. The certificate is specific to the organization that has jurisdiction over your system.
Physicochemical Criteria	Criteria used to ensure that the candidate simulant is a close match for the relevant physical and chemical properties of an agent.
Screening Criteria	Basic criteria used to reduce the number of candidate simulants. For example, limits on boiling point and melting point can be used to screen out compounds that are not of the correct phase.
Simulant Selection Team	The team of individuals responsible for the simulant selection process from beginning to end.
Simulant Assessment Panel	A panel composed of the simulant selection team, DAT, and additional SMEs that convenes to select simulants.
Usability Criteria	Criteria that ensures a simulant is usable. Criteria include safety, material compatibility, cost, etc.
Weights	A number between 0 and 100 given to represent the relative importance of a measure. All weights must add to 100.

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APPENDIX B. ABBREVIATIONS.

AFFF	aqueous fire-fighting foam
ASK	agent simulant knowledgebase
ASR	agent-simulant relationship
atm	atmosphere
BFC	battlefield contaminant
BWA	biological warfare agent
C2	command and control
CAS	Chemical Abstract Service
CB	chemical/biological
CBRNIAC	Chemical, Biological, Radiological and Nuclear Defense Information Analysis Center
CO ₂	carbon dioxide
ColPro	collective protection
COTS	commercial off-the-shelf
DAT	Data Analysis Team
decon	decontamination
DEET	N,N-diethyl-meta-toluamide
DIPPR	Design Institute for Physical Properties
DoD	Department of Defense
DPG	US Army Dugway Proving Ground
DTP	detailed test plan
ECBC	Edgewood Chemical Biological Center
FPD	flame photometric detector
GD	soman
HD	distilled mustard
HR	health rating
IAW	in accordance with
IP	individual protection
IR	infrared
JECP	Joint Expeditionary Collective Protection
JP-8	jet propulsion fuel, type 8
LDW	Logical Decisions for Windows

APPENDIX B. ABBREVIATIONS.

MINICAMS®	a miniature, automatic, continuous air-monitoring system
MSDS	material safety data sheet
NFPA	National Fire Protection Agency
NIST	National Institute of Standards and Technology
PM	Program Manager
QA	quality assurance
QC	quality control
R2	rest and relaxation
SAR	same as report
SME	subject-matter expert
SOP	Standing Operating Procedure
SPET	selection for protective equipment testing
TOP	Test Operations Procedure
V&V	verification and validation
VX	persistent nerve agent

APPENDIX C. REFERENCES.

1. DPG Fiscal Year 2006 (FY06) Annual Report for Simulant Selection for Protective Equipment (CA06TAS438), Document Number: WDTC-XX-09-084, 2006.
2. DPG Fiscal Year 2007 (FY07) Annual Report for Simulant Selection for Protective Equipment Testing (SPET ((CA06TAS438)), Document Number: WDTC-XX-09-083, November 2007.
3. DPG Final Test Report for Joint Expeditionary Collective Protection (JECF) Simulant Selection, Document Number: WDTC-TR-09-070, 2010 (Draft).
4. DPG Final Test Report for The Joint Expeditionary Collective Protection (JECF) Battlefield Contaminant (BFC) Selection Process, Document Number: WDTC-TR-09-028, November 2009.

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Forward comments, recommended changes, or any pertinent data which may be of use in improving this publication to the following address: Test Business Management Division (TEDT-TMB), US Army Developmental Test Command, 314 Longs Corner Road Aberdeen Proving Ground, MD 21005-5055. Technical information may be obtained from the preparing activity: Commander, West Desert Test Center, US Army Dugway Proving Ground, ATTN: TEDT-DPW, Dugway, UT 84022-5000. Additional copies can be requested through the following website: <http://itops.dtc.army.mil/RequestForDocuments.aspx>, or through the Defense Technical Information Center, 8725 John J. Kingman Rd., STE 0944, Fort Belvoir, VA 22060-6218. This document is identified by the accession number (AD No.) printed on the first page.