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Risk Management Analysis

Blue Grass Chemical Agent-Destruction Pilot Plant (BGCAPP) VX Hydrolysate Transportation Risk Assessment

Site: BGCA/BGCAPP	Study Number: RM-20-013

An evaluation of the risk of transporting treated VX hydrolysate from BGCAPP to a treatment, storage, and disposal facility (TSDF) was conducted. The regulations for hazmat classification, handling, loading, and transport were reviewed for safe transport of the hydrolysate in tanker trucks. A transportation risk assessment was conducted for the BGCAPP VX hydrolysate using the accepted Army risk management approach by determining accident frequency and event consequences for (1) an accident/incident with a release/leak and (2) an accident with a release and a fuel fire. Overall, the results determined from modeling indicate that the transportation risk is *Low.*

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1 INTRODUCTION

1.1 Background

Neutralization of nerve agent O-ethyl S-2-(diisopropylamino)ethyl methylphosphonothioate (VX), a chemical warfare agent at the Blue Grass Chemical Agent-Destruction Pilot Plant (BGCAPP), generates a hydrolysate waste stream. The generated hydrolysate is pH-adjusted to between 13 and 14 by the addition of sodium hydroxide (NaOH) to prevent a reverse reaction. The term "hydrolysate" in this transportation risk assessment (TRA) refers to the caustic-adjusted hydrolysate, unless otherwise noted. The hydrolysate was originally intended to be treated onsite by the supercritical water oxidation (SCWO) process. In its review of the criteria for successful treatment of the hydrolysate, the National Academies of Sciences, Engineering, and Medicine (NASEM 2015) considered offsite treatment of the hydrolysate in the event that the SCWO underperformed or failed altogether. The offsite treatment would help reduce the risk to the community by enabling timely completion of treatment operations at BGCAPP.

The decision was made in August 2020 to not use the SCWO system due to multiple issues discovered during testing that raised reliability concerns. Offsite treatment of VX hydrolysate at a commercial treatment, storage, and disposal facility (TSDF) is being considered as an alternative to onsite disposal, as addressed above. Shipment of the waste to a TSDF is a viable option if the potential risk to the public in the event of a transportation accident is acceptable. A TRA identifies and assesses potential risks to the public due to accidents during transport of hazardous waste. The Army previously performed TRAs to support planned shipment of certain types of agent-contaminated secondary waste from specific Army facilities to permitted TSDFs. These shipments subsequently have been completed safely and without incident.

As described in the relevant sections, this TRA uses some of the methodology and/or certain information/data presented in the following previously published risk assessment studies:

- *Bounding Transportation Risk Assessment for >1 Vapor Screening Level (VSL) Waste* (CMA 2014) (hereinafter Bounding TRA)
- *Risk Assessment for Storage and Processing of VX Hydrolysate at the Blue Grass Chemical Agent-Destruction Pilot Plant* (SAIC 2006) (hereinafter BGCAPP Risk Assessment)
- *Newport Chemical Agent Disposal Facility, Transport Safety Plan and Risk Evaluation for Shipment of NECDF Caustic Hydrolysate* (CMA 2007) (hereinafter Newport Chemical Agent Disposal Facility [NECDF] Transport Safety Plan)

- *Transportation Analysis for the Off-Site Shipment of Liquid Process Effluent from the Newport Chemical Agent Disposal Facility at the Newport Chemical Depot, Indiana* (Zimmerman et al. 2003) (hereinafter Zimmerman Transport Analysis)
- *Transportation Safety Assessment and Risk Management Plan, Shipments of Newport (Indiana) Caustic Hydrolysate (NCH) Newport IN to Deepwater NJ* (Burke 2004) (hereinafter Burke Transportation Safety Assessment)
- *Review of the U.S. Army Proposal for Off-site Treatment and Disposal of Caustic VX Hydrolysate from the Newport Chemical Agent Disposal Facility* (CDC 2005) (hereinafter Centers for Disease Control and Prevention [CDC] Off-Site VX Hydrolysate Treatment Review)

This TRA does not consider risk from potential accidents during handling, loading, or unloading the wastes at BGCAPP or at the TSDF. Documents that address hazards during these activities, such as job hazard analyses or monitoring plans, will be developed independently from this TRA. In addition, this TRA is just one element of the Army's program to ensure protection of the public, workers, and the environment during shipment operations. Other documents will be prepared to cover (1) monitoring and characterization of the waste, (2) packaging and segregation of the waste, (3) loading and unloading operations, (4) transportation planning and procedures, and (5) emergency response planning and procedures.

1.2 Objective

The objective of this TRA is to assess the risk related to offsite shipment—via a commercial hazardous waste carrier—of treated VX hydrolysate from the BGCAPP site in Richmond, Kentucky, to a TSDF.

2 DESCRIPTION OF WASTE TO BE SHIPPED

The hydrolysate is composed of a number of VX degradation products, NaOH, and water. Table 2-1 lists the constituent characteristics and estimated concentrations (i.e. weight fractions). The data is based on an average of up to 82 samples of hydrolysate from NECDF, as summarized in the VX Hydrolysate Characterization memo from Bechtel Parsons Blue Grass (BPBG 2020). The concentration of VX is based on the hydrolysate clearing limit of 80 parts per billion from the neutralization reactor. The concentration of S-2-(diisopropylaminoethyl) methylphosphonothioic acid (EA-2192) is based on the hydrolysate clearing limit of 1 part per million from the neutralization reactor.

The samples discussed in the VX Hydrolysate Characterization memo were well-mixed samples taken from the reactor, which had static mixers and recirculation loops. VX hydrolysate, when not being mixed, separates into two layers: an upper organic layer and a lower aqueous layer. The memo estimated the top organic layer to be 1.18 percent of the hydrolysate on average.

The constituents in the top layer are flammable, although the mixed hydrolysate is not flammable.

Table 2-1. Hydrolysate Constituent Characteristics and Estimated Concentrations

Chemical Compound [a,b]	Abbreviation	Structural Formula [b]	Molecular Weight (grams per mole)	Average Concentration [a] (weight fraction)
O-ethyl S-2-(diisopropylamino)ethyl methylphosphonothioate	VX	$C_{11}H_{26}NO_2PS$	267.4	8.0×10^{-8} [c]
S-2-(diisopropylaminoethyl) methylphosphonothioic acid	EA-2192	$C_9H_{22}NO_2PS$	239.3	1.0×10^{-6} [d]
Ethyl methylphosphonic acid	EMPA	$C_3H_9O_2PS$	124.1	7.7×10^{-2}
Methylphosphonic acid	MPA	CH_5O_3P	96	9.7×10^{-3}
Diisopropyl ethyl mercaptoamine	Thiolamine	$C_8H_{19}NS$	161.3	6.3×10^{-2}
Bis(2-diisopropylaminoethyl) disulfide	Disulfide	$C_{16}H_{36}N_2S_2$	320	1.4×10^{-2}
Diisopropylamine	DIPA	$C_6H_{15}N$	101	5.3×10^{-3}
Ethanol	–	C_2H_5OH	46.1	1.6×10^{-3} [e]
Sodium hydroxide	NaOH	NaOH	40	3.5×10^{-2} [e]
Water	H_2O	H_2O	18	7.94×10^{-1}
Total				**1.0**

Notes:

a Bechtel Parsons Blue Grass. 2020. *VX Hydrolysate Characterization*. Memorandum to John Barton from Clara Galbis-Reig. 24915-00-LBT-GAM-00815. Table 2, Summary of NECDF Characterization Data. September.
b Munro, N.B., S.S. Talmage, G.D. Griffin, L.C. Waters, A.P. Watson, J.F. King, and V. Hauschild. 1999. "The Sources, Fate, and Toxicity of Chemical Warfare Agent Degradation Products." *Environmental Health Perspectives* 107 (12), 933–974. https://doi.org/10.1289/ehp.99107933.
c VX concentration based on the hydrolysate clearing limit of 80 parts per billion
d EA-2192 concentration based on the hydrolysate clearing limit of 1 part per million
e Hullman, David. 2020. Leidos. Blue Grass Chemical Agent-Destruction Pilot Plant Field Office. Email dated 1 July 2020, with Battelle Calculation Spreadsheet Attachment, *Expected Hydrolysate Waste Profile*.

Each batch produced in the Agent Neutralization System will be checked for flammability before it is transferred out to the Hydrolysate Storage System (HSS). The mixing system in the HSS tanks ensures that the tank stays mixed up to the point the hydrolysate is pumped into tankers. The line to transfer the hydrolysate to the truck loading system is downstream of the static mixer, to ensure a representative sample of the HSS tank. Stratification is not a concern to the TSDF, as it is able to accept a wide range of organic percentages.

Based on a discussion with BGCAPP Field Office, Bechtel Parsons, and Battelle representatives (Leidos 2020), the following relevant points were noted:

- Ethyl methylphosphonic acid (EMPA), methylphosphonic acid (MPA), and diisopropyl ethyl mercaptoamine (thiolamine) exist almost completely as sodium salts in the aqueous layer and, therefore, have very low vapor pressures.
- Based on an analysis of residual VX in caustic decontamination solutions (ERDEC 1998), the organic layer indicated through nuclear magnetic resonance (NMR) analysis that it consisted mainly of the VX sulfides and disulfides, which have a very low vapor pressure.
- Diisopropylamine (DIPA) would be expected to be in the organic layer and in the vapor space above the organic layer. The NMR analysis did not identify DIPA because it would have completely evaporated due to its high vapor pressure.
- The DIPA content in the NECDF hydrolysate was much higher than would be expected at BGCAPP because the NECDF reactor was run for much longer periods, which breaks down the thiolamine to DIPA. Therefore, the average value of 0.0053 weight fraction should be considered a bounding value.

VX hydrolysate is designated as a listed hazardous waste in Kentucky, with waste code N302 – Agent hydrolysate associated with VX munitions.

In addition, the following Resource Conservation and Recovery Act characteristic hazardous waste codes may apply (Hullman 2020):

- D002 (Corrosive)
- D004 (Arsenic)
- D005 (Barium)
- D006 (Cadmium)
- D007 (Chromium)
- D008 (Lead)
- D009 (Mercury)
- D010 (Selenium)
- D011 (Silver)

VX hydrolysate is classified as a Department of Transportation (DOT) hazardous material (hazmat) belonging to Class 8 (corrosive material) category, due to its pH (between 13.0 and 14.0). It has been determined through testing and generator knowledge based on available data that the hydrolysate does not possess any other DOT hazard class (CMA 2007). The proper shipping name and description under DOT regulations is one of the following:

- *If the flash point is <200°F:* Waste Corrosive Liquid, Basic Organic, n.o.s., 8, UN3267, PG II, RQ (Sodium Hydroxide)

- *If the flash point is >200°F:* Waste Corrosive Liquid, Basic Organic, n.o.s., 8, UN3266, PG II, RQ (Sodium Hydroxide)

As referenced in the NECDF Transport Safety Plan, since there is no specific listing for this hydrolysate in the DOT materials table, a "not otherwise specified" (or n.o.s.) description is used for VX hydrolysate. The hazard class (8) and UN number are used to identify the correct response actions from the Emergency Response Guidebook (ERG 2016). The Packing Group is a relative indication of the degree of hazard associated with the material. PG I indicates a high degree of hazard, PG II a lesser degree, and PG III a minor degree. In this case, the hydrolysate has a PG II designation and a medium degree of corrosivity to human tissue, based on tests prescribed by the DOT. The "RQ" notation identifies any constituent (in this case, NaOH) that is designated a hazardous substance and is present at or above the reportable quantity of 1,000 pounds.

3 PACKAGING AND TRANSPORTATION REQUIREMENTS

3.1 DOT Transport Regulations

49 Code of Federal Regulations (CFR) 172 prescribes the requirements for shipping papers, package marking, labeling, and transport vehicle placarding applicable to the shipment and transportation of each class of hazmat. In addition, it prescribes requirements for emergency response, training, and safety and security plans.

49 CFR 173 prescribes requirements for preparing the hazmats for shipment, including packaging requirements and quantity limitations. 49 CFR 173.50 prescribes requirements for packaging of Class 1 hazmats.

49 CFR 177 prescribes requirements for transportation via public highway by motor vehicle, including inspections, driver training, segregation and separation, and loading and unloading requirements for each class of hazmat.

49 CFR 178 prescribes testing requirements for packaging and containers used for transportation of hazmats.

3.2 Transport Vehicle

The transport vehicle has the following specifications:[1]

- DOT-412 tanker – 5,000 gallon

[1] Source: www.Barrgo.com

- Specially built to carry corrosives
- Typically made from stainless steel
- Maximum allowable working pressure (MAWP): 5 – 25 pounds per square inch gauge (psig)
- Equipped with pressure relief devices
- Pressure relief devices activate at 1.5 times the MAWP

3.3 Description of General Transport Requirements

Transport requirements for hazmats are governed by DOT regulations, as described in Section 3.1. General provisions applicable during the transportation phase (49 CFR 177.800, 177.801, 177.804, 177.810, 177.816, 177.817, and 177.823) include the following:

- Transport without unnecessary delay, from and including the time of commencement of the loading of the hazmat until its final unloading at destination
- Availability of records, equipment, packaging, and containers under the control of a motor carrier, insofar as they affect safety in transportation of hazmats
- Compliance with safe clearance requirements for highway-rail grade crossings in 49 CFR 392.12
- Prohibition of texting and use of handheld telephones while driving, in accordance with 49 CFR 392.80 and 392.82
- Compliance with requirements of hazmat transport restrictions in vehicular tunnels
- Driver training in accordance with 49 CFR 177.816 and 49 CFR 390 through 397, including:
  - Pre-trip safety inspection
  - Use of vehicle controls and equipment, including operation of emergency equipment
  - Operation of vehicle, including turning, backing, braking, parking, handling, and vehicle stability
  - Procedures for maneuvering tunnels, bridges, and railroad crossings

  - Requirements pertaining to attendance of vehicles, parking, smoking, routing, and incident reporting
  - Loading and unloading of materials, including compatibility, segregation, package handling, and load securement
  - Specialized training for cargo tanks and portable tanks including emergency control features of the tank, center of gravity, fluid-load surge on braking, properties and hazards of material transported, and retest and inspection requirements for cargo tanks
- Availability of shipping papers to authorities in the event of accident or inspection
- Marking and placarding a transport vehicle containing a hazardous waste in accordance with 49 CFR 172
- Prohibition on moving a transport vehicle containing a hazardous waste during an emergency unless:
  - The vehicle is escorted by a representative of a state or local government
  - The carrier has permission from the DOT
  - Movement of the vehicle is necessary to protect life or property.

3.4 Loading and Unloading

The hydrolysate will be transferred from the hydrolysate storage tanks into the tanker truck in accordance with the BGCAPP Standing Operating Procedure. This TRA assumes that prior to transfer, the truck will be inspected to ensure all safety features are present and functioning as intended. The TRA also assumes that, at the conclusion of the transfer operation, the truck will be inspected per the Standing Operating Procedure to ensure that valves are closed, caps secured, and pressure relief devices present to ensure that the tanker truck is ready to begin transporting the hydrolysate.

Although this TRA does not address the risk of accidents during loading and unloading, general regulatory requirements (49 CFR 177.834) applicable during hazmat loading and unloading operations include the following:

- No loading or unloading should occur unless the handbrake is securely set and all other reasonable precautions are taken to prevent motion of the motor vehicle.
- A qualified person must attend the cargo tank at all times during loading and unloading.
- A qualified person must be within 25 feet of the cargo tank.

- Cargo motor vehicles must not be driven unless all manholes are closed and secured, and all valves and other closure devices are closed and free of leaks.

3.5 Description of Additional Specific Transport Requirements

Additional operational measures will be implemented that will further increase the safety and security of the shipments. Some measures may overlap with the general procedures outlined in Section 3.3. The requirements/operational measures outlined in this section were originally developed for the NECDF Transport Safety Plan in 2007, but are currently considered valid as representative requirements. However, as stated in Section 1.1, separate documents will be prepared to cover transportation and emergency response planning and procedures. As such, a project-specific Transportation Plan for shipping the BGCAPP VX hydrolysate—incorporating specific requirements, if any, from the state, CDC, and/or community—will be prepared by the selected transporter and submitted to Program Executive Office, Assembled Chemical Weapons Alternatives prior to shipment.

- Trucks will remain in visual contact with each other.
- Trucks will endeavor to drive and/or park on paved surfaces at all times.
- Trucks will be attended at all times in accordance with DOT requirements and in compliance with all motor carrier safety regulations.
- Trucks will stop approximately every 2 hours to conduct a vehicle safety inspection and inspect the security of the load.
- Trucks will always be driven using team drivers. Trucks will be driven “straight through,” according to the prescribed route. Breaks will be limited to required safety/security inspections, lavatory breaks, and reasonable rest stops for meals.
- Each truck will carry a copy of emergency response notification numbers with the shipping papers.
- Each truck will be tracked using satellite GPS methods, be equipped with cellular phones, and maintain routine contact with company dispatch.
- Trucks will observe prescribed travel routes and observe posted speed limits at all times. Any variation of more than 1 mile from the prescribed route must be reported to dispatch.
- Trucks will be equipped with basic spill kits.
- Drivers will receive specific training regarding hydrolysate, leak recognition, spill defensive measures, immediate hazard assessment, and site control. At a minimum, drivers will be trained to the Occupational Safety and Health Administration (OSHA)

Hazardous Waste Operations and Emergency Response (HAZWOPER) Emergency Responder Awareness Level. Drivers will be capable of evacuating the area and summoning additional resources.

- Safety, environmental/technical, and medical services support, as provided by the TSDF, will be on call during the hydrolysate transportation activities.

Qualifications of drivers for hydrolysate transport will include the following:

- Drivers will have current commercial driver's license (CDL), with the necessary endorsements to haul hazmats.
- Drivers will be DOT certified for hazmat transport.
- Drivers will be trained, at a minimum, to the OSHA HAZWOPER Emergency Responder Awareness Level and will complete the prescribed training regarding the Transportation Safety Plan and hydrolysate. Drivers will be current on all training required by DOT and Federal Motor Carrier Safety Administration regulations.
- Drivers will participate in random drug/alcohol testing in accordance with their company policy and DOT/Federal Motor Carrier Safety Administration regulations.
- Drivers will receive training in the Emergency Response Plan developed by the emergency response company contracted to support the hydrolysate transport.

4 METHODOLOGY

4.1 Overview of Methodology

The general methodology used in this TRA relies on the accepted Army risk management approach. The methodology is similar to that used in the Bounding TRA (for example, the same hazard probability categories, severity descriptions, and equivalent hazard severity definitions are used).

Historically, Department of the Army Pamphlet (DA PAM) 385-61 (DA 2002) has been the basis for the Army risk management program for chemical-agent-related hazards. Appendix F of DA PAM 385-61 (2002 version) provides an overview of the Army strategy for a risk management program. It states in part:

> Risk assessment, as a part of risk management, provides a useful tool for estimating the effectiveness of existing and proposed safeguards against chemical agent mishaps. The potential for and consequences of mishaps must be carefully analyzed. The risk assessment must consider not only the traditional MCEs [Maximum Credible Events] and resulting consequences, but also the probabilities and consequences of any realistic accident scenario that could present a risk to worker, the environment or the public.

The risk management requirements cited in the 2002 version of DA PAM 385-61 were rolled into DA PAM 385-30, *Mishap Risk Management* (DA 2007), which was subsequently revised and retitled as *Risk Management* (DA 2014).

As outlined in DA PAM 385-30, the risk assessment is used to establish priorities for corrective action and resolution of identified hazards. Consistent with these objectives, this TRA evaluates the risk of the potential accident and release scenarios based on the combination of hazard probability and severity.

Figure 4-1 provides the Department of the Army model for risk acceptance according to DA PAM 385-30. Risk categories range from *Low* to *Extremely High*. Low risks are generally considered acceptable without mitigation, whereas higher risk categories generally require mitigation. The decision to mitigate or accept specific hazards is left to the discretion of Army authorities.

Severity (expected consequence)	**Probability (expected frequency)**				
	Frequent A	**Likely B**	**Occasional C**	**Seldom D**	**Unlikely E**
Catastrophic I	Extremely High				
Critical II		High			
Moderate III			Medium		
Negligible IV				Low	

Figure 4-1. Qualitative Risk Evaluation Matrix (adapted from DA PAM 385-30)

The probabilities and severities in Figure 4-1 may be categorized—as shown in Tables 4-1 and 4-2, respectively—using schemes provided in DA PAM 385-30. The 2014 version of DA PAM 385-30 no longer specifies the probability values for each category and states that it is often hard to determine objective or numerical probability values but efforts should be made to use the numerical probability values. This TRA uses the values provided in 2007 version, as shown in Table 4-1, as a guide in determining the risk level for the accident scenario.

Table 4-1. Probability Categories per DA PAM 385-30

Description	Level	Single Item or Activity
Frequent	A	Likely to occur often in the life of an item, with a probability of occurrence greater than 10^{-1} in that life.
Probable or Likely	B	Will occur several times in the life of an item, with a probability of occurrence less than 10^{-1} but greater than 10^{-2} [1 time/100 opportunities] in that life.
Occasional	C	Likely to occur some time in the life of an item, with a probability of occurrence less than 10^{-2} but greater than 10^{-3} [1 time/1,000 opportunities] in that life.
Seldom or Remote	D	Unlikely but possible to occur in the life of an item, with a probability of occurrence less than 10^{-3} but greater than 10^{-6} [1 time/1,000,000 opportunities] in that life.
Unlikely or Improbable	E	So unlikely, it can be assumed occurrence may not be experienced, with a probability of occurrence less than 10^{-6} in that life.

Source: Department of the Army (DA), DA Pamphlet (DA PAM) 385-30, *Mishap Risk Management*, Headquarters, Washington, D.C., 10 October 2007.

Table 4-2. Hazard Severity Descriptions in DA PAM 385-30

Hazard Severity	Level	Description
Catastrophic	I	*Definition:* Death, unacceptable loss or damage, mission failure, or unit readiness eliminated. *Quantitative Value:* One or more deaths or permanent total disabilities.
Critical	II	*Definition:* Severe injury, illness, loss, or damage; significantly degraded unit readiness or mission capability. *Quantitative Value:* One or more permanent partial disabilities or hospitalization of at least three personnel.
Moderate	III	*Definition:* Minor injury, illness, loss, or damage; degraded unit readiness or mission capability. *Quantitative Value:* One or more injuries or illnesses resulting in lost time.
Negligible	IV	*Definition:* Minimal injury, loss, or damage; little or no impact to unit readiness or mission capability. *Quantitative Value:* One or more injuries or illnesses requiring first aid or medical treatment.

Source: Department of the Army (DA), DA Pamphlet (DA PAM) 385-30, *Risk Management*, Headquarters, Washington, D.C., 2 December 2014.

4.2 Hazard Definition

The approach outlined in this section defines hazard severity based on two response zones: (1) the initial isolation zone and (2) the secondary control zone. The distance to the boundary of these zones depends on the chemical spilled, as specified in the Emergency Response Guidebook (ERG 2016). The guidebook defines distances for small spills and large spills—this TRA considers a large spill, which is defined in the guidebook as a spill that involves quantities greater than 208 liters (55 US gallons) for liquids and greater than 300 kilograms (660 pounds) for solids.

Since the VX hydrolysate will be shipped as a DOT Class 8 corrosive liquid, Guide 154 (from ERG 2016) is applicable. This guide addresses toxic and/or corrosive (non-commercial) substances. The evacuation criteria for this category of chemicals are not listed in the Isolation Distances table (Table 1 in ERG 2016), but instead refer to the *Public Safety* requirements specified in Guide 154, which call for an immediate isolation distance of 50 meters for a spill, regardless of whether it is a small or large spill. The secondary control zone distance is not specified.

In the event of an accident, personnel involved in the convoy will initially isolate and evacuate the area within the Emergency Response Guidebook recommended distance of 50 meters of the site. This TRA assumes isolation and evacuation will be accomplished within 30 minutes of the accident. The TRA also assumes that it will take up to 2 hours for first responders to arrive at the accident scene, evacuate the secondary zone, and terminate the vapor release. Although the Emergency Response Guidebook (ERG 2016) does not specify a secondary control zone distance for this substance, this TRA assumes a distance of 200 meters, which is typically the shortest secondary zone distance value for other chemicals in Table 1 of the guidebook.

The hazard is characterized in terms of hazard distances, which are the distances necessary for the chemical concentration to fall below specific concentration levels, as it disperses. For VX, the concentration levels are based on established Acute Exposure Guideline Levels (AEGLs). For example, the 30-minute AEGL-1 hazard distance is the distance required for the VX concentration to fall below the 30-minute AEGL-1 concentration. Hazard distances are calculated using a plume dispersion model, specifically, the Army-sponsored D2PC software (Whitacre et al. 1987).

For the other chemical constituents, this TRA uses concentration levels based on established Protective Action Criteria (PAC) levels[2] for each chemical since AEGLs are not established for these chemicals. PAC for chemicals are essential components for planning and response to uncontrolled releases of hazardous chemicals.

[2] https://www.energy.gov/ehss/protective-action-criteria-pac-aegls-erpgs-teels

The benchmark values established for VX (AEGL-1, AEGL-2, and AEGL-3) and for each of the other chemicals (PAC-1, PAC-2, and PAC-3) represent the following health impacts:

- AEGL-1: Notable discomfort, irritation, or certain asymptomatic non-sensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure
- AEGL-2: Irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape
- AEGL-3: Life-threatening health effects or death
- PAC-1: Mild transient health effects
- PAC-2: Irreversible or other serious health effects that could impair the ability to take protective action
- PAC-3: Life-threatening health effects

The established AEGL values are based on 10-minute, 30-minute, 60-minute, 4-hour, and 8-hour exposure. Since 2-hour AEGL concentrations are not available, they were derived using the procedures described in Appendix A of *Acute Exposure Guideline Levels for Selected Chemicals* (NRC 2003).

The established PAC values are based on a 1-hour exposure. For this TRA, PAC concentrations were needed for two exposure durations: 30 minutes (establishing the initial isolation zone) and 2 hours (establishing the secondary control zone). Appendix C describes the derivation of these PAC values.

Table 4-3 presents a set of hazard severity definitions that provide the same acceptable exposure levels both inside and outside the initial isolation zone, the only difference being the duration of the exposure in these two areas. The hazard severity definitions reference AEGL-1, -2, -3, and PAC-1, -2, and -3 concentrations for 30-minute and 2-hour exposures. Exposures at greater than the AEGL-3/PAC-3 concentration could lead to life-threatening effects for susceptible receptors. Exposures at greater than the AEGL-2/PAC-2 concentration, but less than the AEGL-3/PAC-3 concentration, could result in irreversible or other serious health effects. Exposures at greater than the AEGL-1/PAC-1 concentration, but less than the AEGL-2/PAC-2 concentration, could result in mild transient health effects. Table 4-4 presents the 30-minute and 2-hour AEGL concentrations for VX and PAC concentrations for each chemical evaluated for this TRA (see Sections 6.1 and 6.2).

Table 4-3. Hazard Severity Definitions Used for TRA

Hazard Severity	Level	Proposed Definition and Rationale
Negligible	IV	*Proposed Definition:* a. 2-hour AEGL-1/PAC-1 hazard distance < distance to secondary control zone boundary (200 meters) b. 30-minute AEGL-1/PAC-1 hazard distance < distance to initial isolation zone boundary (50 meters) *Rationale:* a. Ensuring that the 2-hour AEGL-1/PAC-1 hazard distance does not reach the nearest member of the public ensures that there are negligible health effects. b. Ensuring that the 30-minute AEGL-1/PAC-1 hazard distance does not extend beyond the initial isolation zone would likely ensure negligible health effects for bystanders.
Moderate	III	*Proposed Definition:* a. 2-hour AEGL-2/PAC-2 hazard distance < distance to secondary control zone boundary (200 meters) b. 30-minute AEGL-2/PAC-2 hazard distance < distance to initial isolation zone boundary (50 meters) *Rationale:* a. Ensuring that the 2-hour AEGL-2/PAC-2 concentration does not reach the nearest member of the public ensures that injuries are minor. b. Ensuring that 30-minute AEGL-2/PAC-2 hazard distance does not extend beyond the initial isolation zone would likely ensure only minor injuries for bystanders.
Critical	II	*Proposed Definition:* a. 2-hour AEGL-3/PAC-3 hazard distance < distance to secondary control zone boundary (200 meters) b. 30-minute AEGL-3/PAC-3 hazard distance < distance to initial isolation zone boundary (50 meters) *Rationale:* a. Ensuring that the 2-hour AEGL-3/PAC-3 concentration does not reach the nearest member of the public ensures that injuries are not fatal, although they may be serious. b. Ensuring that the 30-minute AEGL-3/PAC-3 hazard distance does not extend beyond the initial isolation zone would likely ensure that injuries are not fatal, although they may be serious.

Notes:

AEGL Acute Exposure Guideline Level
PAC Protective Action Criteria

Table 4-4. AEGL and PAC Concentrations for Chemicals

Chemical/Hazard Level [a]	30-minute Concentration [b] (mg/m^3)	2-hour Concentration [b] (mg/m^3)
O-ethyl S-2-(diisopropylamino)ethyl methylphosphonothioate (VX)		
AEGL-1	0.00033 [c]	0.0001 [d]
AEGL-2	0.0042 [c]	0.002 [d]
AEGL-3	0.015 [c]	0.007 [d]
Diisopropylamine (DIPA)		
PAC-1	78.1	31
PAC-2	884	351
PAC-3	5,205	2,066
Bis(2-diisopropylaminoethyl) disulfide (Disulfide)		
PAC-1	121	48
PAC-2	1,370	544
PAC-3	8,062	3,200

Notes:

a EMPA, MPA, thiolamine, EA-2192, and ethanol are not included, per discussion in Section 6.1. NaOH is not included because it is not an organic compound.
b All PAC values are derived values. See discussion in Appendix C.
c Established values from NRC 2003, Appendix D
d Concentration derived as $(K/2)^{0.5}$ (formula and K values are from NRC 2003, Appendix A)

AEGL Acute Exposure Guideline Level
mg/m^3 milligrams per cubic meter
PAC Protective Action Criteria

Source: NRC (National Research Council). 2003. *Acute Exposure Guideline Levels for Selected Chemicals.* Volume 3. Washington, DC: The National Academies Press. https://doi.org/10.17226/10672.

4.3 Technical Approach

Section 4.1 presents a brief discussion of the methodology for this TRA. This technical approach describes the specific steps taken to complete this assessment and identifies key assumptions made in the analysis for a fire scenario. Sections 5 and 6 detail the analysis approach.

The following steps were completed to determine the transportation risks during shipment:

- Develop the transportation accident scenario to be assessed.
- Determine the hazard probability by estimating the probability of a truck accident that results in a spill and a fire, using available data for hazmat transportation accidents.
- Assess the hazard consequences from inhalation (using D2PC), dermal contact, and aquatic impacts.
- Determine the risk level based on the hazard probability and consequences in accordance with Section 5.2.

5 WASTE TRANSPORT TRUCK ACCIDENT PROBABILITY

5.1 Transportation Routing

Different transportation routes could be used to ship the VX hydrolysate from BGCAPP to the TSDF. The transporter will select a shipment route based on consideration of several factors, such as avoiding major population centers/sensitive land areas and ensuring adequate emergency response capabilities. The transporter will also ensure that the route is selected in accordance with the National Hazardous Materials Route Registry (80 Federal Register [FR] 23859). The selected route often will not be the shortest route available. A distance of 2,000 miles is assumed for this TRA. This distance would cover potential TSDFs in most states.

5.2 Truck Accident Probability Estimation

A baseline frequency for truck accidents was obtained from a Battelle study of hazmat truck shipments (Battelle 2001, Tables 24 and 25). Data are provided for accidents involving a vehicle crash and for all incidents related to hazmat transport. Incidents include vehicle crashes as well as non-accident leaks that occur during loading, unloading, and transport. Only releases resulting from vehicle accidents and leaks during transport are considered in this TRA.

The accident rate from the 2001 Battelle study for transportation of Class 8 materials is 1.32×10^{-7} accidents per mile. The accident/incident rate (incidents include leaks en route with no accident) from the 2001 Battelle study for transportation of Class 8 materials is 4.092×10^{-7} accidents or incidents per mile.

This TRA evaluates the following scenarios:

- Scenario 1 – Accident/incident occurs, causing a release
- Scenario 2 – Accident occurs, causing a release and a fuel fire.

The fire is assumed to be the result of a fuel release. The event tree in Figure 5-1 depicts the modeled scenarios. Table 5-1 summarizes the basis for the event frequencies and probabilities. Sections 5.2.1 and 5.2.2 describe the calculation methodology used to determine the event frequencies for the scenarios shown in Figure 5-1.

Initiating Event	Release	Fire	Outcome
Accident Occurs	No Release		Accident – No Release
	Release	No Fire	Accident with Release (Scenario 1)
		Fire	Accident with Release and Fire (Scenario 2)
Incident Occurs	No Leak		Incident – No Release
	Leak		Incident – Release (Scenario 1)

Figure 5-1. Event Tree for Class 8 Materials

Table 5-1. Basis for Event Frequencies and Probabilities

Parameter	Reference	Value
Accident frequency per mile for Class 8 materials	Battelle 2001, Table 24	1.32×10^{-7} accidents per mile
Accident/incident frequency per mile for Class 8 materials (includes leaks en route)	Battelle 2001, Table 25	4.092×10^{-7} accidents/incidents per mile
Event tree conditional probability of a release, given an accident, for Class 8 materials	Battelle 2001, Table 6	0.284
Event tree conditional probability of no fire, given a release, for Class 8 materials	Battelle 2001, Table 6	0.973
Event tree conditional probability of fire, given a release (fuel), for Class 8 materials	Battelle 2001, Table 6	0.027
Number of accidents for Class 8 materials	Battelle 2001, Table 9	257
Number of en route incident leaks for Class 8 materials	Battelle 2001, Table 9	539
Total number of incidents plus accidents for Class 8 materials	Battelle 2001, Table 9	4,926
Miles per shipment	Assumption	2,000 miles

Reference: Battelle, *Comparative Risks of Hazardous Materials and Non-hazardous Materials Truck Shipment Accidents/Incidents*, Columbus, Ohio, March 2001.

5.2.1 Scenario 1 Calculation Methodology

For Scenario 1, a release can occur as a result of an accident or other incident that results in a leak en route. Therefore, the total probability of a release for Scenario 1 is determined by adding the probability of a release due to an accident and the probability of a release due to an incident other than an accident that results in a release.

The frequency of a release due to an accident is determined by multiplying the accident rate (1.32×10^{-7} per mile) by the conditional probability of a release given an accident (0.284), multiplied by the conditional probability of no fire given a release (0.973) (see Figure 5-1), which equals 3.65×10^{-8} per mile ($1.32 \times 10^{-7} \times 0.284 \times 0.973$).

Next, the conditional probability of a leak from an en route incident is determined by dividing the number of en route leaks (539) by the total number of accidents and incidents (4,926) minus the number of accidents (257), which equals 0.115 (539 ÷ (4,926 – 257)). Then, the accident frequency (1.32×10^{-7}) was subtracted from the accident/incident frequency (4.092×10^{-7}) to give the incident-only frequency of 2.77×10^{-7} ($4.092 \times 10^{-7} - 1.32 \times 10^{-7}$). The

frequency of an en route leak was then determined by multiplying the incident-only frequency (2.77×10^{-7}) by the conditional probability of an en route leak (0.115) to give a probability of 3.19×10^{-8} per mile ($2.77 \times 10^{-7} \times 0.115$).

Finally, to obtain the total probability for Scenario 1, the two frequencies (3.65×10^{-8} and 3.19×10^{-8}) are summed to give 6.84×10^{-8}, which is the per mile frequency of a release/leak given an accident/incident. This value was then multiplied by the shipping distance (2,000 miles) to give the frequency of an accident/incident with a release/leak per shipment to the TSDF ($6.84 \times 10^{-8} \times 2{,}000 = 1.37 \times 10^{-4}$).

5.2.2 Scenario 2 Calculation Methodology

For Scenario 2, since a fire results primarily from an accident causing a leak or rupture of the fuel tank, only the accident rate of 1.32×10^{-7} is used. (The incident leak rate is not relevant.) The conditional probability of a release given an accident is 0.284, as in Scenario 1. The accident release rate of 0.284 applies to both the hydrolysate being transported and the fuel in the fuel tank. The data offer no easy way to distinguish between the probability of a hydrolysate release versus a fuel release versus both a hydrolysate and a fuel release. Therefore, to be conservative, the accident release rate (0.284) is applied to hydrolysate in Scenario 1 and to hydrolysate and fuel in Scenario 2. Thus, the accident rate is multiplied by the conditional rate of release given an accident (0.284), and by the conditional rate of a fire given a release (0.027) and then by the distance (2,000 miles) for shipment to the TSDF to give the frequency of 2.02×10^{-6} for an accident with a fuel release and a fire per shipment ($1.32 \times 10^{-7} \times 0.284 \times 0.027 \times 2{,}000$).

5.2.3 Calculated Event Frequencies

Table 5-2 summarizes the results of the accident/incident event frequencies per shipment from BGCAPP to the TSDF for the two scenarios.

Table 5-2. Calculated Event Frequencies per Shipment from BGCAPP to TSDF

Event	Scenario 1 Frequency	Scenario 2 Frequency
Accident/incident per shipment	1.37×10^{-4}	2.02×10^{-6}

6 HAZARD AND CONSEQUENCE ASSESSMENT

This TRA evaluates the following types of hazards associated with a tanker truck accident/incident:

- Injuries/fatalities due to exposure (vapor inhalation) to a release/leak of hydrolysate
- Injuries/fatalities due to exposure (vapor inhalation) to a fuel-spill fire
- Injuries/fatalities due to dermal contact with the hydrolysate
- Aquatic impacts due to release of hydrolysate into water bodies

Injuries or fatalities from exposure to a hydrolysate release are based on either the corrosive or the toxicity characteristics of the hydrolysate, as determined from the composition and the toxicity of the individual constituents and of the mixture as a whole. A liquid mixture spill releases the more volatile constituents through evaporation. Exposure to individuals occurs through inhalation of the vapors or through dermal contact with the liquid.

6.1 Exposure via Vapor Inhalation from Spill

Based on the chemical composition of the hydrolysate, as shown in Table 2-1, and the discussion provided in Section 2, the following constituents represent organic compounds that are not expected to evaporate readily because they are present as sodium salts in the bottom aqueous layer with very low volatility:

- EMPA
- MPA
- Thiolamine
- EA-2192[3]

Ethanol is very soluble in water, is a commercially available household product, and has very low toxicity; therefore, it is not considered in this TRA.

DIPA is present in the upper organic layer and is very volatile; therefore, it is included in this TRA. Disulfide is also present in the organic layer and is included in the TRA, even though it has low volatility because evaporation will occur first from the organic layer.

Although VX is miscible in water, it is included in this TRA due to its extreme toxicity even though its vapor pressure (volatility) is very low.

[3] A 1999 National Academy of Sciences report, *Review and Evaluation of Alternative Chemical Disposal Technologies* (Chapter 8), indicates that EA-2192 is also a sodium salt under alkaline conditions.

The model used in this TRA was also used for the baseline chemical agent disposal facility quantitative risk assessments (QRAs), as described in BGCAPP Risk Assessment.

The QRA evaporation model uses Equation 1 for calculating the evaporation rate of each chemical for outdoor spills:

$$E_m = \frac{3.53 \times 10^3 \, u^{0.78} \, MW \, P_v}{Sc^{0.67} \, d^{0.11} \, P_a \, T} \tag{1}$$

where:

E_m	=	evaporation rate (grams per second-square meter [g/s m^2])
Sc	=	Schmidt number = μ/(Dρ) (dimensionless)
D	=	diffusivity of the vapor in air (square centimeter per second [cm^2/s])
μ	=	dynamic viscosity of air (grams per centimeter second [g/cm-s])
ρ	=	density of air (grams per cubic centimeter [g/cm^3])
u	=	wind speed (meters per second)
d	=	length of spill surface in the downwind direction (meters)
P_v	=	vapor pressure at temperature T (standard atmosphere [atm])
T	=	temperature at the surface of liquid (kelvin [K])
P_a	=	total ambient pressure at the liquid surface (atm)
MW	=	molecular weight

Equation 1 requires that the diffusivity of the evaporating chemical be calculated. The manual for the ALOHA® model (USEPA 2007) provides the following simple equation (Equation 2) for calculating the diffusivity:

$$D_E = D_{H2O} \sqrt{\frac{MW_{H2O}}{MW_E}} \tag{2}$$

where D_{H2O} and MW_{H2O} are the diffusivity and molecular weight of water (2.4×10^{-5} square meters per second and 18 grams per mole, respectively), and D_E and MW_E are the diffusivity and molecular weight of the evaporating chemical.

The vapor pressure used in Equation 1 is the partial pressure of the chemicals of interest. The vapor pressures of VX at the temperatures of interest are estimated using the Antoine equation (Buchanan 1999) (Equation 3):

$$P_v = \frac{1}{133.322} \, e^{[A - B/(C+T)]} \tag{3}$$

Where P_v is the vapor pressure (millimeters of mercury [mm Hg]); e (exponential constant) = 2.718; A, B, and C are VX-specific constants (A = 23.72, B = 6154.91, C = -60.165); and T = temperature (K). The equation also includes a conversion from Pascals to mm Hg.

The vapor pressures for DIPA and disulfide are estimated from a combination of Trouton's rule and the Clausius-Clapeyron equation (Castellan 1971) (Equation 4):

$$\ln(P_v) = 19\left(1 - \frac{T_{bp}}{T_0}\right) + 8.5\ln\left(\frac{T_{bp}}{T_0}\right) \tag{4}$$

where P_v is the vapor pressure of the compound in pure form (atm), T_{bp} is the boiling point (K), and T_0 is the reference temperature (298 K).

To calculate the partial pressure of each chemical of interest, the mole fraction of each chemical is calculated using Raoult's law (Equation 5). To use Raoult's law, the mole fraction of each constituent X_i is first determined based on its concentration (weight fraction) in the mixture and its molecular weight:

$$X_i = \frac{\frac{W_i}{MW_i}}{\sum_{i=0}^{n} \frac{W_i}{MW_i}} \tag{5}$$

where W_i and MW_i are the weight fraction and molecular weight for each constituent in the mixture.

The partial pressure of each constituent in the mixture is then calculated using Equation 6:

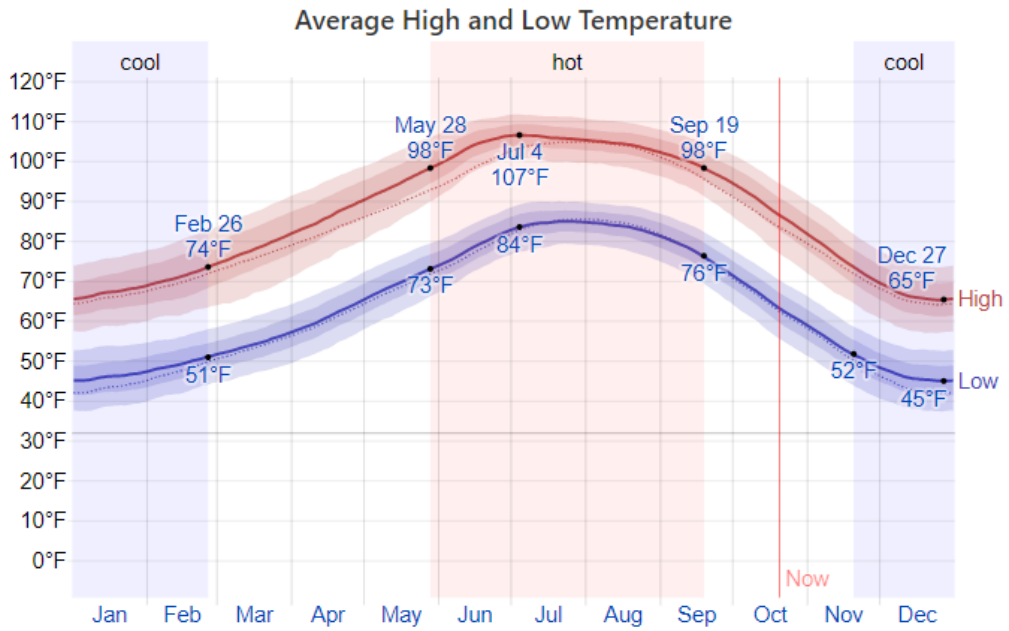
$$P_{vm,i} = P_{vp,i}\, X_i \tag{6}$$

where $P_{vm,i}$ is partial pressure of constituent *i* in the mixture, and $P_{vp,i}$ is the vapor pressure of constituent *i* in pure form. The calculated partial pressures are substituted for P_v in Equations 1 and 2.

Equations 1 through 6 are used to calculate the evaporation rates for each constituent of the hydrolysate under consideration. The calculations show that, overall, DIPA is the dominant contributor (approximately 100 percent) to the evaporative release in terms of mass.

Since the evaporation rate estimate using Equation 1 requires the temperature of the surface of the liquid and the wind speed, these parameters were determined using meteorological data from a worst-case (relative to temperature) location in the U.S. (Phoenix, Arizona). Figures 6-1 and 6-2 show the average temperature and wind speed. The highest average daytime temperature is 107°F (41.7°C). The corresponding average nighttime temperature is 84°F (29°C) during the same period. The wind speed corresponding to the time of the highest average temperature is approximately 7.0 miles per hour (from Figure 6-2) (or 3.1 meters per second).[4]

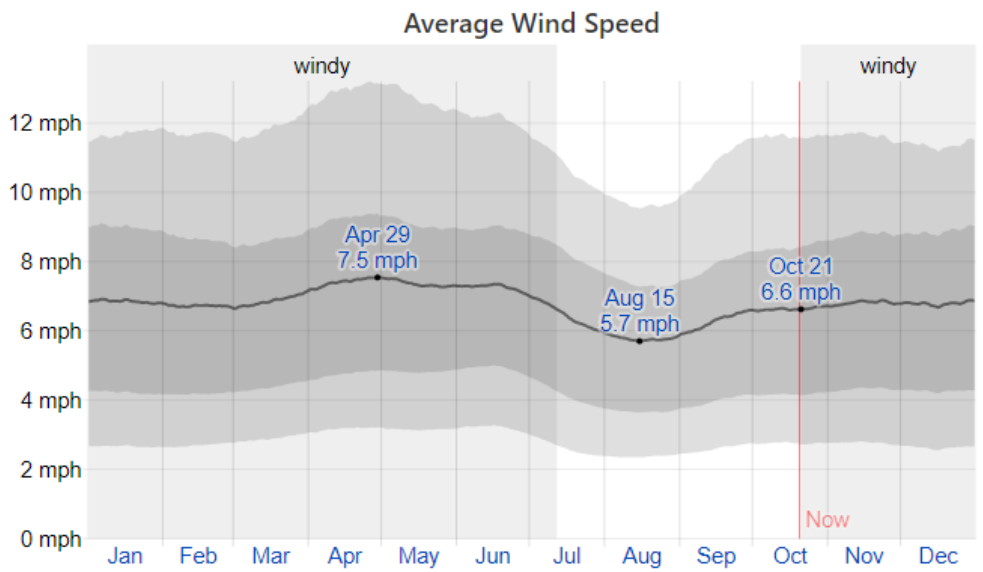
[4] Calculations show that 3.1 meters per second is conservative. Using a lower wind speed produces a lower downwind hazard because of reduced evaporation.



The daily average high (red line) and low (blue line) temperature, with 25th to 75th and 10th to 90th percentile bands. The thin dotted lines are the corresponding average perceived temperatures.

Source: www.weatherspark.com

Figure 6-1. Average Temperatures in Phoenix, Arizona



The average of mean hourly wind speeds (dark gray line), with 25th to 75th and 10th to 90th percentile bands.

Source: www.weatherspark.com

Figure 6-2. Average Wind Speeds in Phoenix, Arizona

Table 6-1 summarizes the results showing the evaporated masses of each constituent.

Table 6-1. Calculated Mass of Chemical Released Due to Evaporation from 5,000-gallon Hydrolysate Spill

Liquid Temp. (°C)	Wind Speed (m/s)	VX (g)	DIPA (g)	Disulfide (g)
41.7	3.1	2.27×10^{-5}	8.33×10^{4}	1.75×10^{-3}
29	3.1	6.65×10^{-6}	5.0×10^{4}	1.83×10^{-3}

Notes:

DIPA diisopropylamine
Disulfide bis(2-diisopropylaminoethyl) disulfide
g grams
m/s meters per second
VX O-ethyl S-2-(diisopropylamino)ethyl methylphosphonothioate

This analysis assumes that aerosol droplets will not be produced during a spill because no explosions or high-pressure releases (such as from a large tank rupture) will occur. The tanker truck will likely develop a breach and the hydrolysate will be released non-vigorously from the tanker. Therefore, exposure from aerosol droplets is not modeled.

The calculated mass of the chemicals from Table 6-1 is then input into D2PC, an atmospheric dispersion model. D2PC is a Gaussian plume model that calculates the distance to specified exposures or concentrations. To determine the potential health effects from exposure to a vapor release, the model calculates the downwind ground distance to reach the 30-minute and 2-hour AEGL-1/PAC-1 concentrations, which are compared to Table 4-3 to determine the hazard consequence. (It was not necessary to calculate the corresponding AEGL-2/PAC-2 and AEGL-3/PAC-3 distances based on the results of the AEGL-1/PAC-1 distances).

As with any computer model, there are a number of variables that must be input in order to model a specific accident scenario. In D2PC, these inputs are referred to as *dispersion control characteristics*. Table 6-2 lists the control characteristics that represent worst-case conditions for the evaporation scenario.

The D2PC model was run at the same temperatures and wind speed (as shown in Table 6-1), using D stability factor for daytime and F stability factor for nighttime release in order to generate the AEGL-1/PAC-1 distances. Table 6-3 summarizes the results. The results indicate that the criteria shown in Table 4-3 for a *Negligible* hazard severity (2-hour AEGL-1/PAC-1 less than 200 meters and 30-minute AEGL-1/PAC-1 less than 50 meters) are met for both daytime and nighttime transport.

Table 6-2. D2PC Dispersion Control Characteristics for Evaporative Release

Control Characteristic	Input Values Used	Rationale
Location	NDF	Not defined because location is not fixed
Height of Mixing Layer	400 meters	Daytime mixing layer height based on average conditions for summer
	250 meters	Nighttime mixing layer height is lower than daytime. A lower mixing height results in a greater ground level concentration.
Munition Type	NON	Non-munition for hydrolysate
Agent Type	VX	Nerve agent VX
	NA	Non-agent chemical (for DIPA and disulfide)
Release Type	EVP	Evaporation from an unconfined spill
Stability Type	D	D stability for worst-case daytime release
	F	F stability for worst-case nighttime release
Wind Speed	3.1 m/s	From Figure 6-2, corresponding to time of highest average temperature (7.0 miles per hour = 3.1 m/s)
Spill Source	mg	Iteratively determined such that the D2PC calculated airborne mass equals the evaporated mass in Table 6-1.
Surface Temperature	41.7°C	Based on highest average daytime temperature (107°F = 41.7°C) from Figure 6-1
	29°C	Based on nighttime average low temperature corresponding to the highest daytime temperature period, from Figure 6-1 (29°C = 84°F)
Atmospheric Pressure	760 mm Hg	Default sea level
Surface Code	CON	Concrete is worst case as compared to gravel or other surface
Release Duration	120 minutes	Corresponds to time for cleaning up the spill

Table 6-2. D2PC Dispersion Control Characteristics for Evaporative Release

Control Characteristic	Input Values Used	Rationale
FMW, FMV, VAP, BPT	DIPA: 101, 140.3, 0.214 (0.123), 355	• FMW = molecular weight • FMV = molecular volume (FMW/density in g/cm^3) [a] • VAP = vapor pressure in terms of partial pressure (mm Hg) at 41.7°C. (Value in parenthesis is for 29°C) • BPT = boiling point (K) [a]
	Disulfide: 320, 400, 2.09×10^{-9} (2.09×10^{-9}), 726	
IMA	1	Method of assessment control
NCI	2	Number of concentrations of interest
CI	VX: 0.0001 0.00033	30-minute and 2-hour AEGL-1 (for VX/PAC-1 concentrations in ascending order
	DIPA: 31 78.1	
	Disulfide: 48 121	

Notes:

a Density and boiling point data were obtained from the following sources:
- Taminco. 2019. *Diisopropylamine.* Safety Data Sheet. Revision 1.3. August.
- Boiling point for disulfide derived from structural formula based on www.chemeo.com/cid/17-687-1/Bis%28diiospropylaminoethyl%29disulfide
- Specific gravity of disulfide estimated as 0.8 due to its presence in the hydrolysate upper layer

AEGL Acute Exposure Guideline Level
DIPA diisopropylamine
Disulfide bis(2-diisopropylaminoethyl) disulfide
g/cm^3 grams per cubic centimeter
K kelvin
m/s meters per second
mg milligrams
mm Hg millimeters of mercury
PAC Protective Action Criteria
VX O-ethyl S-2-(diisopropylamino)ethyl methylphosphonothioate

Table 6-3. D2PC Modeling Results for 5,000-gallon Hydrolysate Spill

Chemical	Surface Temp. (°C)	Wind Speed (m/s)	Atmospheric Stability Factor	Mass Released (g)	2-hour AEGL-1/ PAC-1 Distance (m)	30-minute AEGL-1/ PAC-1 Distance (m)
VX	41.7	3.1	D (daytime)	2.27×10^{-5}	0	0
	29	3.1	F (nighttime)	6.65×10^{-6}	0	0
DIPA	41.7	3.1	D (daytime)	8.33×10^{4}	29	9
	29	3.1	F (nighttime)	5.0×10^{4}	29	7
Disulfide	41.7	3.1	D (daytime)	1.75×10^{-3}	0	0
	29	3.1	F (nighttime)	1.83×10^{-3}	0	0

Notes:

AEGL Acute Exposure Guideline Level
DIPA diisopropylamine
Disulfide bis(2-diisopropylaminoethyl) disulfide
g grams
m meters
m/s meters per second
PAC Protective Action Criteria
VX O-ethyl S-2-(diisopropylamino)ethyl methylphosphonothioate

6.2 Exposure via Vapor Inhalation from Fire

Fires occur in a small percentage of accidents involving hazmat releases. In the case of hydrolysate transport, the fire is unlikely to be sustained because the fuel source (truck fuel) would quickly deplete and the fire would be extinguished. If the spilled hydrolysate were subjected to a fire, assuming that separation of the layers occurs, the organic upper layer would catch on fire but would quickly extinguish because of the small quantity (approximately 1 percent of the spill mass). The remaining liquid would heat very slowly and would reach a maximum at the boiling point of water.

This TRA evaluates the following two cases as worst-case scenarios:

- Case 1: The hydrolysate remains in the tanker and the burning fuel heats up the hydrolysate to its boiling point.
- Case 2: The hydrolysate is spilled from the tanker and the burning fuel is intermixed with the spilled hydrolysate

6.2.1 Case 1

The pressure increase in the tanker is approximated using the following process. Water and NaOH comprise approximately 83.5 percent of the hydrolysate. DIPA is the only highly volatile chemical in the remaining organic mixture, and is present in approximately 0.5 weight percent. The partial pressure exerted by DIPA at this concentration would be negligible. Therefore, it is assumed that water vapor in the air space would be the dominant material exerting pressure in the tanker. Although water vapor does not behave like an ideal gas,[5] the ideal gas equations can still be used to approximately estimate pressure inside the tanker using Equation 7.

$$P_1/T_1 = P_2/T_2 \tag{7}$$

where:

P_1 = Initial pressure = 14.7 pounds per square inch absolute (psia) (atmospheric)
P_2 = Final pressure
T_1 = Initial temperature = 274 K (1°C, worst-case temperature of the tank contents)
T_2 = Final temperature = 382 K (109°C is the boiling point of water at an estimated higher pressure of 20 psia[6])

Solving for P_2 gives 20.5 psia. The pressure increase equals 5.8 psig (20.5 – 14.7).

The MAWP of a DOT-412 tanker is between 5 to 25 psig (see Section 3.2). The pressure relief valve activates at 1.5 times the MAWP. Based on the lower MAWP of 5 psig, the pressure relief valve would activate at 1.5 times 5 psig, or 7.5 psig. A worst-case pressure increase of 5.8 psig will not cause the pressure relief device to release any vapor.

6.2.2 Case 2

The standard fuel tank capacity for large trucks is between 120 and 150 gallons.[7] Long-haul trucks may carry a fuel tank on each side. It is not likely that this amount of fuel could be intermixed fully with the 5,000 gallons of spilled hydrolysate. Therefore, as a worst case, it is assumed that only half of the hydrolysate is exposed to the burning fuel. The other half will be subject only to evaporation. In addition, because of the small quantity, it is assumed that a fire will be 30 minutes in duration. The flammable organics in the top layer will catch on fire and be consumed. The other organics will be released into the fire. Based on the criteria used in the WebPuff dispersion model (WebPuff Version 5.4) for VX, it is estimated that 97.5 percent of the total organic mass released will be consumed, and only 2.5 percent will be released.

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5 https://chemistry.stackexchange.com/questions/103724/can-ideal-gas-law-be-applied-to-water-vapour
6 https://www.engineeringtoolbox.com/boiling-point-water-d_926.html
7 https://www.truckloadindexes.com/data-commentary/how-many-gallons-does-it-take-to-fill-up-a-big-rig

The burning fuel will float on top of the spilled hydrolysate due to its lower specific gravity. The temperature of the spilled hydrolysate will rise to 100°C. Therefore, the evaporative release is modeled at 100°C for the portion of the hydrolysate exposed to the fire. The other portion is modeled at the temperatures determined in Table 6-1 (41.7°C and 29°C). At a liquid temperature of 100°C, the evaporation model indicates that 100 percent of the highly volatile DIPA is released, even if present in a mixture rather than in a separate top layer. Therefore, in either case, all of the DIPA vapors will be released and will combust in the fire and be consumed to 97.5 percent.

Table 6-4 provides the results showing the evaporated masses of each constituent. Table 6-5 lists the D2PC input parameters used for the fire scenario. Table 6-6 provides the results of the fire and evaporation dispersion modeling.

Table 6-4. Calculated Mass of Chemical Released Based on 2,500-gallon Hydrolysate Spill

Liquid Temp. (°C)	Wind Speed (m/s)	VX (g)	DIPA (g)	Disulfide (g)
100 [a]	3.1	2.17×10^{-5}	1.39×10^{3}	1.85×10^{-5}
41.7	3.1	1.13×10^{-5}	4.17×10^{4}	8.77×10^{-4}
29	3.1	3.33×10^{-6}	2.5×10^{4}	9.14×10^{-4}

Notes:

a All masses for the 100°C (fire case) are adjusted to 2.5 percent of evaporated mass to account for consumption in the fire.

DIPA diisopropylamine
Disulfide bis(2-diisopropylaminoethyl) disulfide
g grams
m/s meters per second
VX O-ethyl S-2-(diisopropylamino)ethyl methylphosphonothioate

Table 6-5. D2PC Dispersion Control Characteristics for Fire Case 2 Scenario

Control Characteristic	Input Values Used	Rationale
Location	NDF	Not defined because location is not fixed
Height of Mixing Layer	400 meters	Daytime mixing layer based on average conditions for summer
	250 meters	Nighttime mixing layer height is lower than daytime. A lower mixing height results in a greater ground level concentration
Munition Type	NON	Non-munition for hydrolysate
Agent Type	VX	Agent VX
	NA	Non-agent chemical (for DIPA and disulfide)
Release Type	FIR	Fire
	EVP	Evaporation from an unconfined spill
Stability Type	D	D stability for worst-case daytime release
	F	F stability for worst-case nighttime release
Wind Speed	3.1 m/s	From Figure 6-2, corresponding to time of highest average temperature (7.0 miles per hour = 3.1 m/s)
Surface Temperature	41.7°C	Based on highest average daytime temperature (107°F = 41.7°C) from Figure 6-1
	29°C	Based on nighttime average temperature corresponding to the highest daytime temperature period, from Figure 6-1 (29°C = 84°F)
NQI, Q (mg), TQ (min)	Fire: 1, Q, 30	Number of source intervals = 1. Q = mass based on Table 6-4. Duration of release = 30 minutes due to limited quantity of fuel.
	Evaporation: 1, Q, 120	Number of source intervals = 1. Q = iteratively determined such that the D2PC calculated airborne mass equals the evaporated mass in Table 6-4. Duration of release = 120 minutes.
Atmospheric Pressure	760 mm Hg	Default sea level
Surface Code	CON	Concrete is worst case as compared to gravel or other surface.
FMW, FMV, VAP, BPT	DIPA: 101, 140.3, 0.214 (0.123), 355	• FMW = molecular weight • FMV = molecular volume (FMW/density in g/cm^3) [a] • VAP = vapor pressure in terms of partial pressure (mm Hg) at 41.7°C. (Value in parenthesis is for 29°C.) • BPT = boiling point (K) [a]
	Disulfide: 320, 400, 2.09×10^{-9} (2.09×10^{-9}), 726	

Table 6-5. D2PC Dispersion Control Characteristics for Fire Case 2 Scenario

Control Characteristic	Input Values Used	Rationale
Output Control Code	1	Lists diffusion parameters in the output
Heat Released	238,846 cal/s (1 MW) [b]	A low heat release value results in lower plumes and, therefore, higher ground level concentrations.
Cloud Radius	Not applicable	Default
IMA	1	1 = Concentration (mg/m^3) for evaporation case 0 = Dosage (mg-min/m^3) for fire case
	0	
NCI	2	Number of concentrations of interest
NDI	2	Number of dosages of interest
CI	VX: 0.0001 0.00033	Concentrations for evaporation case: 30-minute and 2-hour AEGL-1 (for VX)/PAC-1 concentrations in ascending order
	DIPA: 31 78.1	
	Disulfide: 48 121	
DI	VX: 0.0048 0.0099	Dosages for fire case: Concentration × 30 min = mg-min/m^3
	DIPA: 930 2,343	
	Disulfide: 1,440 3,630	

Notes:

a Density and boiling point data were obtained from the following sources:
- Taminco. 2019. *Diisopropylamine.* Safety Data Sheet. Revision 1.3. August.
- Boiling point for disulfide derived from structural formula based on www.chemeo.com/cid/17-687-1/Bis%28diiospropylaminoethyl%29disulfide
- Specific gravity of disulfide estimated as 0.8 due to its presence in the hydrolysate upper layer

b A heat release rate of 1 megawatt (MW) was selected to represent a typical truck fire. Studies have shown that heat release rates could be over 100 MW depending on the type and amount of material being transported. (Reference: Lönnermark, A. and Ingason, H., 2004. "Recent Achievements Regarding Heat Release and Temperatures during Fires in Tunnels." *First International Symposium and Safe and Reliable Tunnels, Innovative European Achievements.* Prague, Czech Republic.) Choosing a lower heat release rate is conservative because it reduces the rise height of the buoyant plume.

AEGL	Acute Exposure Guideline Level
cal/s	calories per second
DIPA	diisopropylamine
Disulfide	bis(2-diisopropylaminoethyl) disulfide
g/cm^3	grams per cubic centimeter
K	kelvin
m/s	meters per second
mg	milligrams
mg-min/m^3	milligram-minutes per cubic meter
mg/m^3	milligrams per cubic meter
min	minutes
mm Hg	millimeters of mercury
PAC	Protective Action Criteria
VX	O-ethyl S-2-(diisopropylamino)ethyl methylphosphonothioate

Table 6-6. D2PC Modeling Results for Fire Case 2 Scenario

Chemical	Release	Surface Temp. (°C)	Wind Speed (m/s)	Atmospheric Stability Factor	Mass Released (g)	2-hour AEGL-1/ PAC-1 Distance (m)	30-minute AEGL-1/ PAC-1 Distance (m)
VX	Fire	41.7	3.1	D (daytime)	2.17×10^{-5}	0	0
	Fire	29	3.1	F (nighttime)	2.17×10^{-5}	0	0
	Evaporation	41.7	3.1	D (daytime)	1.13×10^{-5}	0	0
	Evaporation	29	3.1	F (nighttime)	3.33×10^{-6}	0	0
DIPA	Fire	41.7	3.1	D (daytime)	1.39×10^{3}	0	0
	Fire	29	3.1	F (nighttime)	1.39×10^{3}	0	0
	Evaporation	41.7	3.1	D (daytime)	4.17×10^{4}	19	6
	Evaporation	29	3.1	F (nighttime)	2.5×10^{4}	19	4
Disulfide	Fire	41.7	3.1	D (daytime)	1.85×10^{-5}	0	0
	Fire	29	3.1	F (nighttime)	1.85×10^{-5}	0	0
	Evaporation	41.7	3.1	D (daytime)	8.77×10^{-4}	0	0
	Evaporation	29	3.1	F (nighttime)	9.14×10^{-4}	0	0

Notes:

AEGL Acute Exposure Guideline Level
DIPA diisopropylamine
Disulfide bis(2-diisopropylaminoethyl) disulfide
g grams
m meters
m/s meters per second
PAC Protective Action Criteria
VX O-ethyl S-2-(diisopropylamino)ethyl methylphosphonothioate

The results indicate that, for the fire scenario, the chemical concentration does not reach the AEGL-1/PAC-1 at any distance due to the plume rise and atmospheric dispersion of the release. For the evaporation case, the hazard severity is *Negligible* (2-hour AEGL-1/PAC-1 is less than 200 meters and 30-minute AEGL-1/PAC-1 is less than 50 meters).

Based on the calculated results, the criteria shown in Table 4-3 for a *Negligible* hazard severity (2-hour AEGL-1/PAC-1 less than 200 meters and 30-minute AEGL-1/PAC-1 less than 50 meters) are met for both daytime and nighttime transport.

6.3 Exposure via Dermal Contact

Impacts of hydrolysate exposure from dermal contact are based on pH. The amount of NaOH present in the hydrolysate, as shown in Table 2-1, is 3.5 weight percent [$100 \times (3.5 \times 10^{-2})/1 = 3.5$]. According to National Institute for Occupational Safety and Health (NIOSH) Skin Profiles (2011), a 1 percent aqueous solution of NaOH has a pH of about 13. Concentrations equal to or greater than this are considered corrosive to the skin.

Impacts from a dermal exposure to a hydrolysate release have previously been evaluated, as summarized in the following:

- Zimmerman Transport Analysis – Mentions contact hazards (i.e., damage caused by physical contact with the process effluent), but does not elaborate further.

- Burke Transportation Safety Assessment– States that the hydrolysate is considered to be a DOT classified corrosive material due to the presence of NaOH (pH 12 – 14), and that it "presents no unique physical or chemical hazards as compared to other corrosive sodium hydroxide (lye) waste materials."

- CDC Off-Site VX Hydrolysate Treatment Review – Reviews Burke Transportation Safety Assessment and states, "the major potential human exposure pathway for the material is dermal contact that could result in severe, possibly irreversible, burns to the skin or eyes. Overall, the risk from an accidental spill appears to be compatible to that expected for any highly corrosive material with high pH."

- NECDF Transport Safety Plan – Acknowledges that the hydrolysate is a DOT Class 8 corrosive material and states that the hazard is similar in many ways to other corrosive materials shipped daily in the U.S. and throughout the world.

Individual drivers will be required to keep the following in their individual gear bags:

- NIOSH-approved respirator with organic vapor cartridges
- Safety goggles or glasses
- Steel-toed shoes
- Hard hats

In addition, the truck spill kits and driver safety equipment will include, among other equipment, the following items:

- Chemical-resistant gloves
- Chemical-resistant coveralls
- Chemical-resistant show covers or "booties"

In the event of a spill, the driver training and spill/safety equipment will reduce the probability or severity of any dermal exposure from a hydrolysate spill. Based on the statements in the previously referenced dermal-exposure evaluations, the drivers' training, and the availability of safety/spill equipment, the impact of dermal exposure will likely meet *Negligible* hazard severity in Table 4-2 of "one or more injuries or illnesses requiring first aid or medical treatment."

6.4 Aquatic Impacts

Impacts from a hydrolysate release to surface waters have previously been evaluated, as summarized in the following:

- Zimmerman Transport Analysis – "All the aforementioned degradation products [EMPA, MPA, thiolamine] are believed to be mobile in water due to their high solubilities. In the event of an accident during transport, spills of liquid effluent might reach surface waters; however, these highly soluble compounds would rapidly disperse to undetectable levels."

- Burke Transportation Safety Assessment – "As an environmental hazard, the NCH [Newport caustic hydrolysate] is again similar to sodium hydroxide or other caustic solutions. Vegetation may be burned due to the caustic nature. Spills into water may kill fish in the concentrated area due to the increase in pH until mixing has occurred. Sodium hydroxide solution is not classified as a marine pollutant by the U.S. Department of Transportation (DOT)."

- NECDF Transport Safety Plan – "In a worst-case scenario (small river at a low flow condition), the LC50 of 29 mg/L for thiolamine (primary source of toxicity) would be exceeded for no more than 7 hours. The 7 hour period is far shorter than the 96 hour exposure period typically used to determine the LC50 for fish. However, thiolamine will oxidize to the disulfide form when in contact with atmospheric oxygen, reducing the concentration of thiolamine to less than the LC50 in less than 7 hours. The disulfide is soluble in water and although its concentration may increase, it will not increase the duration of the toxicity period. After an instantaneous discharge into a river with a flow velocity of 1 meter per second, the length of river where fish and other biological entities would be killed or stressed could be up to 15 miles."

6.5 Risk Evaluation

The event frequencies given in Table 5-2 are on a per-shipment basis. In order to determine the total frequency and consequence of an accident or incident during hydrolysate transport from BGCAPP over the life of the transport operation, it is necessary to multiply each by the total number of planned shipments.

The number of shipments is determined by dividing the estimated VX hydrolysate to be shipped offsite (195,000 gallons) (Hullman 2020) by the tanker truck capacity. Tanker truck capacities for chemical transport are usually about 5,000 gallons. This capacity translates into 39 shipments.

Table 6-7 summarizes the results of the total frequencies and consequences. Table 6-8 summarizes the information from Table 6-7 in qualitative terms, in accordance with Tables 4-1, 4-2, and 4-3. For all scenarios, the consequence is considered to be *Negligible.* In accordance with the Qualitative Risk Evaluation Matrix (Figure 4-1), the results indicate that the risk level is *Low.*

Table 6-7. Total Frequencies and Consequence Results

Scenario	Total Frequency [a]	Consequence [b]
1 – Accident/Incident Release/Leak	5.34×10^{-3}	*Inhalation:* • 2-hour AEGL-1/PAC-1 hazard distance < secondary control zone distance of 200 meters • 30-minute AEGL-1/PAC-1 hazard distance < initial isolation zone distance of 50 meters *Dermal:* One or more injuries or illnesses requiring first aid or medical treatment
2 – Accident with Fuel Release and Fire	7.89×10^{-5}	*Inhalation:* • 2-hour AEGL-1/PAC-1 hazard distance < secondary control zone distance of 200 meters • 30-minute AEGL-1/PAC-1 hazard distance < initial isolation zone distance of 50 meters

Notes:

a Results are based on 39 shipments multiplied by the frequencies in Table 5-2.
b The concentration of VX and relevant chemicals does not reach the 30-minute/2-hour AEGL-1/PAC-1 concentrations at 50/200 meters, respectively.

AEGL Acute Exposure Guideline Level
PAC Protective Action Criteria

Table 6-8. Risk Level Determination

Scenario	Frequency	Consequence	Risk
1 – Accident/Incident Release/Leak	C – Occasional	IV – Negligible	Low
2 – Accident with Fuel Release and Fire	D – Seldom or Remote	IV – Negligible	Low

7 RISK MITIGATION

The authority for acceptance of the risk lies with the BGCAPP Site Project Manager, and any risk mitigation efforts or required actions will be determined by the BGCAPP Site Project Manager.

8 SUMMARY AND CONCLUSIONS

An evaluation of the risk of transporting treated VX hydrolysate from BGCAPP to a TSDF was conducted. The regulations for hazmat classification, handling, loading, and transport were reviewed for safe transport of the hydrolysate in tanker trucks. A TRA was conducted for the BGCAPP VX hydrolysate using the Army approach by determining accident frequency and event consequences for (1) an accident/incident with a release/leak and (2) an accident with a release and a fuel fire. Overall, the results indicate that the transportation risk is *Low.*

APPENDIX A. ABBREVIATIONS

AEGL	Acute Exposure Guideline Level
atm	standard atmosphere
BGCAPP	Blue Grass Chemical Agent-Destruction Pilot Plant
CDC	Centers for Disease Control and Prevention
CDL	commercial driver's license
CFR	Code of Federal Regulations
cm^2/s	square centimeters per second
DA PAM	Department of the Army Pamphlet
DIPA	diisopropylamine
DOT	Department of Transportation
EA-2192	S-2-(diisopropylaminoethyl) methylphosphonothioic acid
EMPA	ethyl methylphosphonic acid
FR	Federal Register
g/cm^3	grams per cubic centimeter
g/cm-s	grams per centimeter second
$g/s\ m^2$	grams per second-square meter
hazmat	hazardous material
HAZWOPER	Hazardous Waste Operations and Emergency Response
HSS	Hydrolysate Storage System
K	kelvin
MAWP	maximum allowable working pressure
mm Hg	millimeters of mercury
MPA	methylphosphonic acid
NaOH	sodium hydroxide
NECDF	Newport Chemical Agent Disposal Facility
NIOSH	National Institute for Occupational Safety and Health
NMR	nuclear magnetic resonance
OSHA	Occupational Safety and Health Administration
PAC	Protective Action Criteria
psia	pounds per square inch absolute
psig	pounds per square inch gauge
QRA	quantitative risk assessment
SCWO	supercritical water oxidation
TEEL	Temporary Emergency Exposure Limit
thiolamine	diisopropyl ethyl mercaptoamine
TRA	transportation risk assessment
TSDF	treatment, storage, and disposal facility
VX	O-ethyl S-2-(diisopropylamino)ethyl methylphosphonothioate

APPENDIX B. REFERENCES AND SOURCE MATERIALS

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APPENDIX C. DERIVATION OF 2-HOUR AND 30-MINUTE PROTECTIVE ACTION CRITERIA (PAC) CONCENTRATIONS

PAC concentrations for chemicals are established for a duration of 1 hour.[8] For this transportation risk assessment (TRA), PAC concentrations were needed for two exposure durations: 30 minutes and 2 hours.

Data for chemical toxicity of hazardous compounds often can be plotted using an equation (NRC 2003) of the following form:

$$C^n t = k \tag{C-1}$$

where:

- C = concentration for an observed toxic endpoint
- t = exposure duration (minutes)
- n = exponent determined based on the toxicity data
- k = constant

The approach outlined in this appendix is consistent with the default approach used in Acute Exposure Guideline Level (AEGL) and Temporary Emergency Exposure Limit (TEEL) development.

Assumption: $C^n t$ = constant, where n=1 for times greater than 1 hour and n=3 for times less than 1 hour (conservative).

The *n* values for many vapors and gases are derived from experimentally determined miosis and lethality data, and range from 0.8 to 3.5 (NRC 2003). For example, for chemical agents, the *n* value derived is 2 for extrapolation to a time less than 1 hour. Using a higher *n* value is conservative as it results in a lower derived concentration. Therefore, this TRA uses an *n* value of 3 for the derivation of the 30-minute concentration.

Table C-1 shows the calculated values of $C^n t$ for both cases for diisopropylamine (DIPA). As an example, $k = (62)^3 \times 60 = 1.43 \times 10^7$.

[8] https://www.energy.gov/ehss/protective-action-criteria-pac-aegls-erpgs-teels

Table C-1. Calculation of the Constant k for DIPA

Calculation Expression	PAC-1 (mg/m^3)	PAC-2 (mg/m^3)	PAC-3 (mg/m^3)
Established 1-hour PAC value [a]	62	702	4,131
$k = C^n t$ (n=3)	1.43×10^7	2.08×10^{10}	4.23×10^{12}
$k = C^n t$ (n=1)	3,720	42,120	247,860

Notes:

a Established values from https://www.energy.gov/ehss/protective-action-criteria-pac-aegls-erpgs-teels, converted from parts per million to mg/m^3.

mg/m^3 milligrams per cubic meter
PAC Protective Action Criteria

Using the calculated value of k, the PAC concentration for 30-minute exposure is:

$C = (k/t)^{(1/n)}$

As an example, $C = (1.43 \times 10^7 /30)^{(1/3)} = 78.1$.

Table C-2 shows the calculated 30-minute and 2-hour PAC values for DIPA.

Table C-2. Calculated 30-minute and 2-hour PAC Values for DIPA

Calculation Expression	30-minute Exposure Value (mg/m^3)			2-hour Exposure Value (mg/m^3)		
	PAC-1	PAC-2	PAC-3	PAC-1	PAC-2	PAC-3
$C= (k/t)^{(1/n)}$	78.1	884	5,205	31	351	2,066

Notes:

mg/m^3 milligrams per cubic meter
PAC Protective Action Criteria

Check if results match the k value:

$k = C^n t = 78.1^3 \times 30 = 1.43 \times 10^7$, which matches the value in Table C-1.

Similarly, Table C-3 summarizes the 30-minute and 2-hour PAC values for bis(2-diisopropylaminoethyl) disulfide (disulfide).

Table C-3. Calculated 30-minute and 2-hour PAC Values for Disulfide

Established 1-hour Exposure Value [a] (mg/m^3)			Calculated 30-minute Exposure Value (mg/m^3)			Calculated 2-hour Exposure Value (mg/m^3)		
PAC-1	PAC-2	PAC-3	PAC-1	PAC-2	PAC-3	PAC-1	PAC-2	PAC-3
96.04	1,087	6,399	121	1,370	8,062	48	544	3,200

Notes:

a For disulfide, established 1-hour PAC values were not available; therefore, PAC values were estimated based on the ratio of the RfCs of disulfide over DIPA times the PAC value. PAC-2 and PAC-3 values were based on the ratio of DIPA PAC-2 over PAC-1 and DIPA PAC-3 over PAC-1:

- PAC-1 = Disulfide RfC/DIPA RfC x DIPA PAC-1 = 7.9/5.1 x 62 = 96.04 mg/m^3
- PAC-2 = DIPA PAC-2/PAC-1 x Disulfide PAC-1 = 680/62 x 96.04 = 1,087 mg/m^3
- PAC-3 = DIPA PAC-3/PAC-1 x Disulfide PAC-1 = 4,100/62 x 96.04 = 6,399 mg/m^3

RfC data from Munro, N.B., S.S. Talmage, G.D. Griffin, L.C. Waters, A.P. Watson, J.F. King, and V. Hauschild. 1999. "The Sources, Fate, and Toxicity of Chemical Warfare Agent Degradation Products." *Environmental Health Perspectives* 107 (12), 933–974. https://doi.org/10.1289/ehp.99107933.

DIPA diisopropylamine
mg/m^3 milligrams per cubic meter
PAC Protective Action Criteria
RfC Reference Concentration