

Let's Take A PEEK at the PEAC Software

by S. Bruce King

This month our example is Vinyl Carbinol, which has a chemical formula of (C₃H₆O). Vinyl Carbinol is listed under the UN # (United Nations Number) by the US Department of Transportation: UN 1098. Vinyl Carbinol is listed as CAS# (Chemical Abstract Service Number) 107-18-6. The Vinyl Carbinol molecular structure is shown in Figure 1 and is also represented by CH₂=CHCH₂OH.

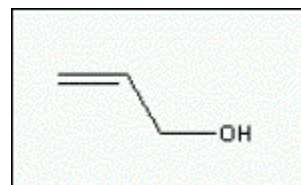


Figure 1 – Vinyl Carbinol molecular structure

Vinyl Carbinol is a colorless liquid, pungent, mustard-like odor, lachrymator.

Uses: Manufacture of flavorings, perfumes, to denature alcohol, fungicides, and herbicides.

Physical Properties:

Molecular Weight: 58

Melting Point: -128°C (-200°F)

Boiling Point: 97°C (205°F)

Vapor Density: 2.0 (air = 1.0)

Flash Point: 21°C (70°F)

Lower Explosion Limit: 2.5%

Upper Explosion Limit: 18%

Synonyms: Allyl Alcohol, chloroethene, chloroethylene, 1-chloroethylene, ethylene monochloride, monochloroethylene, monoVinyl Carbinol, MVC, VC, VCM, and Vinyl Carbinol monomer.

Incompatibilities: Oxidizing agents, strong acids, acids, alkali metals, aluminum, amines, coatings, magnesium, plastics, rubber, sodium hydroxide, isocyanates, sodium, carbon tetrachloride, chlorosulfonic acid, oleum, metallic halides, and diallyl phosphide.

Hazards and Protection:

Storage - Keep away from heat, sparks, and flame. Keep away from sources of ignition. Store in a cool, dry, well-ventilated area away from incompatible substances. Flammables-area.

Handling - Wash thoroughly after handling. Wash hands before eating. Use only in a well ventilated area. Ground and bond containers when transferring material. Use spark-proof tools and explosion proof equipment. Do not get in eyes, on skin, or on

clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Avoid contact with heat, sparks and flame. Do not ingest or inhale. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames.

Protection - Eyes: Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166. Skin: Wear appropriate gloves to prevent skin exposure. Clothing: Wear appropriate protective clothing to prevent skin exposure.

Respirators - Follow the OSHA respirator regulations found in 29CFR 1910.134 or European Standard EN 149. Always use a NIOSH or European Standard EN 149 approved respirator when necessary.

Small spills/leaks - Absorb spill with inert material, (e.g., dry sand or earth), then place into a chemical waste container. Avoid runoff into storm sewers and ditches which lead to waterways. Clean up spills immediately, using the appropriate protective equipment. Remove all sources of ignition. Use a spark-proof tool. A vapor suppressing foam may be used to reduce vapors.

Stability - May form explosive peroxides. May polymerize. Forms explosive mixture with air (flash point 70 degrees F).

Decomposition - Carbon monoxide, irritating and toxic fumes and gases, carbon dioxide.

Health:

Exposure limit(s) - OSHA PEL: TWA 2 ppm (5 mg/m³) skin

NIOSH REL: TWA 2 ppm (5 mg/m³)

NIOSH IDLH: 20 ppm

Exposure effects - May cause liver and kidney damage. Effects may be delayed.

Ingestion - Harmful if swallowed. Causes gastrointestinal irritation with nausea, vomiting and diarrhea. May cause central nervous system depression, characterized by excitement, followed by headache, dizziness, drowsiness, and nausea. Advanced stages may cause collapse, unconsciousness, coma and possible death due to respiratory failure.

Inhalation - Harmful if inhaled. May cause severe irritation of the respiratory tract with sore throat, coughing, shortness of breath and delayed lung edema. May cause pulmonary edema and severe respiratory disturbances. Vapors may cause dizziness or suffocation.

Skin - Causes skin irritation. May be fatal if absorbed through the skin.

First aid:

Inhalation - Get medical aid immediately. Remove from exposure to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. DO NOT use mouth-to-mouth respiration.

Ingestion - Do NOT induce vomiting. If victim is conscious and alert, give 2-4 cupfuls of milk or water. Never give anything by mouth to an unconscious person. Get medical aid immediately.

Skin - Get medical aid immediately. Immediately flush skin with plenty of soap and water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse.

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

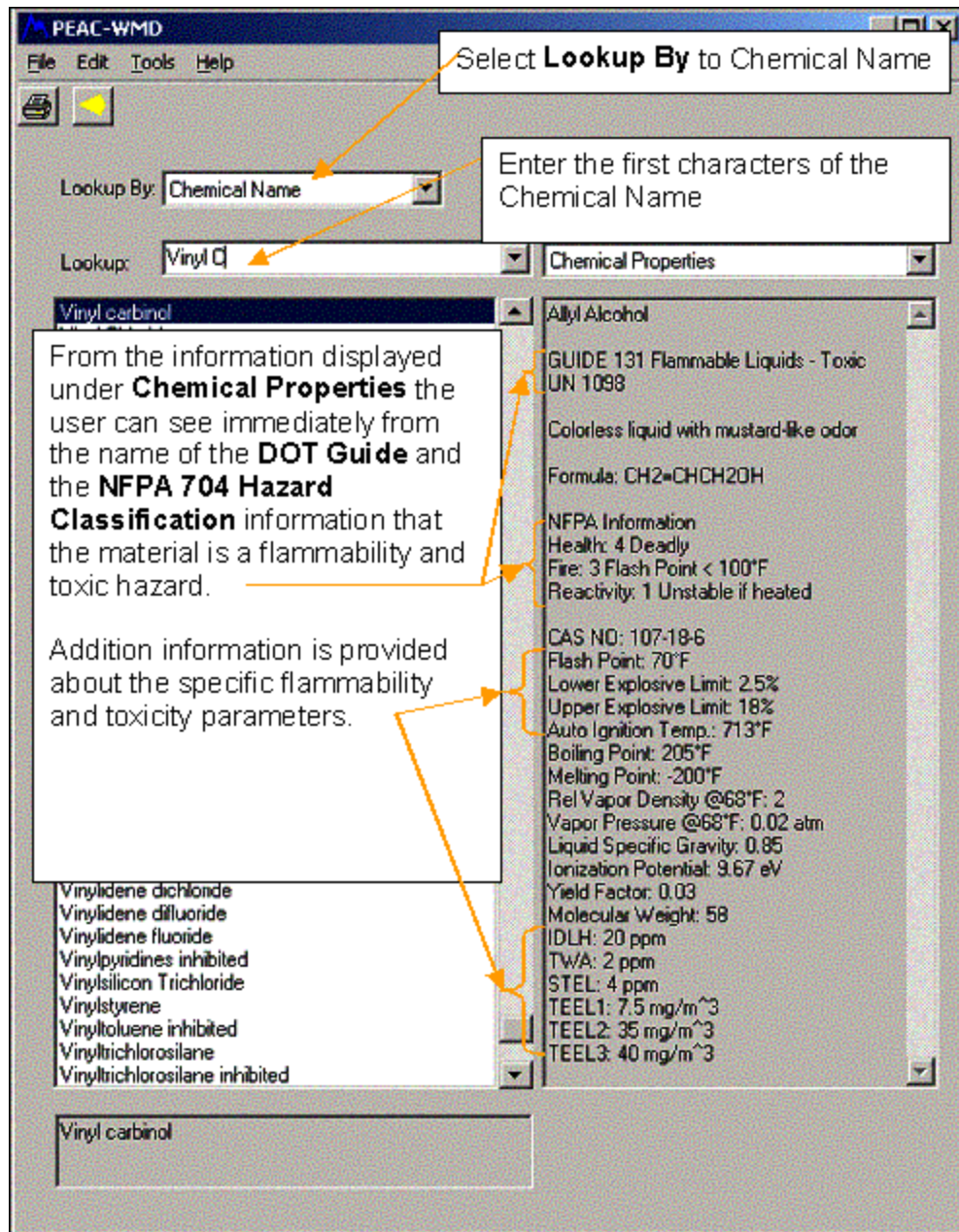


Figure 2 - Using the Lookup By: Name for Vinyl Carbinol using the PEAC-WMD for Windows application

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 below, the published toxicity values, e.g., IDLH, STEL, 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 Protective Action Distance (PAD) a little later.



Figure 3 – Selecting Vinyl Carbinol using the PEAC-WMD for Pocket PC application

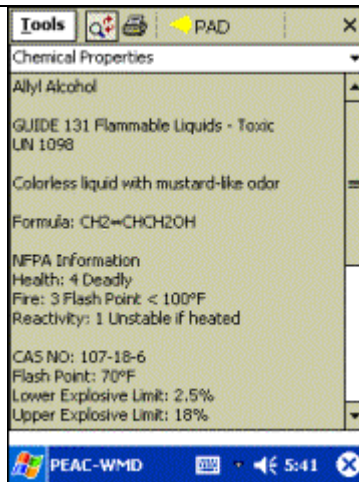


Figure 4 – The top portion of the Chemical Properties Data Display Screen

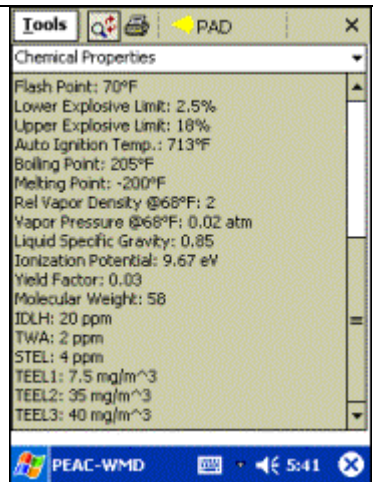


Figure 5– The bottom portion of the Chemical Properties Data Display Screen

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. 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 Vinyl Carbinol as the involved chemical we'll set the location to be fragrance-manufacturing facility located outside Baltimore, MD. The date is April 14, 2004, about 6:00 PM with a temperature of 55°F, wind speed of 2 mph and a clear sky. The hypothetical release involves a drum that contains Vinyl Carbinol and it has fallen off a truck, ruptured and formed a pool about 10' 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 Baltimore and set the date and time to the proper values, otherwise you'll compute different values. We'll use a terrain type of urban/forest since this is a manufacturing facility and has buildings and processing equipment in the immediate area.

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

<p>Meteorology</p> <p>It's Baltimore in April and the temperature about 55°, wind is set for 2 mph, clear skies and the terrain is Urban/Forest since it's a processing facility setting.</p>	<p>Container</p> <p>We have selected from our list of container sizes the Drum/Barrel selection. This gets us a quick estimate of how much material might be involved.</p>	<p>Source</p> <p>We have selected a Large Rupture, and since the liquid boils at 205°F it will form a liquid pool. So the application asks for a pool depth and diameter.</p>

Figure 6 – Calculating a PAD using the PEAC-WMD System for March 11th

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** the IDLH of 20 ppm. This evacuation or standoff distance is based on the toxicity of Vinyl Carbinol, **not** the flammability.

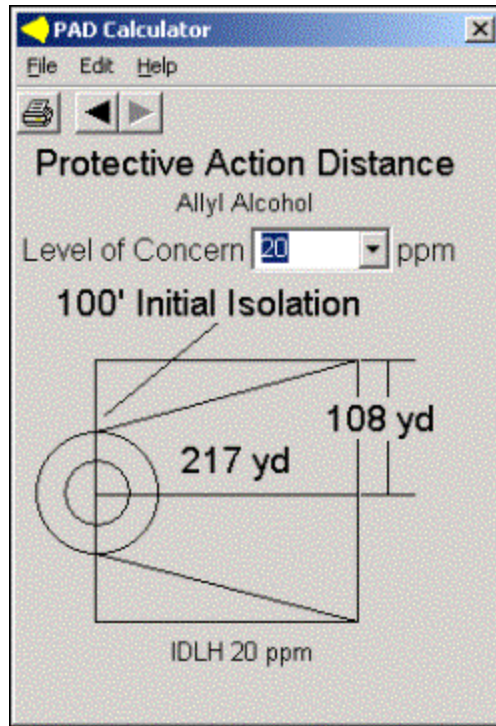


Figure 7 – Default PAD for Vinyl Carbinol using the IDLH of 20 ppm

If we want to calculate a PAD based on a toxicity level other than the IDLH, we can enter a value in the field for **Level of Concern** or we can select a value from our list of toxicity values shown in Figure 8. In this figure we select the STEL value or 4 ppm.

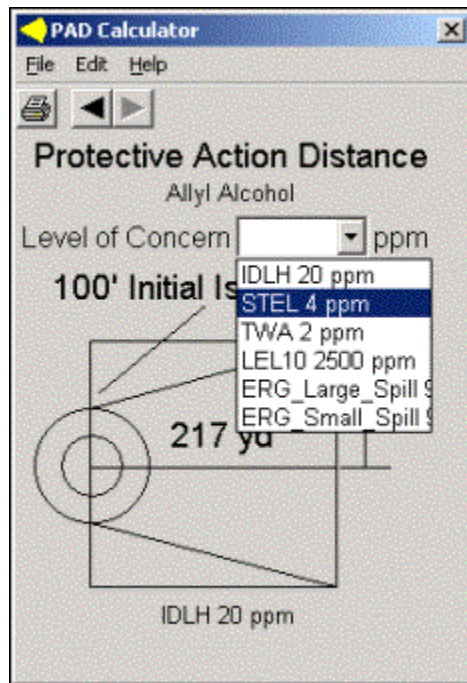


Figure 8 – Selecting another Level of Concern

The calculated PAD will be displayed, see Figure 9.

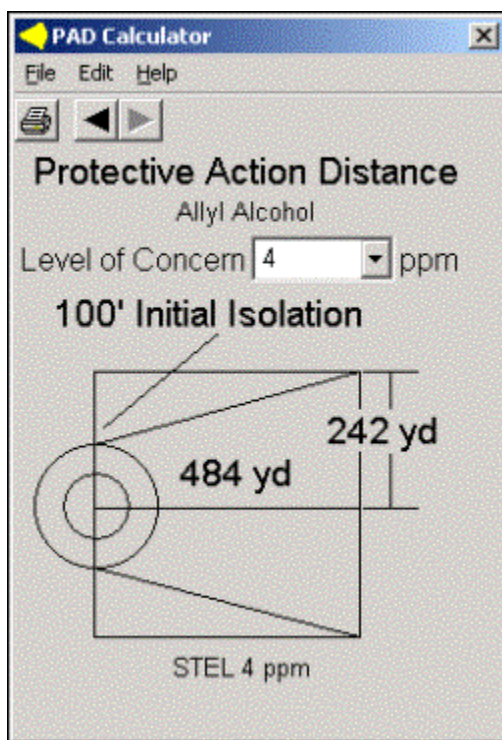


Figure 9 – Calculated PAD using the STEL Level of Concern

In addition to the toxicity of the released material, the user should also remember the flammability issue with Vinyl Carbinol and eliminate all ignition sources.

Substantial portions of this discussion were adapted from:

1. IPCS INCHEM web site, <http://www.inchem.org/>,
2. Chemfinder web site, <http://chemfinder.cambridgesoft.com/>, and
3. University of Akron web site, <http://ull.chemistry.uakron.edu/erd/chemicals1/6/5986.html>.