Let's Take a PEEK at the PEAC Software

PEAC Example--Diborane

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This month our example is Diborane, which has a chemical formula of B_2H_6. Diborane is listed under the UN # (United Nations Number) by the US Department of Transportation: UN 1911 and has a CAS # of 19287-45-7.

Persons exposed only to Diborane gas pose little risk of secondary contamination. Diborane is a colorless highly flammable gas with a repulsive, sickly sweet odor. At high concentrations, it ignites spontaneously in moist air at room temperature. It reacts with water to form hydrogen and boric acid. Diborane vapors are heavier than air and may collect in low-lying areas. Diborane is highly irritant when it contacts moist tissues such as the eyes, skin, and upper respiratory tract and can cause thermal burns. Burns are caused by the exothermic reaction of hydrolysis.

It is generally shipped in pressurized cylinders diluted with hydrogen, argon, nitrogen, or helium. It mixes well with air and explosive mixtures are easily formed. At high concentrations, it will ignite spontaneously in moist air at room temperature. The main toxic effect of exposure to Diborane is irritation of the respiratory airway, skin, and eyes.

Inhalation is the major route of exposure to Diborane. An odor threshold between 2 and 4 ppm has been reported for Diborane, which is higher than the OSHA permissible exposure limit (PEL) of 0.1 ppm. Prolonged, low-level exposures, such as those that occur in the workplace, can lead to olfactory fatigue and tolerance of Diborane's irritant effects. **Odor does not provide adequate warning of hazardous concentrations.**

Children exposed to the same levels of Diborane as adults may receive larger dose because they have a greater lung surface area:body weight ratios and higher minute volume: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 Diborane found nearer to the ground.

Direct contact with concentrated Diborane vapors may cause severe eye or skin burns, leading to cell death and ulceration. Ingestion is unlikely to occur because Diborane is a gas at room temperature.

Physical Properties

Description: Colorless gas at room temperature

Warning properties: odor does not provide adequate warning of hazard

Molecular weight: 27.7 daltons

Boiling point: (760 mm Hg) = -135 °F (-92.8 °C)

Freezing point: -264.8 °F (-164.9 °C)

Specific gravity (liquid): 0.210 at 15 °C

Vapor pressure: @62°F: 39.5 atm

Relative Vapor Density: @68°F: 1

Water solubility: Decomposes in water

Flammability: Auto Ignition temperature 104°F

Flammable Range: 0.8 % to 88 % (concentration in air)

Sources/Uses Diborane is produced by the reaction of lithium hydride with boron trifluoride catalyzed by ether at 25 °C. Diborane is used in rocket propellants and as a reducing agent, as a rubber vulcanizer, as a catalyst for olefin polymerization, as a flame-speed accelerator, and as a doping agent in the manufacture of semiconductor devices.

Synonyms include boroethane, boron hydride, diboron hexahydride.

Standards and Guidelines

NIOSH REL (recommended exposure limit) = 0.1 ppm

NIOSH IDLH (immediately dangerous to life or health) = 15 ppm

AIHA ERPG-2 (maximum airborne concentration below which it is believed that nearly all persons could be exposed for up to 1 hour without experiencing or developing irreversible or other serious health effects or symptoms that could impair their abilities to take protective action) = 1 ppm.

Incompatibilities Diborane is incompatible with oxidizers, aluminum, halogens, and water.

Acute Exposure The toxic effects of Diborane are primarily due to its irritant properties. The local irritant action of Diborane is due to the heat released as a consequence of its reaction with water and products formed by the hydrolysis reaction, such as boron oxide. Symptoms may be apparent immediately or delayed for a few hours. Children do not always respond to chemicals in the same way that adults do. Different protocols for managing their care may be needed.

Respiratory Exposure to Diborane can cause a sensation of tightness of the chest leading to diaphragmatic pain, shortness of breath, cough, and wheezing. These signs and symptoms, which may be delayed for up to 24 hours, can be seen for 3 to 5 days after an exposure. Children may be more vulnerable to gas exposure because of higher minute ventilation per kg and failure to evacuate an area promptly when exposed.

Dermal Skin irritation manifested as reddened skin may occur from exposure to Diborane vapors.

Ocular/Ophthalmic High concentrations of Diborane can cause eye irritation, pain, swelling, lacrimation, or photophobia.

Neurologic Dizziness, headache, weakness, central nervous system depression, and incoordination have been seen following exposure to Diborane.

Potential Sequelae Weakness and fatigue may follow exposure to Diborane. Damage to liver and kidneys may occur in some cases during metabolism and excretion.

Chronic Exposure Chronic exposure to low concentrations of Diborane were reported to have caused seizures, convulsions, fatigue, drowsiness, confusion, altered EEG responses, and spasms of the voluntary muscles. Others have reported headache, vertigo, chills, and sometimes fever. Asthmatic bronchitis can also occur. Chronic exposure may be more serious for children because of their potential for a longer latency period.

Carcinogenicity Diborane has not been classified for carcinogenic effects.

Reproductive and Developmental Effects No information is available regarding reproductive or developmental effects of Diborane in experimental animals or humans. Diborane 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 Diborane in the database. The following figures show the screens displayed for chemical properties, Figure 1 for the *PEAC-WMD for Windows* application and Figure 2-5 for the *PEAC-WMD for the Pocket PC* application.

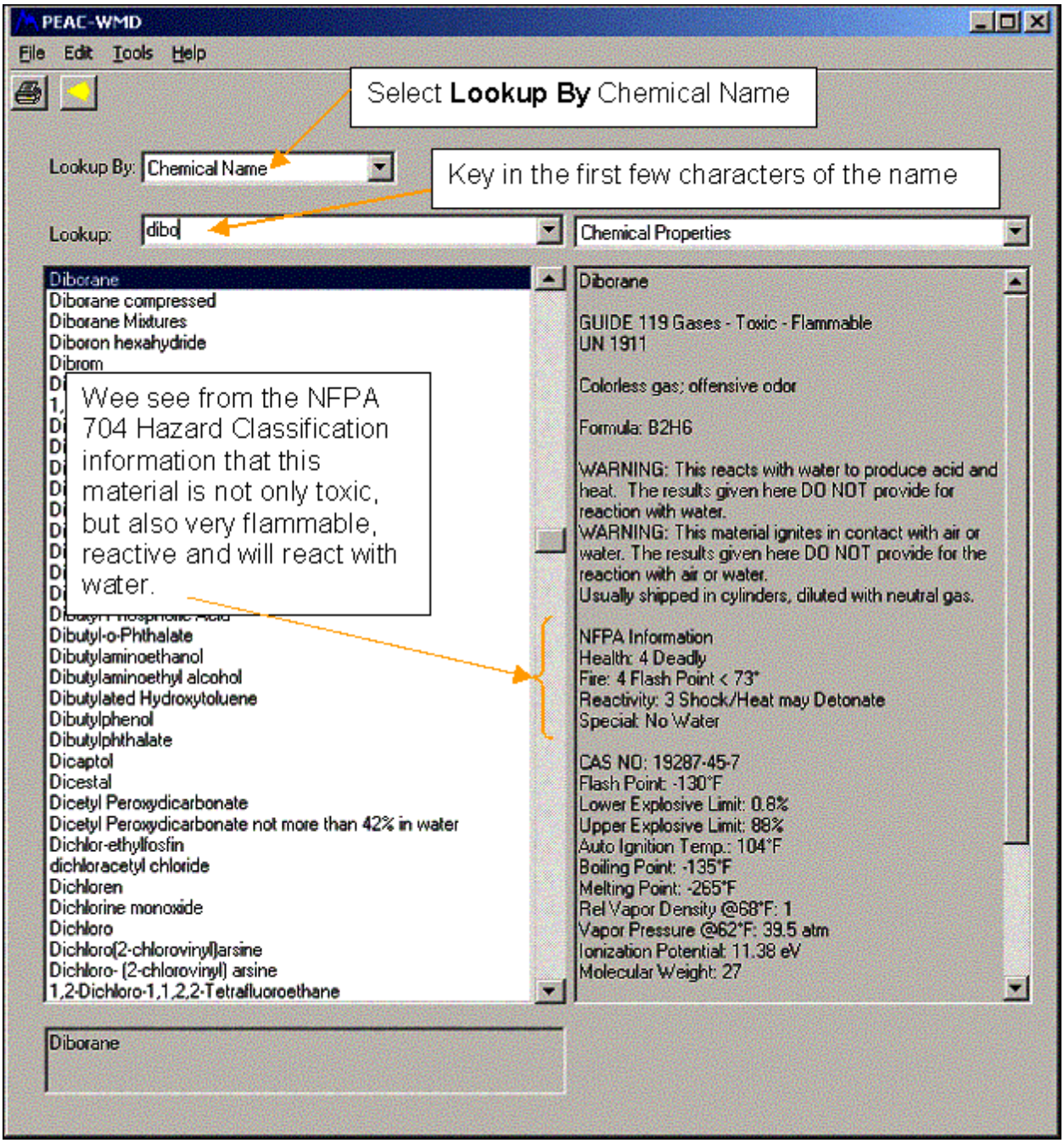


Figure 1 - Using the Lookup By: Name for Diborane using the PEAC-WMD for Windows application

Review of the information displayed in the chemical properties screen whether in Figure 1 (above) or Figures 2-5 (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.

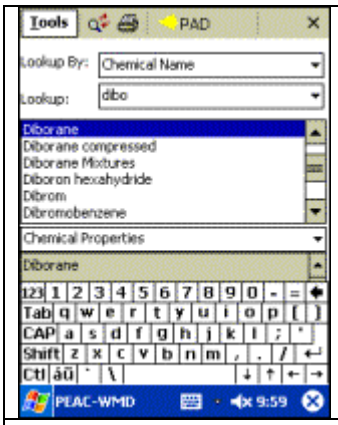


Figure 2 – Selecting Diborane using the PEAC-WMD for Pocket PC application

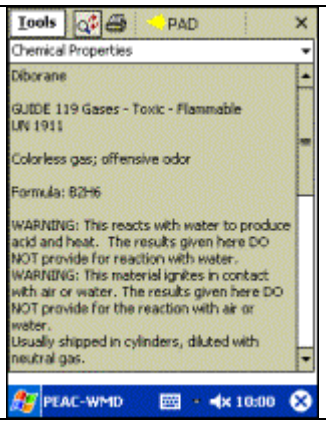


Figure 3 – The top portion of the Chemical Properties Data Display Screen

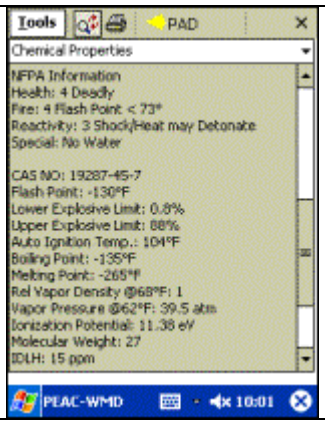


Figure 4– The middle portion of the Chemical Properties Data Display Screen

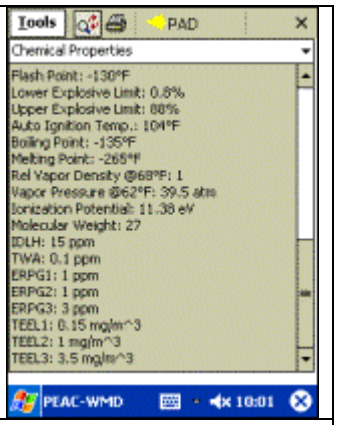


Figure 5– The bottom portion of the Chemical Properties Data Display Screen

The PEAC-WMD application provides more than just the **Chemical Properties** for the identified material, the **Chemical Properties** are just the default information screen displayed, by clicking (if running the Windows version, see Figure 6) or tapping (if running the Pocket PC version, see Figure 7) on the drop-down box where **Chemical Properties** is displayed on the screen, the user is provided with a list of other databases that provide information for the selected chemical (Diborane in our current example). So the search is done once, and the user is indexed into the different databases easily and quickly.

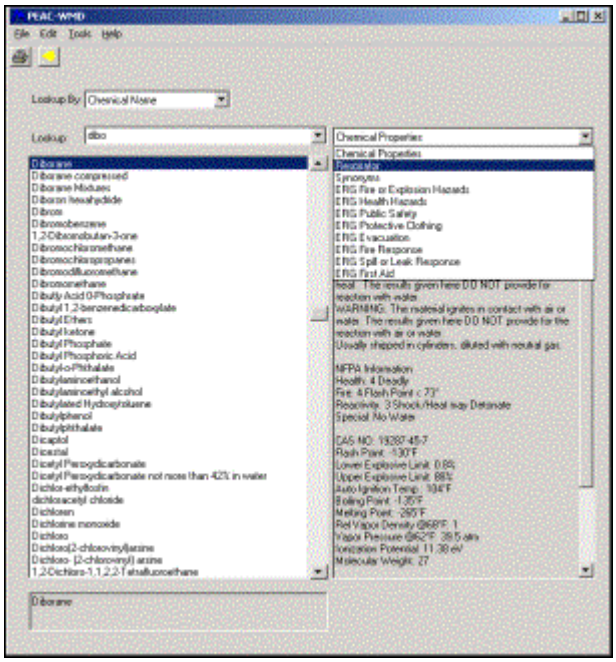


Figure 6 – Accessing other databases from the PEAC-WMD for Windows application

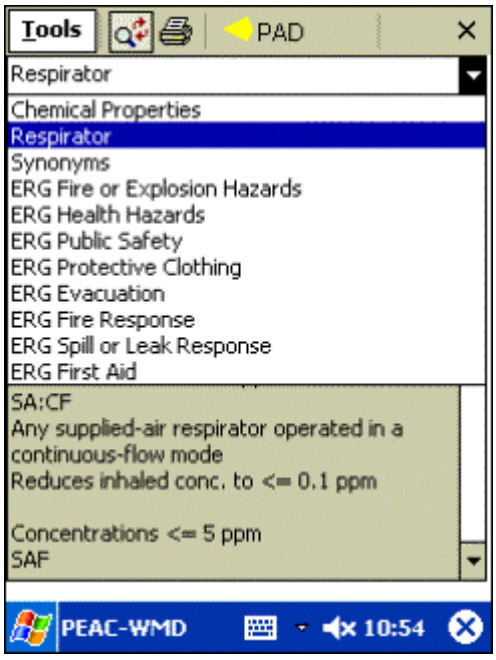


Figure 7 – Accessing other databases from the PEAC-WMD for Pocket PC application

A quick review or sampling of the type of information available in each of these screens is now provided. First is access to **Respirators Recommendations**, these are primarily taken from the NIOSH Pocket Guide and provide the user with different types of respirators for increasing concentrations. A sample of the information is provided in Figure 8.

One of the other databases provided in the PEAC-WMD tool is access to Chemical Protective Clothing (CPC). As shown in Figure 7 above, there was no listing shown for Chemical Protective Clothing in the list of databases available and the reason is that there are no CPC entries in the PEAC-WMD database for Diborane. The reason is that the CPC manufacturers have not tested their products against Diborane. Then the question is why not? The most likely answer is that Diborane reacts with moisture to form Hydrogen and Boric Acid. If using a full-face respirator that protects the eyes and respiratory system as indicated in the respirator database entries, then the minimal irritation to the skin due to contact with Diborane vapors doesn't require CPC.

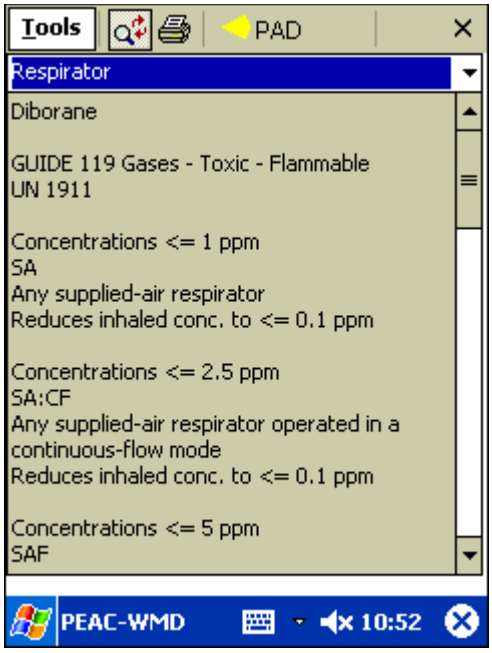


Figure 8 – Respirator Recommendations for Diborane

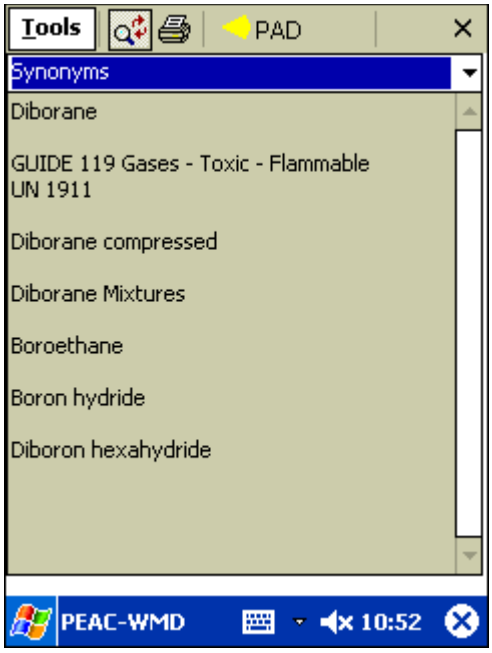


Figure 9 – Synonyms

The IC (Incident Commander) will typically utilize more than a single resource for developing a response plan but sometimes the information in other resources will use a different name for the same substance. Clicking on the **Synonyms** selection will provide a quick list of other names the substance may be referenced by in other resources as shown in Figure 9. To further assist the responder in initiating the best response plan, PEAC-WMD also provides the generic guidelines found in the 'orange pages' of the DOT Emergency Response Guidebook (ERG). These are categorized into different types of procedures depending on the incident and the problem to be mitigated. An example for **Spill or Leak Response** is shown in Figure 10.

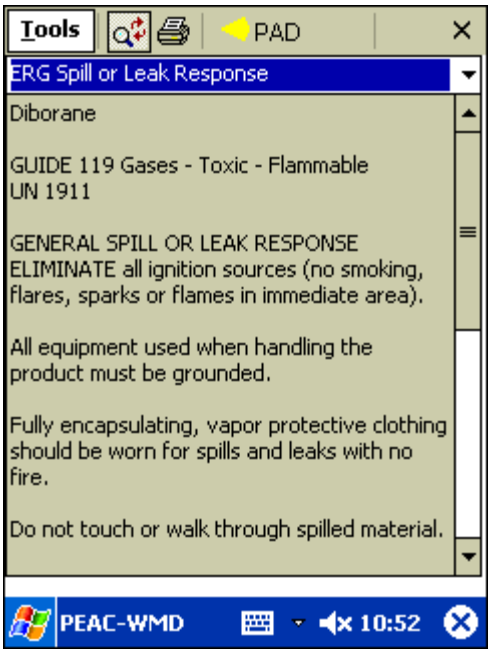


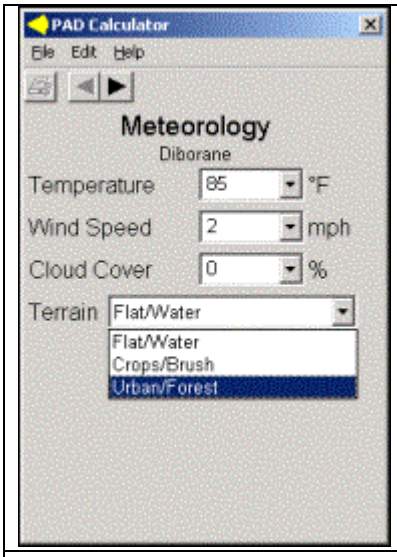
Figure 10 – ERG Spill or Leak Response

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. Because of its boiling point Diborane will be released from a container as a vapor or aerosol or a liquid that will rapidly vaporize. 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 hypothetical scenario using Diborane as the involved chemical we'll set the location to be a manufacturing facility located in Akron, OH. The local fire department knows that the facility has regular deliveries of Diborane cylinders to the facility and that the cylinders are stored outside. The cylinders are moved as needed from their storage location and this movement can be during the day or night since the production facility runs around the clock 24/7. Developing plans for what might happen, the fire department decides to take a look at what impact on surrounding areas if an accident occurred during one of these movements and the contents of a cylinder were released. The HAZMAT Coordinator decides that they'll look at both a daytime (noon) and a midnight release. They select a temperature of 85°F and a date of July 1st and a wind speed of 2 mph with a clear sky for the daytime release. For the nighttime release they select a temperature of 30°F, a date of January 1st and a wind speed of 2 mph and clear skies. In both cases they select an urban/forest terrain type since the manufacturing facility is located in an industrial section of the city. The PEAC tool can provide guidance with regards to toxic vapor clouds that are released.

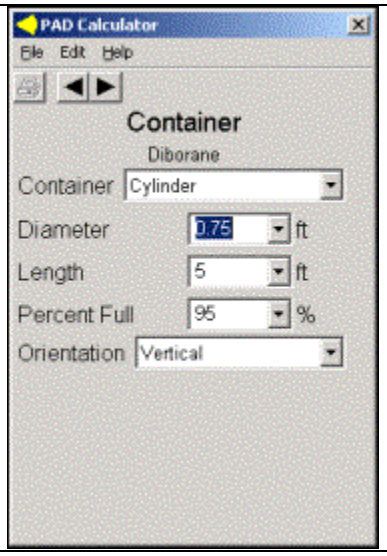
If you decide to follow along as we proceed through these examples, remember to set the location to Akron and set the date and time to the proper values, otherwise you'll compute different values. Also it should be understood that the examples shown below assume that no explosion or fire is involved, otherwise the Diborane would ignite and not form a toxic cloud. In addition, the reader should also understand that the PEAC-WMD system makes no allowance for reaction of the Diborane with moisture in the air.

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 11. 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 two different cases to see what effect they have on our Protective Action Distance.



Meteorology

It's Akron in July and the temperature about 85°, wind is set for 2 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 **Cylinder** selection.

Source

We have selected a **Large Rupture** for the type of release.

Figure 11 – Calculating a PAD using the PEAC-WMD System for daytime (July 1st)

By pressing the right arrow at the top of the screen, the PEAC system will display a screen as shown in Figure 12. This calculates a **PAD** (Protective Action Distance) based on the default **Level of Concern** the IDLH of 15 ppm. This evacuation or standoff distance is based on the toxicity of Diborane.

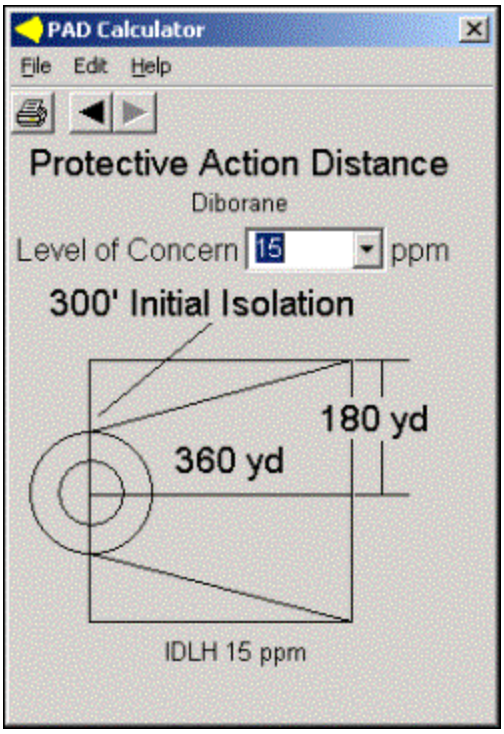


Figure 12 – Default PAD for Diborane on July 1 and using the IDLH of 15 ppm

Now we can re-evaluate but for a night time release on January 1st around midnight, winds of 2 mph and clear skies.

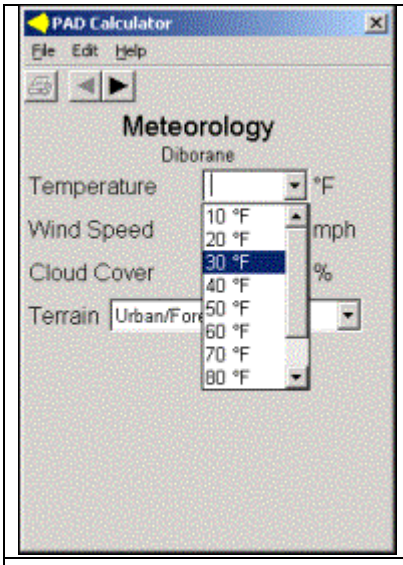
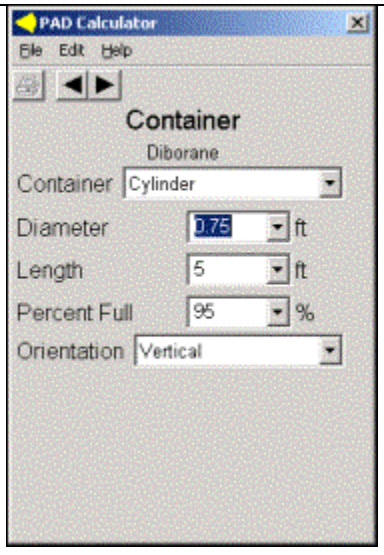
		
Meteorology Now we set the temperature to 30°F and leave everything else unchanged.	**Container** We don't need to change the **Container** type.	**Source** We leave the **Large Rupture** as the Source type.

Figure 13 – Calculating a PAD using the PEAC-WMD System for nighttime (January 1st)

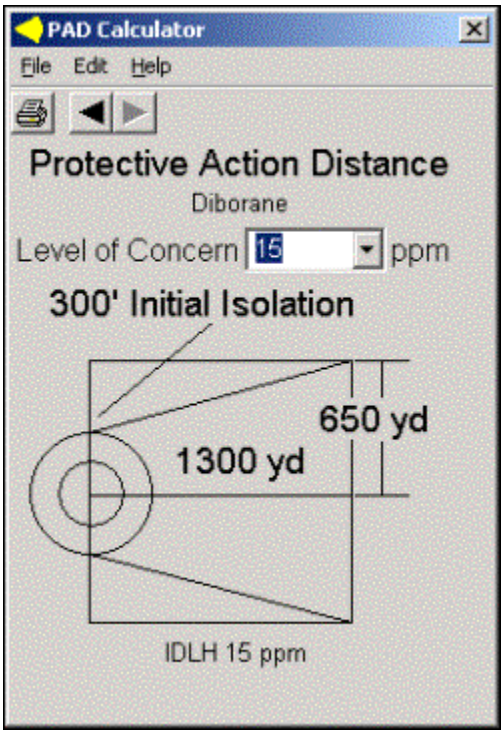


Figure 14 – Default PAD for Diborane on January 1 and using the IDLH of 15 ppm

The obvious effect of nighttime conditions and the associated stable atmospheric conditions found at nighttime increase the size of the PAD. The fire department now knows that for a single cylinder of Diborane, a nighttime release is going to affect a much larger area than a daytime release.

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/.