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Information Store for Chemical Security

July 2010

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Abstract

Preparedness for natural and man-made chemical events requires mitigation of potential consequences, which are driven by the toxicological, chemical, and physical properties of the on-site materials. Threat scenarios include release to the environment; theft and diversion, sabotage and contamination. This work includes the identification of 56 important-to-chemical-security properties. These properties are not available from any one (or even a few sources), so this work also identifies 34 authoritative data sources. This work focuses on development of an Information Store with guidance for mitigation of vulnerabilities for 1,267 unique chemicals, including "chemicals of interest," mission critical items, and economically critical materials. The central components of the Information Store include: 1) collection of chemical properties; 2) quantification of consequences on the basis of historical events; and 3) identification and compilation of key process safety information for vulnerability mitigation. The advantages of this Information Store include: all of the information in a central authoritative repository rather than many disparate sources; retention of the information in a stand-alone, secure system; and access to the information only by authorized users.

1. Introduction

A list of 324 important chemicals was published in the Federal Register (6 CFR Part 27, Appendix to Chemical Facility Anti-Terrorism Standards, Final Rule, published 20 November 2007). Appendix A showing each chemical along with the corresponding screening threshold quantity (STQ) and concentration for toxic release, theft, diversion, and sabotage/contamination scenarios. There is a second list of 199 mission-critical (MC) items, which have 123 unique identification numbers and 178 distinct names. We have analyzed this mission-critical list for naming consistency, duplication, etc. There is also a third list of 974 economically-critical (EC) items, which has been similarly analyzed. After resolution of redundancies and naming inconsistencies, the complete list (1,497 items) is reduced to 1,267 unique chemicals.

The focus of this work is collection and archiving of the chemical, physical, and toxicological properties of these materials. These properties are relevant to the potential consequences of a chemical event. Specifically, this work 1) identifies sources of the chemical properties, 2) acquires the relevant properties for each chemical, 3) archives the information, and 4) provides secure access for subject matter experts to this information.

This report is organized as follows. Section 2 explains a typical risk-based approach to provide an objective basis for chemical facility vulnerability determination. Section 3 elucidates the chemical-properties information that underlies the effort. Section 4 discusses the methods, scope, and validation of the chemical-properties component of the Information Store. Section 4 explains the information collection and repository. Section 5 describes the concept, organization, operational requirements, justification, and inter-operability of the Information Store. Section 6 discusses the application of this Information Store, along with its conformance to modern systems engineering principles and standards of construction.

2. Risk-Based Approach

One approach for quantifying a chemical facility's vulnerability to a chemical event uses a risk-based approach. In order to calculate this risk, it is necessary first to quantify the potential consequences of such attacks. The consequences of an attack are measured in terms of human life — both loss of life (fatalities) and bodily harm (casualties). Specific chemical events include release, theft, sabotage, loss or interruption in national-security-critical production, and diversion/disruption of economically important chemicals. Table 1 summarizes the relationship between chemical properties and chemical security.

Table 1: Relationship Between Chemical Properties and Chemical Security

Feature	Description in terms of information usefulness
Identity	Cross reference among information sources (e.g., NIOSH, DOT quick reference guides) for access to supplemental information.
Toxicity	Quantification of health effects for various acute exposure scenarios.
Chemical Potential	Measures of compound's inherent potential energy, as well as its capacity for thermo-physical response to heat and energy.
Reactivity	Compound's inherent energy content via interactions (e.g., combustion, reactive mixtures) with air, water, structures, and other adjacent material, resulting in an energy release that can alter facility temperatures and pressures (e.g., combustion, reactive mixtures).
Temperature & Pressure	Relationships between release of inherent or reactive energy on temperatures and pressure that can arise at the facility.
Dispersion	Propagation (e.g., via air, water, projectile) of toxic and/or energetic materials as a result the site conditions.

One reliable way to estimate attack consequences is analysis of real events. The Chemical Attack Data Acquisition Tool (CADAT) is a Java-based program that collects data on events involving Federally-identified chemicals of interest (COI). CADAT collects and analyzes relevant Internet-archived news articles, extracts pertinent data from these articles, and provides statistical summaries of the results. (See Appendix B for further details about a typical risk-based approach for determination of a chemical site's vulnerability. Appendix C lists chemicals that are associated with frequent industrial accidents; this list is not inconsistent with the important items in Appendix A.) Although future work is required to improve CADAT's ability to extract all relevant data, a preliminary run of the code produced noteworthy results. Internet searches for chemical events were divided into four categories: casualties from attacks, fatalities from attacks, casualties from accidents, and fatalities from accidents. (Accidents were analyzed in addition to attacks because an accident could trivially serve as a surrogate for an attack, if an attacker should choose to repeat an accident process.) The cumulative distribution functions (CDFs) for these four categories showed great similarity between attack fatalities and accident fatalities; the CDFs for attack casualties and accident casualties likewise showed great similarity. These similarities suggest that the consequences of chemical attacks and chemical accidents may be comparable. Furthermore, for almost every COI in the list, the average number of fatalities is less than 100 for both attacks and accidents. This finding could indicate that, historically, the COI are not highly fatal when used or targeted in attacks. However, it could also indicate that the most lethal use of these chemicals has yet to be successful, in which case an additional method of quantifying potential consequences may need to be implemented.[39]

To date, the emphasis of the project has been on individual chemicals. In the future, attention should be paid to chemical mixtures and to the physical layout of the chemical facility, its vulnerability to surreptitious introduction of flammables, and the geospatial distribution of heat-of-reaction energy on the site. The state of repair and quality of maintenance also bears significantly on site vulnerability and potential consequences of attacks. Other factors are nearby population centers and industrial facilities.

Chemical mixtures are frequently involved in terrorism or natural disasters. For example, urea is an inexpensive, non-detonable material that reacts with nitric acid to produce explosive urea nitrate. Hydrogen peroxide reacts with acetone to produce TATP (an explosive). Additional examples include a highly flammable liquid mixture that evaporates and explodes[1]; unstable chemicals that explode[2] under excessive heating; a heat-generated reaction among chemicals, either causing container over-pressurization or a boiling liquid expanding vapor explosion[3-4]; spread of a localized fire (or explosion) to nearby tanks/containers[5]; mixing of chemicals, which react to create a lethal release[6]. A 2002 study by the Chemical Safety Board[6] identified 167 reactive incidents, which caused 108 deaths over a 21-year period. More than half of those incidents involved chemicals that are not covered by the U.S. Occupational Safety and Health Administration (OSHA) and EPA process safety regulations. Even seemingly safe materials can create deadly mixtures, such as air-borne flammable dust (e.g., wood, coal, grain, flour, sugar, polyethylene)[7], which can explode in confined spaces. Appendix D provides more details about chemical mixtures[36].

A possible attack scenario begins with a sewer-release of a highly flammable liquid, which eventually ignites and explodes. This scenario actually occurred on 22 April 1992 in Guadalajara, Mexico, due to galvanic corrosion of two in-contact, dissimilar-metal, underground pipelines (sewer and gasoline) that allowed the entry of gasoline into a sewer. Numerous gasoline-in-sewer explosions over four hours destroyed kilometers of streets, killed at least 206, injured nearly 500, and left 15,000 homeless. Pipeline releases at U.S. chemical facilities frequently involve a subsequent explosion (2241 major US pipeline accidents in the last 10 years, resulting in 226 deaths and $700M in damage)[38]. Terrorists could use an off-site sewer release to get flammables into a chemical facility; a subsequent in-sewer explosion could be disastrous. Deterrence of an in-sewer event depends on the specific chemical (e.g., liquid gasoline versus gaseous hydrogen), which might necessitate the chemical facility's use of a sewer that is accessible only on-site.

More generally, the on-site chemical potential energy distribution can be determined as a function of the relative location of in-storage and in-process compounds. A geo-spatial map of reactive energy would thus enable subject-matter experts to focus their effort in terms of specific COI and their location(s) within a facility.

3. Chemical-Properties Information

Appendix E is a dictionary of chemical properties[8-25] that was compiled from many professional sources (Appendix F). We excluded Material Safety Data Sheets (MSDS). The chemical-security features in Table 1 arise from the properties in Appendix E. The COI-list (Appendix A) includes sub-categories of chemical security threat issues, which are driven by specific chemical properties, as shown in Table 2.

Table 2: Pertinent Chemical Properties for Each Chemical-Security Sub-Category

Sub-Category of Chemical Security	Chemical Properties That Affect This Sub-Category
Release - Explosive	adiabatic flame temperature, auto-ignition temperature, ID numbers (CAS, EC/EINECS, NA/DOT/UN, RTECS), chemical formula, chemical name, decomposition temperature, density, diffusion coefficient, enthalpy, entropy, explosive or flammability limit, flash point, heat of combustion (*et al.*), Joule-Thomson (Kelvin) coefficient, molecular structure, molecular weight, NFPA rating, (specific) surface area, sublimation point, surface tension, thermal expansion coefficient, vapor density, vapor pressure, viscosity, volatility
Release - Flammable	adiabatic flame temperature, Antoine's equation, auto-ignition temperature, boiling point, chemical formula, chemical name, coefficient of thermal expansion, compressibility, critical point (temperature, pressure, volume), decomposition temperature, density, diffusion coefficient, enthalpy, entropy, explosive/flammability limit, flash point, heat of combustion (*et al.*), ID numbers (CAS, EC/EINECS, NA/DOT/UN, RTECS), Joule-Thomson (Kelvin) coefficient, molecular structure, molecular weight, NFPA rating, (specific) surface area, sublimation point, surface tension, thermal expansion coefficient, vapor density, vapor pressure, viscosity, volatility
Release - Toxic	AEGL, chemical formula, chemical name, coefficient of thermal expansion, compressibility, critical point (temperature, pressure, volume) , decomposition temperature, density, diffusion coefficient, EC_{50}, ERPG, enthalpy, entropy, explosive/flammability limit, flash point, heat of combustion (*et al.*), IDLH, ID numbers (CAS, EC/EINECS, NA/DOT/UN, RTECS), Joule-Thomson (Kelvin) coefficient, LC_{50}, molecular structure, molecular weight, NFPA rating, STEL, surface tension, TEEL, thermal expansion coefficient, TLV-TWA, vapor density, vapor pressure, viscosity, volatility
Theft - Chemical Weapon (Precursor)	chemical formula/name, ID numbers (CAS, EC/EINECS, NA/DOT/UN, RTECS), molecular structure, NFPA rating
Theft - Weapon of Mass Effect	chemical formula/name, ID numbers (CAS, EC/EINECS, NA/DOT/UN, RTECS), molecular structure, NFPA rating
Theft - Explosive/IED precursor	chemical formula/name, ID numbers (NA/DOT/UN, EC/EINECS, CAS, RTECS), melting point, molecular structure, NFPA rating
Sabotage - Contamination	chemical formula/name, Henry's law, ID numbers (CAS, EC/EINECS, NA/DOT/UN, RTECS), molecular structure, NFPA rating, partition coefficient, reactivity, solubility, (specific) surface area, sublimation point, surface area, surface tension

One category of chemical security is a release (first three rows of Table 2) that would affect people in or near the facility, due to a toxic cloud, a flammable-vapor explosion, a pool fire, or an intentional detonation. A second category is theft/diversion (fourth, fifth, and sixth rows of Table 2) with three sub-categories: chemical weapons or CW precursors; chemicals that could be used directly as a weapon of mass effect; and chemicals that could be used as an explosive or as a precursor to an improvised explosive

device (IED). The third category (last row in Table 2) is sabotage/contamination, involving chemicals that could be mixed with other readily available material to create adverse consequences to human life and health. Table 3 shows the relationship between sub-categories of chemical security (Table 2) and features of the various chemical properties (Table 1). Table E.1 (end of Appendix E) provides more details.

Table 3: Relationship Between Chemical Security Sub-Categories and Property Features

Sub-Category of Chemical Security	Identity	Toxicity	Chemical Potential	Reactivity	Temperature & Pressure	Dispersion
Release - Explosive	X	X	X	X	X	
Release - Flammable	X	X	X	X	X	
Release - Toxic	X	X		X		X
Theft - Chemical Weapon Precursor	X	X	X	X	X	X
Theft - Weapon of Mass Effect	X	X	X	X	X	X
Theft - Explosive/IED precursor	X		X	X	X	
Sabotage - Contamination	X	X		X		X

A chemical release can affect the nearby population in several ways, including life-threatening effects, which are characterized and quantified by the scientific discipline of toxicology. Different sources of toxicological assessment exist, each with their own standards (established and enforced by government regulators) or guidelines (non-enforceable). While guidelines are "voluntary," some organizations use them in mandatory orders and procedures. Table 4 summarizes these standards and guidelines.

Table 4: Summary of Toxicological Guidelines and Standards

Name	Sponsor/Developer
AEGL (Acute Exposure Guideline Level)	EPA, National Research Council
ERGP (Emergency Response Planning Guidelines)	American Industrial Hygiene Association
IDLH (Immediately Dangerous to Life and Health)	National Institute of Occupational Safety & Health
TEEL (Temporary Emergency Exposure Limits)	U.S. Department of Energy
TLV (Threshold Limit Values)	American Conf. of Governmental Indus. Hygienists

Life-threatening effects can occur at air concentrations at (or above) the following levels: AEGL-3, which is tabulated for exposure durations of 10 minutes, 30 minutes, 1 hour, 4 hours, and 8 hours; ERPG-3 with a 1-hour exposure; IDLH for 30 minutes of exposure; and a TEEL-3 for one hour of exposure. Appendix E provides further discussion of these values. The chemical properties compilation includes values for AEGL-3, ERPG-3, IDLH, and TEEL-3 for estimation of deaths from an airborne COI release.

Table 5 shows that no single source in Appendix F provides all of the chemical properties. Table 5 omits rarely useful sources. The columns in Table 5 correspond to each chemical property, and the rows show the sources. The green cells indicate that a property can be obtained from a specific source; the red cells show that the property is unavailable from that source. See Appendices E – F for definitions of acronyms.

Table 5: Information Availability Matrix

Sources of Data	Chemical Formula	CAS Number	Structural image	Common synonyms	RTECS #, UN#, DOT guide	EC #	Molecular weight	Color/form	Flash point	Explosive limits	Auto-ignition temp	Melting point	Boiling point	Decomposition pt	Critical temp, Critical	Critical volume	Vapor pressure	Antoine parameters	Density	Water solubility	Henry's law constant	Heat of solution	Heat of combustion	Heat of melting	Heat of vaporization	Heat of sublimation	Heat of decomposition	Adiabatic flame temp	DOT class, NFPA reactivity	Viscosity	Surface tension	Compressibility	Acid/base constants	Partition coefficient	Joule-Thomson coefficient	Diffusion coefficient	Coefficient of thermal	Electrical conductivity	HSC data	Miscellaneous warnings
AEGLs	G	G	R	G	R	R	G	G	G	G	G	G	G	R	R	R	G	R	G	G	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R
Akron	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G	R	G	R	G	G	R	R	G	G	G	R	R	R	G	G	G	R	G	G	R	R	G	R	R	G
ATSDR	G	G	R	G	G	G	G	G	G	G	G	G	G	R	R	R	G	R	G	G	G	R	R	R	R	R	R	R	R	R	R	R	R	G	R	R	R	R	R	G
CAMEO	G	G	R	G	R	R	G	G	G	G	G	G	G	R	R	R	G	R	G	G	R	R	R	R	R	R	R	R	G	R	R	R	R	R	R	R	R	R	R	G
ChemSpider	G	G	G	G	G	G	G	G	G	R	R	G	G	R	R	R	G	R	G	G	G	R	R	R	G	R	R	R	R	R	G	R	R	G	R	R	R	R	R	G
CHRIS	G	G	R	G	R	R	G	G	G	G	G	R	G	R	G	R	R	R	G	G	R	Y	Y	G	G	R	R	Y	G	G	G	R	R	R	R	R	R	R	R	G
CRC	G	G	G	R	R	R	G	G	G	G	G	G	G	Y	G	G	G	R	G	G	Y	Y	G	G	G	G	R	Y	R	G	G	Y	G	G	R	Y	Y	Y	R	R
Dean	G	G	R	R	R	R	G	R	Y	Y	Y	G	G	R	G	R	G	G	G	G	R	G	R	G	G	R	R	R	R	G	G	Y	G	R	R	R	Y	Y	R	R
ESIS	G	G	G	G	R	G	R	R	G	G	G	G	G	R	R	R	G	R	G	G	R	R	R	R	R	R	R	R	R	R	G	R	R	G	R	R	R	R	R	G
HSC	G	G	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	G	R	R	R	R	R	G	R	R	R	R	R	R	R	R	R	R	R	R	R	G	R
HSDB	G	G	R	G	R	R	G	G	G	G	G	G	G	G	G	Y	G	R	G	G	G	G	G	G	G	Y	Y	R	G	G	G	R	G	G	R	Y	Y	Y	R	G
INCHEM	G	G	R	G	G	G	G	G	G	G	G	G	G	R	R	R	G	R	G	G	R	R	R	R	R	R	R	R	G	R	R	R	R	G	R	R	R	R	R	G
Knovel	G	G	R	G	R	R	G	G	G	G	G	G	G	Y	G	G	G	G	G	G	R	R	G	G	G	G	Y	R	R	G	G	R	Y	G	R	G	G	Y	R	G
NFPA	G	G	R	G	R	R	G	R	G	G	G	G	G	Y	R	R	G	R	R	G	R	R	R	R	R	R	R	R	G	R	R	R	R	R	R	R	R	R	R	G
NIOSH	G	G	R	G	G	R	G	G	G	G	R	R	G	R	R	R	G	R	G	G	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	G
NIST	G	G	G	G	R	R	G	R	R	R	R	G	G	R	G	G	G	G	G	R	G	R	G	G	G	Y	R	R	R	G	G	R	R	R	Y	R	R	R	R	R
PhysProp	G	G	R	R	R	R	G	R	R	R	R	G	G	R	R	R	G	R	R	G	G	R	R	R	R	R	R	R	R	R	R	R	G	G	R	R	R	R	R	R

G	Sometimes available from this data sourc
R	Not available from this data source
Y	Rarely available from this data source

4. Information Collection and Repository

A spreadsheet template was prepared to begin the information collection process. This Excel structure was also used as an initial repository, while a relational database was being designed and implemented. The template includes chemical and physical properties for a compound. The relational database software subsequently could support information entry by multiple users, plus simultaneous viewing of information, as discussed in the next section. Appendix G (first page) shows a portion of the Information Store entries for chlorine. Appendix H discusses information consistency issues for the chemical properties.

The repository tables were loaded using Microsoft™ Excel™, Microsoft™ Access™, and SQLLoader™. The information was initially put into Excel™ spreadsheets, which were then imported into Access™. The Access™ tables were then exported as tab-delimited plaintext. SQLLoader™ was used with the appropriate control file to load these text files into Oracle™ database tables. SQLDeveloper™ was used to check the tables after they were loaded, and to make small changes. Appendix H shows the important repository tables for the Information Store (first diagram). The second diagram in Appendix H shows the relationships among these tables, in terms of entity relationships. The third page of Appendix H is a tabular summary of the repository tables.

Information quality assurance is vital, thus requiring rigorous peer-review for completeness, correctness, and consistency. Consequently, a random sample of 40 compounds was selected. A PhD chemist (Burnett) compared the Information Store properties with another authoritative source in Appendix F (WISER, which was compiled by the National Library of Medicine for emergency responders, and does not contain all of the COIs nor all of the chemical properties in Appendix E). In every case, the property values were identical. In a few cases, additional properties were found that are not in the Information Store (e.g., dipole moment, spectral information), but this information is unimportant for the purposes of this work. This comparison provides high confidence that the selected chemical properties are reliable.

Data for the Information Store include the COI from the Appendix A list, MC List, and the EC List. Nine other chemicals were included in the April 2007 version of Appendix A, but were omitted from the final list. The specific chemicals in this "other" category are: Acetone, Urea, Carbon Monoxide, Urea Nitrate, Sulfur Monochloride, Toluene 2,4-diisocyanate, Toluene diisocyanate (mix), Toluene 2,6-diisocyanate, and Diesel Oil #2. The Information Store includes a total of 1,267 chemicals, of which 149 have no available properties, as summarized in Table 6. Table 7 shows the reason that properties could not be found for the three COI chemicals in Appendix A. The data are recorded into Excel™ spreadsheet files.

Table 6: Summary of Chemicals in Information Store

Chemical List	Number of Chemicals	Number with No Data
Appendix A	339	3
MC	128	17
EC	791	129
Other	9	0
Totals	1267	149

Table 7: Chemicals from Appendix A with No Data Found

Chemical with No Data	Reason No Data Found
Propylphosphonyl Difluoride	Acute Toxin (too dangerous to test)
Ethyl Phosphonyl Difluoride	Precursor for Chemical Weapons (too dangerous to test)
Isopropylphosphonyl Difluoride	Precursor for Chemical Weapons (too dangerous to test)

5. Information Store Design and Construction

The Information Store must contain all of the detailed information harvested from the chemical searches. Thus, a companion effort created a conceptual model of the different entities inherent in the information and their attributes and interrelationships. The information features involve many-to-many relationships, as well as inherent hierarchies, making a "flat" spreadsheet approach difficult at best.

In order to design the back end database, a search was made of existing chemical repositories, in order to make use of lessons learned by other systems that exist for general chemical information. The National Oceanographic and Atmospheric Administration (NOAA), in collaboration with the Environmental Protection Agency (EPA) and the Coast Guard, designed a tool for first responders and emergency planners who are involved in hazardous materials incident response and planning[26]. The tool, called Computer-Aided Management of Emergency Operations (CAMEO) Chemicals, contains some information of interest for this effort. The CAMEO staff was contacted, and they were willing to provide insight on lessons they had learned over the years in the design and maintenance of the tool. They also were willing to share with us a list of the chemical fields contained in the CAMEO back-end database[27], which was used for guidance in designing parts of the Information Store.

Other issues involve database encoding or storing of reference citations, and Greek/mathematical notation. The ORNL reference library was consulted on types of information that are stored by electronic tools for referencing. Exporting formats from various tools including EndNote[28], Procite[29], RefWorks[30], and several others were compared. Notes of their field categories, as well as a spreadsheet comparing them were prepared and stored on the internal share point.

The database must encode different units of measure from several different systems of measurement (e.g. SI, English). The chemical formulas and units may contain superscripts and subscripts, the property names may be denoted by Greek symbols, and the units may contain other mathematical notation. MathML[31] is a Markup Language (ML) that is recommended by World Wide Web Consortium (W3C). However, MathML seemed too cumbersome and unsuitable for the initial entries, since custom programming is needed, which would impede the first-phase implementation. A National Institute of Technology (NIST) effort is under way to produce an ML just for units – UnitsML[32]. This approach would be useful, but is just in the development stage. A third alternative was ASCIIMathML[33], which consists of JavaScript functions that convert a simple American Standard Code for Information Interchange (ASCII) text notation into MathML. This option may be a solution for encoding and storing the mathematical notation. ASCIIMathML is similar to TeX[34] notation and uses certain prefix characters (e.g., use of ^ for superscript, and _ for subscript) for encoding and storing in the database.

A modeling tool (xCase[35]) was used to model the structure of the Information Store that would allow easy implementation, via tool-generated Data Definition Language (DDL). The Entity Relationship Diagram (ERD) of this model (Appendix H) was updated as needed and stored on the internal share point. The modeling tool was used to keep documentation on each entity and attribute.

The xCase modeling tool was used to generate DDL to make a SQL Server™ database. This approach was chosen for the initial database, primarily because of the ease in creating a Microsoft Access database as a prototype. Additional insight into the information entry needs arose from experience in the ongoing collection. Consequently, the xCase model was enhanced, and used to generate an Oracle schema (chemical_characterization) hosted on web2u.ornl.gov to provide a development location for this part of the Information Store.

6. Typical Applications of the Information Store

The disastrous consequences of accidents and terrorism are identical, implying that chemical process safety is also important for prevention, protection, and mitigation. Chemical incidents also arise from natural disasters (e.g., fire, flood, hurricane, tornado, lightning, flooding, and storm surge). A chemical incident can release and mix nearby chemicals, for which water solubility and reactivity are important.

The chemical industry has accumulated a vast knowledge of operations and process safety over more than a century. Chemical safety also reduces the vulnerability to terrorism, increases resilience to such incidents, and lowers the impact of real events. Such information has been developed by many disparate private sources, such as the, American Chemical Society (acs.org), American Institute of Chemical Engineers (aiche.org), Mary Kay O'Connor Process Safety Center (process-safety.tamu.edu), American National Standards Institute (ansi.org), Synthetic Organic Chemical Manufacturers Association (socma.com), National Fire Protection Association (nfpa.org), American Petroleum Institute (api.org), E. I. du Pont de Nemours and Company (dupont.com), Dow Chemical Company (dow.com), Archer Daniels Midland Company (admworld.com), and Bayer (bayer.com). Federal contributors include the Chemical Safety Board (csb.gov), Environmental Protection Agency (epa.gov), and Occupational Safety and Health Administration (osha.gov), along with their State and local counterparts. Moreover, major chemical associations have adopted strong security and safety protocols, such as the American Chemistry Council's "ResponsibleCare," the National Association of Chemical Distributors's "Responsible Distribution Code," the Synthetic Organic Chemical Manufacturers Association's "ChemStewards," and the National Paint and Coatings Association's "CoatingsCare." Use of these best practices by the chemical facilities (e.g., inherently safety processing) reduces the vulnerability to terrorism. Such improvements also increase a facility's long-term economic viability, thus motivating information sharing. Consequently, a future component of this Information Store effort could be collection of these chemical-industry protocols to facilitate event prevention, vulnerability reduction, and assessment of event root causes.

Many examples[37] exist for vulnerability reduction from chemical safety: process modification (e.g., lower temperature and/or pressure), substitution with less hazardous chemicals (e.g., less energetic, lower toxicity), production of hazardous material on an as-needed basis via mini-reactors, elimination of transportation and bulk storage of hazardous substances, separation of reactive compounds, approaches for suppression of events, and inventory control. Incident reports are helpful (e.g., events involving the site, COI, COI precursors, or their process intermediates), in terms of known initiators, vulnerabilities that can make an event more severe (e.g., cascade of explosions that damage additional critical infrastructure, such as pipelines and hospitals), and lessons learned about process vulnerabilities and event mitigation methods. Moreover, COI co-location in single or adjacent facilities (e.g., fuel/oxidizer, cyanide/acid) can produce a cascading event (e.g., explosion or toxic release). Geographical, population, and weather information are not part of this present work. Other features of vulnerability reduction include physical and cyber security, emergency planning, operations and engineering support, and collaboration with State and local law enforcement. The bottom line is that chemical vulnerability risk involves many factors.

The source term for specific chemical hazards is typically related to process intermediates, like isocyanates (the toxic source in the 1984 Bhopal accident), ethylene oxide, and many others. Ubiquitous chlorine use is a major vulnerability. Chemical inventory is the prime factor in catastrophic events. Mixtures and reactions among a site's extensive inventory are very challenging to model; potential additions by a terrorist or insider are even more difficult. Other important issues are a dispersible physical form and proximity of the public. Many sites are land-locked by surrounding developments and high property costs. Facilities are typically crowded and close to public assets with minimal separation between storage, processing equipment, private property, and residences. The number (more than 40,000) and complexity of these sites compounds the modeling challenge.

The vulnerability of the U.S. chemical industry is exacerbated by economic pressures and lax policies towards infrastructure maintenance. Supply-side economics and the reliance on foreign suppliers promote the hoarding of key intermediates. Without substitutes, industries must balance costs and availability against the liability of a release. Larger companies are shedding their liability by transferring these toxic chemicals to under-staffed, mid-sized companies that usually operate on the edge of safety in order to maintain profitability. This approach has increased their vulnerability to accidents and has resulted in a proliferation of small- and mid-sized facilities for regulation. Chemical facilities are generally older, and their equipment is pushed to or beyond their life-cycle limits, because of the high capital costs with low returns. Older equipment frequently is used for newer processes, for which they were not designed and are operated beyond their limits for pressure relief and heat removal. Inadequate separation typically exists in crowded facilities for fire protection and deluge systems. Therefore, many processes are not safety-resilient and are prone to cascading catastrophic events with or without external initiators.

This work suggests a simple, defensible way to identify chemical facilities with the potential for very severe consequences from an unmitigated event. We propose the following three parameters to facilitate this distinction:

(1) Total chemical potential energy = (on-site COI in kg) x (heat of combustion per kg);

(2) Number of lethal doses from acute toxicity = (on-site COI in kg)/ (lethal dose in kg);

(3) Population = maximum people within a one-mile radius of the site.

These equations must also be summed over the on-site COIs. The heat of combustion and the lethal dose are a function only of the specific COI. Gosselin's book, "Clinical Toxicology of Commercial Products[40]" (1984), is a standard reference for lethal dose, which is given in milligrams of ingested dose per kilogram of body mass (~70 kg as a typical value). Other toxicity factors involve availability of the chemical, likelihood of its synthesis, and probability of weaponization. These factors are not included, because they have already been considered in the choice of COI compounds. Another measure of toxicity is "reportable quantity" (RQ) under US Environmental Protection Agency regulations. However, RQ relates more to chronic toxicity and carcinogenicity, rather than to acute effects. The maximum population is taken over day-versus-night and weekday-versus-weekend time frames. These three parameters give a bounding estimate of chemical risk to nearby population by the total chemical potential energy and the total toxicity, independent of facility characteristics, local geography, chemical processing, etc. Facilities with large values of all three parameters clearly have the highest unmitigated potential consequences. This analysis would use the chemical properties in Appendix E that are readily available in the Information Store. A check list for site-specific COI (and processes) may be helpful. For example, the check list could include observational questions, such as, "If you see xxx, then is yyy near?"

In summary, potential consequences of chemical events involve 56 specific toxicological, chemical, and physical properties of the on-site materials. This work identifies 34 authoritative data sources for these properties, which are unavailable from any one authoritative source. This work develops an Information Store for 1,267 unique chemicals, including Federally-identified "chemicals of interest," mission critical items, and economically critical materials. The Information Store components include: 1) collection of chemical properties; 2) quantification of consequences on the basis of historical events; and 3) identification and compilation of key process safety information for vulnerability mitigation. The advantages of this Information Store include: all of the information in a central authoritative repository rather than many disparate sources; retention of the information in a stand-alone, secure system; and access to the information only by authorized users.

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Appendix A: Chemicals of Interest [Appendix A of 6CFR27 in *Federal Register* 72 (#223, 20 Nov 2007) pages 65421-65435]

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
Acetaldehyde		75-07-0	1.00	10,000						X					
Acetone cyanohydrin, stabilized		75-86-5					ACG	APA							X
Acetyl bromide		506-96-7					ACG	APA							X
Acetyl chloride		75-36-5					ACG	APA							X
Acetyl iodide		507-02-8					ACG	APA							X
Acetylene	[Ethyne]	74-86-2	1.00	10,000						X					
Acrolein	[2-Propenal] or Acrylaldehyde	107-02-8	1.00	5,000					X						
Acrylonitrile	[2-Propenenitrile]	107-13-1	1.00	10,000						X					
Acrylyl chloride	[2-Propenoyl chloride]	814-68-6	1.00	10,000						X					
Allyl alcohol	[2-Propen-1-ol]	107-18-6	1.00	15,000					X						
Allylamine	[2-Propen-1-amine]	107-11-9	1.00	10,000						X					
Allyltrichlorosilane, stabilized		107-37-9					ACG	APA							X
Aluminum (powder)		7429-90-5			ACG	100								X	
Aluminum bromide, anhydrous		7727-15-3					ACG	APA							X
Aluminum chloride, anhydrous		7446-70-0					ACG	APA							X
Aluminum phosphide		20859-73-8					ACG	APA							X
Ammonia (anhydrous)		7664-41-7	1.00	10,000					X						
Ammonia (conc. 20% or greater)		7664-41-7	20.00	20,000					X						
Ammonium nitrate, [with more than 0.2 percent combustible substances, including any organic substance calculated as carbon, to the exclusion of any other added substance]		6484-52-2	ACG	5,000	ACG	400					X			X	

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
Ammonium nitrate, solid [nitrogen concentration of 23% nitrogen or greater]		6484-52-2			33.00	2000								X	
Ammonium perchlorate		7790-98-9	ACG	5,000	ACG	400					X			X	
Ammonium picrate		131-74-8	ACG	5,000	ACG	400					X			X	
Amyltrichlorosilane		107-72-2					ACG	APA							X
Antimony pentafluoride		7783-70-2					ACG	APA							X
Arsenic trichloride	[Arsenous trichloride]	7784-34-1	1.00	15,000	30.00	2.2			X			X			
Arsine		7784-42-1	1.00	1,000	0.67	15			X				X		
Barium azide		18810-58-7	ACG	5,000	ACG	400					X			X	
1,4-Bis(2-chloroethylthio)-n-butane		142868-93-7			CUM 100g							X			
Bis(2-chloroethylthio)methane		63869-13-6			CUM 100g							X			
Bis(2-chloroethylthiomethyl)ether		63918-90-1			CUM 100g							X			
1,5-Bis(2-chloroethylthio)-n-pentane		142868-94-8			CUM 100g							X			
1,3-Bis(2-chloroethylthio)-n-propane		63905-10-2			CUM 100g							X			
Boron tribromide		10294-33-4			12.67	45	ACG	APA					X		X
Boron trichloride	[Borane, trichloro]	10294-34-5	1.00	5,000	84.70	45			X				X		
Boron trifluoride	[Borane, trifluoro]	7637-07-2	1.00	5,000	26.87	45			X				X		
Boron trifluoride compound with methyl ether (1:1)	[Boron, trifluoro [oxybis (methane)]-,T-4-]	353-42-4	1.00	15,000					X						
Bromine		7726-95-6	1.00	10,000					X						
Bromine chloride		13863-41-7			9.67	45							X		
Bromine pentafluoride		7789-30-2					ACG	APA							X
Bromine trifluoride		7787-71-5			6.00	45	ACG	APA					X		X
Bromotrifluorethylene	[Ethene, bromotrifluoro-]	598-73-2	1.00	10,000						X					

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
1,3-Butadiene		106-99-0	1.00	10,000						X					
Butane		106-97-8	1.00	10,000						X					
Butene		25167-67-3	1.00	10,000						X					
1-Butene		106-98-9	1.00	10,000						X					
2-Butene		107-01-7	1.00	10,000						X					
2-Butene-cis		590-18-1	1.00	10,000						X					
2-Butene-trans	[2-Butene, (E)]	624-64-6	1.00	10,000						X					
Butyltrichlorosilane		7521-80-4					ACG	APA							X
Calcium hydrosulfite	[Calcium dithionite]	15512-36-4					ACG	APA							X
Calcium phosphide		1305-99-3					ACG	APA							X
Carbon disulfide		75-15-0	1.00	20,000					X						
Carbon oxysulfide	[Carbon oxide sulfide (COS); carbonyl sulfide]	463-58-1	1.00	10,000						X					
Carbonyl fluoride		353-50-4			12.00	45							X		
Carbonyl sulfide		463-58-1			56.67	500							X		
Chlorine		7782-50-5	1.00	2,500	9.77	500			X				X		
Chlorine dioxide	[Chlorine oxide, (ClO2)]	10049-04-4	1.00	1,000			ACG	APA	X						X
Chlorine monoxide	[Chlorine oxide]	7791-21-1	1.00	10,000						X					
Chlorine pentafluoride		13637-63-3			4.07	15							X		
Chlorine trifluoride		7790-91-2			9.97	45							X		
Chloroacetyl chloride		79-04-9					ACG	APA							X
2-Chloroethylchloro-methylsulfide		2625-76-5			CUM 100g							X			
Chloroform	[Methane, trichloro-]	67-66-3	1.00	20,000					X						
Chloromethyl ether	[Methane, oxybis(chloro-)]	542-88-1	1.00	1,000					X						
Chloromethyl methyl ether	[Methane, chloromethoxy-]	107-30-2	1.00	5,000					X						
1-Chloropropylene	[1-Propene, 1-chloro-]	590-21-6	1.00	10,000						X					
2-Chloropropylene	[1-Propene, 2-chloro-]	557-98-2	1.00	10,000						X					

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
Chlorosarin	[o-Isopropyl methylphosphonochloridate]	1445-76-7			CUM 100g							X			
Chlorosoman	[o-Pinacolyl methylphosphonochloridate]	7040-57-5			CUM 100g							X			
Chlorosulfonic acid		7790-94-5					ACG	APA							X
Chromium oxychloride		14977-61-8					ACG	APA							X
Crotonaldehyde	[2-Butenal]	4170-30-3	1.00	10,000						X					
Crotonaldehyde, (E)-	[2-Butenal], (E)-]	123-73-9	1.00	10,000						X					
Cyanogen	[Ethanedinitrile]	460-19-5	1.00	10,000	11.67	45				X			X		
Cyanogen chloride		506-77-4	1.00	10,000	2.67	15			X				X		
Cyclohexylamine	[Cyclohexanamine]	108-91-8	1.00	15,000					X						
Cyclohexyltrichlorosilane		98-12-4					ACG	APA							X
Cyclopropane		75-19-4	1.00	10,000						X					
DF	Methyl phosphonyl difluoride	676-99-3			CUM 100g							X			
Diazodinitrophenol		87-31-0	ACG	5,000	ACG	400					X			X	
Diborane		19287-45-7	1.00	2,500	2.67	15			X				X		
Dichlorosilane	[Silane, dichloro-]	4109-96-0	1.00	10,000	10.47	45				X			X		
N,N-(2-diethylamino)ethanethiol		100-38-9			30.00	2.2						X			
Diethyldichlorosilane		1719-53-5					ACG	APA							X
o,o-Diethyl S-[2-(diethylamino)ethyl] phosphorothiolate		78-53-5			30.00	2.2						X			
Diethyleneglycol dinitrate		693-21-0	ACG	5,000	ACG	400					X			X	
Diethyl methylphosphonite		15715-41-0			30.00	2.2						X			
N,N-Diethyl phosphoramidic dichloride		1498-54-0			30.00	2.2						X			
N,N-(2-diisopropylamino)ethanethiol	N,N-diisopropyl-(beta)-aminoethane thiol	5842-07-9			30.00	2.2						X			

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
Difluoroethane	[Ethane, 1,1-difluoro-]	75-37-6	1.00	10,000						X					
N,N-Diisopropyl phosphoramidic dichloride		23306-80-1			30.00	2.2						X			
1,1-Dimethylhydrazine	[Hydrazine, 1, 1-dimethyl-]	57-14-7	1.00	10,000						X					
Dimethylamine	[Methanamine, N-methyl-]	124-40-3	1.00	10,000						X					
N,N-(2-dimethylamino)ethanethiol		108-02-1			30.00	2.2						X			
Dimethyldichlorosilane	[Silane, dichlorodimethyl-]	75-78-5	1.00	10,000			ACG	APA		X					X
N,N-Dimethyl phosphoramidic dichloride	[Dimethylphosphoramido-dichloridate]	677-43-0			30.00	2.2						X			
2,2-Dimethylpropane	[Propane, 2,2-dimethyl-]	463-82-1	1.00	10,000						X					
Dingu	[Dinitroglycoluril]	55510-04-8	ACG	5,000	ACG	400					X			X	
Dinitrogen tetroxide		10544-72-6			3.80	15							X		
Dinitrophenol		25550-58-7	ACG	5,000	ACG	400					X			X	
Dinitroresorcinol		519-44-8	ACG	5,000	ACG	400					X			X	
Diphenyldichlorosilane		80-10-4					ACG	APA							X
Dipicryl sulfide		2217-06-3	ACG	5,000	ACG	400					X			X	
Dipicrylamine [or] Hexyl	[Hexanitrodiphenylamine]	131-73-7	ACG	5,000	ACG	400					X			X	
N,N-(2-dipropylamino)ethanethiol		5842-06-8			30.00	2.2						X			
N,N-Dipropyl phosphoramidic dichloride		40881-98-9			30.00	2.2						X			
Dodecyltrichlorosilane		4484-72-4					ACG	APA							X
Epichlorohydrin	[Oxirane, (chloromethyl)-]	106-89-8	1.00	20,000					X						
Ethane		74-84-0	1.00	10,000						X					
Ethyl acetylene	[1-Butyne]	107-00-6	1.00	10,000						X					
Ethyl chloride	[Ethane, chloro-]	75-00-3	1.00	10,000						X					
Ethyl ether	[Ethane, 1,1-oxybis-]	60-29-7	1.00	10,000						X					
Ethyl mercaptan	[Ethanethiol]	75-08-1	1.00	10,000						X					

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
Ethyl nitrite	[Nitrous acid, ethyl ester]	109-95-5	1.00	10,000						X					
Ethyl phosphonyl difluoride		753-98-0			CUM 100g							X			
Ethylamine	[Ethanamine]	75-04-7	1.00	10,000						X					
Ethyldiethanolamine		139-87-7			80.00	220						X			
Ethylene	[Ethene]	74-85-1	1.00	10,000						X					
Ethylene oxide	[Oxirane]	75-21-8	1.00	10,000						X					
Ethylenediamine	[1,2-Ethanediamine]	107-15-3	1.00	20,000					X						
Ethyleneimine	[Aziridine]	151-56-4	1.00	10,000						X					
Ethylphosphonothioic dichloride		993-43-1			30.00	2.2						X			
Ethyltrichlorosilane		115-21-9					ACG	APA							X
Fluorine		7782-41-4	1.00	1,000	6.17	15			X				X		
Fluorosulfonic acid		7789-21-1					ACG	APA							X
Formaldehyde (solution)		50-00-0	1.00	15,000					X						
Furan		110-00-9	1.00	10,000						X					
Germane		7782-65-2			20.73	45							X		
Germanium tetrafluoride		7783-58-6			2.11	15							X		
Guanyl nitrosaminoguanylidene hydrazine			ACG	5,000	ACG	400					X			X	
Hexaethyl tetraphosphate and compressed gas mixtures		757-58-4			33.37	500							X		
Hexafluoroacetone		684-16-2			15.67	45							X		
Hexanitrostilbene		20062-22-0	ACG	5,000	ACG	400					X			X	
Hexolite	[Hexotol]	121-82-4	ACG	5,000	ACG	400					X			X	
Hexyltrichlorosilane		928-65-4					ACG	APA							X
HMX	[Cyclotetramethylene-tetranitramine]	2691-41-0	ACG	5,000	ACG	400					X			X	

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
HN1 (nitrogen mustard-1)	[Bis(2-chloroethyl)ethylamine]	538-07-8			CUM 100g							X			
HN2 (nitrogen mustard-2)	[Bis(2-chloroethyl)methylamine]	51-75-2			CUM 100g							X			
HN3 (nitrogen mustard-3)	[Tris(2-chloroethyl)amine]	555-77-1			CUM 100g							X			
Hydrazine		302-01-2	1.00	10,000						X					
Hydrochloric acid (conc. 37% or greater)		7647-01-0	37.00	15,000					X						
Hydrocyanic acid		74-90-8	1.00	2,500					X						
Hydrofluoric acid (conc. 50% or greater)		7664-39-3	50.00	1,000					X						
Hydrogen		1333-74-0	1.00	10,000						X					
Hydrogen bromide (anhydrous)		10035-10-6			95.33	500							X		
Hydrogen chloride (anhydrous)		7647-01-0	1.00	5,000	ACG	500			X				X		
Hydrogen cyanide	[Hydrocyanic acid]	74-90-8			4.67	15							X		
Hydrogen fluoride (anhydrous)		7664-39-3	1.00	1,000	42.53	45			X				X		
Hydrogen iodide, anhydrous		10034-85-2			95.33	500							X		
Hydrogen peroxide (concentration of at least 35%)		7722-84-1			35.00	400								X	
Hydrogen selenide		7783-07-5	1.00	10,000	0.07	15				X			X		
Hydrogen sulfide		7783-06-4	1.00	10,000	23.73	45			X				X		
Iodine pentafluoride		7783-66-6					ACG	APA							X
Iron, pentacarbonyl-	[Iron carbonyl (Fe (CO)5), (TB5-11)-]	13463-40-6	1.00	10,000						X					
Isobutane	[Propane, 2-methyl]	75-28-5	1.00	10,000						X					
Isobutyronitrile	[Propanenitrile, 2-methyl-]	78-82-0	1.00	20,000					X						
Isopentane	[Butane, 2-methyl-]	78-78-4	1.00	10,000						X					
Isoprene	[1,3-Butadiene, 2-methyl-]	78-79-5	1.00	10,000						X					

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
Isopropyl chloride	[Propane, 2-chloro-]	75-29-6	1.00	10,000						X					
Isopropyl chloroformate	[Carbonochloridic acid, 1-methylethyl ester]	108-23-6	1.00	15,000					X						
Isopropylamine	[2-Propanamine]	75-31-0	1.00	10,000						X					
Isopropylphosphonothioic dichloride		1498-60-8			30.00	2.2						X			
Isopropylphosphonyl difluoride		677-42-9			CUM 100g							X			
Lead azide		13424-46-9	ACG	5,000	ACG	400					X			X	
Lead styphnate	[Lead trinitroresorcinate]	15245-44-0	ACG	5,000	ACG	400					X			X	
Lewisite 1	[2-Chlorovinyldichloroarsine]	541-25-3			CUM 100g							X			
Lewisite 2	[Bis(2-chlorovinyl)chloroarsine]	40334-69-8			CUM 100g							X			
Lewisite 3	[Tris(2-chlorovinyl)arsine]	40334-70-1			CUM 100g							X			
Lithium amide		7782-89-0					ACG	APA							X
Lithium nitride		26134-62-3					ACG	APA							X
Magnesium (powder)		7439-95-4			ACG	100								X	
Magnesium diamide		7803-54-5					ACG	APA							X
Magnesium phosphide		12057-74-8					ACG	APA							X
MDEA	[Methyldiethanolamine]	105-59-9			80.00	220						X			
Mercury fulminate		628-86-4	ACG	5,000	ACG	400					X			X	
Methacrylonitrile	[2-Propenenitrile, 2-methyl-]	126-98-7	1.00	10,000					X						
Methane		74-82-8	1.00	10,000						X					
2-Methyl-1-butene		563-46-2	1.00	10,000						X					
3-Methyl-1-butene		563-45-1	1.00	10,000						X					
Methyl chloride	[Methane, chloro-]	74-87-3	1.00	10,000						X					
Methyl chloroformate	[Carbonochloridic acid, methyl ester]	79-22-1	1.00	10,000						X					
Methyl ether	[Methane, oxybis-]	115-10-6	1.00	10,000						X					
Methyl formate	[Formic acid Methyl ester]	107-31-3	1.00	10,000						X					

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
Methyl hydrazine	[Hydrazine, methyl-]	60-34-4	1.00	15,000					X						
Methyl isocyanate	[Methane, isocyanato-]	624-83-9	1.00	10,000					X						
Methyl mercaptan	[Methanethiol]	74-93-1	1.00	10,000	45.00	500				X			X		
Methyl thiocyanate	[Thiocyanic acid, methyl ester]	556-64-9	1.00	20,000					X						
Methylamine	[Methanamine]	74-89-5	1.00	10,000						X					
Methylchlorosilane		993-00-0			20.00	45							X		
Methyldichlorosilane		75-54-7					ACG	APA							X
Methylphenyldichlorosilane		149-74-6					ACG	APA							X
Methylphosphonothioic dichloride		676-98-2			30.00	2.2						X			
2-Methylpropene	[1-Propene, 2-methyl-]	115-11-7	1.00	10,000						X					
Methyltrichlorosilane	[Silane, trichloromethyl-]	75-79-6	1.00	10,000			ACG	APA		X					X
Sulfur mustard (Mustard gas (H))	[Bis(2-chloroethyl)sulfide]	505-60-2			CUM 100g							X			
O-Mustard (T)	[Bis(2-chloroethylthioethyl)ether]	63918-89-8			CUM 100g							X			
Nickel Carbonyl		13463-39-3	1.00	10,000						X					
Nitric acid		7697-37-2	80.00	15,000	68.00	400			X					X	
Nitric oxide	[Nitrogen oxide (NO)]	10102-43-9	1.00	10,000	3.83	15			X				X		
Nitrobenzene		98-95-3			ACG	100								X	
5-Nitrobenzotriazol		2338-12-7	ACG	5,000	ACG	400					X			X	
Nitrocellulose		9004-70-0	ACG	5,000	ACG	400					X			X	
Nitrogen mustard hydrochloride	[Bis(2-chloroethyl)methylamine hydrochloride]	55-86-7			30.00	2.2						X			
Nitrogen trioxide		10544-73-7			3.83	15							X		
Nitroglycerine		55-63-0	ACG	5,000	ACG	400					X			X	
Nitromannite	[Mannitol hexanitrate, wetted]	15825-70-4	ACG	5,000	ACG	400					X			X	
Nitromethane		75-52-5			ACG	400								X	
Nitrostarch		9056-38-6	ACG	5,000	ACG	400					X			X	
Nitrosyl chloride		2696-92-6			1.17	15							X		

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
Nitrotriazolone		932-64-9	ACG	5,000	ACG	400					X			X	
Nonyltrichlorosilane		5283-67-0					ACG	APA							X
Octadecyltrichlorosilane		112-04-9					ACG	APA							X
Octolite		57607-37-1	ACG	5,000	ACG	400					X			X	
Octonal		78413-87-3	ACG	5,000	ACG	400					X			X	
Octyltrichlorosilane		5283-66-9					ACG	APA							X
Oleum (Fuming Sulfuric acid)	[Sulfuric acid, mixture with sulfur trioxide]	8014-95-7	1.00	10,000					X						
Oxygen difluoride		7783-41-7			0.09	15							X		
1,3-Pentadiene		504-60-9	1.00	10,000						X					
Pentane		109-66-0	1.00	10,000						X					
1- Pentene		109-67-1	1.00	10,000						X					
2-Pentene, (E)-		646-04-8	1.00	10,000						X					
2-Pentene, (Z)-		627-20-3	1.00	10,000						X					
Pentolite		8066-33-9	ACG	5,000	ACG	400					X			X	
Peracetic acid	[Ethaneperoxic acid]	79-21-0	1.00	10,000						X					
Perchloromethylmercaptan	[Methanesulfenyl chloride, trichloro-]	594-42-3	1.00	10,000					X						
Perchloryl fluoride		7616-94-6			25.67	45							X		
PETN	[Pentaerythritol tetranitrate]	78-11-5	ACG	5,000	ACG	400					X			X	
Phenyltrichlorosilane		98-13-5					ACG	APA							X
Phosgene	[Carbonic dichloride] or [carbonyl dichloride]	75-44-5	1.00	500	0.17	15			X				X		
Phosphine		7803-51-2	1.00	10,000	0.67	15				X			X		
Phosphorus		7723-14-0			ACG	400								X	
Phosphorus oxychloride	[Phosphoryl chloride]	10025-87-3	1.00	5,000	80.00	220	ACG	APA	X			X			X
Phosphorus pentabromide		7789-69-7					ACG	APA							X
Phosphorus pentachloride		10026-13-8					ACG	APA							X
Phosphorus pentasulfide		1314-80-3					ACG	APA							X

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
Phosphorus trichloride		7719-12-2	1.00	15,000	3.48	45	ACG	APA	X				X		X
Picrite	[Nitroguanidine]	556-88-7	ACG	5,000	ACG	400					X			X	
Piperidine		110-89-4	1.00	10,000						X					
Potassium chlorate		3811-04-9			ACG	400								X	
Potassium cyanide		151-50-8					ACG	APA							X
Potassium nitrate		7757-79-1			ACG	400								X	
Potassium perchlorate		7778-74-7			ACG	400								X	
Potassium permanganate		7722-64-7			ACG	400								X	
Potassium phosphide		20770-41-6					ACG	APA							X
Propadiene	[1,2-Propadiene]	463-49-0	1.00	10,000						X					
Propane		74-98-6	1.00	60,000						X					
Propionitrile	[Propanenitrile]	107-12-0	1.00	10,000					X						
Propyl chloroformate	[Carbonchloridic acid, propylester]	109-61-5	1.00	10,000						X					
Propylene	[1-Propene]	115-07-1	1.00	10,000						X					
Propylene oxide	[Oxirane, methyl-]	75-56-9	1.00	10,000						X					
Propyleneimine	[Aziridine, 2-methyl-]	75-55-8	1.00	10,000					X						
Propylphosphonothioic dichloride		2524-01-8			30.00	2.2						X			
Propylphosphonyl difluoride		690-14-2			CUM 100g							X			
Propyltrichlorosilane		141-57-1					ACG	APA							X
Propyne	[1-Propyne]	74-99-7	1.00	10,000						X					
QL	[o-Ethyl-o-2-diisopropylaminoethyl methylphosphonite]	57856-11-8			CUM 100g							X			
RDX	[Cyclotrimethylenetrinitramine]	121-82-4	ACG	5,000	ACG	400					X			X	
RDX and HMX mixtures		121-82-4	ACG	5,000	ACG	400					X			X	
Sarin	[o-Isopropyl methylphosphonofluoridate]	107-44-8			CUM 100g							X			
Selenium hexafluoride		7783-79-1			1.67	15							X		

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
Sesquimustard	[1,2-Bis(2-chloroethylthio)ethane]	3563-36-8			CUM 100g							X			
Silane		7803-62-5	1.00	10,000						X					
Silicon tetrachloride		10026-04-7					ACG	APA							X
Silicon tetrafluoride		7783-61-1			15.00	45							X		
Sodium azide		26628-22-8			ACG	400								X	
Sodium chlorate		7775-09-9			ACG	400								X	
Sodium cyanide		143-33-9					ACG	APA							X
Sodium hydrosulfite	[Sodium dithionite]	7775-14-6					ACG	APA							X
Sodium nitrate		7631-99-4			ACG	400								X	
Sodium phosphide		12058-85-4					ACG	APA							X
Soman	[o-Pinacolyl methylphosphonofluoridate]	96-64-0			CUM 100g							X			
Stibine		7803-52-3			0.67	15							X		
Strontium phosphide		12504-16-4					ACG	APA							X
Sulfur dioxide (anhydrous)		7446-09-5	1.00	5,000	84.00	500			X				X		
Sulfur tetrafluoride	[Sulfur fluoride (SF4), (T-4)-]	7783-60-0	1.00	2,500	1.33	15			X				X		
Sulfur trioxide		7446-11-9	1.00	10,000					X						
Sulfuryl chloride		7791-25-5					ACG	APA							X
Tabun	[o-Ethyl-N,N-dimethylphosphoramido-cyanidate]	77-81-6			CUM 100g							X			
Tellurium hexafluoride		7783-80-4			0.83	15							X		
Tetrafluoroethylene	[Ethene, tetrafluoro-]	116-14-3	1.00	10,000						X					
Tetramethyllead	[Plumbane, tetramethyl-]	75-74-1	1.00	10,000					X						
Tetramethylsilane	[Silane, tetramethyl-]	75-76-3	1.00	10,000						X					
Tetranitroaniline		53014-37-2	ACG	5,000	ACG	400					X			X	
Tetranitromethane	[Methane, tetranitro-]	509-14-8	1.00	10,000						X					
Tetrazene	[Guanyl nitrosaminoguanyltetrazene]	109-27-3	ACG	5,000	ACG	400					X			X	

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
1H-Tetrazole		288-94-8	ACG	5,000	ACG	400					X			X	
Thiodiglycol	[Bis(2-hydroxyethyl)sulfide]	111-48-8			30.00	2.2						X			
Thionyl chloride		7719-09-7					ACG	APA							X
Titanium tetrachloride	[Titanium chloride (TiCl4) (T-4)-]	7550-45-0	1.00	2,500	13.33	45	ACG	APA	X				X		X
TNT	[Trinitrotoluene]	118-96-7	ACG	5,000	ACG	400					X			X	
Torpex	[Hexotonal]	67713-16-0	ACG	5,000	ACG	400					X			X	
Trichlorosilane	[Silane, trichloro-]	10025-78-2	1.00	10,000			ACG	APA		X					X
Triethanolamine		102-71-6			80.00	220						X			
Triethanolamine hydrochloride		637-39-8			80.00	220						X			
Triethyl phosphite		122-52-1			80.00	220						X			
Trifluoroacetyl chloride		354-32-5			6.93	45							X		
Trifluorochloroethylene	[Ethene, chlorotrifluoro]	79-38-9	1.00	10,000	66.67	500				X			X		
Trimethylamine	[Methanamine, N,N-dimethyl-]	75-50-3	1.00	10,000						X					
Trimethylchlorosilane	[Silane, chlorotrimethyl-]	75-77-4	1.00	10,000			ACG	APA		X					X
Trimethyl phosphite		121-45-9			80.00	220						X			
Trinitroaniline		26952-42-1	ACG	5,000	ACG	400					X			X	
Trinitroanisole		606-35-9	ACG	5,000	ACG	400					X			X	
Trinitrobenzene		99-35-4	ACG	5,000	ACG	400					X			X	
Trinitrobenzenesulfonic acid		2508-19-2	ACG	5,000	ACG	400					X			X	
Trinitrobenzoic acid		129-66-8	ACG	5,000	ACG	400					X			X	
Trinitrochlorobenzene		88-88-0	ACG	5,000	ACG	400					X			X	
Trinitrofluorenone		129-79-3	ACG	5,000	ACG	400					X			X	
Trinitro-meta-cresol		602-99-3	ACG	5,000	ACG	400					X			X	
Trinitronaphthalene		55810-17-8	ACG	5,000	ACG	400					X			X	
Trinitrophenetole		4732-14-3	ACG	5,000	ACG	400					X			X	
Trinitrophenol		88-89-1	ACG	5,000	ACG	400					X			X	
Trinitroresorcinol		82-71-3	ACG	5,000	ACG	400					X			X	
Tritonal		54413-15-9	ACG	5,000	ACG	400					X			X	
Tungsten hexafluoride		7783-82-6			7.10	45							X		

Appendix A: Chemicals of Interest (continued)

Chemicals of Interest (COI)	Synonym	Chemical Abstract Service (CAS) #	Release		Theft		Sabotage		Security Issue						
			Minimum Concentration (%)	Screening Threshold Quantities (in pounds)	Minimum Concentration (%)	Screening Threshold Quantities (in pounds unless otherwise noted)	Minimum Concentration (%)	Screening Threshold Quantities	Release -- Toxic	Release -- Flammables	Release -- Explosives	Theft -- CW/CWP	Theft -- WME	Theft -- EXP/IEDP	Sabotage/Contamination
Vinyl acetate monomer	[Acetic acid ethenyl ester]	108-05-4	1.00	10,000						X					
Vinyl acetylene	[1-Buten-3-yne]	689-97-4	1.00	10,000						X					
Vinyl chloride	[Ethene, chloro-]	75-01-4	1.00	10,000						X					
Vinyl ethyl ether	[Ethene, ethoxy-]	109-92-2	1.00	10,000						X					
Vinyl fluoride	[Ethene, fluoro-]	75-02-5	1.00	10,000						X					
Vinyl methyl ether	[Ethene, methoxy-]	107-25-5	1.00	10,000						X					
Vinylidene chloride	[Ethene, 1,1-dichloro-]	75-35-4	1.00	10,000						X					
Vinylidene fluoride	[Ethene, 1,1-difluoro-]	75-38-7	1.00	10,000						X					
Vinyltrichlorosilane		75-94-5					ACG	APA							X
VX	[o-Ethyl-S-2-diisopropylaminoethyl methyl phosphonothiolate]	50782-69-9			CUM 100g							X			
Zinc hydrosulfite	[Zinc dithionite]	7779-86-4					ACG	APA							X

[1] The acronyms used in this appendix have the following meaning: ACG = A Commercial Grade; APA = A Placarded Amount; CW/CWP = Chemical Weapons/Chemical Weapons Precursors; WME = Weapons of Mass Effect; EXP/IEDP = Explosives/Improvised Explosive Device Precursors

Appendix B: Risk-Based Approach to Chemical Facility Anti-Terrorism Standards[39]

Across the nation there are numerous facilities that contain potentially dangerous chemicals. Decision makers are interested in calculating the risk of terrorist attacks at those facilities in order to prevent such attacks and save human lives. The risk of an attack is given by the statistical formula:

$$R = (\textit{probability of attack}) \times (\textit{probability of success, given an attack}) \times (\textit{consequences, given success})$$

A particular concern is the consequences of potential terrorist attacks. Thus, it is important to develop a method that will quantify these potential consequences. One measure of the consequences of an event is the resultant human casualties and fatalities. (Another measure of consequences is the monetary cost of damage resulting from an event. Monetary cost is not a parameter that CADAT addresses, and this is a subject of Future Work.) By analyzing the consequences of previous attacks, it is possible to achieve an estimate of the potential consequences of future events. Accidents should also be analyzed because an accident could serve as a surrogate for an attack, since an attacker could repeat an accident process.

In order to automate the process of gathering data on chemical attacks and accidents, the Chemical Attack Data Acquisition Tool (CADAT) was created. CADAT is a Java-based program that parses Internet news articles about real chemical attacks and accidents. CADAT retrieves the text of these articles, searches for and extracts relevant data from the text, creates a tabular summary of the data, and calculates meaningful statistics.

Methodology

The basic process for a single run of CADAT is as follows:

1. Import list of all COI.
2. Create a main folder to index all information from this run of CADAT.
3. Acquire data for each chemical in the list. For a given chemical:
    a. Create a subfolder to index all information for this chemical.
    b. Search "new.google.com" for articles about *attacks* with this chemical.
    c. Retrieve text of each article found.
    d. Check relevance of each article and discard irrelevant articles.
    e. Parse relevant articles for data (number of casualties, number of fatalities).
    f. Create tabular summary of data from all articles found for this search.
    g. Repeat steps b-f, for *accidents* with this chemical.
4. Repeat step 3 for each COI.
5. Summarize data, by chemical, in a table showing number of events, average, and standard deviation for each of four event categories: casualties from attacks, fatalities from attacks, casualties from accidents, fatalities from accidents.

We next discuss Step 3 in greater detail. To retrieve information about real chemical attack consequences, it is most efficient to search only news reports. Thus, all Internet searches were conducted via the Google News Archives ("news.google.com"). Using this site helps in several ways. First, searching Google News ensures that all results of a search are news articles, which increases the chances of seeing relevant web pages in the search results. For example, a regular Google search for "chlorine attack" (with the specific search string shown in italics below) gives

approximately 72,100 results. However, when the same search is performed using Google News, the search returns a more manageable 4,950 results. With the regular Google search, 10 out of the first 40 results are actual news articles about a specific chlorine attack, whereas with the Google News search, 18 out of the first 40 results are pertinent. Thus, using Google News, the number of unwanted pages has been greatly reduced, making the process of parsing articles for data much more efficient. Furthermore, each article from the Google News Archives is clearly dated, making extraction of the article date quite simple.

In searching for data about chemical attack consequences, it is necessary to analyze only those articles that contain terms such as "deaths" and "injuries." There are many ways to say "this many people died" and "this many people were injured," so it is important to consider each possibility in a search. The "~" operator in Google (and Google News) signals the search engine to find either the exact word following the "~" or to find a synonym of that word. With this operator and other Google search syntax, the following search string was constructed:

> *chlorine attack ~killed OR ~died OR ~death OR ~injury OR ~sicken OR suffer OR hospital*

This string tells Google News to find articles containing both the words "chlorine" and "attack" and also containing at least one of the words "killed," "died," "death," "injury," "sicken," "suffer," or "hospital," or any synonym of "killed," "died," "death," "injury," or "sicken."

After the Google News search is performed for a chemical attack or accident, CADAT extracts the html source code from each of the first 40 results. (These searches were limited to 40 results in order to limit the time needed for CADAT to complete a full run over all chemicals. A subject of Future Work is to look at more than 40 results.) Next, for each chemical, CADAT uses Lucene, an open-source Java-based text search engine library, to organize the contents of each page into "fields" (title, text, url, etc.) and index each page (now a collection of fields) as a document in the subfolder for the specific chemical.

Once the indexing process is complete for one Internet search, CADAT uses Lucene to check the documents for relevance. Each document is deemed relevant or not relevant, and only relevant documents are parsed for data. It is necessary to exclude information from "blogs" in data calculations, because such information may not be trustworthy. Thus, documents that include the word "blog" in the URL or in the page title are marked as not relevant. Similarly, articles about worst-case scenarios, plans/preparedness for chemical attacks, or any other fictional case should be excluded from the results, because only data from real events are desired. To exclude fictional articles, CADAT uses Lucene to analyze the language of each article. Specifically, CADAT first counts the number of "conditional" words in an article ("could," "would," "might," etc.). Then it counts the number of words that signal a real event ("happened," "killed," "caused," etc.). CADAT compares the number of "conditional" words to the number of "real event" words. After a human reading of a sampling of articles, it was determined that a ratio of 1.0 "conditional" to "real event" words is an appropriate threshold to eliminate unwanted pages. An article with a ratio greater than 1.0 is deemed not relevant, and articles with a ratio less than 1.0 are relevant. Any article published before 1980 is marked as irrelevant, because events that occurred in the past 30 years are more likely to represent near-future events than those that occurred more than 30 years ago. (This number was chosen simply because it seemed like a reasonable cut-off. Trying other cut-off dates is a subject of Future Work.) Currently, there is no method for determining whether multiple articles are found for a single event. This issue is also a subject of Future Work.

After each document has been labeled either "relevant" or "not relevant," CADAT begins searching for pertinent data in the relevant articles only. First, all written numbers (such as "five" or "thirty") are converted to the appropriate integer value ("5" or "30"). Thus, CADAT can parse the document for integers and not miss a number because it is spelled out. The next step is to find and extract the integers that correspond to a number of casualties. There are many ways to make a statement such as "six people were injured." For example, an article could say, "the attack injured six people," "six injuries resulted from the attack," "six people were hospitalized," "six soldiers were wounded," and so on. To account for as many phrasing variations as possible, CADAT uses an array of words that could signal casualties:

{injur, wound*, casualt*, sicken*, suffer*, hospital*, treat*, harm*, hurt}*

(The asterisk at the end of a word root indicates that it could have any ending.) CADAT also needs an array of words that signify a human life:

{people, person, civilian*, soldier*}*

Next, CADAT uses regular expressions (a pattern matching language) with Lucene to check for numbers appearing in specific textual patterns with a word from the "casualties" array, and sometimes with a word from the "human" array. The regular expressions patterns will match any of the following:

i. number followed by casualty ("4 wounded" or "500 hospitalized")
ii. casualty followed by number ("injured 50" or "sickened 300")
iii. number followed by human, followed by a free word space, followed by casualty ("27 people wounded" or "20 civilians were hurt")

When a match is found, the integer in the match is saved in an array of "casualties" data for that specific chemical search (such as "chlorine attack"). CADAT then calculates the average and standard deviation of the values in the "casualties" data array and saves these statistics.

Next, the pattern matching process described above is repeated, this time parsing the documents for integers corresponding to fatalities. Now, CADAT uses an array of words that could signal fatalities:

{death, dead, die*, kill*, fatalit*}*

CADAT uses the same array of "human" words and the same regular expressions as before, replacing the "casualties" array with the "fatalities" array. Every time a match is found, the integer in the match is saved into an array of "fatalities" data. Statistics are calculated from this array and are saved for later use. (A subject of Future Work is to look at matching more textual patterns with more sophisticated regular expressions and more possibilities in the arrays of words for "casualties," "fatalities," and "human life.") The following two excerpts come from two relevant articles in the search for "chlorine attack." The underlined phrases are those that CADAT will recognize, and the highlighted numbers are extracted.

3 Killed, 25 Injured In Chlorine Attack
Insurgents Appear to Try New Tactics
By Ernesto Londoño/ Washington Post Staff Writer /

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Thursday, February 22, 2007; A12

BAGHDAD, Feb. 21 -- A tank truck carrying chlorine
exploded in western Baghdad on Wednesday, killing
three people and wounding at least 25 in the second
such attack in as many days, according to a spokesman
for Iraq's Interior Ministry.
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Chlorine Attack in Iraq Kills 20
By KIRK SEMPLE and JON ELSEN
Published: April 6, 2007

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BAGHDAD, April 6 — Twenty people were killed and 30
wounded in Ramadi today when a suicide bomber
detonated a truck loaded with explosives and chlorine
gas near a residential complex, police said. Another
50 had trouble breathing after the attack.
```

In the first excerpt, the regular expressions matched the number "3" twice, and in the second excerpt, the number "20" is matched twice. Multiple matches of the same data could cause a problem with calculating statistics later. To solve this problem, any repeated numbers in the same document are recorded only once.

At this point in the analysis, all documents for a given chemical search (such as "chlorine attack") have been indexed, marked relevant or not relevant, and the relevant documents have been parsed for data. CADAT will now move on to the next search ("chlorine accident") and repeat the same process. When this search is complete, CADAT moves to the next chemical and the entire process runs again. The output from each search is saved in a table in the indexing folder for that chemical. Tables B1 and B2 show the results for chlorine.

Table B1. Chlorine Attack Output (16 entries)

ID#	Casualties	Fatalities	Date	URL
1	350, 16, 55	8, 16, 5, 2	18-Mar-07	http://www.sptimes.com/2007/03/18/Worldandnation/Chlorine_attacks_sick.shtml
2	30, 4	20	6-Apr-07	http://www.nytimes.com/2007/04/06/world/middleeast/06cnd-iraq.html
3	3, 9, 25	3	22-Feb-07	http://www.washingtonpost.com/wp-dyn/content/article/2007/02/21/AR2007022100225_pf.html
4	31, 35, 150	13	21-Feb-07	http://www.usatoday.com/news/world/iraq/2007-02-21-iraq-helicopter_x.htm
8	1	--	8-Apr-07	http://abclocal.go.com/wpvi/story?section=nation_world&id=5191014
9	28	20	19-Mar-07	http://www.usatoday.com/printedition/news/20070319/a_iraqnews19.art.htm
10	12	3, 4, 27	6-Apr-07	http://www.usatoday.com/news/world/iraq/2007-04-06-efp_N.htm
11	350, 4, 5	4, 7, 2	18-Dec-08	http://www.thestandard.com.hk/news_detail.asp?pp_cat=17&art_id=40445&sid=127260348&con_type=1
16	--	--	2-Sep-92	http://docs.newsbank.com/g/GooglePM/ST/lib00155,0EAF8EB2C873D0C6.html
18	--	--	23-Mar-07	http://www.accessmylibrary.com/premium/0286/0286-30097685.html
22	250	9	26-Feb-07	http://www.redorbit.com/news/science/853361/chlorine_attacks_raise_specter_of_chemical_war/index.html
25	--	--	11-Jul-04	http://www.accessmylibrary.com/premium/0286/0286-8157675.html
27	--	--	29-Mar-88	[illegible]
28	75	2	16-May-07	http://www.guardian.co.uk/Iraq/Story/0,,2080864,00.html?gusrc=rss&feed=networkfront
37	--	7, 2	28-Feb-08	http://www.cbc.ca/world/story/2008/02/27/israel-palestine.html
39	6, 50, 2	4, 32, 5	20-May-07	http://news.bbc.co.uk/mobile/bbc_news/world/americas/667/66743/story6674319.shtml

Table B2. Chlorine Accident Output (18 entries)

ID#	Casualties	Fatalities	Date	URL
2	17	--	13-Jun-92	http://docs.newsbank.com/g/GooglePM/KC/lib00144,0EAF3DD3C484195B.html
3	--	27	30-Mar-05	http://www.cbc.ca/world/story/2005/03/30/chlorine050330.html
4	--	9	10-Jan-05	http://www.nytimes.com/2005/01/10/national/10train.html
7	--	8	7-Jan-05	http://www.nytimes.com/2005/01/07/national/07derail.html
13	240, 2	8, 81, 1	6-Jan-05	http://www.usatoday.com/news/nation/2005-01-06-trains_x.htm
14	30, 4	20	6-Apr-07	http://www.nytimes.com/2007/04/06/world/middleeast/06cnd-iraq.html
18	--	--	8-Jan-05	http://www.accessmylibrary.com/premium/0286/0286-7777557.html
20	31, 148	16, 9, 13, 28	22-Feb-07	http://www.sptimes.com/2007/02/22/Worldandnation/US_troops_rescued_in_.shtml
24	17	--	18-Oct-03	http://cities.expressindia.com/fullstory.php?newsid=66033
26	--	9	7-Jan-06	http://www.accessmylibrary.com/premium/0286/0286-12262824.html
27	--	--	16-Jan-04	http://www.chinadaily.com.cn/en/doc/2004-01/16/content_299661.htm
28	--	--	18-Jul-02	http://www.accessmylibrary.com/premium/0286/0286-25991609.html
32	70	--	13-Aug-04	http://news.xinhuanet.com/english/2004-08/13/content_1774471.htm
33	7	--	20-Jun-98	http://www.cnn.com/US/9806/20/briefs/train.derail/index.html
34	--	--	27-Jun-06	http://docs.newsbank.com/g/GooglePM/CO/lib00111,11288AC3F4377A38.html
35	50	--	15-Aug-02	http://docs.newsbank.com/g/GooglePM/SL/lib00170,0F584FA940F339DE.html
39	14	8	26-Feb-07	http://www.accessmylibrary.com/premium/0286/0286-29751081.html
40	--	3	7-Jul-96	http://docs.newsbank.com/g/GooglePM/SJ/lib00189,0EB71FC8385A2AE5.html

Some entries in the output tables show that no data were found for casualties or fatalities. These entries remain visible in the table, however, to indicate that a relevant article was found at the given URL. Even though no data were extracted by CADAT, there could be data in the article that CADAT was unable to find with its specific required textual patterns.

Output tables, like those shown above, were integral to the development of CADAT. In its preliminary stages, CADAT performed only one search at a time, on the chemical *chlorine* and only searching for *attack*. These search terms give a manageable number of results, which was helpful in validating the data that CADAT collected. First, it was necessary to ensure that CADAT was indexing all relevant articles and discarding all irrelevant articles. As explained above, a comparison was done between the articles that CADAT determined to be relevant and those articles that were actually relevant, according to a human interpretation of the article. For the *chlorine attack* search parameters, CADAT achieved 81% agreement with the human determination of which articles should be relevant.

It is also important to ensure that CADAT extracts the correct data from the articles. Another comparison was done between the data extracted by CADAT and the data that a human reader found. The results of this comparison (for *chlorine attack*) are shown in Table B3.

For *casualties* found by CADAT, the average and standard deviation are 67.8 and 108.1, respectively. For the actual *casualties* data, as found by a human reader, the average and standard deviation are 105.2 and 105.8, respectively. For *fatalities* found by CADAT, the average and standard deviation are 9.3 and 8.8, respectively. For the actual *fatalities* data, the average and standard deviation are 14.6 and 15.5, respectively. These discrepancies between data gathered by CADAT and actual data are relatively modest for a first attempt. The need for continued data validation is critical. Once CADAT has finished the data collection process for each COI, the statistics for each chemical are organized into a summary table and this table is saved in the main index. The summary table may be opened in Microsoft Excel, where further statistical analysis can take place.

Table B3. Comparison of CADAT Results with Human-Reader Values

ID#	CADAT Casualties	actual Casualties	CADAT Fatalities	actual Fatalities	URL
1	350, 16, 55	100, 250	8, 16, 5, 2	2	http://www.sptimes.com/2007/03/18/Worldandnation/Chlorine_attacks_sick.shtml
2	30, 4	30	20	20	http://www.nytimes.com/2007/04/06/world/middleeast/06cnd-iraq.html
3	3, 9, 25	25	3	3	http://www.washingtonpost.com/wp-dyn/content/article/2007/02/21/AR2007022100225_pf.html
4	31, 35, 150	150	13	9	http://www.usatoday.com/news/world/iraq/2007-02-21-iraq-helicopter_x.htm
8	1	6	--	--	http://abclocal.go.com/wpvi/story?section=nation_world&id=5191014
9	28	--	20	--	http://www.usatoday.com/printedition/news/20070319/a_iraqnews19.art.htm
10	12	30	3, 4, 27	27	http://www.usatoday.com/news/world/iraq/2007-04-06-efp_N.htm
11	350, 4, 5	356	4, 7, 2	2	http://www.thestandard.com.hk/news_detail.asp?pp_cat=17&art_id=40445&sid=12726034&con_type=1
16	--	--	--	--	http://docs.newsbank.com/g/GooglePM/ST/lib00155,0EAF8EB2C873D0C6.html
18	--	--	--	--	http://www.accessmylibrary.com/premium/0286/0286-30097685.html
22	250	150, 55	9	5	http://www.redorbit.com/news/science/853361/chlorine_attacks_raise_specter_of_chemical_war/index.html
25	--	--	--	--	http://www.accessmylibrary.com/premium/0286/0286-8157675.html
27	--	--	--	--	[illegible]
28	75	60	2	45	http://www.guardian.co.uk/Iraq/Story/0,,2080864,00.html?gusrc=rss&feed=networkfront
37	--	--	7, 2	--	http://www.cbc.ca/world/story/2008/02/27/israel-palestine.html
39	6, 50, 2	50	4, 32, 5	1, 32	http://news.bbc.co.uk/mobile/bbc_news/world/americas/667/66743/story6674319.shtml

Results

Table B4 shows the results from one full run of CADAT over all COI. This run was performed on April 15, 2009. The table is organized by chemical, showing the results of the searches for attacks and accidents with that chemical. The pink column shows all data found for casualties resulting from attacks; the red column shows data for fatalities resulting from attacks; the light blue column shows data for casualties resulting from accidents; and the teal column shows data for fatalities resulting from accidents. For a specific search, CADAT reports *n* (the number of data values found), *average* (the mean of the data values), and *standard deviation* (a measure of the variation in the data). Chemicals for which no data were found have not been included in this summary. The notation, "--" indicates that no data were found for that specific search.

It is useful to visualize these data in order to gain a better understanding of how lethal and injurious chemical attacks and accidents tend to be. Figure B1 shows four plots of cumulative distribution function (CDF) versus the average across all COI. Separate plots were created for each of the four categories of chemical searches: attack casualties (a), attack fatalities (b), accident casualties (c), and accident fatalities (d). The CDF is a measure of how data accumulate as (in this case) the average increases. For example, a point *(x,y)* signifies that *y* occurrences of data were found with an average less than or equal to *x*. All four plots are depicted on the same scale for direct comparison. A CDF that increases rapidly [as in plot (b) or (d)] indicates that most of the chemicals have a low average value in that search category. A CDF that increases more gradually [like plot (a)] indicates that the average values in that category are more dispersed-some low, some high, and some in the middle.

Table B4. Results from One Run of CADAT over All COI

	ATTACKS						ACCIDENTS					
	casualties			*fatalities*			*casualties*			*fatalities*		
chemical name	**n**	**average**	**std dev**	**n**	**average**	**std dev**	**n**	**average**	**std dev**	**n**	**average**	**std dev**
Acetaldehyde	0	--	--	0	--	--	3	11	13.4412	0	--	--
Acetyl chloride	0	--	--	0	--	--	0	--	--	1	6	0
Acetylene OR Ethyne	7	39.1429	36.8178	15	48	74.0738	3	16.6667	7.4087	5	44.2	82.9106
Acrylonitrile OR 2-Propenenitrile	0	--	--	0	--	--	6	3.5	1.70783	3	1	0
Allyl alcohol OR 2-Propen-1-ol	0	--	--	0	--	--	0	--	--	3	44.3333	39.7185
Aluminum	1	266	0	9	58.7778	92.3156	2	5.5	0.5	3	1.33333	0.4714
Aluminum chloride	1	111	0	3	18.6667	23.5844	1	3	0	6	2.5	1.38444
Aluminum phosphide	0	--	--	2	5.5	0.5	0	--	--	1	0	0
Ammonia	1	4	0	1	2	0	0	--	--	0	--	--
Anhydrous ammonia	0	--	--	0	--	--	1	20	0	3	1.66667	0.94281
Ammonium nitrate	6	50.8333	59.8398	19	91.1579	84.3715	7	40.4286	55.2213	9	34.5556	43.8003
solid Ammonium nitrate	5	172.4	196.935	12	57.5833	68.305	1	500	0	5	43.2	63.2784
Ammonium perchlorate	1	250	0	2	1.5	0.5	6	159.167	157.042	11	2.18182	1.33609
Arsine	0	--	--	0	--	--	2	97.5	2.5	0	--	--
Bromine	1	1	0	1	5	0	2	3.5	2.5	1	9	0
1-3-Butadiene	0	--	--	0	--	--	3	18.6667	9.87702	2	2.5	0.5
Butane	7	19.2857	21.6314	15	12.0667	14.9954	3	6.33333	6.18241	2	56	55
Butene OR Butylene	0	--	--	0	--	--	2	4	1	1	1	0
Calcium phosphide	0	--	--	1	34	0	1	1	0	0	--	--
Carbon disulfide	0	--	--	0	--	--	0	--	--	1	1	0
Carbon oxysulfide OR Carbon oxide sulfide	0	--	--	0	--	--	2	150	150	3	5	5.09902
Chlorine	22	67.7727	105.569	21	9.28571	8.56984	12	52.5	68.6373	14	17.1429	19.3275
Chlorine dioxide	3	170	233.351	13	5	2.48069	3	69.6667	92.1822	3	5	3.26599
Chlorine monoxide OR Chlorine oxide	2	251.5	248.5	10	5.3	2.64764	9	25.5556	61.7038	1	1	0
Chloroform OR Trichoromethane	1	18	0	2	1.5	0.5	0	--	--	0	--	--
Cyanogen OR Ethanedinitrile	0	--	--	0	--	--	2	14	13	4	9	10.4163
Cyanogen chloride	0	--	--	0	--	--	1	1	0	0	--	--
Cyclohexylamine OR Cyclohexanamine	0	--	--	0	--	--	1	11	0	1	4	0
Difluoroethane	0	--	--	0	--	--	0	--	--	2	3	2
Dinitrophenol	0	--	--	0	--	--	0	--	--	1	9	0
Ethane	3	145	48.9898	4	26.25	33.9513	6	56.1667	71.9523	15	22.7333	22.3322
Ethyl chloride OR Chloroethane	0	--	--	3	3.33333	1.24722	1	12	0	4	2.75	1.47902
Ethyl ether	0	--	--	4	9.25	7.36122	2	6.5	5.5	5	3.8	3.18748
Ethylene OR Ethene	1	66	0	2	2	0	12	36.75	97.8307	8	3.75	3.69966
Ethylene oxide OR Oxirane	0	--	--	0	--	--	10	15	18.1714	4	1	0
Ethyleneimine OR Aziridine	0	--	--	0	--	--	1	9	0	0	--	--
Fluorine	1	10	0	3	50	55.1604	8	3.125	1.61536	5	32	48.4107
Formaldehyde	2	15.5	3.5	3	9.66667	7.03957	0	--	--	0	--	--
Germane	0	--	--	0	--	--	0	--	--	6	73	108.809
HMX	8	30.5	13.2004	14	48.7143	74.7839	1	3	0	5	60	105.157

Table B4 (cont'd)

	ATTACKS						ACCIDENTS					
	casualties			*fatalities*			*casualties*			*fatalities*		
chemical name	**n**	**average**	**std dev**	**n**	**average**	**std dev**	**n**	**average**	**std dev**	**n**	**average**	**std dev**
Hydrazine	1	8	0	1	168	0	3	46	38.8844	2	2	0
Hydrochloric acid	7	112.429	127.168	2	16	7	9	95	124.317	13	5.76923	5.63169
Hydrocyanic acid	0	--	--	2	149.5	139.5	0	--	--	4	73.75	124.281
Hydrofluoric acid	1	28	0	0	--	--	3	8.33333	4.98888	4	8.75	6.25999
Hydrogen	2	32	20	5	36	19.5959	0	--	--	0	--	--
Hydrogen bromide	0	--	--	1	100	0	2	8	5	0	--	--
Hydrogen cyanide	1	12	0	6	19.5	18.715	3	6.66667	6.01849	10	32.3	72.363
Hydrogen fluoride	1	144	0	4	7.25	2.94746	9	3.77778	1.81217	6	30	35.4024
Hydrogen peroxide	3	35.3333	23.5702	15	57.2667	38.1636	6	9.83333	10.2862	6	45.5	49.1825
Hydrogen sulfide	2	63	57	4	14.25	18.1297	4	85.75	124.476	6	113	110.49
Isobutane OR 2-Methylpropane	0	--	--	0	--	--	8	36	33.3766	10	7.4	7.22772
Isopentane OR 2-Methylbutane	1	2	0	0	--	--	1	9	0	4	11.5	6.06218
Isopropyl chloride OR 2-Chloropropane	0	--	--	0	--	--	1	12	0	1	1	0
Lead azide	0	--	--	4	9.75	7.62807	0	--	--	0	--	--
Lewisite 1	0	--	--	1	12	0	2	50	0	0	--	--
Lewisite 2	7	54.2857	69.3227	5	64.8	117.641	2	50	0	0	--	--
Lewisite 3	6	60.8333	72.8455	4	6	3.4641	0	--	--	0	--	--
Magnesium	0	--	--	0	--	--	1	8	0	6	9.83333	9.47658
Magnesium phosphide	0	--	--	0	--	--	1	4	0	1	30	0
Mercury fulminate OR 2-methyl-2-propenenitrile	1	79	0	1	3	0	1	18	0	1	60	0
Methane	4	36.25	11.3661	7	20.8571	21.6889	7	25.7143	16.0954	28	30.5	26.024
Methyl chloride OR Chloromethane	1	36	0	0	--	--	7	8.14286	11.482	0	--	--
Methyl ether OR Oxybismethane	0	--	--	0	--	--	2	8.5	3.5	4	14.5	8.17007
Methyl formate	0	--	--	0	--	--	0	--	--	1	22	0
Methyl isocyanate	2	19	17	6	94.1667	181.662	8	7.25	10.9972	4	79.75	132.366
Methyl mercaptan OR Methanethiol	2	46.5	23.5	4	20	0	2	16	7	9	4.88889	5.34258
Sulfur mustard OR mustard gas	0	--	--	3	14.6667	12.3918	1	19	0	0	--	--
Nickel Carbonyl	0	--	--	2	18.5	15.5	0	--	--	0	--	--
Nitric acid	5	60.6	71.3627	16	111.5	91.5847	5	32.4	35.3361	3	55.3333	50.7302
Nitric oxide OR Nitrogen oxide	0	--	--	0	--	--	8	3.625	1.49478	2	20	15
Nitrobenzene	1	6	0	3	6.33333	6.18241	8	30.125	28.9846	21	35.4286	71.0068
Nitrocellulose OR Pyroxylin	4	97	94.0106	6	98.3333	92.6888	1	20	0	6	22.1667	45.5427
Nitrogen trioxide OR Dinitrogen trioxide	0	--	--	0	--	--	2	23	16	0	--	--
Nitroglycerine	1	168	0	2	194	26	0	--	--	0	--	--
Nitromethane	0	--	--	5	136.8	62.4	0	--	--	0	--	--
Oleum OR Fuming Sulfuric acid	1	20	0	0	--	--	4	89	144.943	2	1.5	0.5
Oxygen difluoride	1	144	0	2	9.5	2.5	1	5	0	1	20	0
Pentane	0	--	--	1	48	0	2	12	3	8	14.125	14.2165
PETN OR Pentaerythritol tetranitrate	0	--	--	0	--	--	1	3	0	2	119.5	110.5
Phosgene OR Carbonic dichloride	0	--	--	0	--	--	7	3	2	0	--	--

Table B4 (cont'd)

	ATTACKS						ACCIDENTS					
	casualties			*fatalities*			*casualties*			*fatalities*		
chemical name	**n**	**average**	**std dev**	**n**	**average**	**std dev**	**n**	**average**	**std dev**	**n**	**average**	**std dev**
Phosphine	0	--	--	0	--	--	1	2	0	0	--	--
Phosphorus	2	32.5	20.5	7	16.2857	22.5814	2	78.5	45.5	5	20.6	25.4998
Potassium chlorate	5	104.6	59.0579	14	77.6429	91.0334	4	58.25	82.5784	9	44.3333	53.9176
Potassium cyanide	6	7	4.12311	11	5.27273	3.04783	3	10.3333	8.21922	3	4.66667	1.24722
Potassium nitrate	2	160	140	14	34.2857	31.1962	3	210	164.866	3	33	26.1661
Potassium perchlorate	4	93.25	60.9564	15	97.8667	94.4774	5	46.8	77.3289	5	61	67.0015
Potassium permanganate	0	--	--	1	15	0	1	1	0	1	9	0
Potassium phosphide	0	--	--	0	--	--	1	0	0	1	0	0
Propane	9	34.2222	45.1314	19	16.3158	18.041	3	6.66667	5.90668	4	9	4.30116
Propylene OR 1-Propene	3	72.6667	56.5351	10	27.1	58.6028	3	7.66667	6.2361	8	5.375	6.55625
Propylene oxide OR Methyloxirane	0	--	--	0	--	--	0	--	--	3	14.6667	3.29983
RDX OR Cyclotrimethylenetrinitramine	0	--	--	0	--	--	6	38.6667	32.5252	14	47.5	70.9112
RDX HMX	1	10	0	6	69.8333	82.0882	1	3	0	2	140	130
Sarin	6	112	180.632	20	11.75	4.06048	0	--	--	10	64.7	72.5356
Silane	0	--	--	2	42	40	4	4.5	1.65831	8	49.375	48.1299
Silicon tetrachloride	0	--	--	1	3	0	1	6	0	0	--	--
Silicon tetrafluoride	0	--	--	1	3	0	0	--	--	0	--	--
Sodium azide	1	5	0	7	50.4286	71.394	3	5	2.16025	3	90.6667	126.808
Sodium chlorate	1	8	0	5	36.2	65.9315	3	9.66667	10.873	10	26.2	42.1753
Sodium cyanide	1	168	0	9	26	50.3477	2	93.5	89.5	5	11.6	16.2555
Sodium hydrosulfite OR Sodium dithionite	0	--	--	0	--	--	4	169.5	158.639	11	11.9091	18.8316
Sodium nitrate	2	160	140	6	68.1667	70.279	0	--	--	5	8.2	11.4263
Soman	1	67	0	3	10.3333	2.35702	1	2	0	5	6.6	6.62118
Sulfur dioxide	0	--	--	1	14	0	4	121	164.2	5	7	6.03324
Sulfur trioxide	0	--	--	0	--	--	6	41.3333	36.7181	2	2.5	0.5
Tabun	0	--	--	3	135.667	107.939	3	60.6667	34.1207	5	9.2	5.34416
Tetrafluoroethylene OR Tetrafluoroethene	0	--	--	0	--	--	0	--	--	2	3	1
Thiodiglycol	0	--	--	2	16.5	14.5	0	--	--	0	--	--
TNT OR Trinitrotoluene	15	54.9333	47.8922	36	45.6667	62.996	1	13	0	1	6	0
Trichlorosilane	0	--	--	0	--	--	1	6	0	1	1	0
Trimethylchlorosilane OR Chlorotrimethylsilane	0	--	--	0	--	--	1	15	0	1	111	0
Trimethyl phosphite	0	--	--	0	--	--	3	18.3333	12.7105	4	3	1.73205
Trinitrophenol OR Picric acid	2	4	0	7	7.85714	6.55588	0	--	--	0	--	--
Tritonal	0	--	--	3	25	16.8721	0	--	--	0	--	--
Vinyl acetate monomer	0	--	--	0	--	--	2	8	2	4	8	7.17635
Vinyl acetylene	0	--	--	0	--	--	1	6	0	2	13	7
Vinyl chloride OR Chloroethene	2	19.5	16.5	2	5.5	0.5	8	7.5	10.8743	7	46.5714	107.147
Vinyl fluoride OR Fluoroethene	0	--	--	0	--	--	6	3.5	1.70783	0	--	--
VX	2	74	70	6	13.8333	7.90394	1	25	0	0	--	--

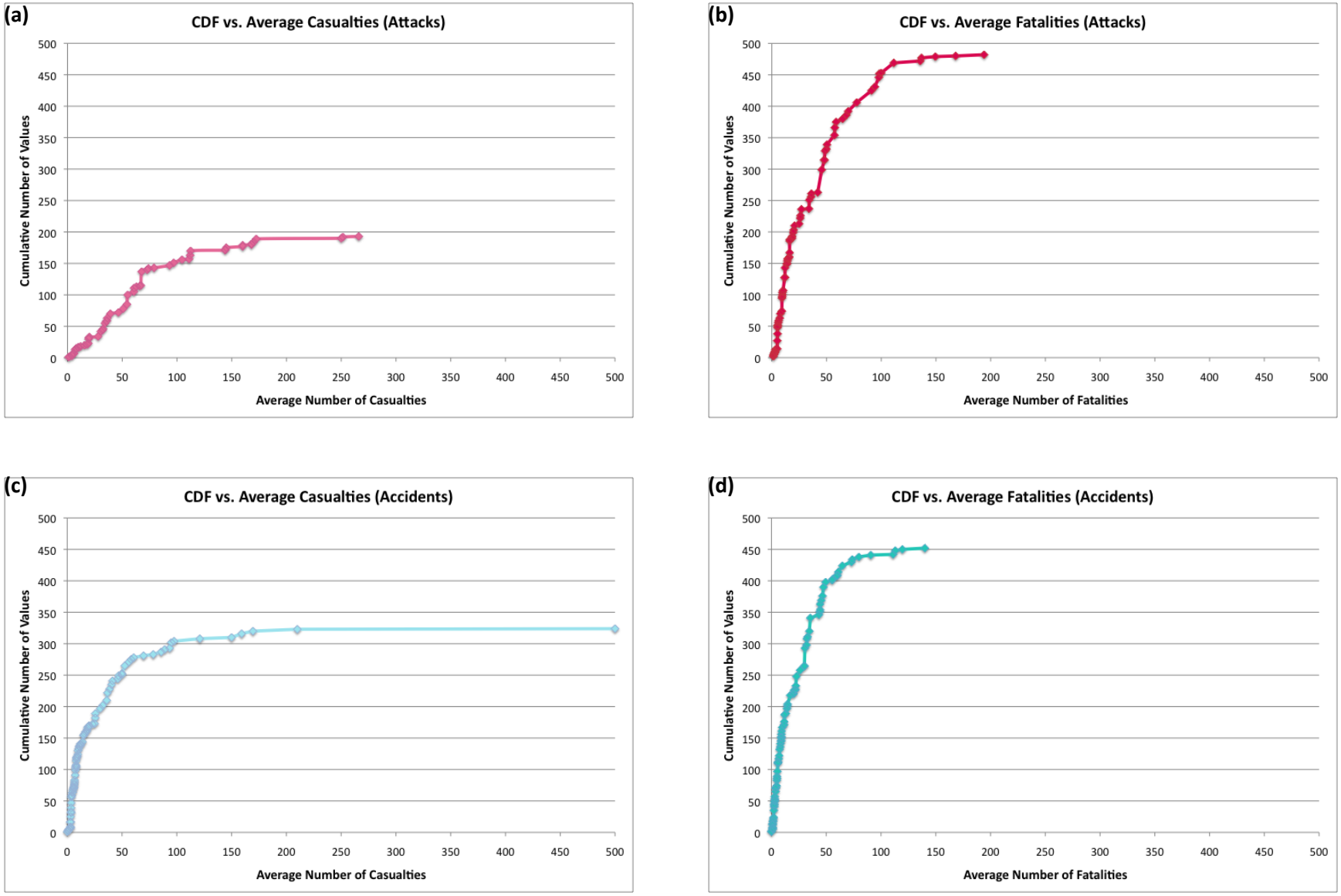


Figure B1. CDF vs. Average for Attack Casualties (a), Attack Fatalities (b), Accident Casualties (c), and Accident Fatalities (d)

Discussion

Table B4 shows that the average is of the same order of magnitude as the standard deviation in almost all cases. Assuming that the news articles found represent a realistic sampling of chemical events, and assuming that the data collected are accurate and true, then this statistical finding would indicate that an attack with a given chemical has relatively unpredictable results. It would be possible to assess whether an attack is likely to injure 200 people or closer to 10, but such an assessment would not necessarily be an accurate prediction due to the large variability in the estimates.

It is no surprise that the data for a given chemical show such great variation. In considering a chemical attack or accident, there are many factors other than the chemical itself that could skew the calculated consequences. For example, if all chlorine attacks occurred in the same way (say, a truck bomb), with the same volume of chlorine, with the same weather conditions, with the same terrain, and with the same surrounding population density and distribution, there would likely be less variation in the number of people injured or killed by chlorine attacks. Of course, no two attacks will occur in exactly the same way, which introduces large variability into the data. However, even with such variability in the data for a given chemical, an assessment could still be made about the probable relative danger of that chemical as compared to another.

Another potentially useful finding is that, with the exception of eleven chemicals (Hydrazine, Hydrocyanic acid, Hydrogen bromide, Hydrogen sulfide, Nitric acid, Nitroglycerine, Nitromethane, PETN or Pentaerythritol tetranitrate, RDX HMX, Tabun, and Trimethylchlorosilane), the average number of fatalities from chemical attacks and accidents is less than 100. The chemicals that have greater than 100 fatalities also have at most 5 data values, and the standard deviations are comparable in magnitude to the average. This result indicates that past chemical attacks and accidents have tended to kill less than 100 people. This result could also mean that the COI are not particularly lethal when used as agents of attack. Or, the result could indicate that the most lethal uses of the COI have not yet been implemented, in which case it could be necessary to analyze how the chemicals could be used. Such factors could be taken into consideration in other parts of the equation that quantifies Risk (such as the "probability of success, given an attack").

Conclusions

Notably, the CDF's for attack casualties and accident casualties appear to be quite similar in shape, initial rate of increase, and maximum value. The same is true for the CDF's of attack fatalities and accident fatalities. This result indicates that the consequences of attacks and accidents are comparable with regard to the distribution of data. This finding upholds the notion that accidents could serve as a surrogate for attacks. Not only could the processes be identical, but the results are also remarkably similar.

All conclusions that may be drawn at this time are, of course, somewhat speculative. In order to reach sound conclusions, it is imperative to verify that the data gathered by CADAT are relevant and true. As the code is developed further, the process of verifying the data gathered will be vital. CADAT has the potential to be a useful tool, but it will only become usable if it provides verifiably accurate results.

We deem these results as helpful and worthy of continuing development, despite several limitations which we discuss next. First, CADAT excludes sidebar links to other articles, but variability in html source code still allows extraction of irrelevant (and sometime inconsistent) information from the body of the news article. Second, the search for each chemical should include more news stories. The present limit of 40 articles requires 4.5 hours to search the entire list of 321 chemicals of interest on a personal computer with a 2.4 GHz processor using a 1.0 Gb/sec Ethernet connection. Third, the present work focuses on methodology development, not better computational efficiency (e.g., Lucene's indexing).

Fourth, an exhaustive list of synonyms is needed to extract deaths and injuries. Fifth, better parsing is needed for text like, "15 people were hospitalized with lacerations and another 30 suffered severe burns," which presently is converted into two separate incidents with injuries of 15 and 30. Sixth, large numbers are presently excluded to avoid confusion with a year ("the attack in 2003 killed…") or a worst-case scenario. Seventh, generation of the CDF plots should be automated. Eighth, these results are from 1980 to present, and should be compared to other cutoff dates. Ninth, these results do not capture the event location, which may be correlated to chemical types, days of the week, etc. Tenth, the present method does not check for more than one article about a single event. Eleventh, the accuracy of *RelevanceChecker* still needs improvement to avoid false positives and false negatives. The only authoritative means of accuracy verification is a human reader who presently limits the speed of test-mode analysis. Twelfth, the CADAT does not return any results for some chemicals that have no associated news articles; this approach cannot quantify the consequences of a chemical attacks in such cases. Finally, this approach cannot quantify the consequences in terms of monetary cost, for which news articles typically provide little if any information.

Appendix C: 1994-1999 Accidents in RMP*Info by Chemical, involving 10 or more Incidents

(P.R. Kleindorfer, "Industrial Ecology and Risk Analysis," Risk Management and Decision Processes Center, University of Pennsylvania (November 2000) in Handbook of Industrial Ecology, ed. by L. Ayers and R. Ayers.)

Chemical Name	Chemical ID	Number of Accidents
Ammonia (anhydrous)	56	656
Chlorine	62	518
Hydrogen fluoride/Hydrofluoric acid	55	101
Flammable Mixture	155	99
Chlorine dioxide [Chlorine oxide (ClO2)]	71	55
Propane	98	54
Sulfur dioxide (anhydrous)	49	48
Ammonia (conc 20% or greater)	57	43
Hydrogen chloride (anhydrous) [Hydrochloric acid]	54	32
Hydrogen	149	32
Methane	93	30
Butane	118	26
Ethylene oxide [Oxirane]	9	19
Hydrogen sulfide	63	19
Formaldehyde (solution)	1	17
Isobutane [Propane, 2-methyl]	107	17
Pentane	125	17
Titanium tetrachloride [Titanium chloride (TiCl4) (T-4)-]	51	15
Phosgene [Carbonic dichloride]	10	12
Nitric acid (conc 80% or greater)	58	12
Ethane	94	12
Oleum (Fuming Sulfuric acid)	69	11
Ethylene [Ethene]	95	11
Vinyl chloride [Ethene, chloro-]	101	11
Trichlorosilane [Silane, trichloro-]	153	11
Methyl chloride [Methane, chloro-]	5	10
Toluene diisocyanate (unspecified isomer)	77	10
Propylene [1-Propene]	129	10

APPENDIX D: Chemical Mixtures

One type of chemical mixture is a vapor-cloud explosive, which we discuss first as an abridged version of a much longer description at the following URL: http://www.fas.org/man/dod-101/sys/dumb/fae.htm. Vapor cloud explosions (VCE) are important to the refining and chemical processing industry. These explosions cause huge losses (e.g., deaths, injuries, property damage, business interruption, loss of goodwill, and environmental impact). A minimum ratio of fuel-vapor to air exists, below which ignition will not occur, due to insufficient fuel (lower explosive limit, LEL). A maximum ratio of fuel-to-air also exists, above which ignition will not occur, due to inadequate oxygen (upper explosive limit, UEL). For example, these limits for gasoline are 1.3 to 6.0%, and 5 to 15% for methane. Combustion events include pool fires, turbulent vapor jets, and a boiling liquid expanding vapor explosion (BLEVE). VCE damage is driven by the mass and material type, ignition-source strength, release type (e.g., turbulent jet), confinement of the vapor cloud, and turbulence induced in the cloud (e.g., from ambient obstructions).

Conservative assumptions allow calculation of the maximum distance, where an over-pressure or heat effect of concern can be detected. The distances for potential impact can be derived by the following formula, $D = C \times (n\ E)^{1/3}$. Here, D is the distance (meters) that experiences a 1-psi over-pressure; C is a constant with a typical value of 0.15; n is the VCE yield factor, corresponding to the mechanical force from the explosion with a typical value of ~0.1; and E is the explosive energy (Joules). The power of 1/3 arises from dissipation of the explosive energy into a 3-dimensional volume. E can be calculated from the flammable mass (M in kilograms) times the heat of combustion (H_C in Joules per kilogram), $E = M \times H_C$. Combining these two equations gives: $D = 0.15 \times (0.1\ M\ H_C)^{1/3}$. VCE modeling historically has been subject to large uncertainties resulting from inadequate understanding of explosive effects. According to current single-degree of freedom models, blast damage/injury can be represented by Pressure-Impulse (P-I) diagrams, which include the effects of over-pressure, dynamic pressure, impulse, and pulse duration. The peak over-pressure and duration are used to calculate the impulse from shock waves. Some advanced explosion models ignore the effects of blast wave reflection off structures, which can either over- or under-estimate the vulnerability of a structure. Three-dimensional models of VCE effects allow the evaluation of damage to a structure from a primary explosion and any subsequent secondary explosions.

Blast effects depend not only on the amount of fuel, but also on the combustion mode. The deflagration mode has a subsonic flame speed, which increases in restricted areas (higher over-pressure) and decreases in open areas (lower over-pressure). Indeed, the flame-front speed is directly proportional to the amount of blast over-pressure, resulting in a spectrum of flame speeds under complex conditions. High flame-front speeds and resulting high blast over-pressures are seen in accidental VCE, involving significant confinement and congestion that limits flame-front expansion and increases flame turbulence. These conditions are more difficult to achieve in an unconfined environment. Most VCE are deflagrations.

The detonation mode has a supersonic flame speed, and consumes nearly all available flammable vapors. A detonation causes more severe damage than a deflagration, due to a higher peak over-pressure and much higher blast energy. TNT generates >4,000 psi over-pressure in close proximity to the explosive source, along with significant radiant heat effects from the fireball. Conventional high explosives also produce fragments from the munitions case, as well as target fragments that are broken loose by the blast. The duration of the positive phase of a shock wave is an important parameter in the response of structures to a blast. Significant over-pressures can be generated by both detonations and deflagrations.

There are dramatic differences between explosions involving vapor clouds and high explosives at close distances. For the same amount of energy, the high explosive blast over-pressure is much higher and the blast impulse is much lower than that from a VCE. The shock wave from a TNT explosion is of relatively short duration, while the blast wave produced by an explosion of hydrocarbon material displays a relatively long duration.

APPENDIX D: Chemical Mixtures (continued)

A second type of chemical mixture is a fuel-air explosive (FAE), which is ignited by an embedded detonator. The rapidly expanding wave front (over-pressure) flattens all objects near the epicenter with debilitating damage well beyond the epicenter. The FAE's destructive force is high over-pressure, which is useful against soft targets (e.g., minefields, armored vehicles, aircraft in the open, and bunkers).

A third type of mixture is an air-dust cloud, which causes many industrial explosions and fires (e.g., coal mining, grain storage, woodworking, and paper). A 2006 study of dust explosions by the Chemical Safety Board identified 281 incidents between 1980 and 2005 that killed 119 and injured 718 with extensive facility damages. Food processing (e.g., corn, wheat, soybeans, sugar) involved 24% of these explosions. Dust arises from granules abrasion during conveyer-belt transport and shifts between bins. Fine particles form a cloud inside enclosures. Dust explosions depend on three factors. First, smaller dust particles are more reactive and more easily dispersed/suspended, and thus increasing the ignition potential and reaction propagation. Smaller particle sizes also result in more total surface area for ignition. Second, the dust mass per unit volume must be above the lower explosive limit (LEL) and below the upper explosive limit (UEL), as discussed above. Third, an ignition source must be present, for example a spark or a hot bearing on a conveyer belt. Almost all organic dust will ignite at temperatures below 500°C, which is roughly the temperature of a newly extinguished match. When all of these conditions are satisfied, even normally incombustible materials (e.g., cotton, plastics, sugar, flour, cocoa) can create explosions. Explosion prevention includes nitrogen gas purging to keep the oxygen concentration below the combustion limit.

A fourth type of mixture involves different chemical concentrations. Mixtures with the same CAS number can have different UN (United Nations) identifiers, because the properties change significantly with concentration. For example, hydrogen peroxide (H_2O_2) in water has a CAS #7722-84-1. However, the UN identifiers are UN2984 for 8-20% H_2O_2 in water, UN2014 for 20-60% H_2O_2 in water, and UN2015 for >60% H_2O_2 in water. Low concentrations of hydrogen peroxide are used to disinfect minor wounds. However, a high concentration can be used to make explosives. Indeed, pure H_2O_2 is an explosive. Consequently, H_2O_2 is on the COI list for high concentrations. Ammonium nitrate (NH_4NO_3) is also on COI list, as a readily available, strong oxidizing agent that makes an explosive mixture when combined with a hydrocarbon, such as fuel oil or kerosene. Pure ammonium nitrate is an explosive.

Mixtures in general (e.g., chemicals *A* and *B*) can be complex. Some mixtures do not react, but rather can be easily separated, for example by boiling a saline solution to recover the dissolved salt. Other chemicals may react to give a completely new third chemical, *C* via the reaction, $A + B \rightarrow C$. Examples include:

$NH_3 + H_2O \rightarrow NH_4OH$ (anhydrous ammonia + water $\rightarrow$ ammonium hydroxide, a strong base);

$SO_3 + H_2O \rightarrow H_2SO_4$ (sulfur trioxide + water $\rightarrow$ sulfuric acid, a strong acid);

$NO_2 + H_2O \rightarrow HNO_3$ (nitrogen dioxide + water $\rightarrow$ nitric acid, a strong acid).

The above reactions can also be reversed by the addition of heat to decompose the reaction product into the original reactants. Still other reactions are not reversible, but rather the addition of heat creates new compounds, *D*, *E*, *F*, etc. Consequently, a mixture's properties are frequently very different from the initial reactants. For example, urea is a high-volume, inexpensive, non-detonable material that can be reacted with nitric acid to produce urea nitrate, which is an explosive. Another example is hydrogen peroxide, which reacts with acetone to produce the powerful explosive, TATP. In general, the reactivity of two (or more) compounds in a mixture may be significantly greater than each of them separately. Thus, chemical mixtures are a significant potential threat, as illustrated by the above examples.

The State of New Jersey's Administrative Code [NJAC7.31] regulates suspect chemicals that can create highly reactive mixtures. Such mixtures (by proximity or co-location with minimal/no material transport) could be used by terrorists to initiate or sustain violent exothermic reactions for facility disruption and/or

toxin dispersal. The New Jersey regulations set threshold quantities [N.J.A.C. 7:31-6.3(b) and N.J.A.C. 7:31-6.3(c)] on the basis of the chemical energy that is available in the mixture (heat of reaction, ΔH_R, with $\Delta H_R<0$ indicating heat emission). The heat of reaction for a specific compound can be determined by experiments or by using a thermodynamic code (e.g., ASTM's CHETA or Outokumpu's HSC). The New Jersey regulations set threshold quantities on the basis of the heat of reaction, as shown below.

Heat of Reaction ($-\Delta H_R$) (Calories/g of Mixture)	**Threshold Quantity (Pounds)**
$100 \leq -\Delta HR < 200$	13,100
$200 \leq -\Delta HR < 300$	8,700
$300 \leq -\Delta HR < 400$	6,500
$400 \leq -\Delta HR < 500$	5,200
$500 \leq -\Delta HR < 600$	4,400
$600 \leq -\Delta HR < 700$	3,700
$700 \leq -\Delta HR < 800$	3,300
$800 \leq -\Delta HR < 900$	2,900
$900 \leq -\Delta HR < 1{,}000$	2,600
$-\Delta HR \geq 1{,}000$	2,400

Subsequent pages of this Appendix show two lists from selected sections of this New Jersey regulation. The first list shows functional groups of atoms (or moieties) that are responsible for the energetic reactions. The second list shows specific oxidizers, which result in a very energetic mixture with a fuel and/or a COI. See Ref. 36 for further details. Consequently, these (classes of) reactive compounds should be considered in addition to the current COI.

APPENDIX D: Chemical Mixtures (continued)

Table I, Part D, Group II
Reactive Hazard Substance Mixtures Functional Groups
(For Threshold Quantity Determination See N.J.A.C. 7:31-6.3(b) and N.J.A.C. 7:31-6.3(c))

	Functional Group(s)	Reactive Substance Class
1.	-C≡C-	Acetylenic compounds
2.	-C≡C-M	Metal acetylides
3.	-C≡C-X	Haloacetylene derivatives
	N=N \ / C	Diazirines
4.	CN_2	Diazo compounds
5.	-C-N=O -N-N=O	Nitroso compounds
6.	$-C-NO_2$ $Ar-NO_2$, $Ar(NO_2)_n$ $C(NO_2)_n$ $O_2NC-CNO_2$ $HC[OCH_2C(NO_2)_3]_3$, $C[OCH_2(NO_2)_3]_4$	Nitroalkanes, C-nitro and Nitroaryl and Polynitroaryl compounds Polynitroalkyl compounds Trinitroethyl orthoesters
7.	-C-O-N=O	Acyl or alkyl nitrites
8.	$-C-O-NO_2$	Acyl or alkyl nitrates
9.	>C-C< \ / O	1,2-Epoxides
10.	MC≡N→O C=N-O-M	Metal fulminates or aci-nitro salts, oximates
11.	NO_2 -C-F NO_2	Fluorodinitromethyl compounds
12.	-N-M	N-metal derivatives
13.	$-N=Hg^{+}=N-$	Poly(dimercuryimmonium salts)
14.	$-N-NO_2$	N-nitro compounds
15.	$=N^{+}-N-NO_2$	N-Azolium nitroimidates
16.	-C-N=N-C-	Azo compounds
17.	Ar-N=N-O-R	Arenediazoates
18.	ArN=N-S-Ar	Arenediazo aryl sulfides
19.	Ar-N=N-O-N=N-Ar	Bis(arenediazo) oxides
20.	Ar-N=N-S-N=N-Ar	Bis(arenediazo) sulfides
21.	>C-N=N-N-C<< R (R=H, CN, OH, NO)	Trizenes (TCPA note: typographical error, correct spelling is "Triazines"
22.	-N=N-N=N- N-N=N-N=C-	High-nitrogen compounds Tetrazoles
23.	-C-O-O-H O R-C-O-OH	Alkylhydroperoxides Peroxyacids

APPENDIX D: Chemical Mixtures (continued)

	Functional Group(s)	Reactive Substance Class
24.	-C-O-O-C-	Peroxides (cyclic, diacyl, dialkyl,), peroxyesters
	$-\overset{O}{\overset{\Vert}{C}}-O-OR$	
25.	-O-O-M	Metal peroxides, peroxoacid salts
	EOO^-	
	MOO^-	
26.	-O-O-E	Peroxoacids, peroxyesters
27.	$H_3N\rightarrow Cr-OO-$	Amminechromium peroxocomplexes
28.	$-N_3$	Azides (acyl, halogen, nonmetal, organic)
29.	$\overline{C-N_2^+O}^-$	Arenediazonium oxides
30.	$-C-N_2^+S^-$	Diazonium sulfides and derivatives, "Xanthates"
31.	N^+-HZ^-	Hydrazinium salts
	$N^+EO_n^-$	Oxosalts of nitrogenous bases
32.	$-N^+-OH\ Z^-$	Hydroxylaminium salts
33.	$-C-N_2^+Z^-$	Diazonium carboxylates or salts
34.	$[N\rightarrow Metal]^+\ Z^-$	Amminemetal oxosalts
35.	Ar-Metal-X	Halo-arylmetals
	X-Ar-Metal	Haloarenemetal π-complexes
36.	-N-X	Halogen azides
	XN_3	N-halogen compounds
	$\overset{O}{\overset{\Vert}{C}}-\overset{X}{\overset{\vert}{N}}-\overset{O}{\overset{\Vert}{C}}-$	N-haloimides
37.	$-N-F_2$	Difluoroamino compounds
	$-C(NF)NF_2$	*N,N,N*-trifluoroalkylamidines
38.	N-O-	N-O compounds
39.	-O-X	Hypohalites
	XO_n	Halogen oxides
	$-Cl-O_3$	Perchloryl compounds
	ClO_2^-	Chlorite salts
	$R-O-Cl-O_3$	Alkyl perchlorates
	$RN^+H_3ClO_4^-$	Aminium perchlorates
40.	$\left(\overset{\vert}{\underset{\vert}{C}}-\overset{\vert}{\underset{\vert}{C}}\right)_n$	Polymerization, alkene (vinyl) polymers and monomers thereof
41.	$-\left(\overset{\vert}{\underset{\vert}{C}}-C\overset{O}{\underset{N}{\diagdown}}-\right)_n$	Polymerization, polyamide polymers and monomers thereof
42.	$-\left(\overset{\vert}{\underset{\vert}{C}}-C\overset{O}{\underset{O}{\diagdown}}-\right)_n$	Polymerization, polyester polymers and monomers thereof
43.	$S_2O_4^{--}$	Dithionites

Abbreviations: Ar = aromatic (benzene); M = metal; R = organic chain; X = halogen; E = nonmetal; Z = anion; n = integer variable; all other abbreviations are for the element symbols from the periodic table of elements

Note: Not all chemical bond symbols are shown.

APPENDIX D: Chemical Mixtures (continued)

List of Individual Reactive Hazard Substances: Strong Oxidizers

Substance	CAS #	Threshold Quantity (Pounds)	Basis for Listing
1. Acetyl peroxide	110-22-5	2,500	e
2. Butyl hydroperoxide tertiary	75-91-2	2,500	e
3. Butyl hypochlorite tertiary	507-40-4	2,500	b
4. Calcium dithionite or Calcium hydrosulfite	15512-36-4	5,000	b
5. Chlorodinitrobenzenes	97-00-7	2,500	d, e
6. Cumene hydroperoxide	80-15-9	2,500	e
7. Dibenzoyl peroxide	94-36-0	2,500	f
8. Diethyl peroxide	628-37-5	2,500	e
9. Diisopropyl peroxydicarbonate	105-64-6	2,500	e
10. Dinitro phenol, dry or wet,less than 15% water as 2,4	51-28-5	2,500	a
11. Dinitro resourcinol (wetted with not less than 15% water)	35860-51-6	2,500	a
12. Dipicryl sulfide	115937	2,500	a
13. Di-tert-butyl peroxide	110-05-4	2,500	e
14. Divinyl acetylene	821-08-9	2,500	e
15. Ethyl nitrate	625-58-1	2,500	e
16. Ethyl nitrite (solutions)	109-95-5	2,500	d, e
17. Isosorbide dinitrate	87-33-2	2,500	a
18. Magnesium diamide	7803-54-5	2,500	b
19. m-Dinitrobenzene	99-65-0	2,500	d
20. Nitroglycerine (alcohol solution)	55-63-0	2,500	e
21. Nitromethane	75-52-5	2,500	d, e
22. o-Dinitrobenzene	528-29-0	2,500	e
23. p-Dinitrobenzene	100-25-4	2,500	d
24. Peracetic acid (greater than 56% peracetic acid)	79-21-0	2,500	d, e
25. Picric acid (wet, with not less than 10% water)	88-89-1	2,500	d
26. Potassium dithionite or Potassium hydrosulfite	14293-73-3	5,000	b
27. Propargyl bromide (3-Bromopropyne)	106-96-7	2,500	d, e
28. Silver picrate wetted with not less than 30% water	146-84-9	2,500	a
29. Sodium dithionite or Sodium hydrosulfite	7775-14-6	5,000	b
30. Trinitro benzene as 1,3,5 (wetted not less than 30 % water)	99-35-4	2,500	a

Basis for listing: a = DOT 4.1; b = DOT 4.2; c = DOT 4.3; d = NFPA 49; e = NFPA 325; f = NFPA 432.

Appendix E: Dictionary of Chemical Properties

Acid/Base Dissociation Constant (Ka/Kb): relative measure of an acid (Ka) or base (Kb). Larger K (>1) indicates a strong acid (or base). Larger K denotes greater likelihood to dissolve in water. – secondary[I].

Acute Exposure Guideline Levels (AEGLs): concentrations of a chemical vapor, above which different health effects could begin to occur in unprotected civilian populations after single, one-time exposures with a duration of 10 minutes, 30 minutes, 1 hour, 4 hours, and 8 hours. AEGLs are non-mandatory guidelines, which are developed by an extensive, multiple-committee review process (taking years to finalize), including the U.S. Environmental Protection Agency (EPA) and the Committee on Toxicology of the National Research Council, and are published by the National Academy Press. While AEGLs are considered voluntary, several states have incorporated them in their regulations. AEGLs apply to civilians including infants, children, and other sensitive/susceptible individuals. AEGL-1 is a level, above which persons could experience some transient, non-disabling effects of discomfort, irritation, odor, or non-sensory effects. AEGL-2 is the airborne level, above which the general population could experience more serious effects that could be long lasting or permanent or could impair the person's ability to escape. AEGL-3 is an air concentration, above which the population could experience increasingly severe, even life-threatening effects or death, without treatment. These protective guidelines include the precautionary use of multiple uncertainty factors to ensure that the AEGL is below the level at which the critical effect was noted in experimental species – primary[II].

Adiabatic Flame Temperature: The temperature that results from a complete combustion process that occurs without any heat transfer or changes in kinetic or potential energy. The adiabatic flame temperature indicates the maximum temperature that materials can produce in a reaction[9] – primary.

Antoine's Equation: An empirical equation for vapor pressure as a function of temperature, which has the form: $\log P = A - B/(T + C)$, where A, B, and C are experimentally determined – primary.

Auto-ignition Temperature: The temperature at/above which a substance spontaneously burns in air without the presence of a spark or flame (an extremely dangerous condition)[17] – primary.

Boiling Point: The temperature at which the vapor pressure of a liquid is equal to the pressure on the liquid (usually atmospheric pressure). Boiling point is useful for determining how quickly a substance will produce a vapor when heated[8] – primary.

CAS Number: Chemical Abstract Service identifier for the compound – primary. The CAS Number is a unique identifier and is often used as a critical search term.

Chemical Formula: An abbreviated notation that describes the number of atoms for each element in a molecule of the material. For example, the chemical formula for water is H_2O, meaning that a water molecule consists of two atoms of hydrogen (H) and one atom of oxygen (O) – primary.

Chemical Name: Descriptive title for the material (e.g., chlorine), together with common and trade names – primary. Note that the chemical name can vary greatly, especially in international trade. In contrast, the CAS number is a unique, compound-specific identifier.

[I] The chemical properties that are of less importance than the primary properties.

[II] The chemical properties that are of the greatest importance for chemical security.

Appendix E: Dictionary of Chemical Properties (continued)

Coefficient of Thermal Expansion: The fractional change in a substance's dimensions per degree of temperature change. Materials typically expand when heated and contract when cooled. Water has a negative coefficient, and therefore expands when cooled. A large coefficient indicates that the substance's dimensions will change a lot in response to a variance in temperature[10] – primary.

Compressibility (β): A substance's relative volume (*V*) change due to a pressure (*p*) change. A decrease in pressure generally leads to an increase in volume: $\beta = -(1/V)(dV/dp)$[11] – primary.

Critical Point: Temperature and pressure at which a substance's liquid and gaseous phases are indistinguishable. When a liquid passes this point ("goes critical"), the substance in a container expands into a gas, over-pressurizing (and possibly destroying) the tank in the process[11] – primary.

Critical Pressure: Pressure to liquefy a gas at its critical temperature; see Critical Point – primary.

Critical Temperature: Temperature at and above which a vapor cannot be liquefied, regardless of how much pressure is applied;[12] see Critical Point – primary.

Critical Volume: Volume per chemical mass at the critical temperature and pressure[13] – primary.

Decomposition temperature: Temperature at which the substance decomposes into smaller molecules or into its constituent atoms – primary.

Density (ρ): Mass per unit volume, which is temperature- and pressure-dependent. Density determines if a substance will rise or sink when mixed with another substance – primary.

Diffusion Coefficient (D, also Diffusivity): Amount of a substance diffusing through an area of 1 square centimeter (grams per second)[14] – secondary.

DOT Number (same as NA number; see also UN Number): Unique identifier for hazardous chemicals that are issued by the U.S. Department of Transportation. NA Numbers (**N**orth **A**merica) are identical to UN numbers, except that some substances without a UN number may have an NA number. These additional NA numbers use the range NA8000 - NA9999 – primary.

EC_{50}: Median effective concentration, as the statistically estimated airborne concentration associated with a specifically defined effect in 50% of the exposed population – primary.

EC/EINECS Number: Unique identifier for compounds according to the European INventory of Existing Commercial chemical Substances (EINECS). The EINECS number could be useful in identifying chemicals from European sources – primary.

Electrical Conductivity (or conductance): ability to conduce an electrical current – secondary.

Appendix E: Dictionary of Chemical Properties (continued)

Emergency Response Planning Guideline (ERPG): concentration of a vapor in air, above which health effects could occur in unprotected civilians after one-time exposures of 1 hour; intended as temporary guidance until superseded by AEGL estimates (as discussed above). The American Industrial Hygiene Association (AIHA) is a U.S. non-governmental group that develops ERPGs for industrial compounds. Three tiers of effect are defined. ERPG-1 is expected to produce low level/mild transient effects. ERPG-2 levels produce moderate effects that may lead to permanent injury. A 1-hour exposure at the ERPG-3 (most severe) level is the threshold for life-threatening effects. ERPGs are voluntary (not mandated by Federal or State regulatory agencies), as guidelines for planning and emergency response – primary.

Enthalpy (H): The heat content of a thermodynamic (chemical) system, being the maximum amount of thermal energy that can be derived from a simple system at constant pressure.[8] Larger enthalpy indicates that more chemical energy is available from a specific reaction – primary.

Entropy (*S*): Energy to or from a system, divided by the mean absolute temperature during the change, as a measure of the availability of a system's energy. Entropy is essential in predicting whether a complex chemical reaction will proceed as written or in the opposite direction.[8]

Explosive Limit (also Flammability Limits): Concentration range (expressed as a percent of fuel by volume), over which a flammable vapor can produce a fire or explosion in the presence of an ignition source. Above the upper explosive limit (UEL), the air-fuel mixture contains too little oxygen to burn. Below the lower explosive limit (LEL), insufficient fuel exists to burn[17]. Increasing the fraction of inert component(s) in a mixture raises the lower limit and decreases the upper limit. A deflagration is a propagation of a combustion zone at a velocity less than the speed of sound in the unreacted medium. A detonation is a propagation of a combustion zone at a velocity greater than the speed of sound in the unreacted medium. An explosion is the bursting/rupture of an enclosure/container due to the development of internal pressure from a deflagration or detonation – primary. See Appendix D for more details.

Flash Point: Lowest temperature, at which a flammable liquid can ignite when exposed to oxygen.[17] An "open cup" measurement holds the sample in an open cup (hence the name), which is heated, and at intervals a flame is brought over the surface. The flash point in this case varies with the height of the flame above the liquid surface. Alternatively, the sample is sealed inside a "closed cup" container, into which an ignition source is introduced periodically. Closed cup testers give lower values for the flash point (typically 5-10 K), where the vapor pressure reaches the Lower Flammable Limit (LFL).

Heat of Combustion: Amount of heat produced when a substance at constant pressure or volume is oxidized, or burns with the presence of oxygen[14] – primary.

Heat of Decomposition: Amount of heat to decompose a compound into basic elements. This measure is not applicable to all substances, since they do not decompose in the relevant temperature range.

Heat of Melting (also Enthalpy [Change] of Fusion, Heat of Fusion): Amount of thermal energy that must be absorbed for 1 mole of a substance to change from a solid to a liquid – primary.

Heat of Solution: Enthalpy change when one mole of a substance is dissolved completely in a large volume of a solvent at constant pressure – primary.

Heat of Sublimation: Amount of heat to convert one gram of a solid substance into a gas. This amount determines the vapor pressure of the solid[21] – primary.

Appendix E: Dictionary of Chemical Properties (continued)

Heat of Vaporization: Amount of heat to convert a liquid at its normal boiling point into a vapor. A low heat of vaporization indicates that a liquid is more readily released into the air[8] – primary.

Henry's Law: Henry's Law states that solubility of a non-reactive gas in a dilute solution is proportional to its partial pressure above the solution[14], or as an equation, $p = kc$ (p = partial pressure of the solute above the solution; c = concentration of the solute in the solution; and k = Henry's constant)[18] – primary.

Immediately Dangerous to Life and Health (IDLH): Airborne work-place concentration, at which a 30-minute unprotected exposure is expected to compromise self rescue, escape, or be a threat to life. The National Institute for Occupational Safety and Health (NIOSH) develops and publishes these health and safety standards, which are enforced by the U.S. Occupational Safety and Health Administration (OSHA).

Joule-Thomson (Kelvin) Coefficient: Measure of the change in temperature with respect to a change of pressure in a Joule-Thomson process, in which a gas expands freely with no heat transfer or external work. A negative value means the temperature of the gas increases on expansion. The equation has the form: $\mu = (dT/dp)_H$, where T is temperature; p is pressure; and H represents constant enthalpy.[15] This measure determines the temperature of gases expanding through a tank leak – primary.

LC_{50}: median lethal concentration; the statistically-estimated airborne concentration associated with death in 50% of the exposed population.

Melting Point: The temperature at which the solid and liquid phases of a substance are in equilibrium at atmospheric pressure[8] – primary.

Molecular Structure (also Structural Formula): The three-dimensional arrangement of the atoms that make up a molecule. The Structural Formula is a graphical representation of the chemical's molecular structure showing the atoms and the chemical bonds between them, for example via line-angle formulas. Distinct chemicals can have the same chemical formula, but different structural formulas that makes the difference (for example) between stable and highly explosive compounds. Molecular structure determines properties such as color, magnetism, matter phase, polarity, and reactivity[8] – primary.

Molecular Weight (M_r): The weighted average of molecular masses in a substance. Higher-molecular-weight substances are denser, and therefore are less likely to disperse as widely[8] – primary.

NA Number (same as DOT Number; see also UN Number): Unique identifier for hazardous chemicals that are issued by the U.S. Department of Transportation. NA Numbers (**N**orth **A**merica) are identical to UN numbers, except that some substances without a UN number may have an NA number. These additional NA numbers use the range NA8000 - NA9999 – primary.

NFPA Rating: National Fire Protection Association rating for the chemical on the basis of health, flammability, instability, and related hazards – primary.

Partition Coefficient (K_{OW} or K_D, also Distribution Constant): The ratio of concentrations of a compound in a mixture of two immiscible solvents at equilibrium. Hence, this coefficient is a measure of differential solubility of the compound between the two solvents that do not mix homogenously. Since one of the solvents is typically water, the partition coefficient measures how well a substance dissolves in water. Substances with high partition coefficients do not tend to dissolve easily in water. Such materials also tend to be more active and have greater risk of environmental impact – secondary[16].

Appendix E: Dictionary of Chemical Properties (continued)

Reactivity: The rate at which a substance tends to undergo a chemical reaction, as determined by other physical properties. For example, surface area, contaminants, and crystal structure all affect reactivity.[13]

RTECS Number (Registry of Toxic Effects of Chemical Substances): Unique identifier for the material by the National Institute of Occupational Safety and Health (NIOSH). Typical properties include: (1) primary irritation; (2) mutagenic effects; (3) reproductive effects; (4) tumorigenic effects; (5) acute toxicity; and (6) other multiple dose toxicity – secondary. All values should be verified independently due to the presence of errors in this database.

Short Term Exposure Limit (STEL): a 15-minute "ceiling" concentration estimated to ensure that peak workplace exposures are safe. STELs should still be below the daily worker population level (WPL); published by the American Conference of Governmental Industrial Hygienists – primary.

Solubility: The maximum amount of solute that can be dissolved per unit of solvent[8] – primary.

(Specific) Surface Area (meters^2/gram): The total surface area of a solid divided by the mass, as an indicator of reactivity, useful in predicting dust explosions and interactions with liquids and vapors – primary. Typically, the rate of reaction will increase with increased surface area[14] – secondary.

Sublimation Point: Sublimation is a phase transition from a solid to a gas with no intermediate liquid. Sublimation occurs at temperatures (T_S) and pressures (P_S) below the triple point, ($T_S < T_T$, $P_S < P_T$). The sublimation temperature of a material is a function of pressure, $T_S = T_S(P_S)$. The location in temperature-pressure space, (T_S, P_S), is the sublimation point.

Surface Tension: The attractive force between liquid molecules that causes the surface of a liquid to minimize its surface area. Surface tension measures the liquid's ability to penetrate porous materials and predicts its interaction with other materials (e.g., water, oil, and solids). Higher surface tension indicates more energy to disperse the substance into the air[8, 12] – secondary.

Temporary Emergency Exposure Level (TEEL): air-born vapor concentration, above which different health effects could begin to occur in unprotected civilian populations after a single, one-time exposure of 1 hour. The U.S. Department of Energy (USDOE) develops TEELs for chemicals-of-concern at its facilities that have neither ERPG nor AEGL values. TEELs are temporary guidance for emergency planning, hazard evaluation, and consequence assessment for employees, guests, and the population in adjacent communities. Four tiers of effect are defined for TEELs. A TEEL-0 level corresponds to no effect, while a TEEL-3 is the threshold for the most severe (life-threatening) effects – primary.

Threshold Limit Value-Time Weighted Average (TLV-TWA): the time-weighted average airborne concentration, at which nearly all workers are expected to exhibit no effect after repeated daily exposures. The American Conference of Governmental Industrial Hygienists (ACGIH) is a U.S. non-governmental group that develops Threshold Limit Values (TLVs) for work-place exposure to industrial and commercial compounds for assurance of continuous safe conditions in the workplace. TLVs can be further broken down into those suitable for short-term exposure limits (TLV-STELs; for 15-minute exposures that occur no more that four times per day), or for time-weighted averages (TLV-TWAs) over an eight-hour day during a forty-hour work-week. A "ceiling" exposure limit (TLV-C) should not be exceeded under any circumstance. TLVs are copyrighted and "owned" by ACGIH, and can only be applied under the caveats used in their development. ACGIH guidelines are voluntary (non-enforceable).

Appendix E: Dictionary of Chemical Properties (continued)

UN Number: Four-digit number that uniquely identifies a hazardous substance (e.g., explosive, flammable liquid, toxic) in the framework of international transport. For example, the UN Number for acrylamide is UN2074. – primary.

Vapor Density: Relative density of a gas to that of air. Gases with a vapor density above 1 are denser than air and sink if released; gases with a vapor density below one will rise. Dense vapors tend to collect in clouds on the ground, displacing air and creating a significant fire and safety hazard[25] – primary.

Vapor Pressure: The pressure at which a gas is in equilibrium with its liquid or solid state at a given temperature. Substances with high vapor pressure tend to evaporate quickly, and are generally referred to as "volatile"[8] – primary.

Viscosity: A measure of a resistance to mechanical flow. High viscosity means liquids flow slowly (e.g. molasses), while low viscosity chemicals are likely to leak and spread quickly[8] – secondary.

Appendix E (continued)
Table E.1: Contribution of Each Property to Chemical-Security Features in Tables 1 and 3.

Property	Identity	Toxicity	Chemical Potential	Reactivity	Temperature & Pressure	Dispersion
Adiabatic flame temperature				X	X	
Acute exposure guideline levels		X				
Antoine's equation coefficients					X	X
Auto-ignition temperature			X	X	X	
Boiling point					X	X
CAS number	X					
Chemical formula	X	X		X		
Chemical name	X					
Coefficient of thermal expansion					X	
Compressibility (β)					X	
Critical point					X	
Critical pressure					X	
Critical temperature					X	
Critical volume					X	
Decomposition temperature				X	X	X
Density (ρ)			X		X	X
Diffusion coefficient						X
EC50		X				
EC/EINECS Number	X					
Emergency response planning guideline		X		X		X
Enthalpy (H)			X	X		
Entropy (S)			X	X		
Explosive limit				X		X
Flash point				X	X	
Heat of combustion			X	X	X	
Heat of decomposition			X	X	X	
Heat of melting			X	X	X	
Heat of solution			X	X	X	
Heat of sublimation			X	X	X	
Heat of vaporization			X	X	X	
Henry's law constant		X			X	X
Immediately dangerous to life and health		X				
Joule-Thomson coefficient					X	X
LC50		X				
Melting point					X	X
Molecular structure	X		X	X		
Molecular weight	X		X			
NA number (or DOT number)	X					
NFPA rating				X		
Partition coefficient	X					X

Appendix E (continued)

Table E.1: Contribution of Each Property to Chemical Security Features in Tables 1 and 3.

Property	Identity	Toxicity	Chemical Potential	Reactivity	Temperature & Pressure	Dispersion
Reactivity				X		X
RTECS number	X					
Short term exposure limit		X				
Solubility		X				X
Surface area (meter^2/gram)				X		X
Sublimation point					X	X
Surface tension		X				X
Temporary emergency exposure level		X				
Threshold limit value		X				
UN number	X					
Vapor density		X				X
Vapor pressure					X	X
Viscosity						X

Appendix F: Sources of Chemical Properties

This appendix (F) summarizes the 34 information sources (next two pages) that were used to compile the specific chemical properties, as discussed in the previous appendix (E). Peer-reviewed sources are particularly important for authoritative properties and are marked with an asterisk (*) next to the source name in the table below. For example, AEGL properties have been reviewed by the National Research Council. We found that the Hazardous Substances Data Bank was the best initial source. Additional sources were searched in an order that was more by habit and bookmark sequence than anything else. The HSC source involved the following procedure: (a) open the HSC software; (b) click on 'Reaction Equations;' (c) click on 'Peep Database;' (d) enter the chemical formula in the Formula bar; (e) select the appropriate chemical from the list on the left; (f) collect information, plus Reference and Class. The properties from each source were entered into a spreadsheet, along with an indicator that any item was not found (NF), not applicable (NA, e.g., no flash point for a non-combustible compound), or not likely (NL, i.e., the information should exist, but could not be found for that chemical).

An important detail involves the Joule-Thompson coefficient, which requires some effort to extract from the NIST database, as follows. Go to NIST Chemistry WebBook and click on 'Thermophysical Properties of Fluid Systems' under 'Models and Tools.' Select the chemical from the dropdown list and change the units to Celsius and atmospheres (atm). Select 'Isobaric properties' and 'Default for fluid.' On the next screen, enter 1 atm as the pressure. Make the starting temperature the chemical's boiling point and the maximum its critical temperature. The increment should be set to give about 6 values. Click on 'View data in HTML table.' HSC can also be used with some extra effort, as follows. Open the HSC software. Click on 'Reaction Equations.' Click 'Peep Database.' Type the chemical formula in the Formula bar and select the chemical from the list on the left. Collect data from T1 K to D, Reference, and Class. This detail is provided for the sake of thorough documentation of the work.

Appendix F: Sources of Chemical Properties (continued)

Source Name	Identifier	Developer/Maintainer	Online availability (http://)
Acute Exposure Guideline Levels*	AEGLs	USEPA	www.epa.gov/oppt/aegl/pubs/chemlist.htm (publication by National Academy Press)
CAMEO	CAMEO	U.S. National Oceanic and Atmospheric Administration	http://cameochemicals.noaa.gov/ CAMEO=computer aided management of emergency operations
CAS Registry	CAS	Chemical Abstract Service	www.cas.org
ChemFinder	ChemFinder	CambridgeSoft Corporation	chemfinder.cambridgesoft.com
ChemSpider	ChemSpider	ChemZoo, Inc.	www.chemspider.com/
Chemical Book	ChemBook	Chemical Book Inc.	www.chemicalbook.com
Chemical Database		Prof. James K. Hardy	ull.chemistry.uakron.edu/erd/
Chemical Hazards Response Information	CHRIS	US Coast Guard	www.chrismanual.com
Chem. Safety Board	CSB	Chemical Safety Board	www.csb.gov
ChemStewards		Synthetic Organic Chemical Manufacturers Association	www.socma.com/ChemStewards/
Emergency Response Planning Guidelines	ERPGs	American Industrial Hygiene Association (AIHA)	www.aiha.org (includes Workplace Exposure Level Guides, WEELs)
European chemical substances information	ESIS	European Chemicals Bureau	ecb.jrc.it/esis/
Handbook of Chemistry & Physics	CRC	CRC Press	www.hbcpnetbase.com/
Hazardous Substances DataBank*	HSDB	National Library of Medicine	toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB
HSC Chemistry 5	HSC	Outokumpu Research Oy	www.outotec.com/hsc (software)
High Production Volume Information	HPVIS	U.S. Environmental Protection Agency (USEPA)	www.epa.gov/hpvis/ (information for more than 900, high production compounds at >1 million pounds/year)
INCHEM	INCHEM	Int'l Programme Chemical Safety	www.inchem.org/
Integrated Risk Information System	IRIS	USEPA	cfpub.epa.gov/ncea/iris/index.cfm
Knovel	Knovel	Knovel Corporation	www.knovel.com/web/portal/basic_search
Lange's	Lange's	Lange's Handbook of Chemistry	J.A. Dean, 15th edition, McGraw-Hill (1999) www.knovel.com/knovel2/Toc.jsp?BookID=47&VerticalID=0
Mary Kay O'Connor Process Safety	MKOPSC	Center Texas A&M University	process-safety.tamu.edu/

Appendix F: Sources of Chemical Properties (continued)

Source Name	Identifier	Developer/Maintainer	Online availability (http://)
Fire Protection Guide to Hazardous Mat'ls	NFPA	National Fire Protection Association	(book) 12th edition, 1997 (Quincy, MA)
NIST Chemistry WebBook	NIST	National Institute of Standards and Technology (NIST)	webbook.nist.gov/chemistry/ (NIST/TRC Web Thermo Tables, Professional Ed. by subscription)
NIOSH Pocket Guide	NIOSH	National Institute for Occupational Safety and Health (NIOSH)	www.cdc.gov/niosh/npg/
Patty's Industrial Hygiene & Toxicology	Patty's	Wiley InterScience (book)	www.wiley.com/legacy/products/subject/reference/pattys_index.html
PhysProp	PhysProp	Syracuse Research Corporation, Syracuse, NY	www.syrres.com/esc/physprop.htm (peer reviewed)
Protective Action Criteria	PAC	USDOE	hss.energy.gov/HealthSafety/WSHP/chem_safety/ (including Temporary Emergency Exposure Level, TEEL)
Process Safety Incident Database	PSID	American Institute of Chemical Engineers	www.aiche.org/CCPS/ActiveProjects/PSID/index.aspx
Registry of Toxic Effects of Chemical Substances	RTECS	Symyx Technologies, Inc. (Elsevier MDL)	www.mdl.com/products/predictive/toxicity/index.jsp (over 100,000 chemicals)
Responsible Care Management System	Responsible Care	American Chemistry Council www.americanchemistry.com	www.responsiblecaretoolkit.com/management.asp
Responsible Distribution Process	RDP	National Association of Chemical Distributors	www.nacd.com/dist_process/
Threshold Limit Values	TLVs	American Conf. of Governmental Industrial Hygienists (ACGIH)	www.acgih.org/TLV/
Toxicological Profiles	ATSDR	Agency for Toxic Substances and Disease Registry (ATSDR)	www.atsdr.cdc.gov/toxpro2.html
WISER	WISER	National Institute of Health	webwiser.nlm.nih.gov/knownSubstanceSearch.do WISER=wireless information system for emergency responders

Appendix G: Sample (Incomplete) of Information for Chlorine

Priority	Type	Function of	Item	Chlorine-Specific Properties
1	C	n	Formula	Cl2(g)
1	C	n	Chemical Name	Chlorine
2	C	n	Common Chemical Name(s)	Diatomic chlorine; dichlorine; bertholite
1	C	n	CAS No	7782-50-5
1	C	n	NIOSH/RTECS No.	FO2100000
2	C	n	UN No	UN1017
2	C	n	EEC No (EINEC)	231-959-5
1	C	n	DOT Guide	http://hazmat.dot.gov/pubs/erg/g124.pdf
1	P	n	Molecular Weight	70.906 g
3	P	n	Color	Greenish-yellow
1	C	Tp	Flash Point	Nonflammable
			Open cup	NA
			Closed cup	NA
			LEL	NA
			UEL	NA
			Auto Ignition	NA
				1 atm
1	P	p	Melting Point	-105.5 DEG C
1	P	p	Boiling Point	-34.04 DEG C
1	C	p	Decomposition Pt	NA
			Critical Point	
1	P	n	Temperature	144 DEG C
1	P	n	Pressure	76.1 ATM
3	P	n	Volume	1.763 l/kg
1				25 C
	P	T	Vapor Pressure	5830 mm Hg

Appendix H: Information Inconsistencies

ORNL also identified inconsistencies in the chemicals-of-interest information, as follows.

1) Carbon oxysulfide and carbonyl sulfide are two names for the same chemical (CAS# 463-58-1). Appendix A specifically notes the duplication. However, the two entries are in Appendix A for no obvious reason. The entry pages also show separate entries for carbonyl sulfide and carbon oxysulfide. The data entry list of Flammable Release Chemicals shows carbon oxysulfide with a synonyms of carbon oxide sulfide (COS) and carbonyl sulfide, and screening threshold quantities that are consistent with Appendix A. The data entry list for Theft/Diversion WME shows this compound as carbonyl sulfide with no synonyms with screening threshold quantities that are shown in a separate entry of Appendix A (56.67% and 500 lbs). These redundant entries are confusing.

2) Four chemicals have incorrect names, as shown in the following table.

CAS#	Incorrect Name in Appendix A	Correct Names
100-38-9	N,N-(2-diethylamino)ethanethiol	2-(N,N-diethylamino)ethanethiol 2-(Diethylamino)ethanethiol
5842-07-9	N,N-(2-diisopropylamino)ethanethiol	2-(N,N-diisopropylamino)ethanethiol 2-(Diisopropylamino)ethanethiol
108-02-1	N,N-(2-dimethylamino)ethanethiol	2-(N,N-dimethylamino)ethanethiol 2-(Dimethylamino)ethanethiol
5842-06-8	N,N-(2-dipropylamino)ethanethiol	2-(N,N-dipropylamino)ethanethiol 2-(Dipropylamino)ethanethiol

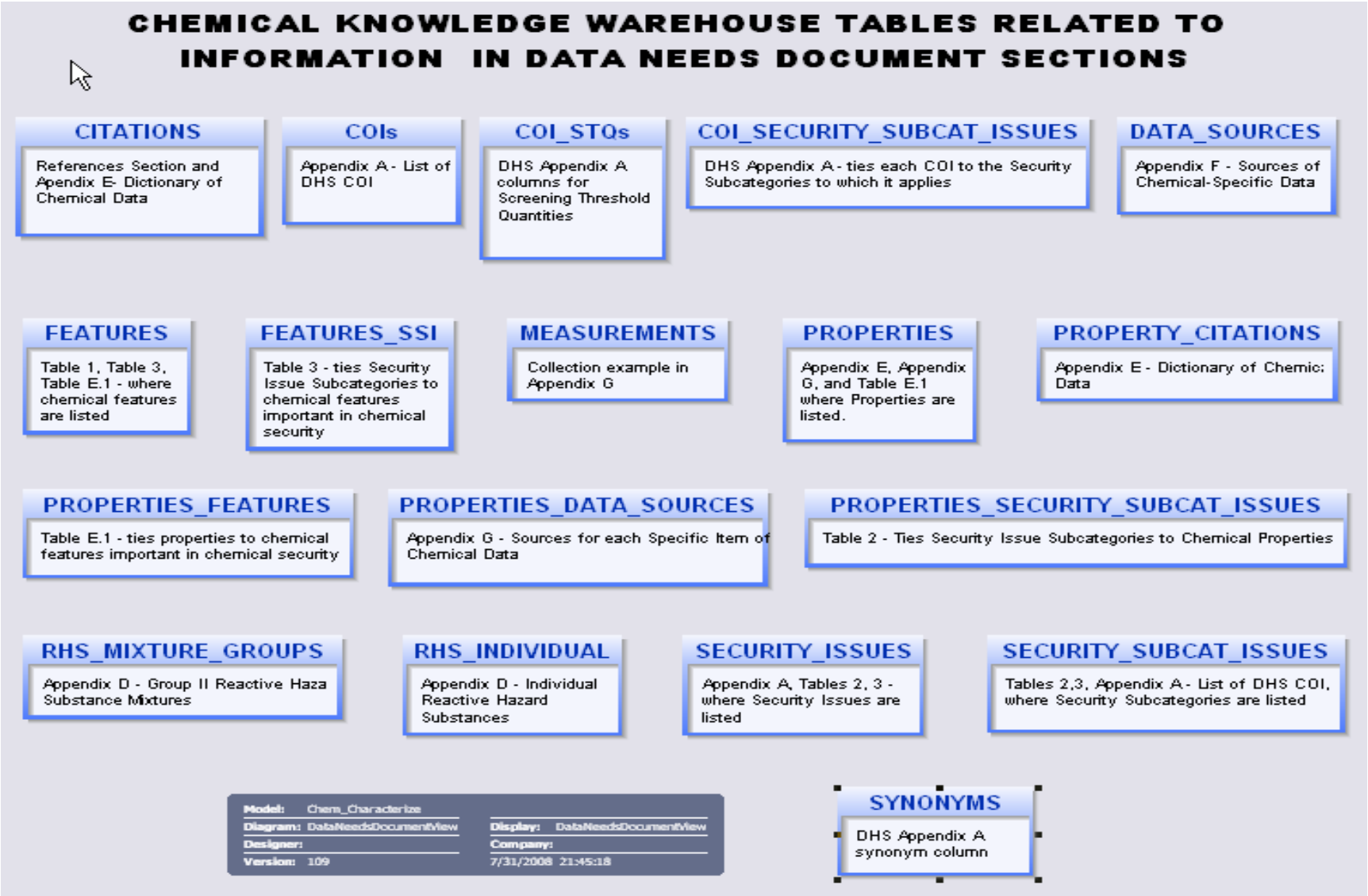
3) Several chemicals in Appendix A should use upper-case, "O-" and "O,O-", instead of lower-case, "o-" and "o,o-". The two cases have different meanings. (The N's and S's in the appendix are correctly shown in uppercase.) The correct chemical names are as follows:

O,O-Diethyl S-[2-(diethylamino)ethyl] phosphorothiolate (CAS# 78-53-5);
O-Isopropyl methylphosphonochloridate (CAS# 1445-76-7);
O-Pinacolyl methylphosphonochloridate (CAS# 7040-57-5);
O-Ethyl-O-2-diisopropylaminoethyl methylphosphonite (CAS# 57856-11-8);
O-Isopropyl methylphosphonofluoridate (CAS# 107-44-8);
O-Pinacolyl methylphosphonofluoridate (CAS# 96-64-0);
O-Ethyl-N,N-dimethylphosphoramido-cyanidate (CAS# 77-81-6);
O-Ethyl-S-2-diisopropylaminoethylmethyl phosphonothiolate (CAS# 50782-69-9).

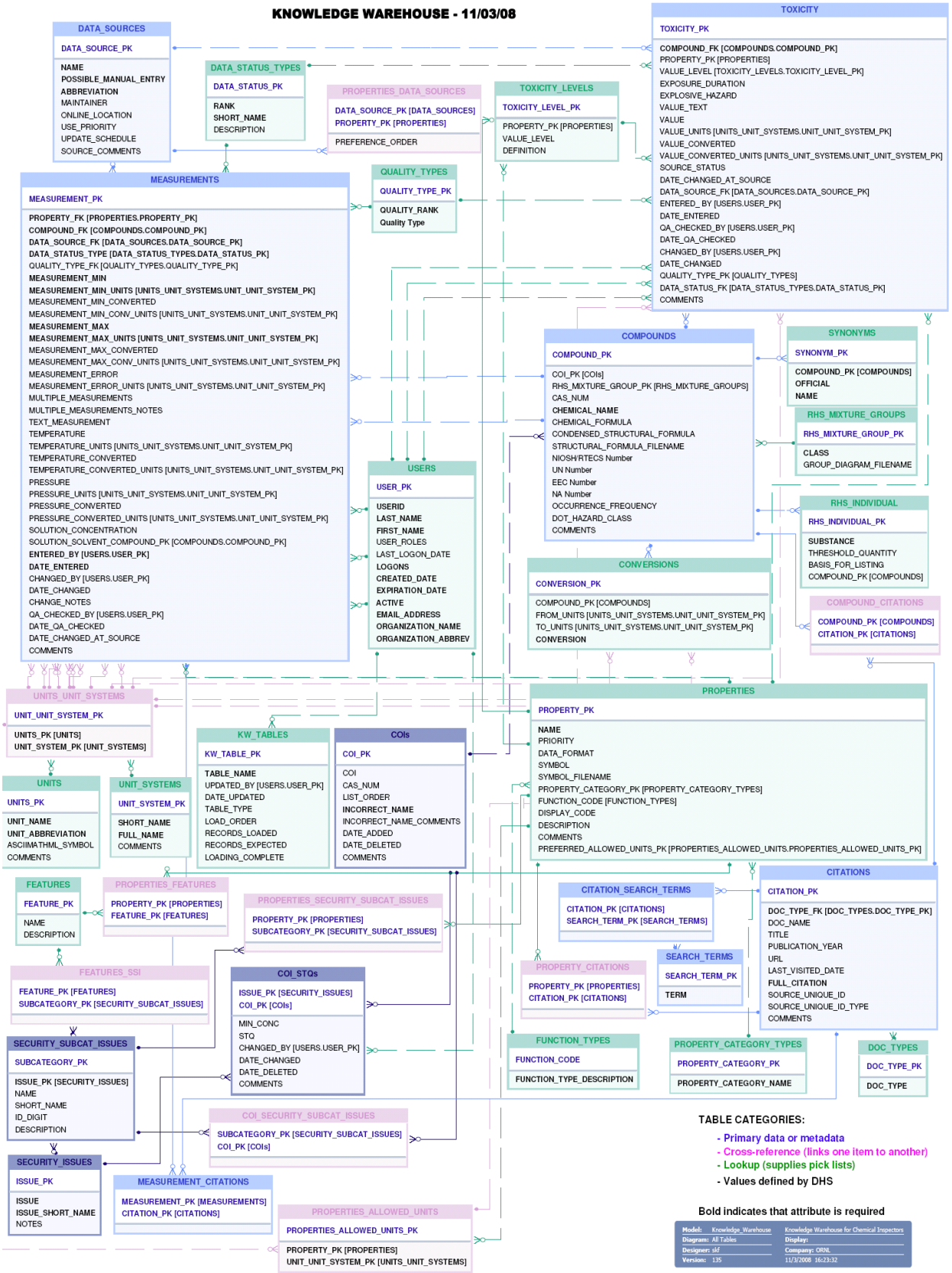
4) Appendix A has "butene" (CAS# 25167-67-3), in addition to its 4 isomers. The purpose is unclear for listing the butene class name (as a mixture?) in addition to the isomers.

5) We found no information for four compounds: N,N-diisopropyl phosphoramidic dichloride (CAS# 23306-80-1); N,N-Dipropyl Phosphoramidic Dichloride (CAS# 40881-98-9); JPA (without a CAS#); JP8 (kerosene-based Jet Propellant "8" without a CAS#).

Appendix I: Prototype of Information Store Design



Appendix I: Prototype of Information Store Design (continued)



Appendix I: Prototype of Information Store Design (continued)

TABLE	BRIEF DESCRIPTION
CITATION_SEARCH_TERMS	Primary data/metadata: terms for searching citations.
CITATIONS	Primary data/metadata: name, title, author, URL, identifiers.
COI_SECURITY_SUBCAT_ISSUES	Cross-reference table: link COI to chemical security subcategories.
COI_STQS	STQs from Appendix A, security issues, comments, and change dates.
COIS	Chemicals of interest from Appendix A with metadata (e.g., date added, date deleted, list order, and CAS number).
COMPOUND_CITATIONS	Cross-reference table: links for COI to its respective citation.
COMPOUNDS	Primary data/metadata: important compounds in addition to the COIs with registration numbers, DOT Hazard classes, chemical name, and COI table primary key.
DATA_SOURCES	Primary data/metadata: source name, URL, maintainer.
DATA_STATUS_TYPES	Lookup table: trustworthiness status for data (rank, rank description, and short name to be used in drop down lists).
DOC_TYPES	Lookup table: document (e.g., journal article) with identifier.
FEATURES	Lookup table: chemical security feature, description, identifier.
FEATURES_SSI	Cross-reference table: chemical security features with their respective security subcategory issues.
FUNCTION_TYPES	Lookup table: property change (temperature, pressure, both, or none).
KW_TABLES	Primary data/metadata: entry and description for each table.
MEASUREMENT_CITATIONS	Cross-reference table: link each measurement to its citation.
MEASUREMENTS	Primary data/metadata: value (minimum, maximum, units).
PROPERTIES	Lookup table: property, format, name, units, and priority.
PROPERTIES_ALLOWED_UNITS	Cross-reference table: unit system(s) for each property.
PROPERTIES_DATA_SOURCES	Cross-reference table: links data_sources table with properties.
PROPERTIES_FEATURES	Cross-reference table: property link chemical security feature.
PROPERTIES_SECURITY_SUBCATS	Cross-reference table: property link to security issue.
PROPERTY_CATEGORY_TYPES	Lookup table: category (chemical, physical, toxicological).
PROPERTY_CITATIONS	Cross-reference table: link each property to its citation(s).
QUALITY_TYPES	Lookup table: source quality ranking (1=best, 4=unknown).
RHS_INDIVIDUAL	Lookup table: compound name and threshold quantity.
RHS_MIXTURE_GROUPS	Lookup table: reactive substance class and functional group.
SEARCH_TERMS	Primary data/metadata: terms for searching the database.
SECURITY_ISSUES	Entries for each security issue, description, and notes.

SECURITY_SUBCAT_ISSUES	Entry for each security subcategory with an identifier, a short name, and a subcategory table primary key.
SYNONYMS	Lookup table: entry for each compound, respective synonyms, and whether that synonym is given by Appendix A.
UNIT_SYSTEMS	Lookup table: entry for each unit system (e.g., SI or CGS), a full name, short name, and comments for each.
UNITS	Lookup table: entry for each unit, abbreviations, comments.
UNITS_UNIT_SYSTEMS	Cross-reference table: links units to unit systems, indicating which units belong to which unit system.
USERS	Lookup table: list of database users, contact information, created date, organization, roles, userID, and name.

Appendix J: List of Acronyms

Acronym	Full Name	Website (If Applicable)
ACG	A Commercial Grade	
ACGIH	American Conference of Governmental Industrial Hygienists	http://www.acgih.org/home.htm
ACS	American Chemical Society	http://portal.acs.org/portal/acs/corg/content
AEGL	Acute Exposure Guideline Level	http://www.epa.gov/oppt/aegl/
AICHE	American Institute of Chemical Engineers	http://www.aiche.org/
AIHA	American Industrial Hygiene Association	http://www.aiha.org/Content
ANSI	American National Standards Institute	http://www.ansi.org/
APA	A Placarded Amount	
API	American Petroleum Institute	http://www.api.org/
ASCII	American Standard Code Information Interchange	
ASTM	American Society for Testing and Materials	http://www.astm.org/
ATSDR	Agency for Toxic Substances and Disease Registry	http://www.atsdr.cdc.gov/
BLEVE	Boiling Liquid Expanding Vapor Explosion	
CADAT	Chemical Attack Data Acquisition Tool	
CAMEO	Computer-Aided Management of Energy Operations	http://cameochemicals.noaa.gov/
CAS	Chemical Abstracts Service	http://www.cas.org/
CDF	Cumulative Distribution Functions	
CGS	Centimeter-Gram-Second Units	
CHETA	The Computer Program for Chemical Thermodynamics and Energy Release Evaluation	http://www.southalabama.edu/engineering/chemical/chetah/index.html
CHRIS	Chemical Hazards Response Information System	http://www.chrismanual.com/
COI	Chemicals of Interest	
CRC	Chemical Rubber Company	http://www.crcpress.com/
CSB	Chemical Safety Board	http://www.chemsafety.gov/
CVI	Chemical Vulnerability Information	
CW/CWP	Chemical Weapons/Chemical Weapons Precursors	
DDL	Data Definition Language	
DOT	United States Department of Transportation	http://www.dot.gov/new/index.htm
EC	Economically Critical	
EC_{50}	Median Effective Concentration	
EC/EINECS	European Commission/European Inventory of Existing Commercial Chemical Substances	http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=ein

EPA	United States Environmental Protection Agency	http://www.epa.gov/
ERD	Entity Relationship Diagram	
ERPG	Emergency Response Planning Guidelines	
ESIS	European Chemical Substances Information System	http://ecb.jrc.ec.europa.eu/esis/
EXP/IEDP	Explosives/Improvised Explosive Device Precursors	
FAE	Fuel-Air Explosion	
FOUO	For Official Use Only	
GEM	Graduate Degrees for Minorities in Engineering, Incorporated	http://www.gemfellowship.org/
GUI	Graphical User Interface	
HERE	Higher Education Research Experiences	http://www.orau.gov/hereatornl/
HPVIS	High Production Volume Information Systems	http://www.epa.gov/hpvis/
HSC	Enthalpy-Entropy-Heat Capacity	
HSDB	Hazardous Substances Data Base	http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB
HTML	Hyper-Text Markup Language	
IDLH	Immediately Dangerous to Life and Health	
IED	Improvised Explosive Device	
INCHEM	International Programme on Chemical Safety	http://www.inchem.org/
IRIS	Integrated Risk Information System	http://www.epa.gov/iris/
LC_{50}	Median Lethal Concentration	
LEL	Lower Explosive Limit	
LFL	Lower Flammable Limit	
MC	Mission Critical	
MKOPSC	Mary Kay O'Connor Process Safety Center	http://process-safety.tamu.edu/
ML	Markup Language	
MSDS	Material Safety Data Sheets	
NA	Not Applicable	
NA#	North America Number	
NF	Not Found	
NFPA	National Fire Protection Association	http://www.nfpa.org/index.asp?cookie%5Ftest=1
NIOSH	National Institute for Occupational Safety and Health	http://www.cdc.gov/niosh/npg/
NIST	National Institute of Standards and Technology	http://www.nist.gov/index.html
NL	Not Likely	
NOAA	National Oceanographic and Atmospheric Administration	http://www.noaa.gov/
ORNL	Oak Ridge National Laboratory	http://www.ornl.gov/
OSHA	United States Occupational Safety and Health	http://www.osha.gov/

PAC	Protection Action Criteria (see also TEEL)	http://hss.energy.gov/HealthSafety/WSHP/chem_safety/teel.html
PSID	Process Safety Incident Database	http://www.psidnet.com/
RDP	Responsible Distribution Process	
RMP	Risk Management Plan	
RQ	Reportable Quantity	
RTECS	Registry of Toxic Effects of Chemical Substances	www.mdl.com/products/predictive/toxicity/index.jsp
SBU	Sensitive But Unclassified	
SC	Search Code	
SI	Système International d'Unités (International System of Units)	
SOCMA	Synthetic Organic Chemical Manufacturers Association	http://www.socma.com/
SQL	Structured Query Language	
STEL	Short Term Exposure Limit	
STQ	Screening Threshold Quantity	
SULI	Science Undergraduate Laboratory Internships	
TATP	Triacetone Triperoxide	
TCPA	Toxic Catastrophe Prevention Act	http://www.state.nj.us/dep//rpp/brp/tcpa/downloads/title13.htm
TEEL	Temporary Emergency Exposure Limits (see also PAC)	Same URL as PAC
TeX	"tek" in English (typesetting system for documents)	http://tug.org/; http://en.wikipedia.org/wiki/TeX
TLV	Threshold Limit Value	
TLV-C	Threshold Limit Value-Ceiling	
TLV-STEL	Threshold Limit Value-Short Term Exposure Limit	
TLV-TWA	Threshold Limit Value-Time Weighted Average	
TNT	2,4,6-Trinitrotoluene	
UN#	United Nations Number	
UEL	Upper Explosive Limit	
URL	Uniform Resource Locator	
USDOE	United States Department of Energy	http://www.energy.gov/
VCE	Vapor Cloud Explosion	
W3C	World Wide Web Consortium	http://www.w3.org/
WISER	Wireless Information System for Emergency Responders	http://wiser.nlm.nih.gov/
WME	Weapons of Mass Effect	