Compound Selection for Battlefield Testing

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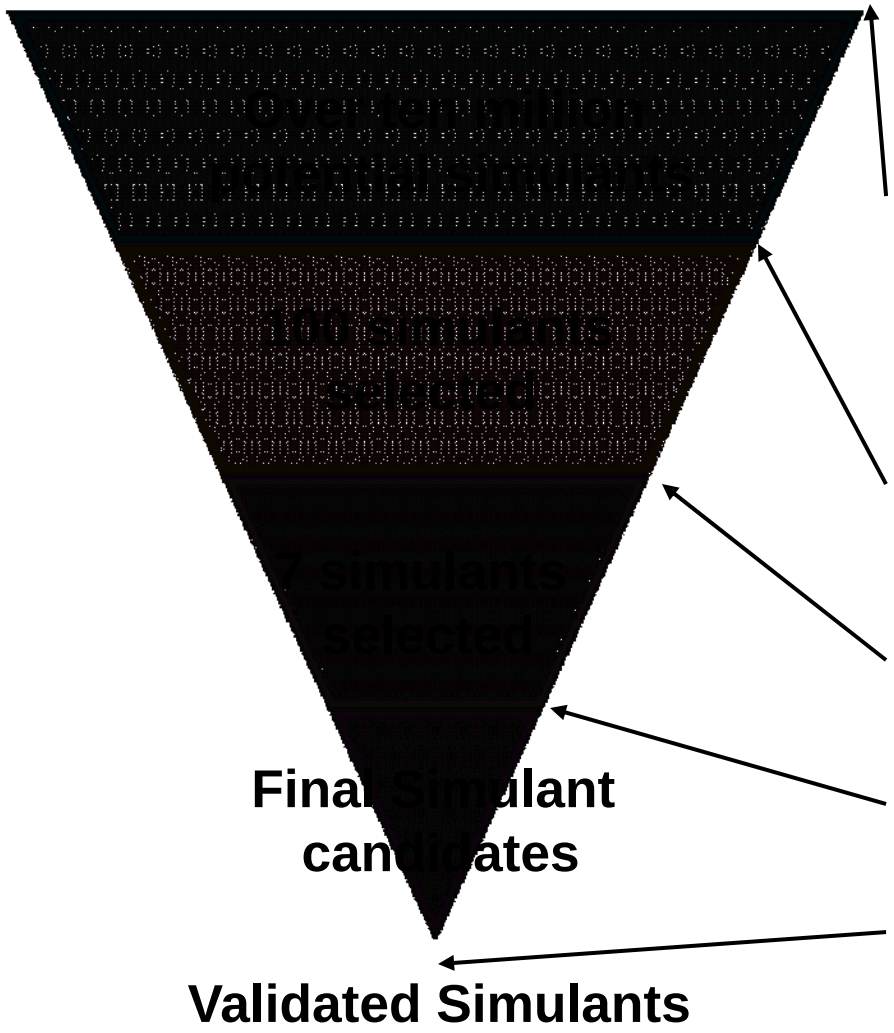
Dugway and CB Testing

- U.S. Army Dugway Proving Ground (DPG) has been a major test and support center for chemical and biological (CB) defense and related programs since 1942.
- DPG physical characteristics:
  - 798,214 acres, 1247 square miles ≅ Rhode Island.
  - In the Great Salt Lake Desert, about 85 miles SW of Salt Lake City, Utah.
  - Level salt flats, sand dunes, and rugged mountains.
- www.wdtc.army.mil

Testing with Simulants

- Military equipment is tested to prove its resistance to chemical warfare agents.
- The life of the warfighter depends upon knowing that the system will perform as expected!
- The use of actual agents is restricted by the Chemical Weapons Convention.
- Therefore, far less toxic substances (simulants) are used for large-scale chamber and field testing.
- Choosing the best simulant is part of the test process.
- For this program, simulants were systematically chosen to test CB protective capabilities of tents:
  - Simulants may be used in laboratory, large test chamber, or field.
  - Should perform similarly to the selected chemical properties of the chemical agents sarin (GB), soman (GD), distilled mustard (HD), and persistent nerve agent (VX).
  - Simulant performance was verified in the laboratory.
- Battlefield contaminants (BFCs) were also chosen.

Simulant Selection Pyramid



1. Defined physical, chemical properties of simulant that affected vapor permeation.
2. Defined usability properties that affected use of simulants in test.
3. Defined scale to convert each property to a number.
4. Weighted properties.
5. Defined screening criteria.
6. Searched for simulants.
7. Selected candidate simulants.
8. Verified candidate simulants.
9. Validated candidate simulants.

Chemical Challenges on Materiel

- Chosen not to be specific for any materiel or agent:
  - Liquid drop and vapor on air-permeable fabric.
  - Liquid drop and vapor on air-impermeable fabric.
  - Aerosol on air-permeable fabric.
  - Vapor on filter.
  - Contamination tracked into the tent by equipment/personnel and evaporating inside the tent.

Selected Chemical Properties to be Searched

Molecular Events	Chemical Parameters found in Databases
Equilibrium solubility, surface site binding, and permeation	Molecular dipole
Evaporation/vapor/threat and surface site binding	Heat of vaporization
Surface site binding	Heat of adsorption on activated carbon
Pore diffusion	Molar volume
Evaporation/vapor/threat	Vapor pressure
Particle diffusion	Particle diameter (aerosol only)
Pore diffusion; droplet contact angle on impermeable materials	Surface tension and viscosity

Sources of Chemical Data

- Obtained agent physical property data.
- Obtained simulant properties using Beilstein, SciFinder, Agent Simulant KnowledgeBase (ASK), HyperChem, and vendor data.
- Searched within a range e.g., heat of vaporization ±5 kcal/mol of agent property value.

Screening Criteria: 1 of 2

- With over 10 million candidates, we had to screen compounds.
- Database searching allowed a query to only return compounds meeting certain criteria:
  - Unambiguous Chemical Abstracts Service (CAS) number.
  - Real-time low-level detection with current instrumentation: must contain phosphorus, sulfur, or chlorine
  - No radioactive atoms.
  - No functional groups that would be unstable in the presence of water or air or light: aldehydes, thiols, organometallic, sulfates, etc.
  - Single compound, no mixtures or polymers; mixture properties were hard to predict, even if component properties were known. Also, composition would change during use.
  - Aprotic, to better resemble agents, which were aprotic.
  - Liquid from 0°C to 60°C at ambient pressure or below.
  - Flash point > 60°C.
  - Available values for most physical properties.

Screening Criteria: 2 of 2

- Further screening criteria:
  - Commercially available from domestic vendor.
  - Field test: bulk cost less than about $.05/g.
  - Acceptable odor in accordance with the Material Safety Data Sheets (MSDS).
  - Not on a Drug Enforcement Agency schedule.
  - Any other reason based on team member experience.
- Once an initial list was obtained, the candidates were sorted by functional group (e.g., alcohol). Only the best candidates within each group were considered.
- Compounds were then sorted by preliminary score based on physicochemical properties (also used for final selection).
- Reduced list to 100 compounds; data were gathered on these.

Usability for Testing

- Team included scientific, military, and test perspectives.
- Stable when stored at room temperature.
- Acceptable lower, upper explosive limits of vapor in air.
- Nonreactive in presence of light, air, water, or materiel.
- Low toxicity in accordance with the MSDS:
  - Use of less toxic simulants is inherently safer.
  - Require less protective clothing and equipment.
- Little environmental impact: fauna, flora, atmosphere.
- These properties were translated to properties for selection and were weighted.

Pulling it Together

- The value of each property was reduced to a number on a 0-100 scale.
- The importance of each chemical or physical property was expressed as a numerical weight, on which subject matter experts reached a consensus:
  - In the laboratory physical properties were more important, to get the best match to agent.
  - In the field, environmental impact and safe handling/safety and cost were paramount.
  - e.g., environmental impact had weight of 0 for laboratory use because simulant was not released to the environment, but weight of 14 for field use.

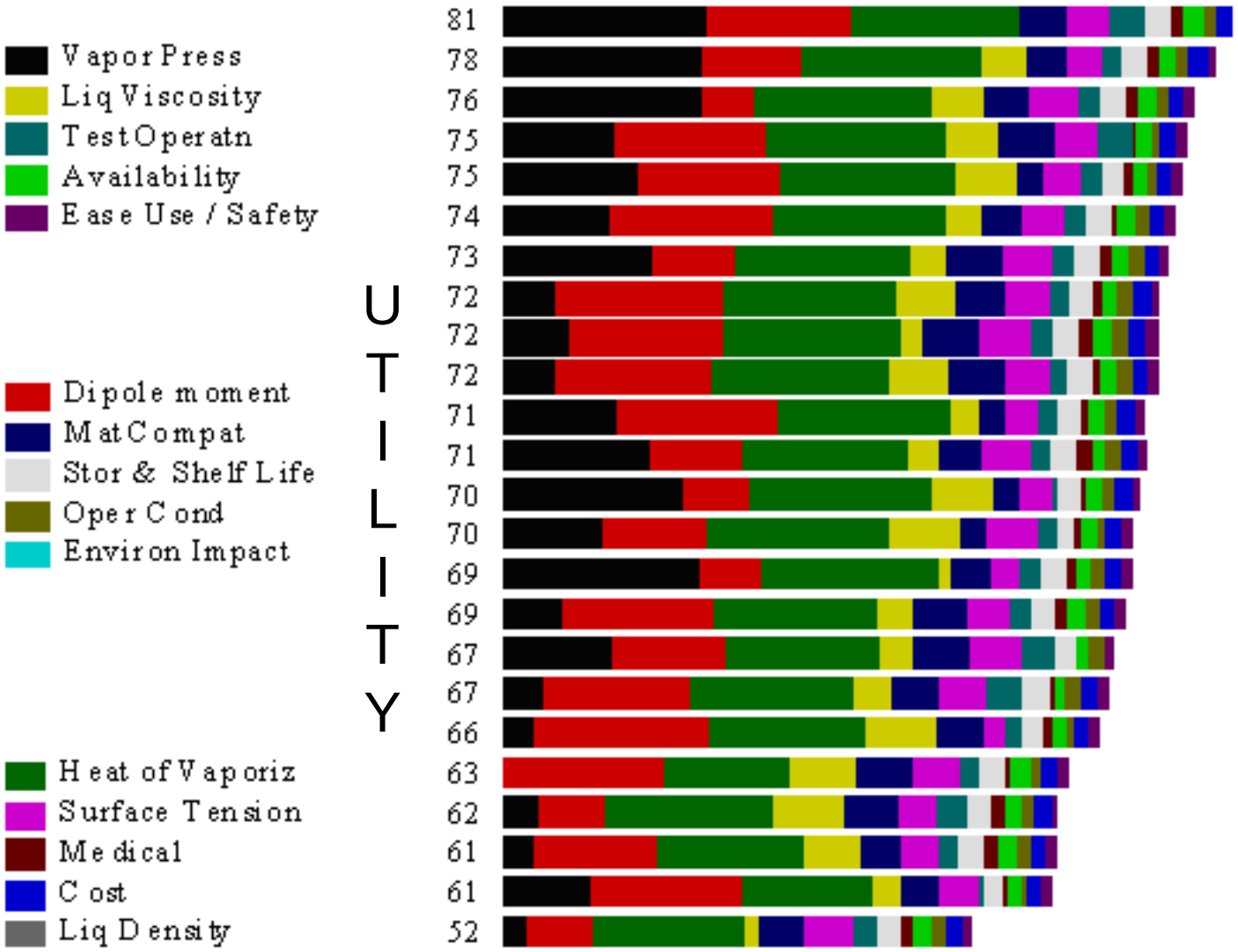
Properties Affecting Choice of Simulant, with Weights

Property	Laboratory Test Weight	Chamber Test Weight	Field Test Weight
Physical/Chemical – Heat of vaporization	8	6	2
Physical/Chemical – Molecular Dipole	20	14	4
Physical/Chemical – Vapor pressure	20	14	4
Physical/Chemical – Surface tension	12	8	2
Physical/Chemical – Viscosity	8	6	2
Physical/Chemical – Molar volume	10	7	1
Medical	2	7	16
Ease of Use/Safety	1	4	7
Material Compatibility	4	4	8
Operating Conditions	6	6	10
Test Operations	5	10	16
Storage and Shelf Life	2	2	2
Environmental Impact	0	7	14
Availability	0	0	0
Cost	2	5	12
TOTAL	100	100	100

Rank Simulants and Prepare Shortlist

- Multiplied score of each simulant for each property (e.g., 80 out of 100) by the weight assigned to that property (e.g., 0.2).
- Product (e.g., 16) represented contribution of that property to the importance of that simulant for test.
- Using decision analysis software:
  - For each simulant, all contributions were added to form a utility value.
  - The higher the utility value, the better it was expected to be for use in testing.
  - Simulants ranked and ordered by utility value.
- Process was not wholly precise due to uncertainties in gathering/assessing numerical data. A priority was
- placed on testing the higher-ranked simulants.
- List was reviewed by technical experts and testers.

Decision Analysis Software Output Rankings



Shortlist of Simulants

- Prepared shortlist of seven candidate simulants, selected based on scores and other factors.
- Candidate simulants were taken to the laboratory for testing.
- Each simulant was ranked against the agent in terms of its ability to permeate a given material.
- The experimental ranking of simulants with respect to agent was quite similar to the model ranking.

Usability for Testing: Laboratory Work

- Vapor does not stick strongly to surfaces (plaquing).
- Detection:
  - At low concentrations.
  - No background presence (no false positive).
  - Substances present during test should not mask simulant (no false negative).
  - Laboratory only: should not cause false alarm in safety air monitoring.
- Can be disseminated.
- Little offgassing from samples of material that represent typical facility surfaces: Portland cement, painted metal, stainless steel, unpainted wood, polyvinyl chloride (PVC).
- Can be decontaminated using various cleanup solutions. Simulant is physically removed intact or reacts rapidly and safely with existing decon solutions. Must test both liquid and adsorbed simulant.

BFC Selection Overview

- Many BFCs exist.
- Some may impair CB protective materiel.
- Used process to prepare short list of BFCs to test:
  - Test filters with only aerosols and gases.
  - Test barrier material with any type of BFC, including liquids, pastes, and solids.
- Selected the top few BFCs from the list.
- Will test each BFC on the short list, to determine reduction in protective capability.

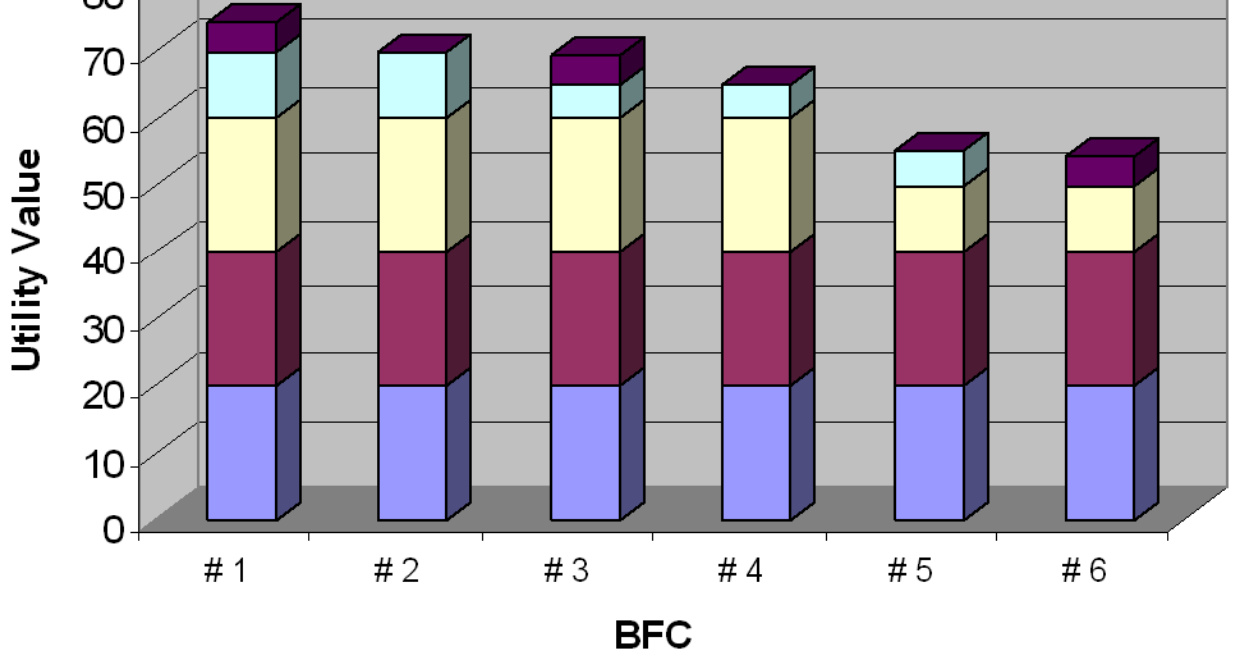
BFC Selection: User Inputs

- Generated draft list from Armed Forces' service representatives and from other programs; over 200 BFCs.
- Defined selection properties that determined whether BFC would impair materiel.
- Surveyed representatives to gather data using different names (e.g., benzene and fuel):
  - Prevalence on battlefield: is it widespread?
  - Likelihood of contacting equipment: will it contact materiel?
  - Duration of contact with test item before cleaning up: how much time will it have to damage materiel?
  - Any other comments.
- Merged the inputs from different services.

BFC Selection: Chemical Data and Test Perspective

- Gathered chemical input data from databases, MSDS. Reviewed by scientists:
  - Physical state i.e., gas, liquid, or solid (also vapor, aerosol, and paste): what part of equipment will it contact and how will the BFC be disseminated?
  - Chemical properties (e.g., corrosive, oxidizing, reactive with plastics): How quickly will it impair the materiel?
  - National Fire Protection Association (NFPA) health rating: risks to DPG test personnel.
- Established numeric weights: chemical properties > prevalence = likelihood = duration > health rating.
- Established numeric scoring: converted both qualitative and quantitative data to numeric values for ranking.
- Used screening criteria to exclude certain BFCs: already tested in other parts of the test program, similar to other BFCs, spontaneously combustible, radioactive, or explosive.
- Ranked BFCs and prepared shortlist.
- Assessing interference with detection, reaction with agent or surfaces of fixture, and potential redesign to existing fixtures.

Selected BFCs for Barrier Materials as a Stacked Chart



Summary

- Simulants and BFCs were systematically chosen for testing.
- Team included scientific, military, and test perspectives.
- Rationale is traceable, defensible.
- Acknowledgments:
  - Threat Agent Science (TAS) office of Defense Threat Reduction Agency (DTRA)/Joint Science and Technology Office (JSTO).
  - Joint Expeditionary Collective Protection Program (JECP).