Let's Take A PEEK at the PEAC Software

PEAC Example–Mustard

by S. Bruce King

This month our example is Mustard also called H, HD (distilled mustard, very pure), or Sulfur Mustard. The chemical name is Bis-(2-chloroethyl)sulfide. This is one of the blister agents; it is yellow to brown oily liquids with a slight garlic or mustard odor. Although volatility is low, vapors can reach hazardous levels during warm weather. Sulfur mustards are absorbed by the skin, causing erythema and blisters. Ocular exposure to these agents may cause incapacitating damage to the cornea and conjunctiva. Inhalation damages the respiratory tract epithelium and may cause death. Its chemical formula is $C_4H_8Cl_2S$, which corresponds to a molecular weight of 159. Mustard has a vapor density greater than air (5.5), so any vapors are going to seek low spots. Mustard has a United Nations # of 2810 and a Chemical Abstract Service # of 505-60-2.

At standard conditions of sea level and 68°F, the chemical has a vapor pressure of 0.072 mm of Mercury, which is equivalent to 0.000095 atmospheres. With a melting point of 58°F and a boiling point of 419°F, it is typically found as a liquid. As with all the chemical warfare agents, the material is extremely toxic. Currently NIOSH has not established an IDLH value but the DOD has established a 30-minute AEGL 2 (acute exposure guideline level 2 defined as irreversible or other serious, long-lasting effects or impaired ability to escape) of 0.03 mg/m^3, which is roughly equivalent to 0.005 ppm. When compared to hazardous substances such as chlorine (IDLH=10 ppm) or Phosgene (IDLH=2 ppm), we can see that Mustard is indeed a very dangerous material and must be handled with a great deal of respect. AristaTek has elected to display the IDLH as 0.003 mg/m^3, which is the same as the TWA in the PEAC-WMD application.

For those instances where the **LOC** is reported as mg/m^3, to convert to ppm, the following equation holds at low concentrations.

$$LOC_{\text{concentration in ppm}} = (LOC_{\text{concentration in mg/m3}} * 24.45)/(\text{molecular weight})$$

Mustard (H) is not your everyday typical industrial chemical; it actually has only one purpose, to be used as a chemical warfare agent. The USA has signed the "Convention on the Prohibition of the Development, Production, Stockpiling and Use of Chemical Weapons and on their Destruction" (Chemical Weapons Convention or CWC). The treaty lists three different schedules of chemicals, with the "recognized" chemical warfare agents, e.g., Sarin, VX, Soman, Mustard, making up the Schedule 1 list. It is **illegal** to possess Mustard and/or manufacture the chemical. It would therefore be expected that Mustard would be encountered in one of two instances: (1) as a munitions device stolen from the United States Military (highly improbable since these materials and their associated devices are under strict security whether in storage or transport for destruction), or (2) in the possession of a terrorist group that has smuggled the chemical into the country or manufactured the material in a clandestine laboratory.

People whose skin or clothing is contaminated with sulfur mustard can contaminate rescuers by direct contact or through off-gassing vapor.

Description: Sulfur mustards are vesicants and alkylating agents. They are colorless when pure but are typically a yellow to brown oily substance with a slight garlic or mustard odor. H contains about 20 to 30% impurities (mostly sulfur); distilled mustard is known as HD and is nearly pure; HT is a mixture of 60% HD and 40% agent T (a closely related vesicant with a lower freezing point). Sulfur mustards evaporate slowly. They are very sparingly soluble in water but are soluble in oils, fats, and organic solvents. They are stable at ambient temperatures but decompose at temperatures greater than 149°C.

Sources/Uses: Sulfur mustards were first developed in the early-to-mid-1800s and were introduced as chemical warfare agents in 1917 during World War I. They have been used extensively in chemical warfare and remain a major threat. More than a dozen countries have sulfur mustard in their chemical arsenals. Destruction of U.S. stockpiles of chemical agents, including sulfur mustards, was mandated by the CWC to take place before April 2007.

Synonyms for Mustard, H and HD are Bis(2-chloroethyl) sulfide; bis(beta-chloroethyl) sulfide; di-2-chloroethyl sulfide; 1-chloro-2(beta-chloroethylthio)ethane; 2,2'-dichloroethyl sulfide; sulfur mustard; Iprit; Kampstoff "Lost"; mustard gas; senfgas, S-yperite; yellow cross liquid; and yperite.

Routes of Exposure:

Inhalation Sulfur mustards are readily absorbed from the respiratory tract; injury develops slowly and intensifies over several days. The pure liquid is colorless and odorless. Agent grade material is yellow to dark brown or black and the odor is variously described as similar to burning garlic, horseradish, a characteristic sweetish odor, or a weak, sweet, agreeable odor. The odor of sulfur mustards **does not** provide adequate warning for detection. The LCt_{50} (the product of concentration times time that is lethal to 50% of the exposed population by inhalation) is approximately 1,500 mg-min/m^3. The vapors are heavier than air. When inhaled, these agents may cause systemic effects. The estimated Ct for airway injury is 100 to 200 mg-min/m^3.

Skin/Eye Contact Mustard vapor and liquid are absorbed through the eyes, skin, and mucous membranes. Clinical effects do not occur until hours after exposure. The median incapacitating dose for the vapor is 200 mg-min/m^3. A Ct of 12 to 70 mg-min/m^3 produces eye lesions. Direct contact with the liquid can cause skin and eye burns that develop an hour or more after exposure. A 10 µg droplet is capable of producing blisters. Skin, eye, and airway exposure to vapor sulfur mustard and skin and eye exposure to liquid mustard may cause systemic toxicity. The lethal dose is about 100 mg/kg or 1 to 1.5 teaspoons of liquid.

Ingestion Ingestion may cause local effects and systemic absorption.

Physical Properties:

Description: Colorless when pure but usually a pale yellow, dark brown or black oily liquid. The vapor is colorless.

Warning properties: Faint garlic or mustard odor (odor threshold 0.6 mg/m^3)

Molecular Weight: 159.08 daltons

Boiling Point: (760 mm Hg) 419°F

Melting Point: 58.1°F

Specific Gravity: 1.27 g/ml

Vapor Pressure: 0.072 mm Hg or 0.000095 atmospheres

Vapor Density: 5.4 50 5.5 (air = 1.0)

Flash Point: 221 °F

Incompatibilities: Sulfur mustards are rapidly corrosive to brass and steel at 149 °F (65 °C); they are destroyed by strong oxidizing agents. These agents hydrolyze to form hydrochloric acid (HCl) and thiodiglycol.

Health Effects:

Sulfur mustards are vesicants causing skin, eye, and respiratory tract injury. Although these agents cause cellular changes within minutes of contact, the onset of pain and other clinical effects are delayed for 1 to 24 hours.

Sulfur mustards are alkylating agents that may cause bone marrow suppression and neurologic and gastrointestinal toxicity.

Acute Exposure: Sulfur mustards are vesicants and alkylating agents; however, the biochemical mechanisms of action are not clearly understood. They are highly reactive and combine rapidly with proteins, DNA, or other molecules. Therefore, within minutes following exposure intact mustard or its reactive metabolites are not found in tissue or biological fluids. Sulfur mustards also have cholinergic activity, stimulating both muscarinic and nicotinic receptors. The onset of clinical symptoms and their time of onset depend on the severity of exposure (Table 1). The death rate from exposure to sulfur mustard is low (2 to 3% during World War I). Death usually occurs between the 5th and 10th day due to pulmonary insufficiency complicated by infection due to immune system compromise.

Ocular The eye is the most sensitive tissue to sulfur mustard effects. Sulfur mustard vapor or liquid may cause intense conjunctival and scleral pain, swelling, lacrimation, blepharospasm, and photophobia; however, these effects do not appear for an hour or more. Miosis due to cholinergic effects may occur. High concentrations of vapor or liquid can cause corneal edema, perforation, blindness, and later scarring.

Dermal Direct skin exposure to sulfur mustards causes erythema and blistering. Generally, a pruritic rash will develop within 4 to 8 hours followed by blistering 2 to 18 hours later. Contact with the vapor may result in first and second degree burns, while contact with the liquid typically produces second and third degree chemical burns. An area of burn covering 25% or more of the body surface area may be fatal.

Respiratory Dose-dependent inflammatory reactions in the upper and lower airway begin to develop several hours after exposure and progress over several days. Burning nasal pain, epistaxis, sinus pain, laryngitis, loss of taste and smell, cough, wheezing, and dyspnea may occur. Necrosis of respiratory epithelium can cause pseudomembrane formation and local airway obstruction.

Gastrointestinal Ingestion may cause chemical burns of the GI tract and cholinergic stimulation. Nausea and vomiting may occur following ingestion or inhalation. Early nausea and vomiting is usually transient and not severe. Nausea, vomiting, and diarrhea occurring several days after exposure indicates damage to the GI tract and thus is a poor prognostic sign.

CNS High doses of sulfur mustards can cause hyperexcitability, convulsions, and insomnia.

Hematopoietic Systemic absorption of sulfur mustard may induce bone marrow suppression and an increased risk for fatal complicating infections, hemorrhage, and anemia.

Delayed Effects Years after apparent healing of severe eye lesions, relapsing keratitis or keratopathy may develop.

Potential Sequelae Persistent eye conditions, loss of taste and smell, and chronic respiratory illness including asthmatic bronchitis, recurrent respiratory infections, and lung fibrosis may persist following exposure to sulfur mustards.

Table 1. Clinical Effects and Time of Onset by Severity of Exposure to Sulfur Mustard

Tissue	Severity of Exposure	Clinical effects	Time to first effect
Eyes	Mild	Tearing, itching, burning, gritty feeling	4-12 hours
	Moderate	Above effects and reddening, lid edema, moderate pain	3-6 hours
	Severe	Marked lid edema, possible corneal damage, severe pain	1-2 hours
Airways	Mild	Rhinorrhea, sneezing, epistaxis, hoarseness, hacking cough	6-24 hours
	Severe	Above effects and productive cough, mild to severe dyspnea	2-6 hours
Skin	Mild	Erythema	2-24 hours
	Severe	Erythema and vesication	2-24 hours

Chronic Exposure: Prolonged or repeated acute exposure to sulfur mustards may cause cutaneous sensitization and chronic respiratory disease. Repeated exposures result in cumulative effects because mustards are not naturally detoxified by the body.

Carcinogenicity The International Agency for Research on Cancer (IARC) has classified sulfur mustard as carcinogenic to humans (Group 1). Epidemiological evidence indicates that repeated exposures to sulfur mustard may lead to cancers of the upper airways.

Reproductive and Developmental Effects There is limited evidence that repeated exposures to sulfur mustards may cause defective spermatogenesis years after exposure. Sulfur mustard has been implicated as a potential developmental toxicant because of its similarity to nitrogen mustard; however, data are inconclusive.

Decontamination:

Patients/Victims: Remove clothes and place contaminated clothes and personal belongings in a sealed double bag. Decontamination of mustard-exposed victims by either vapor or liquid should be performed within the first two minutes following the exposure to prevent tissue damage. If not accomplished within the first several minutes, decontamination should still be performed to ensure any residual liquid mustard is removed from the skin or clothes or to ensure any trapped mustard vapor is removed with the clothing. Removing trapped mustard vapor will prevent vapor off-gassing or subsequent cross-contamination of other emergency responders/health care providers or the healthcare facility. Physical removal of the mustard agent, rather than detoxification or neutralization, is the most important principle in patient decontamination. Mustard is not detoxified by water alone and will remain in decontamination effluent (in dilute concentrations) if hydrolysis has not taken place.

(1) Patients exposed to vapor should be decontaminated by removing all clothing in a clean air environment and shampooing or rinsing the hair to prevent vapor off-gassing.

(2) Patients exposed to liquid should be decontaminated by –

a. Washing in warm or hot water at least three times. Use liquid soap (dispose of container after use and replace), large volumes of water, and mild to moderate friction with a single-use sponge or washcloth in the first and second washes. Scrubbing of exposed skin with a brush is discouraged, because skin damage may occur which may enhance absorption. The third wash should be to rinse with large amounts of warm or hot water. Shampoo can be used to wash the hair. The rapid physical removal of a chemical agent is essential. If warm or hot water is not available, but cold water is, use cold water. Do not delay decontamination to obtain warm water.

b. Rinsing the eyes, mucous membranes, or open wounds with sterile saline or water.

(3) The healthcare provider should –

a. Check the casualty after the three washes to verify adequate decontamination before allowing entry to the medical treatment facility. If the washes were inadequate, repeat the entire process.

b. Be prepared to stabilize conventional injuries during the decontamination process. Careful decontamination can be a time consuming process. The health care provider may have to enter the contaminated area to treat the casualty during this process. Medical personnel should wear the proper PPE and evaluate the exposed workers.

In using the PEAC application we access information for the chemical by first locating Mustard or H or HD in the database. The following figures show the screens displayed for chemical properties, Figure 1 for the *PEAC-WMD for Windows* application and Figure 2-4 for the *PEAC-WMD for the Pocket PC* application.

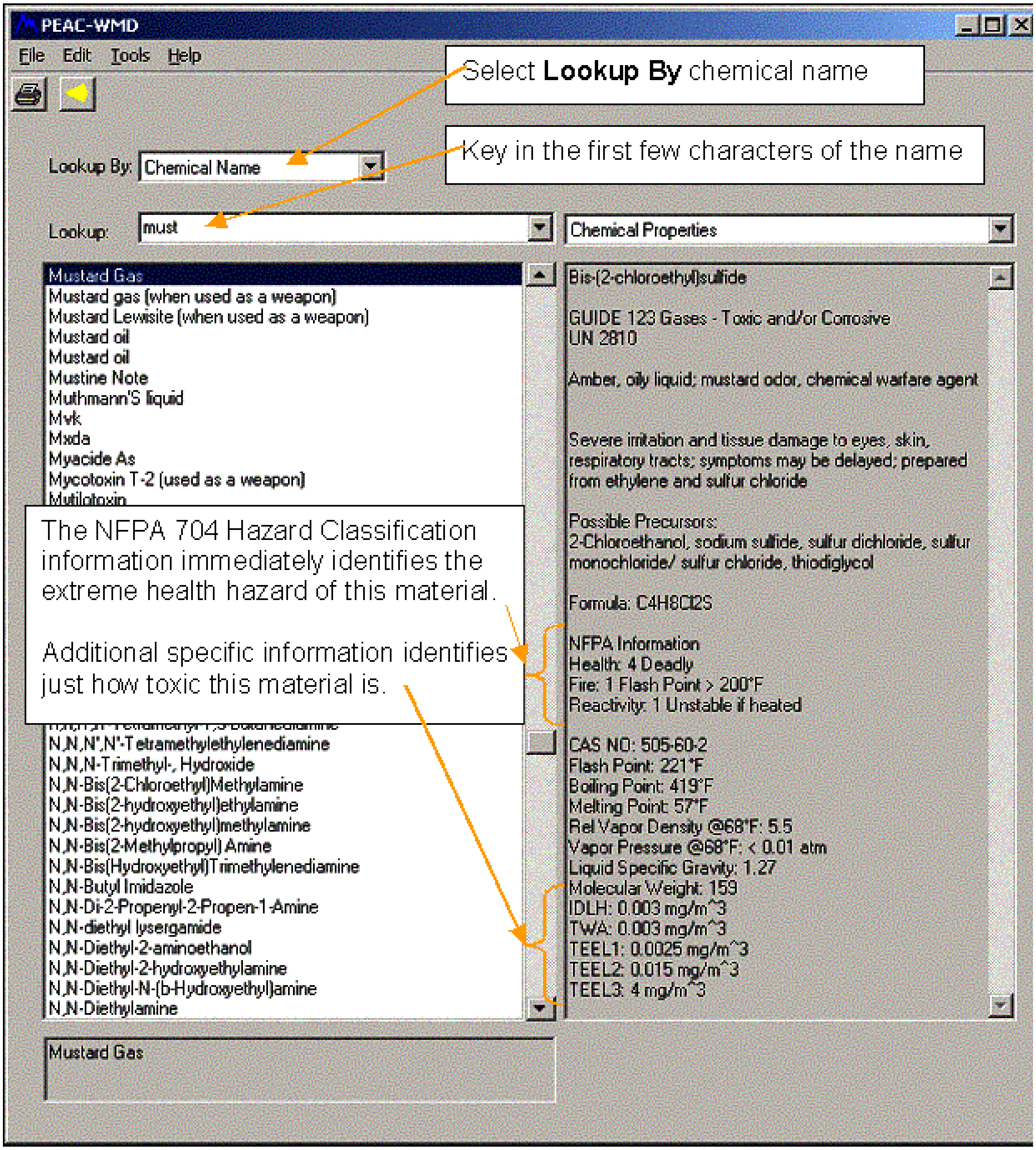

Figure 1 - Using the Lookup By: Name for Mustard using the PEAC-WMD for Windows application

Review of the information displayed in the chemical properties screen whether in Figure 1 (above) or Figures 2-4 (below), show chemical properties values discussed earlier at the top of this discussion. In addition, other values are provided such as the TEELs (Temporary Emergency Exposure Limit) published by Department of Energy.

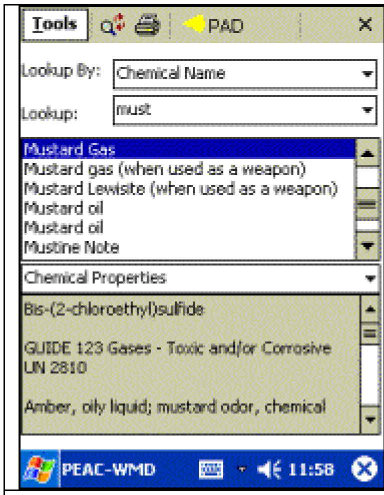

Figure 2 – Selecting Mustard using the PEAC-WMD for Pocket PC application

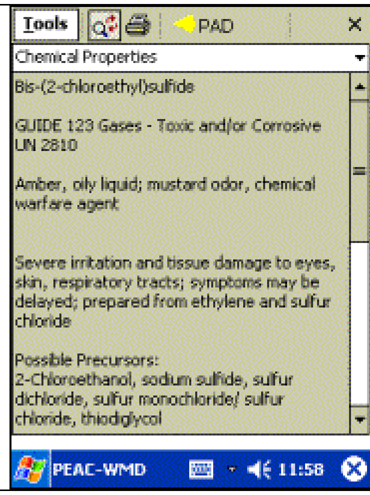

Figure 3 – The top portion of the Chemical Properties Data Display Screen

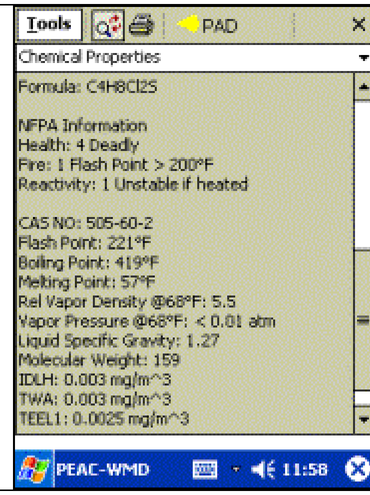

Figure 4 – The bottom portion of the Chemical Properties Data Display Screen

Additional information is available regarding how to prevent skin contact by checking the CPC listing, i.e., **Chemical Protective Clothing**.

An advantage of using the PEAC tool is assistance in the development of an evacuation zone for those chemicals that produce a toxic vapor cloud. Mustard has a very low vapor pressure (0.072 mm Hg), so if a small amount is spilled and forms a puddle, the amount of vapor released is very minimal. Why then is there so much concern with the chemical warfare agents, e.g., Mustard, Tabun, Soman, VX, Lewisite, and Mustard Gas, all of which have very low vapor pressures at standard conditions? The answer has two parts. First, as already discussed above for Mustard, these hazardous substances are very toxic, on the order of 100 or 1,000 times more toxic than the most toxic industrial chemicals. Secondly, if they are released under conditions where more than just a pool or puddle is created, the effect of their low vapor pressure can be overcome. When released as a weapon, e.g., using an explosive charge or atomizer to create an aerosol or tiny droplets, the effective liquid surface area of the resulting released agent is increased several orders of magnitude. This increase in effective surface area increases not only the resulting vapor content in the air to be inhaled by victims; it also increases the opportunity for skin contact and the resulting exposure by victims.

As with all of our examples, AristaTek creates a scenario for a spill or release of the specific chemical and then we work through the development of a PAD (Protective Action Distance) to demonstrate how the PEAC system works. For our scenario using Mustard as the spilled chemical we'll use Coors Baseball Field in Denver as the location and the time as 2:30 PM on June 18th. A small container (estimated at 2-3 quarts in size) with Mustard is released using an explosive charge. The temperature is about 80°F, the winds are 2 mph, and it's a clear day (no clouds).

As seen at the top of the data display screens, there is a yellow icon displayed, this is the PEAC icon for notifying the user that a Protective Action Distance can be calculated. Clicking or tapping on the PAD icon will display a screen as shown in Figure 5. Following through the screens, we provide information on the Meteorology, Container Size, and Type of Release (Source). The last screen displays the PAD based on the provided information.

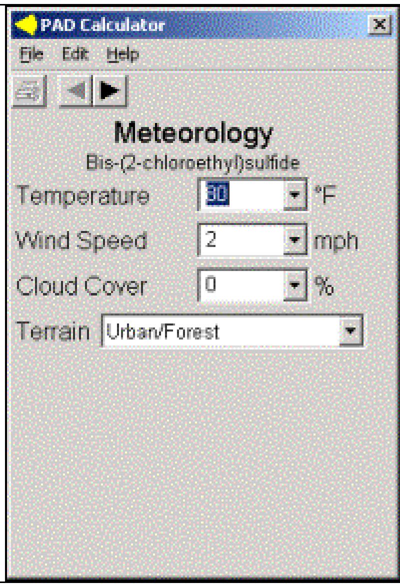	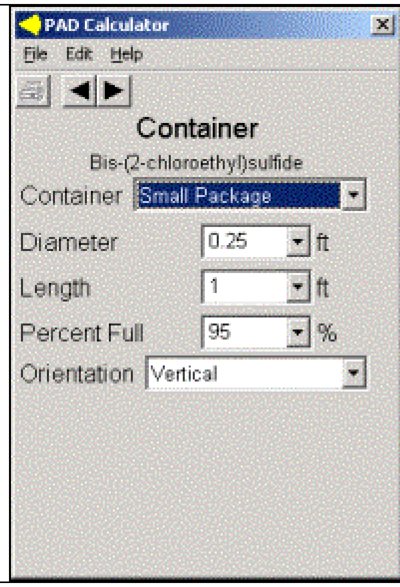	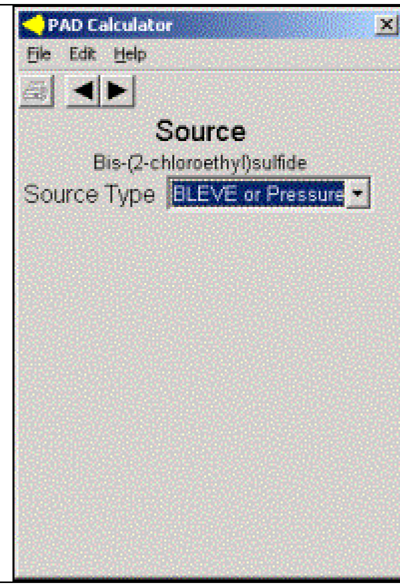
Meteorology It’s Denver in June and the temperature about 80°, light wind is set for 2 mph, clear sky so we’ll set cloud cover to 0%, and the terrain is Urban/Forest since it’s an urban setting (stadium).	**Container** We have selected from our list of container sizes the **Small Package** selection. This provides us with a default size that should get us pretty close to the actual size.	**Source** Since the scenario has Mustard released with an explosive charge, we’ve selected a **BLEVE or Pressure Explosion** as the **Source** type of release.

Figure 5 – Calculating a PAD using the PEAC System

After specifying the release or source is a BLEVE or Pressure Explosion, the user taps the right arrow at the top of the screen and the PAD computation results are displayed, see Figure 6.

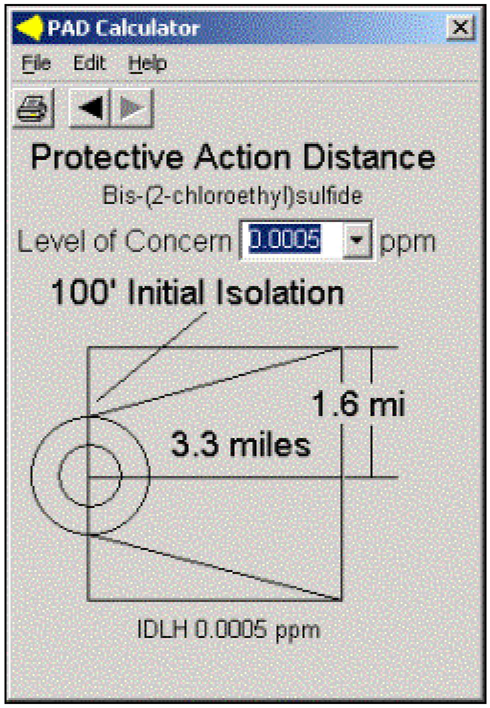

Figure 6 - The PEAC computation for PAD using the IDLH

Since the IDLH and TWA are both listed as 0.003 mg/m^3, the user may also want to calculate a PAD based on a different concentration, e.g., the DOD AEGL 2 discussed earlier which was 0.03 mg/m^3 or ~0.005 ppm. Entering the desired value in the Level of Concern entry field does this. The PEAC-WMD application will recalculate a PAD distance and display the value, as shown in Figure 7.

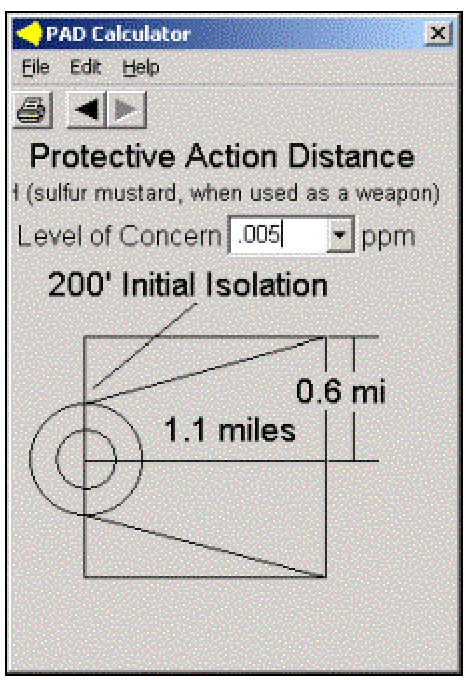

Figure 7 – PAD recalculated using the DOD AEGL 2 value of ~0.005 ppm

Portions of this discussion on Mustard were adapted from the ATSDR Medical Management Guideline document for blister agents, which can be downloaded from the ADSTR web site at: http://www.atsdr.cdc.gov/mmg.html. Additional information was adapted from the CDC web site: http://www.bt.cdc.gov/.