# Let's Take a Peek at the PEAC software

*by S. Bruce King*

This month our example is Dichlorosilane which has a chemical formula of $SiH_2Cl_2$. Its chemical structure is shown in Figure 1. Dichlorosilane is a colorless gas with an irritating, acidic odor. The immediate health hazard is that it is a toxic gas. It is flammable, and may form mixtures with air that are flammable or explosive. Dichlorosilane is reactive with water and it fumes in moist air to form hydrogen chloride and siloxanes. Dichlorosilane is used for deposition of epitaxial silicon and silicon-based alloys. It is normally shipped as a liquefied compressed gas.

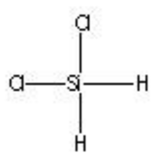


**Figure 1 - Structure**

It has a melting point of -188°F and a boiling point of 47°F. Its molecular weight is 101.01, and has a vapor density is 3.52, so it will seek low areas. It has a vapor pressure of 1,232 mm of Hg at a standard temperature of 70°F. It is extremely flammable with a flash point of -62°F. The lower Explosive Limit (LEL) is 4.7%; the Upper Explosive Limit (UEL) is 96%. Since it forms hydrogen chloride when in contact with water or moisture it should be handled with extreme caution.

There is no established IDLH for Dichlorosilane but Voltaix, Inc., a manufacturer of the material, recommends a Ceiling of 2.5 ppm, which is half the Ceiling specified by ACGIH and OSHA for hydrogen chloride.

The important thing to remember when dealing with Dichlorosilane is that it is both a very flammable substance and its vapors can react with any moisture to form hydrogen chloride. Therefore if the material is released from its container, every effort should be made to eliminate ignition sources and appropriate PPE must be worn to protect from exposure or inhalation.

**Hazards and protection**

**Storage -** Keep separated from incompatible substances. Avoid heat, flames, sparks and other sources of ignition.

**Handling -** All chemicals should be considered hazardous. Avoid direct physical contact. Use appropriate, approved safety equipment. Untrained individuals should not handle this chemical or its container. Handling should occur in a chemical fume hood.

**Protection -** Wear appropriate chemical protective clothing.

**Respirators -** Wear positive pressure self-contained breathing apparatus.

**Small spills or leaks -** Keep sparks, flames, and other sources of ignition away. Keep material out of water sources and sewers. Attempt to stop leak if without undue personnel hazard. Use water spray to knock-down vapors.

**Stability -** May polymerize violently or explosively.

**Incompatibilities -** Reacts with water or moist air to form HCl. Attacks many metals in presence of water.

**Hazardous Decomposition -** The substance may spontaneously ignite on contact with air. Decomposes on heating or on burning producing toxic and corrosive fumes including HCl.

**Health related information**

**Exposure effects**

The toxological properties of this substance have not been fully investigated.

**Ingestion -** Causes burns.

**Inhalation -** Sore throat, cough, burning sensation, shortness of breath, labored breathing. Corrosive to the respiratory tract. May cause lung edema. Exposure to high levels may result in death. Symptoms may be delayed.

**Skin -** Redness, pain, burns, blisters. Exposure to liquid can cause serious frostbite.

**Eyes -** Pain, redness, severe deep burns, loss of vision. Tear drawing.

**First aid**

**Ingestion -** Seek medical assistance.

**Inhalation -** Move victim to fresh air. Apply artificial respiration if victim is not breathing. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; induce artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Administer oxygen if breathing is difficult.

**Skin -** Remove and isolate contaminated clothing and shoes. Immediately flush with running water for at least 20 minutes. In case of contact with liquefied gas, thaw frosted parts with lukewarm water.

**Eyes -** Immediately flush with running water for at least 20 minutes.

In using the PEAC application we access information for the chemical by first locating Dichlorosilane in the database. The following figures show the screens displayed for chemical properties, Figure 2 for the *PEAC-WMD for Windows* application and Figure 3-5 for the *PEAC-WMD for the Pocket PC* application.

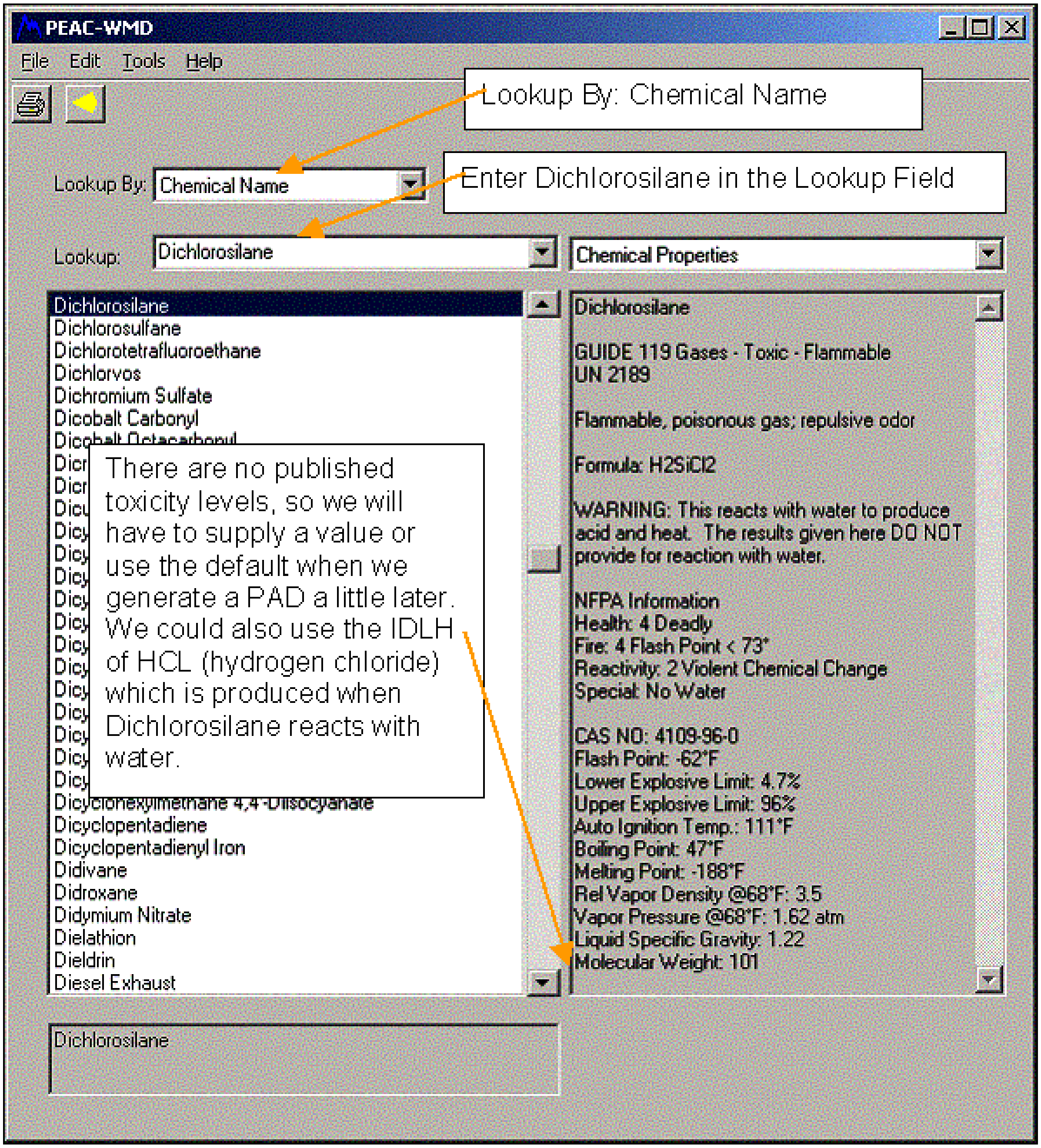


**Figure 2 -** Using the Lookup By: Name for Dichlorosilane using the PEAC-WMD for Windows application

Review of the information displayed in the chemical properties screen whether in Figure 2 (above) or Figures 3-5 (below), show chemical properties values discussed earlier at the top of this discussion. As you can see, there are no published toxicity values, e.g., IDLH, ERPGs, or even the TEELs published by Department of Energy. We will use either the default Level of Concern or enter a value when we develop the PAD a little later.

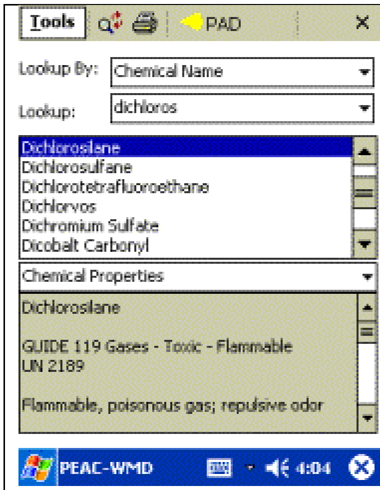


**Figure 3** – Selecting Dichlorosilane using the PEAC-WMD for Pocket PC application

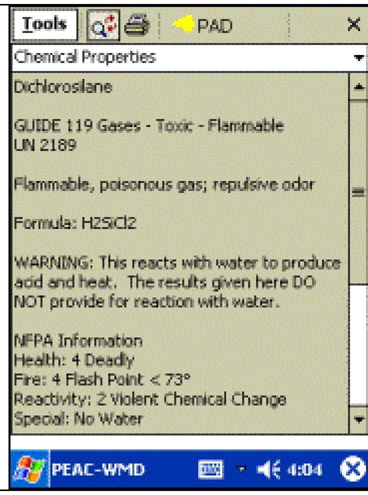


**Figure 4** – The top portion of the Chemical Properties Data Display Screen

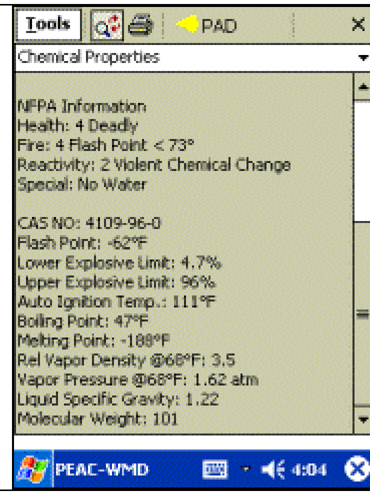


**Figure 5** – The bottom portion of the Chemical Properties Data Display Screen

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. Dichlorosilane has a relatively high vapor pressure (1232 mm Hg) at room temperature, so if the chemical is released it will vaporize rapidly. 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 Dichlorosilane as the spilled chemical we'll set the location to Phoenix and the time as 12:30 PM on February 12th. A transport truck with 40 cylinders of Dichlorosilane has rolled off the Interstate 10 close to the center of the city. At least one of the cylinders has the valve cover knocked off the cylinder and is leaking vapor very rapidly. The temperature is about 70°F, the winds are about 5 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 6. 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. If you decide to follow along on this example, remember to change the location to Phoenix and the time to 12:30 PM, February 12$^{th}$.

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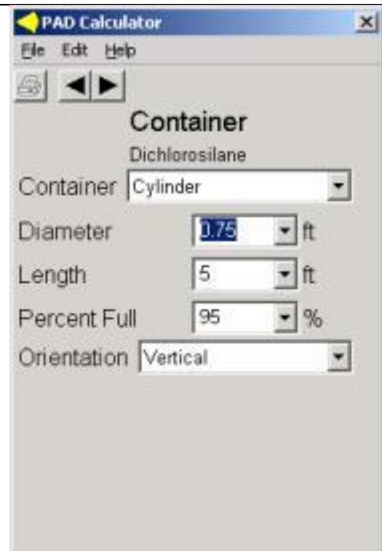
<td>
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<td>Meteorology<br><br>It's Phoenix in February and the temperature about 70°, light wind is set for 5 mph, clear sky so we'll set cloud cover to 0%, and the terrain is Urban/Forest since it's an urban setting.</td>
<td>Container<br><br>We have selected from our list of container sizes the Cylinder selection. This provides us with a default size that should get us pretty close to the actual size.</td>
<td>Source<br><br>Since the scenario has the valve cover knocked off we've assumed a worst-case scenario, we've selected a Large Rupture as the Source type of release.</td>
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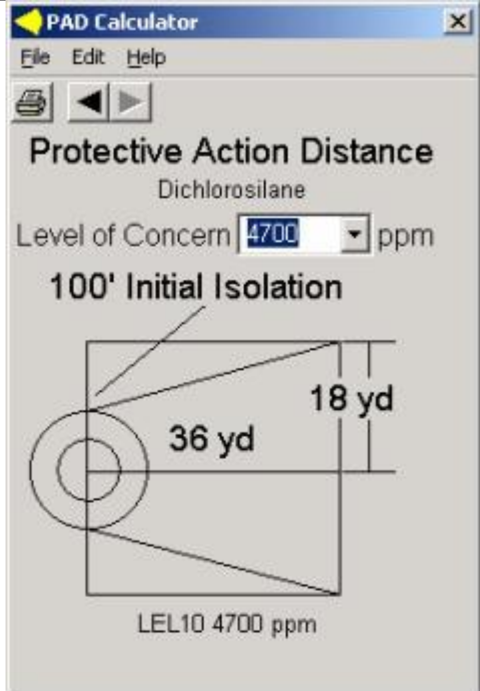
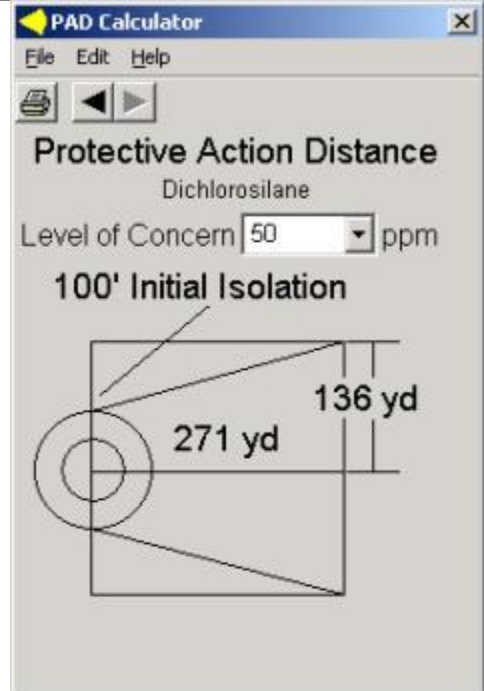
**Figure 6 –** Calculating a PAD using the PEAC System

By pressing the right arrow at the top of the screen, the PEAC system will display a screen as shown in Figure 7. This calculates a **PAD** (Protective Action Distance) based on the default **Level of Concern**, works out to 10% of the LEL or 4700 ppm, since there are no published toxicity levels. Since we know that Dichlorosilane reacts with moisture to form Hydrogen Chloride (HCl), we can also use the IDLH of HCl (50 ppm) as a Level of Concern to calculate a more appropriate PAD (see Figure 8).

|  |  |
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| **Figure 7** – Default PAD for Dichlorosilane based on 10% of the LEL as the Level of Concern. | **Figure 8** – PAD for Dichlorosilane using 50 ppm (the IDLH of Hydrogen Chloride) as the Level of Concern. |

Portions of this discussion were adapted from the WEB site supported by the Hardy Research Group, Department of Chemistry, The University of Akron: http://ull.chemistry.uakron.edu/. Additional information was adapted from Voltaix, Inc., a manufacturer of Dichlorosilane and available at their web site: http://www.voltaix.com/msds/msds-dichlorosilane_sih2cl2.htm.