Let's take a peek at the PEAC-WMD software.
by S. Bruce King

PEAC Example – Vinyl Chloride

This month our example is Vinyl Chloride, which has a chemical formula of (C_2H_3Cl). Vinyl Chloride is listed under the UN # (United Nations Number) by the US Department of Transportation: UN 1086. Vinyl Chloride is listed as CAS# (Chemical Abstract Service Number) 75-01-4. The Vinyl Chloride chemical structure is shown in Figure 1.

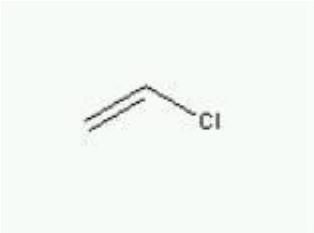


Figure 1 – Vinyl Chloride molecular structure

Persons exposed only to vinyl chloride gas pose no risk of secondary contamination. Persons whose clothing or skin is contaminated with pressurized liquid vinyl chloride can secondarily contaminate rescuers by direct contact or through off-gassing of vapor.

At all ambient temperatures, vinyl chloride is an extremely flammable and potentially explosive gas that is heavier than air. It has a mild, sweet odor, but odor is not an adequate warning of hazardous concentrations.

Inhalation is the major route of vinyl chloride exposure; absorption is rapid and nearly complete. Gastrointestinal absorption is unlikely as vinyl chloride is a gas at room temperature. Dermal absorption is negligible.

Description: At room temperature, Vinyl Chloride is a colorless, highly flammable, potentially explosive gas. It has a faint sweet odor. The odor threshold for Vinyl Chloride is about 3,000 ppm in air, depending on the individual. When confined under high pressure in special containers, Vinyl Chloride exists in a liquefied state. It is shipped and handled this way. When burned or heated to a high enough temperature, Vinyl Chloride decomposes to hydrogen chloride, carbon monoxide, carbon dioxide, and traces of phosgene. Vinyl Chloride should be stored in a cool, dry, well-ventilated location, separate from oxidizing materials and accelerants. Phenol is often added as a stabilizer.

Sources/Uses: Annual production levels of Vinyl Chloride continue to increase, with 14.98 billion pounds produced in the United States in 1995. Vinyl Chloride is produced by chlorinating ethylene to produce 1,2-dichloroethane, which is then subjected to high pressures and temperatures. This causes pyrolysis (thermal cracking) of the 1,2-dichloroethane to produce the Vinyl Chloride monomer. Most Vinyl Chloride is polymerized to form Polyvinyl Chloride (PVC), a material used to manufacture automotive parts and accessories, furniture, packaging materials, pipes, wall coverings, and wire coatings. Vinyl Chloride is also used as an intermediate in the production of other chlorinated compounds and as a component in mixed-monomer plastics. Historically, it was used as a solvent, propellant, and refrigerant, and it was once evaluated as a potential anesthetic.

Physical Properties:

Description: colorless gas with a sweet odor at room temperature; colorless liquid when contained under pressure or cooled.

Warning properties: **inadequate** (odor threshold of about 3,000 ppm; varies significantly among individuals)

Boiling point: 7.9 °F (-13.4 °C)

Freezing Point: -244.8 °F (-153.8 °C) The melting or freezing point value presents an interesting and not infrequent issue that AristaTek has encountered in developing the PEAC-WMD database of chemical properties. The melting point as displayed by CDC's ATSDR, International Programme on Chemical Safety (IPCS) and the CHRIS Manual as shown above, is -244.8°F. Yet in the PEAC-WMD database the value is listed and displayed as -256°F. The lower value –256°F is found in other references (e.g., the NIOSH Pocket Guide and the University of Akron Department of Chemistry's Chemical Database). Usually the values are relatively close but there are some cases where discrepancies of this magnitude do occur. Nevertheless, as described in the PEAC-WMD User's Guide, the value shown in the PEAC-WMD database will display the more conservative value of those found in the public domain literature.

Specific gravity: 0.9106 (liquid) at 68 °F (20 °C) (water = 1.00)

Vapor pressure: 2,530 mm Hg at 68 °F (20 °C)

Vapor density: 2.16 (air = 1.00)

Flammability: highly flammable and explosive gas; flammability range is 3.6% to 33% (concentration in air)

Flash point: -108.4 °F (-78 °C)

Synonyms: chloroethene, chloroethylene, 1-chloroethylene, ethylene monochloride, monochloroethylene, monovinyl chloride, MVC, VC, VCM, and vinyl chloride monomer.

Standards and Guidelines:

OSHA PEL (permissible exposure limit) = 1 ppm (averaged over an 8-hour workshift)

NIOSH IDLH (immediately dangerous to life or health) = not yet determined; vinyl chloride is treated as a human carcinogen.

American Industrial Hygiene Association (AIHA) ERPG values

ERPG-1 = 500 ppm

ERGP-2 = 5,000 ppm

ERPG-3 = 20,000 ppm

The U.S. Department of Energy (DOE) Emergency Management Advisory Committee's Subcommittee on Consequence Assessment and Protective Action (SCAPA) has developed TEEL-(1,2,3) values for Vinyl Chloride as follows:

TEEL-1 = 500 ppm

TEEL-2 = 5,000 ppm

TEEL-3 = 20,000 ppm

Incompatibilities: Vinyl Chloride self-polymerizes explosively if peroxidation occurs (e.g., if heated, exposed to sunlight, or mixed with air and contaminants). Avoid contact with oxygen, strong oxidizing agents (such as perchlorates, peroxides, permanganates, chlorates, nitrates, chlorine, bromine and fluorine), aluminum, copper, iron, steel nitrogen oxides; and acetylide forming metals.

Routes of Exposure:

Inhalation Inhalation is the primary route of exposure, and Vinyl Chloride is readily absorbed from the lungs. **Its odor threshold is too high to provide an adequate warning of hazardous concentrations**. The odor of Vinyl Chloride becomes detectable at around 3,000 ppm and the OSHA PEL is 1 ppm (8-hour TWA). Therefore, workers can be overexposed to Vinyl Chloride without being aware of its presence. A 5-minute exposure to airborne concentrations of 8,000 ppm can cause dizziness. As airborne levels increase to 20,000 ppm, effects can include drowsiness, loss of coordination, visual and auditory abnormalities, disorientation, nausea, headache, and burning or tingling of the extremities. Exposure to higher concentrations of Vinyl Chloride for longer durations can cause death, presumably due to central nervous system (CNS) and respiratory depression. The gas is heavier than air and can cause asphyxiation in poorly ventilated or enclosed spaces.

Children exposed to the same levels of Vinyl Chloride as adults may receive a larger dose 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 Vinyl Chloride found nearer to the ground.

Skin/Eye Contact Direct skin contact with escaping compressed gas or liquid Vinyl Chloride can cause frostbite injury, but systemic absorption is negligible. Direct ocular exposure to Vinyl Chloride vapor can cause localized burns or irritation of the conjunctiva and cornea.

Ingestion Ingestion of vinyl chloride is unlikely because it is a gas at room temperature. Small amounts can dissolve in other liquids, but in such small concentrations that acute toxicity is unlikely.

Health Effects:

The primary target of Vinyl Chloride acute exposure is the CNS. Signs and symptoms include dizziness, ataxia, inebriation, fatigue, numbness and tingling of the extremities, visual disturbances, coma, and death.

Vinyl Chloride can irritate the eyes, mucous membranes, and respiratory tract. Escaping compressed gas or liquid can cause frostbite or irritation of the skin and eyes.

Chronic exposure can cause permanent liver injury and liver cancer, neurologic or behavioral symptoms, and changes to the skin and bones of the hand.

Vinyl Chloride's acute CNS effects are likely to be caused by interaction of the parent compound with neural membranes. Other effects appear to be caused by interaction of reactive intermediates with macromolecules.

Acute Exposure: Vinyl Chloride is thought to depress the CNS via a solvent effect on lipids and protein components of neural membranes that interrupts signal transmission. Reactive metabolic intermediates may also cause specific target organ toxicity by covalently bonding to tissue or initiating destructive chain reactions such as lipid peroxidation. There may be a latent period of hours to days between exposure and symptom onset. Vinyl Chloride is rapidly metabolized and the metabolites are eliminated in the urine.

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

CNS: The CNS is the primary target of Vinyl Chloride acute toxicity. The symptoms reported most commonly stem from the anesthetic properties of vinyl chloride; these symptoms include dizziness, ataxia, fatigue, drowsiness, headache, and loss of consciousness. With inhalation exposure, signs and symptoms increase in severity over a range of 8,000 to 20,000 ppm in air. Exposure to higher concentrations for longer durations can cause death, presumably due to CNS and respiratory depression. Sublethal CNS effects resolve quickly when the victim is removed from further exposure

Respiratory: Vinyl Chloride gas inhalation can cause mild respiratory tract irritation, wheezing, and chemical bronchitis. These effects are transient and resolve quickly following removal from exposure. Death may result from respiratory depression.

Exposure to certain chemicals 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.

Hydrocarbon pneumonitis may be a problem in children.

Cardiovascular: Vinyl Chloride may lower the myocardial threshold to the dysrhythmogenic effects of catecholamines; it might predispose patients to ventricular ectopy and fibrillation. In experimental animals, exposure to vinyl chloride has led to ECG abnormalities, including ventricular ectopy, heart block, and T-wave inversions.

Dermal: Exposure to escaping compressed gas or liquid can cause frostbite injury with redness, blistering, and scaling.

Ocular: Exposure to escaping compressed gas or liquid can cause frostbite injury with corneal and conjunctival irritation or burns. High concentrations of vapor can cause eye irritation.

Potential Sequelae: Patients exposed to significant amounts of Vinyl Chloride may not develop symptoms immediately and should be monitored for CNS and respiratory depression and liver and kidney damage for 24 to 48 hours.

Chronic Exposure: Prolonged absorption of Vinyl Chloride can induce hepatotoxicity and hepatic cancers, including angiosarcoma. Portal hypertension and cirrhosis can occur. Vinyl Chloride toxicity is thought to result from the binding of reactive epoxide metabolites to hepatic DNA. Other effects of chronic exposure include sensory-motor polyneuropathy; pyramidal, extrapyramidal, and cerebellar abnormalities; neuropsychiatric symptoms such as sleep disorders, loss of libido, headaches, and irritability; EEG alterations; and immunopathologic phenomena such as purpura and thrombocytopenia. Vinyl Chloride disease is a syndrome consisting of Raynaud's phenomenon, acroosteolysis (dissolution of the bones of the terminal phalanges and sacroiliac joints), and scleroderma-like skin changes.

Carcinogenicity: The U.S. Department of Health and Human Services (DHHS) and the International Agency for Research on Cancer (IARC) have classified Vinyl Chloride as a known human carcinogen. Vinyl Chloride has caused angiosarcoma of the liver in heavily exposed workers. It is also suspected to cause cancer of the brain, lungs, gastrointestinal tract, and lymphatic/hematopoietic system.

Reproductive and Developmental Effects: Vinyl Chloride is 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. However, there is no conclusive evidence of reproductive or developmental effects in humans. A few case reports describe decreased libido or fertility in men with chronic occupational exposure, and some animal studies also support this finding. Some studies in experimental animals have reported developmental toxicity associated with high-dose exposures, but Vinyl Chloride is not considered a developmental toxicant.

Special consideration regarding the exposure of pregnant women is warranted, since vinyl chloride has been shown to be a genotoxin; thus, medical counseling is recommended for the acutely exposed pregnant women.

In using the PEAC application we access information for the chemical by first locating Vinyl Chloride in the database. The following figures show the screens displayed for chemical properties, Figure 2-3 for the *PEAC-WMD for Windows* application and Figure 4-8 for the *PEAC-WMD for the Pocket PC* application.

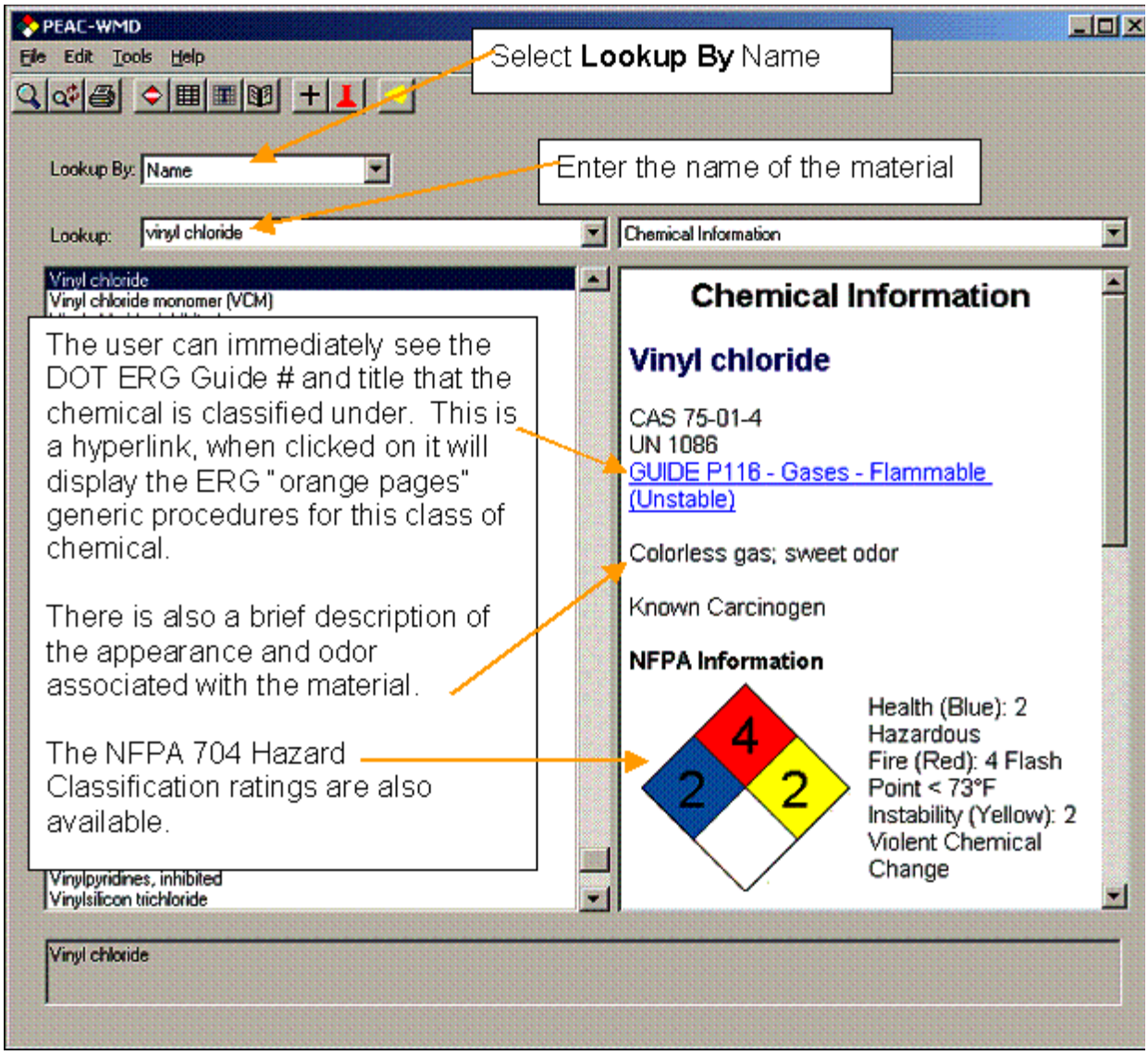


Figure 2 - Using the Lookup By: Name for Vinyl Chloride using the PEAC-WMD for Windows application

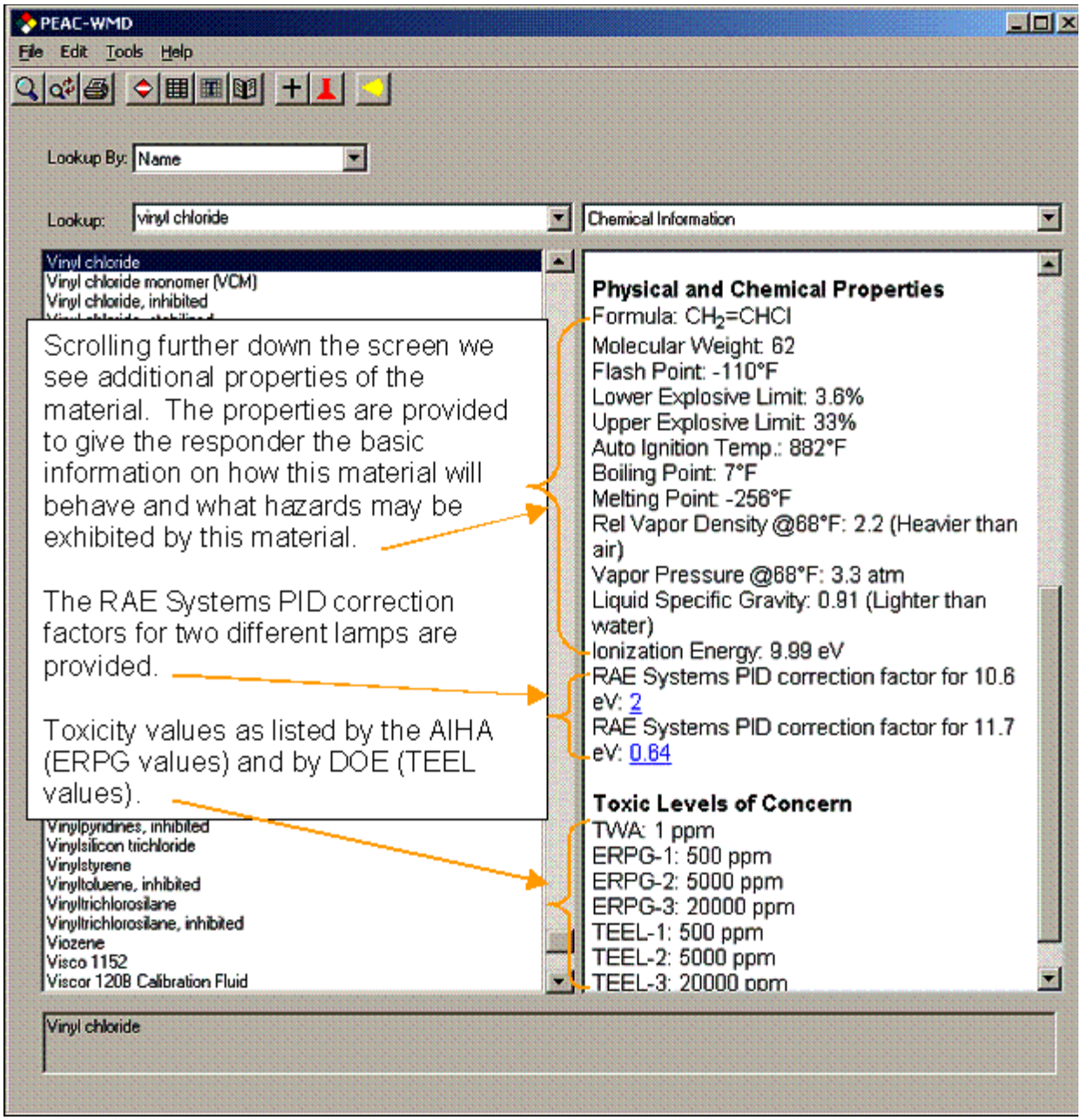


Figure 3 – Bottom portion of the Chemical Information Screen for Vinyl Chloride using the PEAC-WMD for Windows application

Review of the information displayed in the chemical properties screen whether in Figure 2 and 3 (above) or Figures 4-8 (below), show chemical properties values discussed earlier in this discussion. As you can see below, the published toxicity values, e.g., ERPGs (Emergency Response Planning Guidelines) published by the American Industrial Hygiene Association and the TEELs (Temporary Emergency Exposure Limits) published by Department of Energy are provided. We will use the ERPG-1 as the Level of Concern when we develop the Protective Action Distance (PAD) a little later.

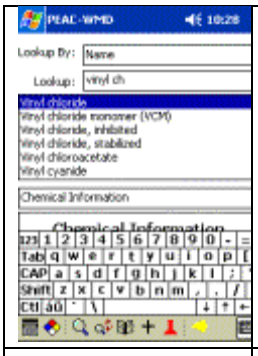
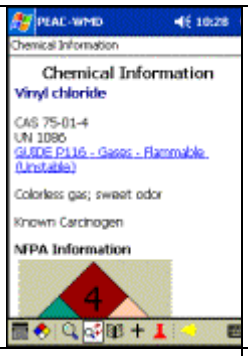
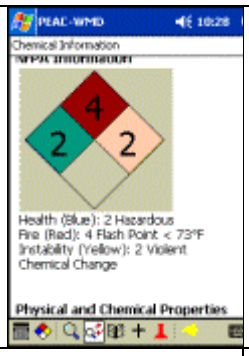
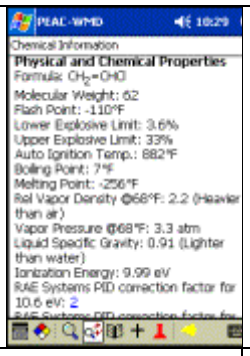
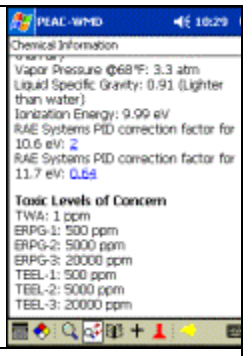
				

Figure 4 **Selecting Vinyl Chloride using the PEAC-WMD for Pocket PC application**	**Figure 5** **The first portion of the Chemical Information screen**	**Figure 6** **The second portion of the Chemical Information screen**	**Figure 7** **The third portion of the Chemical Information screen**	**Figure 8** **The final portion of the Chemical Information screen**

The new release of the PEAC-WMD application provides additional information and features the user can easily access by a simple click on the screen or selection from a screen menu. As an example, the user can toggle on the automatic Glossary feature by clicking on the Glossary icon [] that appears at the top of the screen in the Windows version of the application. With the Glossary toggle ON, those terms that appear in the Glossary portion of the PEAC-WMD application will appear in a different colored font on the display. If the cursor is clicked on the term, a screen will appear that displays the definition of that term. An example is shown in Figure 9, where the term **Carcinogen** is clicked on in the Chemical Information screen and the definition of the term is displayed.

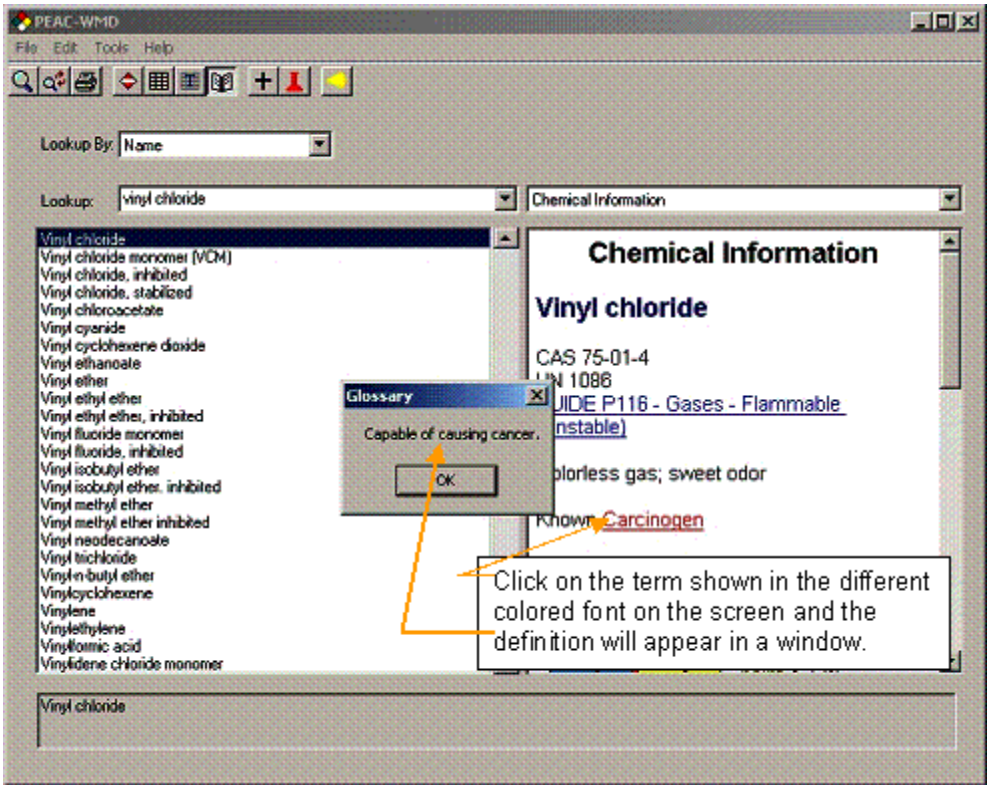


Figure 9 – Example of using the Glossary feature in the PEAC-WMD application

Another example of the additional information provided in the new release is the access to the EPA Reactivity Information. This information is used when two or more chemicals might be mixed or come in contact and the responder wants to assess their potential reactions but it is also a good resource of specific information on documented reactions for a single material. Figure 10 provides a partial display of the EPA Reactivity Information for Vinyl Chloride (the screen is displayed in the Full Screen mode which is toggled by clicking on the [ ] icon at the top left of the screen.

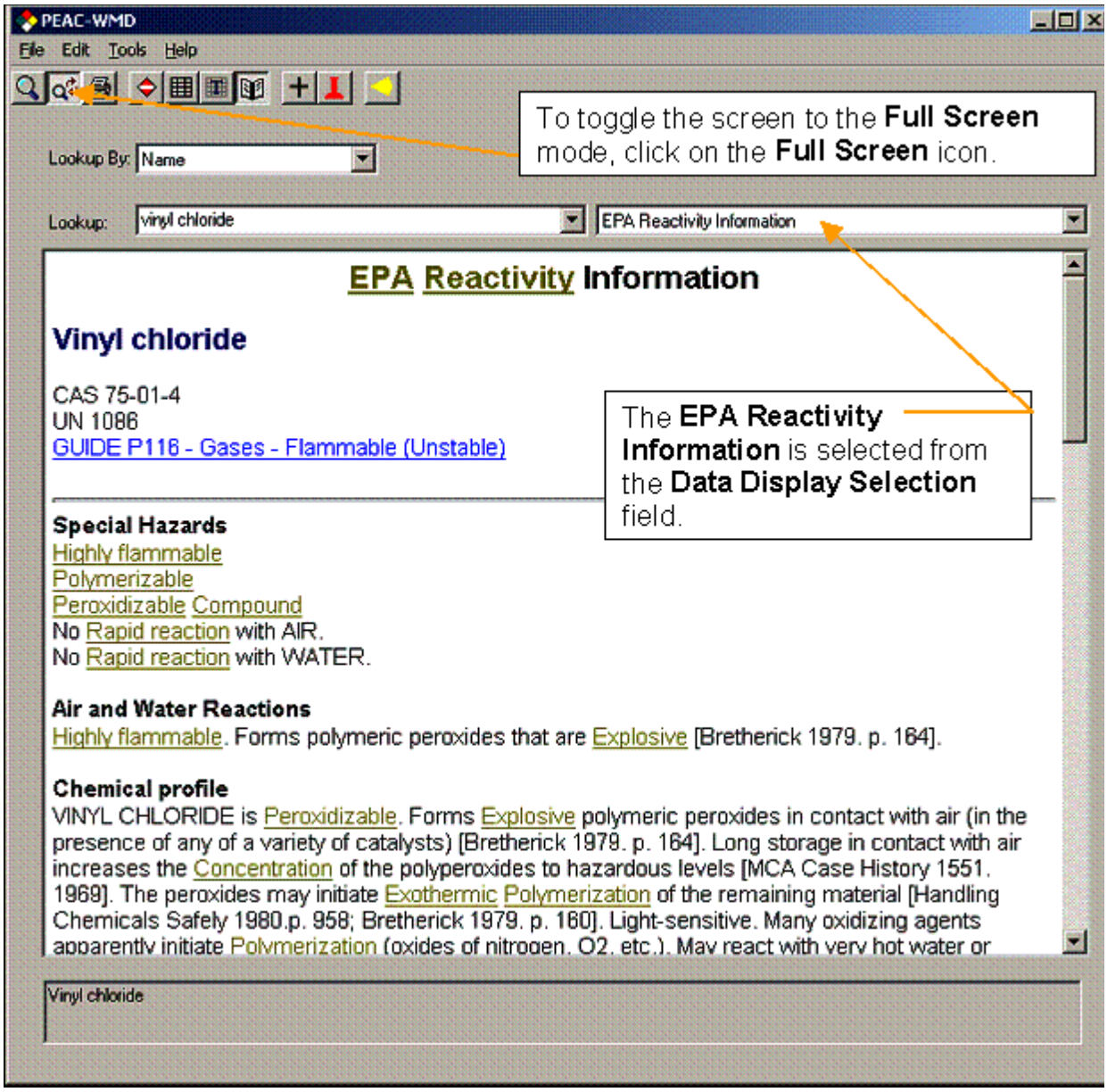


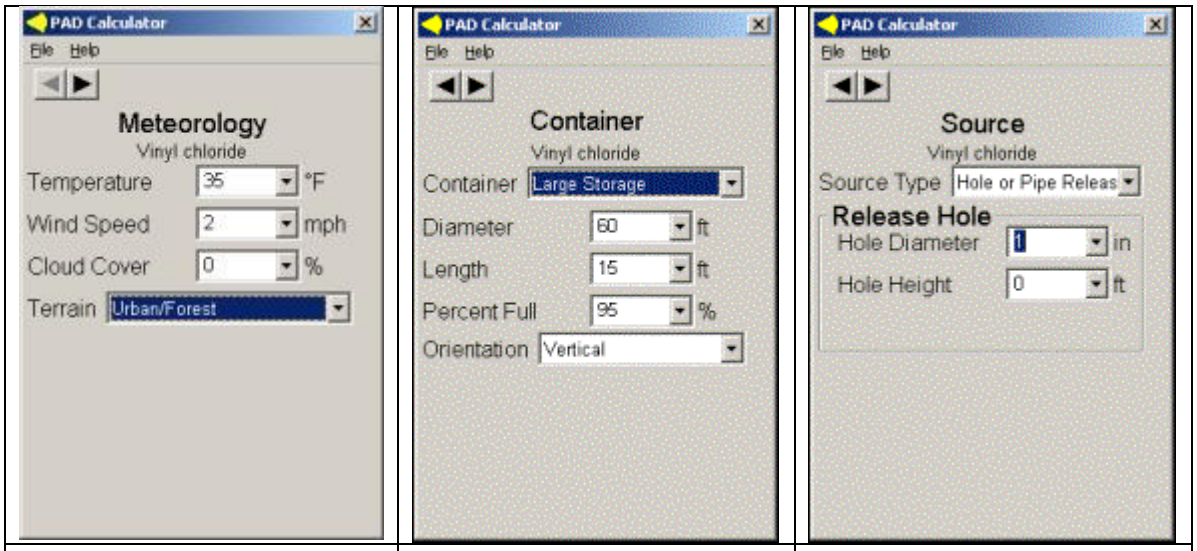
Figure 10 – Viewing the EPA Reactivity Information in the Full Screen mode

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 Chloride as the involved chemical we'll set the location to be plastics manufacturing facility located outside Detroit, MI. The date is February 10, 2005, about 1:30 AM with a temperature of 35°F, wind speed of 2 mph and a clear sky. The hypothetical release involves a large storage tank (15' in diameter and 60' high) that contains Vinyl Chloride and a 1" valve has been knocked off the bottom of the tank. 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 Detroit 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 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 scenario to see what our Protective Action Distance should be.



Meteorology	Container	Source
It's Detroit in February and the temperature about 35°, wind is set for 2 mph, clear skies and the terrain is **Urban/Forest** since it's a processing facility setting.	We have selected from our list of container sizes the **Large Storage** selection with a 15' diameter and a 60' tall. This gets us a quick estimate of how much material might be involved.	We have selected a **Hole or Pipe Release**, and since the liquid boils at 7°F it will be released as a liquid from the bottom of the tank that will flash to an aerosol/vapor mixture very quickly.

Figure 11 – Calculating a PAD using the PEAC-WMD System

By pressing the right arrow at the top of the screen, the PEAC system will calculate a PAD based on the default value of 1 ppm. This will cause a warning window to be displayed letting the user know the PAD exceeds a threshold of 7 miles (11.3 km) and be aware of changes in meteorology and terrain that can vary over extended distances. For our example, we'll select a different Level of Concern (the ERPG-1 or 500 ppm) and the distance will be calculated and displayed as shown in Figure 12.

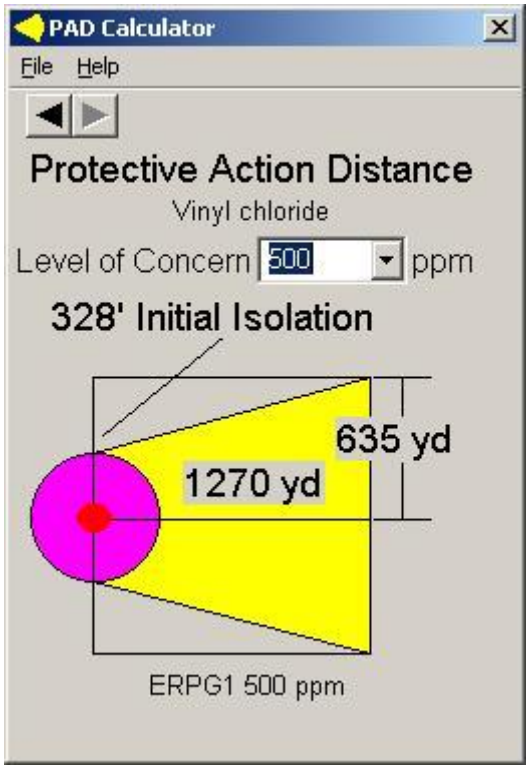


Figure 12 –PAD for Vinyl Chloride using the ERPG-1 of 500 ppm

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

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/