Let's Take A PEEK at the PEAC software

PEAC Example –Phosgene

by S. Bruce King

This month our example is Phosgene, which has a chemical formula of ($COCl_2$). Phosgene is listed under the UN # (United Nations Number) by the US Department of Transportation: UN 1076. Phosgene CAS# is: 75-44-5.

Persons exposed only to phosgene gas do not pose substantial risks of secondary contamination. Persons whose clothing or skin is contaminated with liquid phosgene (ambient temperature below 47 °F) can secondarily contaminate response personnel through direct contact or off-gassing vapor.

At room temperature, phosgene is a colorless, nonflammable gas with a suffocating odor like new mown hay. However, odor provides insufficient warning of hazardous concentrations. At high concentrations it is mildly irritating.

Below 47 °F, it is a colorless, fuming liquid; contact with the liquid can cause frostbite. In the presence of water (sweat, saliva, tears), the liquid or gas slowly hydrolyzes to hydrochloric acid, which can irritate and damage cells.

Phosgene is absorbed to some extent by the lungs, but not by intact skin. Systemic damage is usually a secondary result of anoxia caused by loss of lung function. It is corrosive to the lungs and intact skin.

Description Phosgene is a colorless, fuming liquid below 47 °F (8.2 °C) and a colorless, nonflammable gas above 47 °F. At low concentrations, its odor is similar to that of green corn or new mown hay; at high concentrations, its odor can be sharp and suffocating. Phosgene is slightly soluble in water and is hydrolyzed slowly by moisture to form hydrochloric acid. It is soluble in most liquid hydrocarbons. It is shipped as a liquefied, compressed gas. Large quantities of phosgene should be stored in a dry, cool, well-ventilated, and fireproof room. Phosgene is a combustion product of many household products that contain volatile organochlorine compounds. Therefore, it may contribute to the hazards of smoke inhalation in fire victims and firefighters.

Sources/Uses Phosgene is produced commercially by chlorinating carbon monoxide. It is a combustion or decomposition by-product of most volatile chlorinated compounds; therefore, household substances such as certain solvents, paint removers, and dry-cleaning fluids can produce phosgene when exposed to heat or fire. Phosgene may also be produced during the welding of metal parts that have been cleaned with chlorinated hydrocarbons. Phosgene is used as an intermediate in the manufacture of many chemicals including isocyanates, polyurethane, polycarbonates, dyes, pesticides, and pharmaceuticals.

Physical Properties:

Description: Colorless gas with musty odor at room temperature; a fuming liquid below 47°F (8°C).

Warning properties: Detectable odor following brief emergency releases; odor threshold 0.4 to 1.5 ppm; slightly irritating in high concentration. **Odor provides inadequate warning of harmful concentrations**.

Molecular weight: 98.9 daltons

Boiling point: (760 mm Hg): 47 °F (8 °C)

Freezing point: -198 °F (-127 °C)

Specific gravity: 1.43 (liquid at 32 °F)

Vapor pressure: 1,215 mm Hg at 68 °F (20 °C)

Gas density: 3.48 (air = 1)

Water solubility: Slight

Flammability: Nonflammable gas

Synonyms: carbonic acid dichloride, carbonic dichloride, carbon oxychloride, carbonyl chloride, and chloroformyl chloride.

Standards and Guidelines: OSHA PEL (permissible exposure limit) = 0.1 ppm (averaged over a 8-hour workshift)

NIOSH IDLH (immediately dangerous to life or health) = 2 ppm

AIHA ERPG-2 (emergency response planning guideline) (maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to 1 hour without experiencing or developing irreversible or other serious health effects or symptoms which could impair an individual's ability to take protective action) = 0.2 ppm

Incompatibilities: Phosgene reacts with moisture (water or alcohols). In water, it slowly decomposes to hydrochloric acid and carbon dioxide. When heated to decomposition, it will produce toxic and corrosive fumes. Phosgene reacts violently with various chemicals (e.g., alkalis, ammonia, amines, copper, aluminum); it attacks many metals in the presence of water and can also attack plastic and rubber.

Routes of Exposure:

Inhalation Inhalation is the major route of phosgene exposure. The odor threshold for phosgene is 5 times higher than the OSHA PEL. **Thus, odor provides insufficient warning of hazardous concentrations**. Phosgene's irritating quality can be mild and delayed, which may result in a lack of avoidance leading to exposure for prolonged periods. Phosgene is heavier than air and may cause asphyxiation in poorly ventilated, low-lying, or enclosed spaces.

Children exposed to the same levels of phosgene gas as adults may receive larger doses because they have greater lung surface area:body weight ratios and increased minute volumes:weight ratios. In addition, they may be exposed to higher levels than adults in the same location because of their short stature and the higher levels of phosgene gas found nearer to the ground.

Skin/Eye Contact When phosgene gas contacts moist or wet skin, it may cause irritation and erythema. High airborne concentrations can also cause corneal inflammation and opacification. Direct contact with liquid phosgene under pressure can cause frostbite as well as severe irritation and corrosive effects.

Children are more vulnerable to toxicants affecting the skin because of their relatively larger surface area:body weight ratio.

Ingestion Ingestion of phosgene is unlikely because it is a gas at room temperature.

Health Effects

Phosgene is an irritant to the skin, eyes, and respiratory tract; there may be minimal irritation immediately after exposure, but delayed damage may be severe.

Common initial symptoms include mild irritation of the eyes and throat, with some coughing, choking, feeling of tightness in the chest, nausea and occasional vomiting, headache, and lacrimation.

Phosgene poisoning may cause respiratory and cardiovascular failure, which results from low plasma volume, increased hemoglobin concentration, low blood pressure, and an accumulation of fluid in the lungs. Secondary systemic damage is the result of anoxia.

Acute Exposure Phosgene directly reacts with amine, sulfhydryl, and alcohol groups in cells, thereby adversely affecting cell macromolecules and cell metabolism. Direct toxicity to the cells leads to an increase in capillary permeability, resulting in large shifts of body fluid, decreasing plasma volume. In addition, when phosgene hydrolyzes, it forms hydrochloric acid, which can also damage surface cells and cause cell death in the alveoli and bronchioles. Hydrochloric acid release into the mucosa triggers a systemic inflammatory response. Phosgene stimulates the synthesis of lipoxygenase-derived leukotrienes, which attract neutrophils and causes their massive accumulation in the lungs; this contributes to the development of pulmonary edema. Following phosgene exposure, a patient may be free of symptoms for 30 minutes to 48 hours before respiratory damage becomes evident; the more severe the exposure, the shorter the latency. If the initial concentration of phosgene was high, rapid onset of direct cytotoxicity and enzymatic poisoning may ensue. Because phosgene is not very water soluble and hydrolysis tends to be slow, victims inhaling low concentrations of the gas may experience no irritation or only mild irritation of the upper airway. Lack of irritation allows victims to inhale the gas more deeply into the lungs and for prolonged periods.

Children do not always respond to chemicals in the same way that adults do. Different protocols for managing their care may be needed.

Respiratory Inhaling low concentrations of phosgene may cause no signs or symptoms initially, or symptoms may be due only to mild irritation of the airways; these symptoms (dryness and burning of the throat and cough) may cease when the patient is removed from exposure.

However, after an asymptomatic interval of 30 minutes to 48 hours, in those developing severe pulmonary damage, progressive pulmonary edema develops rapidly with shallow rapid respiration, cyanosis, and a painful paroxysmal cough producing large amounts of frothy white or yellowish liquid. Inadequate, labored respiration, during which abnormal chest sounds are evident, may be accompanied by increased distress and apprehension. Insufficient oxygenation of arterial blood, and massive accumulation of fluid in the lungs may be accompanied by cardiovascular and hematological signs.

Exposure to phosgene has been reported to result in Reactive Airway Dysfunction Syndrome (RADS), a chemically- or irritant-induced type of asthma.

Children may be more vulnerable to corrosive agents than adults because of the relatively smaller diameter of their airways. Children may also be more vulnerable because of increased minute ventilation per kg and failure to evacuate an area promptly when exposed.

Previously exposed persons may develop inflammation of the lungs when reexposed to extremely low levels of Phosgene. Flu-like symptoms such as fever, malaise, shortness of breath, and cough can develop 4 to 6 hours after exposure and persist for 12 hours or longer. Chest x-rays may indicate lung changes.

In sensitized individuals, asthmatic attacks can occur after exposure to extremely low Phosgene air concentrations (0.0001 ppm). Asthmatic reactions can be immediate, delayed (4 to 8 hours), or both.

Exposure to Phosgene can lead to Reactive Airway Dysfunction Syndrome (RADS), a chemically- or irritant-induced type of asthma.

Children may be more vulnerable because of relatively increased minute ventilation per kg and failure to evacuate an area promptly when exposed.

Cardiovascular Cardiovascular collapse may occur if the patient is severely hypovolemic and hypoxemic from accumulation of fluid in the lungs. Destruction of red blood cells in the pulmonary circulation can cause capillary plugging that leads to strain on the right side of the heart and death.

Dermal If the skin is wet or moist, contact with phosgene vapor can cause irritation and redness of the skin. Contact with liquid phosgene under pressure can result in frostbite. Because of their relatively larger surface area:body weight ratio, children are more vulnerable to toxicants affecting the skin.

Ocular High vapor concentrations cause tearing and increased presence of blood in the eye. Contact with liquid phosgene may result in clouding of the cornea and delayed perforation.

Hematologic In severe cases, phosgene may cause hemolysis that results in the plugging of pulmonary capillaries. Most hematologic changes (e.g., hemolysis, methemoglobinemia, bone marrow suppression, and anemia) can be detected by standard blood tests.

Hepatic In cases of high exposures, phosgene may be directly cytotoxic to the liver, causing necrosis and loss of function.

Renal In cases of high exposures, phosgene may be directly cytotoxic to the kidneys, causing necrosis and loss of function.

Gastrointestinal Nausea and vomiting may occur following exposure to phosgene.

Potential Sequelae If the patient survives the initial 48 hours after exposure, recovery is likely. Sensitivity to irritants may persist, causing bronchospasm and chronic inflammation of the bronchioles. Pulmonary tissue destruction and scarring may lead to chronic dilation of the bronchi, lobular emphysema, regions of atelectasis, and increased susceptibility to infection.

Exposure to phosgene has been reported to result in Reactive Airway Dysfunction Syndrome (RADS), a chemically- or irritantinduced type of asthma.

Chronic ExposureA group of workers who were exposed daily to high levels of phosgene showed an increase in mortality and morbidity from inflammation of the lungs, chronic inflammation of the bronchioles, destruction of alveoli, and impaired pulmonary function. Chronic exposures to low levels of phosgene may lead to chronic pneumonitis, which may resolve or lead to pulmonary edema.

Chronic exposure may be more serious for children because of their potential longer latency period.

Carcinogenicity Phosgene has not been classified for carcinogenic effects.

Reproductive and Developmental Effects No information was found pertaining to reproductive or developmental hazards caused by phosgene exposure. Phosgene is not included in *Reproductive and Developmental Toxicants,* a 1991 report published by the U.S. General Accounting Office (GAO) that lists 30 chemicals of concern because of widely acknowledged reproductive and developmental consequences.

In using the PEAC application we access information for the chemical by first locating Phosgene 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.

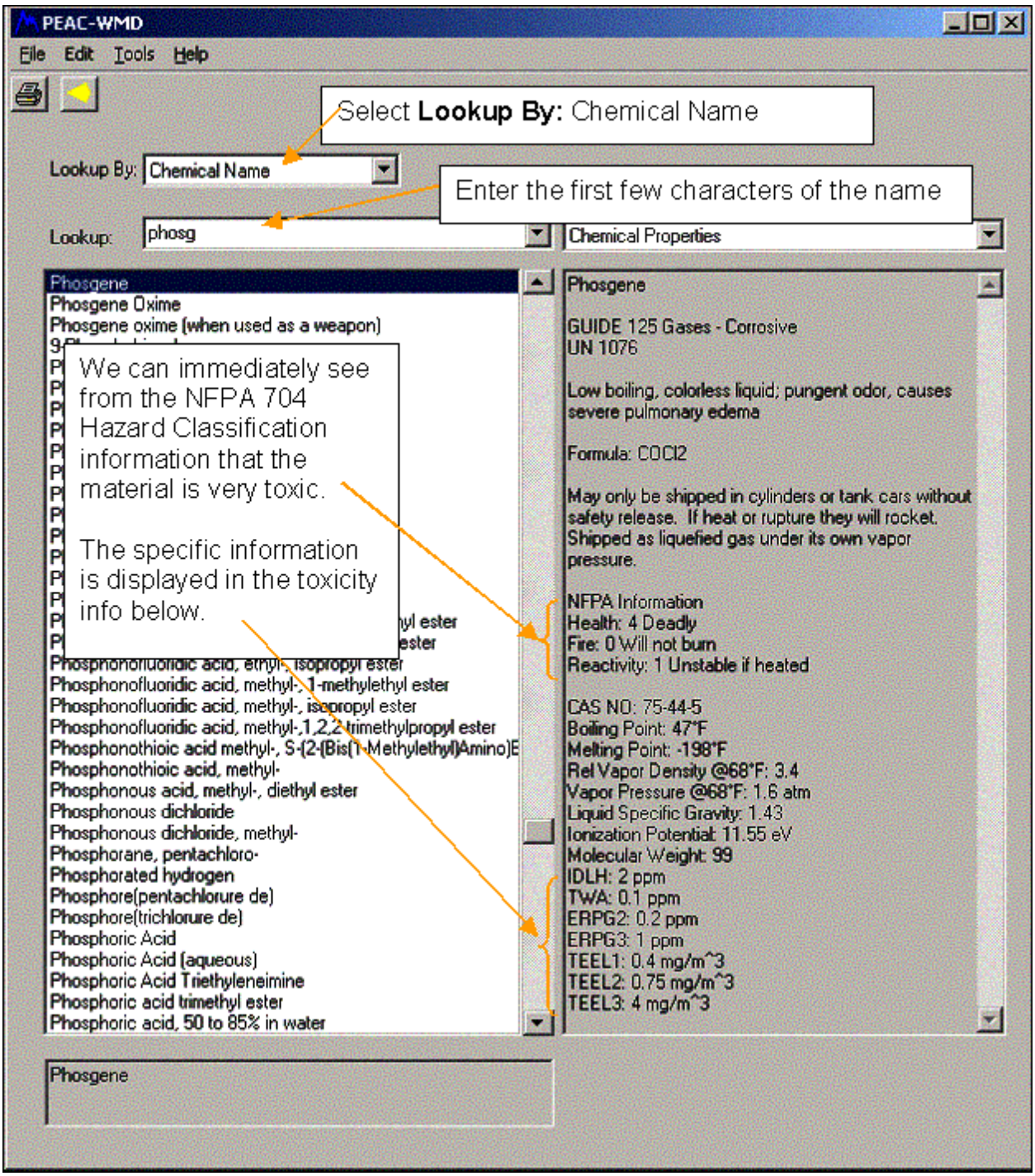

Figure 1 - Using the Lookup By: Name for Phosgene using the PEAC-WMD for Windows application

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. As you can see below, the published toxicity values, e.g., IDLH, ERPGs, and the TEELs (Temporary Emergency Exposure Limits) published by Department of Energy are provided. We will use the IDLH as the Level of Concern when we develop the PAD a little later.

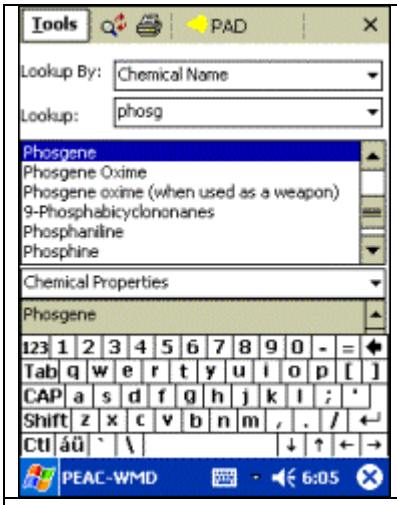

Figure 2 – Selecting Phosgene using the PEAC-WMD for Pocket PC application

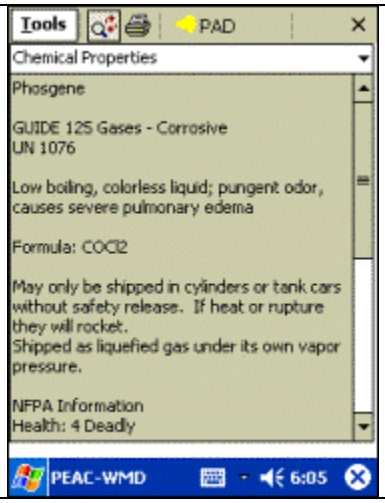

Figure 3 – The top portion of the Chemical Properties Data Display Screen

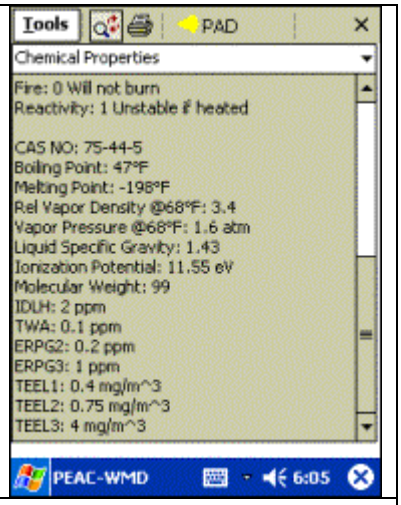

Figure 4– The bottom portion of the Chemical Properties Data Display Screen

A benefit of using the PEAC tool is assistance in the development of an evacuation zone for those chemicals that produce a toxic vapor cloud. If transported as a compressed liquefied vapor it will be released from a container as a vapor or aerosol or a liquid that will rapidly vaporize. As with most 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 hypothetical scenario using Phosgene as the involved chemical we'll set the location to be a chemical manufacturing facility located in Houston, TX. The date is December 11, 2003, about 1:30 AM with a temperature of 55°F, a wind speed of 5 mph with a clear sky. The release involves a portable tank that has a 1-inch transfer valve knocked off by a forklift. The facility response team responds and by the time they have arrived, a pool of liquid has formed about 25' in diameter. The PEAC tool can provide guidance with regards to toxic vapor cloud that is released.

If you decide to follow along as we proceed through these examples, remember to set the location to Houston and set the date and time to the proper values, otherwise you'll compute different values.

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 following figures demonstrate how we would work through our scenario to see what our Protective Action Distance should be.

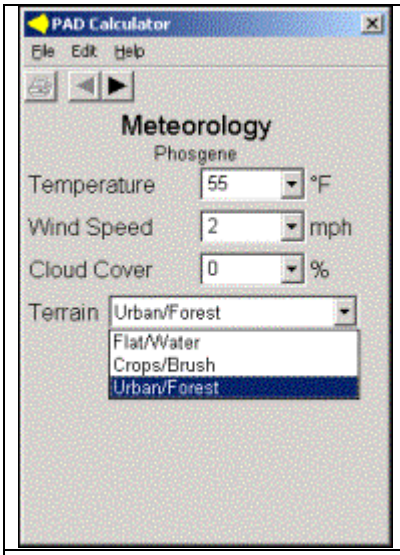	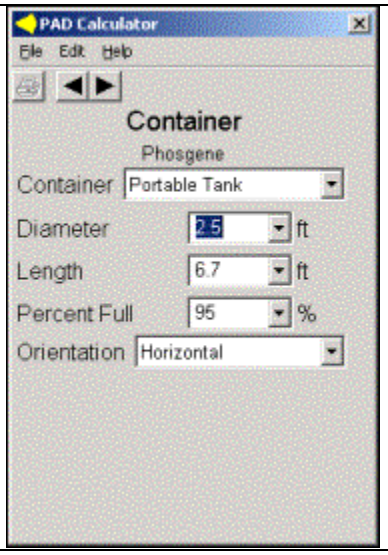	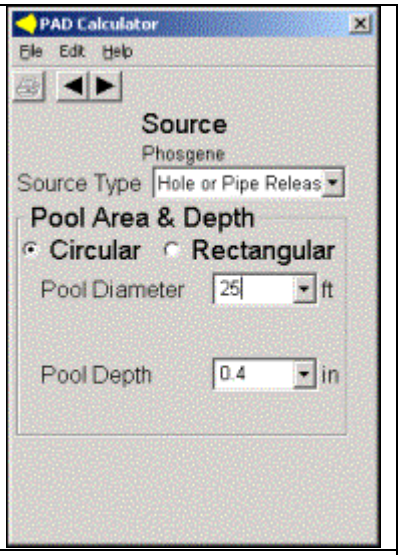
Meteorology It's Houston in December and the temperature about 55°, wind is set for 5 mph, clear skies and the terrain is **Urban/Forest** since it's an industrial setting.	**Container** We have selected from our list of container sizes the **Portable Tank** selection; this gives some quick dimensions that should get us close to the right size.	**Source** We have selected a **Hole or Pipe Release** for the type of release with a **Pool Diameter** of 25 ft and a **Pool Depth** set to the default depth of 0.4".

Figure 5 – Calculating a PAD using the PEAC-WMD System for December 11th

By pressing the right arrow at the top of the screen, the PEAC system will display a screen as shown in Figure 6. This calculates a **PAD** (Protective Action Distance) based on the default **Level of Concern** the IDLH of 2 ppm. This evacuation or standoff distance is based on the toxicity of Phosgene.

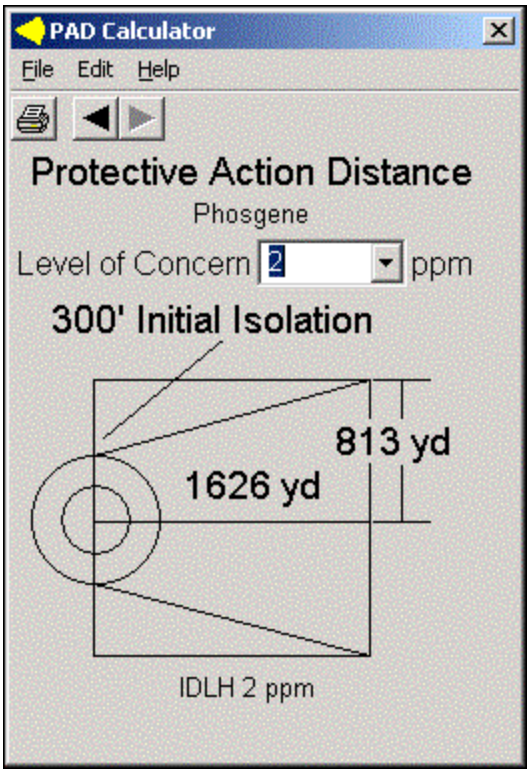

Figure 6 – Default PAD for Phosgene using the IDLH of 2 ppm

With a wind speed of 5 mph the downwind evacuation or PAD extends about 1 mile. If the wind speed was slower so that stable atmospheric conditions were established, the downwind evacuation distance will be impacted. To see the effect, click on the left arrow [◂] at the top of the screen until you return to the meteorological input screen. As shown in Figure 7, select a wind speed of 2 mph rather than 5 mph.

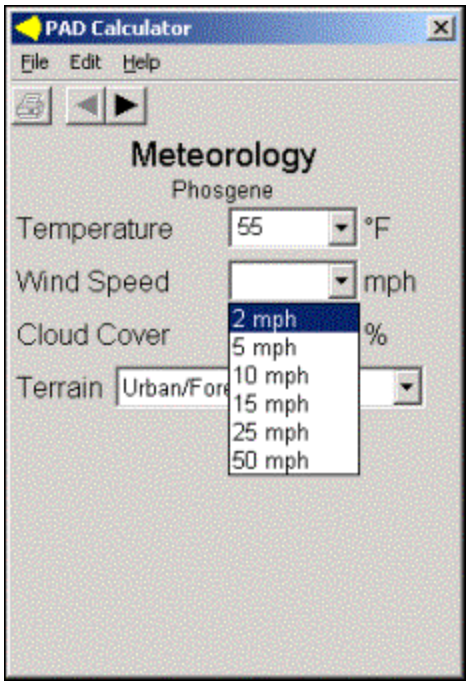

Figure 7 – Change the wind speed to 2 MPH

Then click on the right arrows [▸] at the top of the screen until a new PAD screen is displayed. The results of the new calculations are shown in Figure 8.

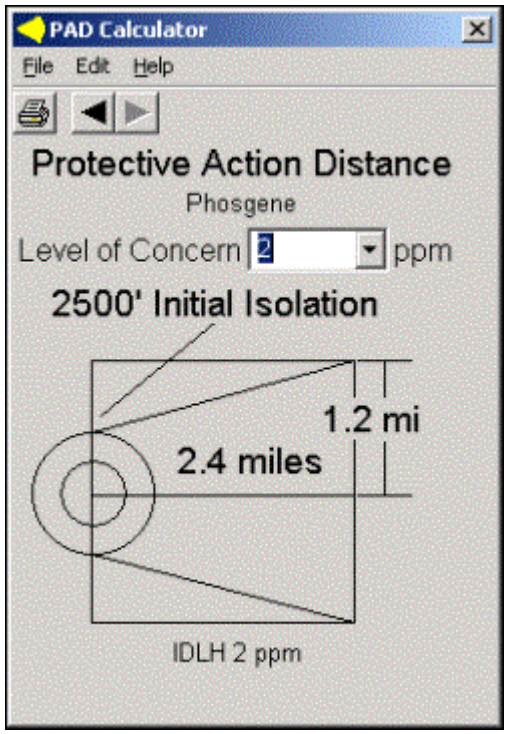

Figure 8 – PAD under stable conditions

As can be seen in Figure 8, the evacuation distance has increased substantially when stable atmospheric conditions are present, hence the term “worst case conditions”.

The user should be aware that stable atmospheric conditions may exist during night with low winds. These conditions can present serious problems with respect to toxic clouds and their behavior.

Substantial portions of this discussion were adapted from the Agency for Toxic Substances and Disease Registry (ATSDR) Web site for Medical Management Guidelines at: http://www.atsdr.cdc.gov/.