Let's Take a PEEK at the PEAC software

by S. Bruce King

This month our example is Acrylonitrile, which has a chemical formula of CH_2=CHCN. Acrylonitrile is a clear, colorless or slightly yellow liquid that is highly volatile and toxic. Acrylonitrile vapor is heavier than air. It has a pungent odor of onion or garlic that but the odor detection level is at a concentration level that does not provide adequate warning of hazardous levels. Acrylonitrile is poisonous by inhalation, ingestion or skin contact. Within the body acrylonitrile releases cyanide.

It is a health hazard because of its toxicity and it is flammable forming mixtures with air that are flammable or explosive. It is shipped as a liquid, since it has a boiling point of 171°F. It is moderately soluble in water (solubility in water is 7.45 g/100 ml) and soluble in most organic solvents.

Acrylonitrile, one of the world's most important industrial chemicals, is produced by catalytic reaction of propylene with ammonia. In 1999, it was reported that approximately 80 plants in 22 countries produce about 10 billion pounds of acrylonitrile each year. It is a raw material in the manufacture of acrylic fibers, styrene plastics, and adhesives. Such fibers and plastics are components of clothing, furniture, appliances, construction materials, motor vehicles, and food packaging. In the past, acrylonitrile was also used as a room fumigant and pediculicide (an agent used to destroy lice).

Synonyms include AN, cyanoethylene, propenenitrile, VCN, vinyl cyanide, carbacryl, fumigain, and ventox. Acrylonitrile reacts with strong oxidizers, acids, alkalies, bromine, amines, and copper. Unless inhibited (usually with methylhydroquinone), acrylonitrile may polymerize spontaneously. It may also polymerize when heated or in the presence of strong alkalies.

OSHA PEL (permissible exposure limit) = 2 ppm (skin) (averaged over an 8-hour workshift).

OSHA STEL (short-term exposure limit) = 10 ppm (over a 15-minute time period).

NIOSH IDLH (immediately dangerous to life or health) = 85 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) = 35 ppm.

Acute Exposure --Some, but not all, of the toxicity of acrylonitrile may be due to the metabolic release of cyanide, which inhibits numerous enzymes, including cytochrome oxidase, resulting in cellular asphyxiation. Toxicity not related to cyanide formation is due to the formation of reactive vinyl groups and epoxide intermediates which can deplete glutathione stores and cause liver damage. The onset of symptoms due to cyanide release may be delayed 4 to 12 hours.

Children do not always respond to chemicals in the same way that adults do. In addition, children of different ages (e.g., *inutero*, infants, toddlers, older children)

may have different responses to certain chemical exposures, and thus, different protocols for managing their care may be needed.

Acrylonitrile has a boiling point of 171°F and a melting point of -116°F. Its molecular weight is 53, and has a relative vapor density is 1.9 (compared to air), so it will seek low areas. It has a vapor pressure of 83 mm Hg at 68°F (0.11 atmosphere). The lower Explosive Limit (LEL) is 3%; the Upper Explosive Limit (UEL) is 17%.

The important thing to remember when dealing with Acrylonitrile is that it is both a very flammable substance and its vapors are toxic. 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 away from heat and flame. Keep away from sources of ignition. Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances. Flammables-area.

Handling - Wash thoroughly after handling. Wash hands before eating. Remove contaminated clothing and wash before reuse. 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. 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 protective 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 or 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. Scoop up with a nonsparking tool, then place into a suitable container for disposal. Remove all sources of ignition. Provide ventilation. Use water spray to reduce vapors or divert vapor cloud drift.

Stability - Stable under normal shipping and handling conditions. However, it may undergo explosive polymerization if uninhibited.

Incompatibilities - Oxidizing agents, acids, bases, copper, copper alloys, heat, light, bromine, silver nitrate, benzyl trimethylammonium hydroxide, peroxides.

Hazardous Decomposition - Hydrogen cyanide, nitrogen oxides, carbon monoxide, carbon dioxide.

Other hazards - Not corrosive to metals.

Health related information - Exposure effects

May cause cancer in humans. Prolonged skin contact results in systemic toxicity and ulceration after a latency period of several hours with the affected skin resembling a second degree thermal burn.

Ingestion - Harmful if swallowed. Symptoms may include: headache, excitement, fatigue, nausea, vomiting, stupor, and coma.

Inhalation - May be fatal if inhaled. Inhalation of high concentrations may cause central nervous system effects characterized by headache, dizziness, unconsciousness and coma. May cause cyanosis, characterized by bluish-colored skin. May cause irritation of the respiratory tract with burning pain in the nose and throat, coughing, wheezing, shortness of breath and pulmonary edema. Exposure to high concentrations may cause weakness, asphyxia, and death.

Skin - Causes skin irritation. Harmful if absorbed through the skin. May cause skin sensitization, an allergic reaction, which becomes evident upon re-exposure to this material. Prolonged and/or repeated contact may cause defatting of the skin and dermatitis. It is toxic in contact with skin.

Eyes - Causes severe eye irritation. May result in corneal injury. Lachrymator. Causes redness and pain.

First aid

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.

Inhalation - Get medical aid immediately. Remove from exposure to fresh air immediately. If breathing is difficult, give oxygen. DO NOT use mouth-to-mouth respiration. If breathing has ceased apply artificial respiration using oxygen and a suitable mechanical device such as a bag and a mask.

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.

Eyes - Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid immediately.

In using the PEAC application we access information for the chemical by first locating Acrylonitrile in the database. The following figures show the screens displayed for chemical properties, Figure 2 for the *PEAC-WMD for Windows* application and Figure 3-6 for the *PEAC-WMD for the Pocket PC* application.

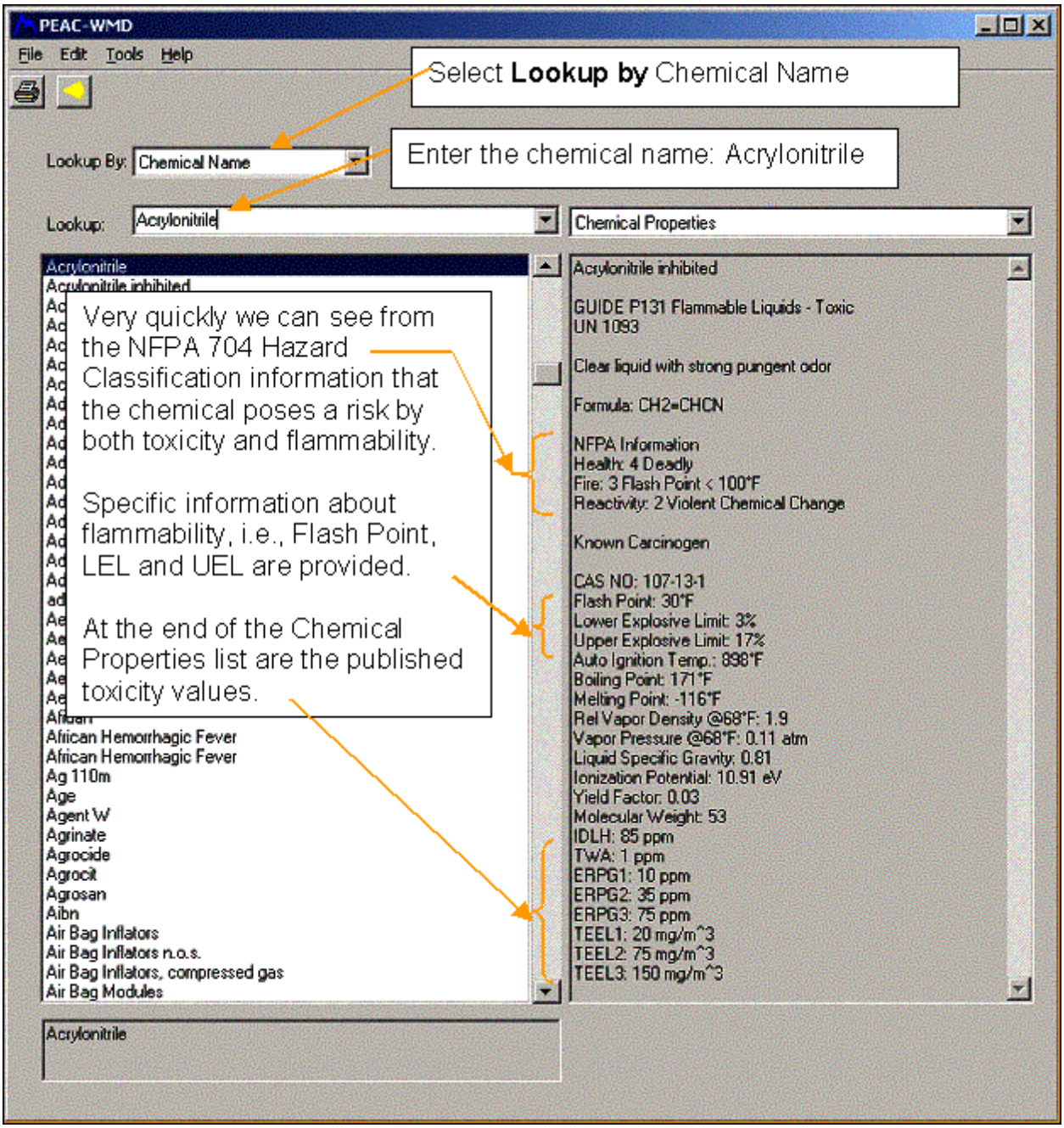


Figure 2 - Using the Lookup By: Name for Acrylonitrile using the PEAC-WMD for Windows application

Review of the information displayed in the chemical properties screen whether in Figure 2 (above) or Figures 3-6 (below), show chemical properties values discussed earlier at the top of this discussion. As you can see, the published toxicity values, e.g., IDLH, ERPGs (Emergency Response Protection Guidelines) published by American Industrial Hygiene Association, 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 3 – Selecting Acrylonitrile using the PEAC-WMD for Pocket PC application

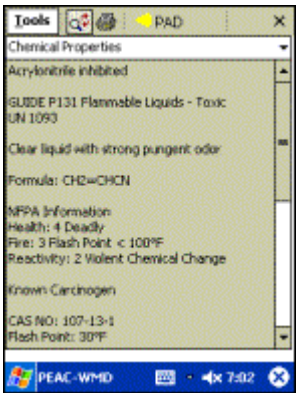


Figure 4 – The top portion of the Chemical Properties Data Display Screen

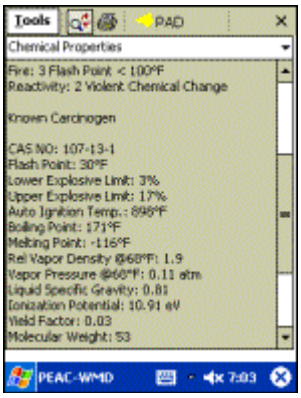


Figure 5 – The middle portion of the Chemical Properties Data Display Screen

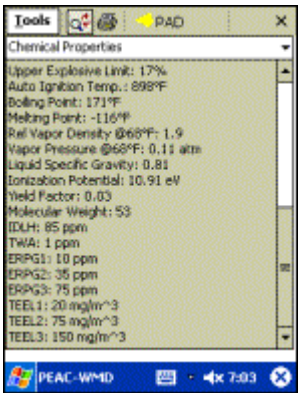


Figure 6 – The lower portion of the Chemical Properties Data Display Screen

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 7) or tapping (if running the Pocket PC version, see Figure 8) 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 (Acrylonitrile in our current example). So the search is done once, and the user is indexed into the different databases easily and quickly.

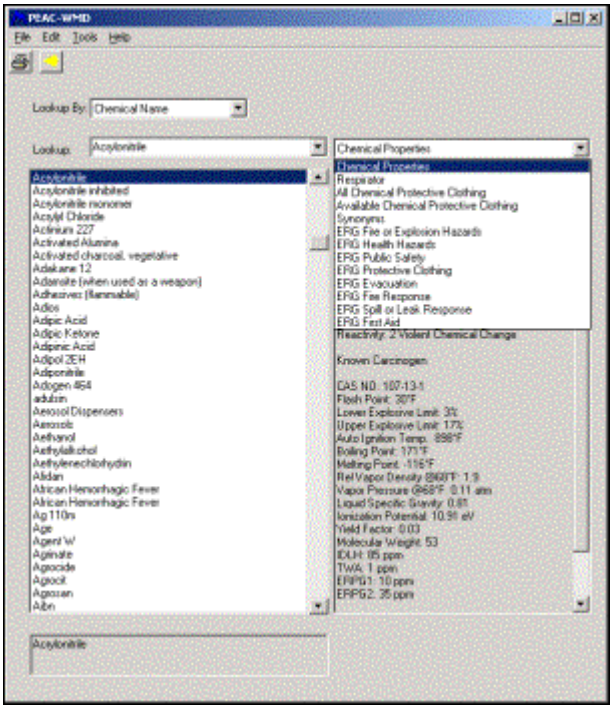


Figure 7 – Accessing other databases from the PEAC-WMD for Windows application

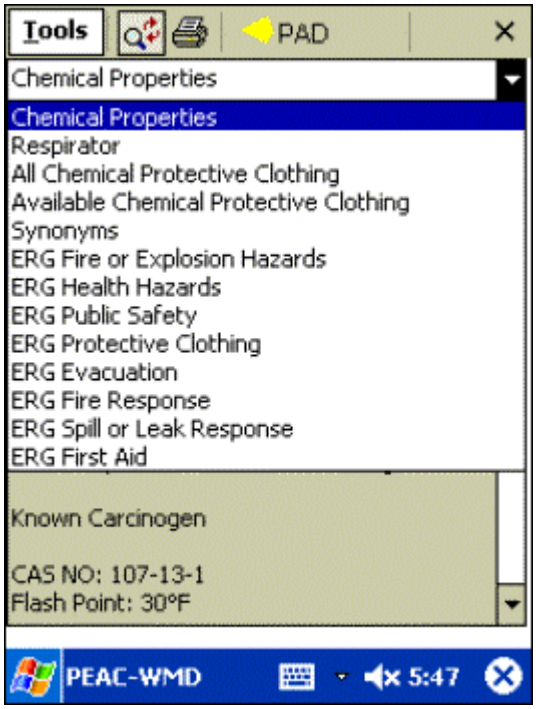


Figure 8 – Accessing other databases from the PEAC-WMD for Pocket PC application

A quick review or sampling of the type of information available in each of these screen 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 9. Likewise the **Chemical Protective Clothing (CPC)** database can be accessed by clicking on either the **All Chemical Protective Clothing** or the **Available Chemical Protective Clothing** selection as shown in Figure 10. The **All Chemical Protective Clothing** displays all the CPC entries in the PEAC-WMD database for the selected chemical vs. the **Available Chemical Protective Clothing** displays just those CPC entries that match the manufacturers the user has previously identified as the products the response organization typically keeps in inventory.

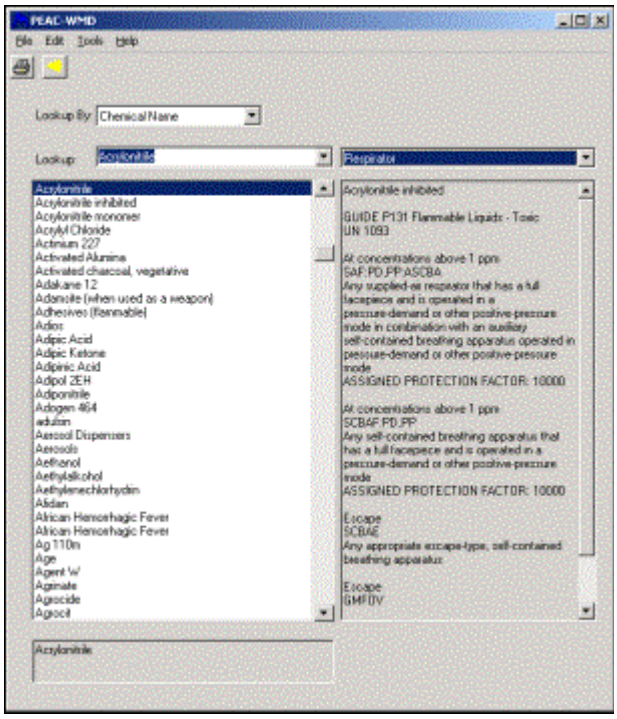


Figure 9 – Respirator Recommendations for Acrylonitrile

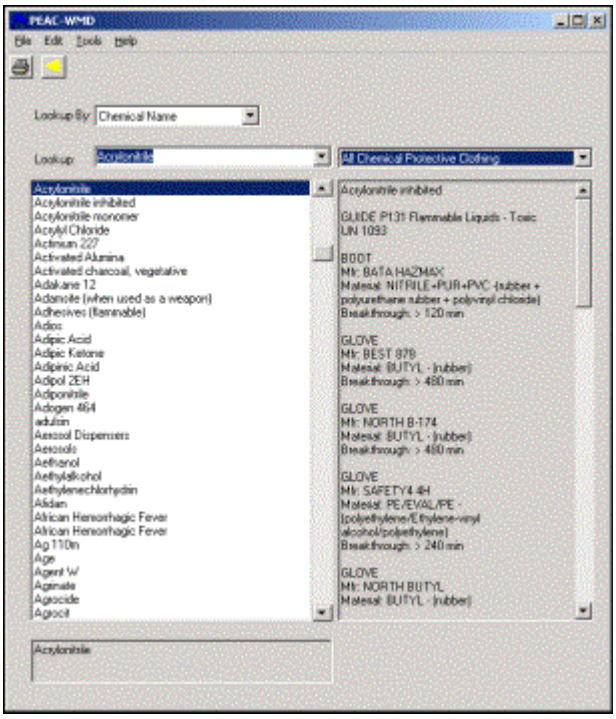


Figure 10 – Chemical Protective Clothing for Acrylonitrile

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 11. 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 12.

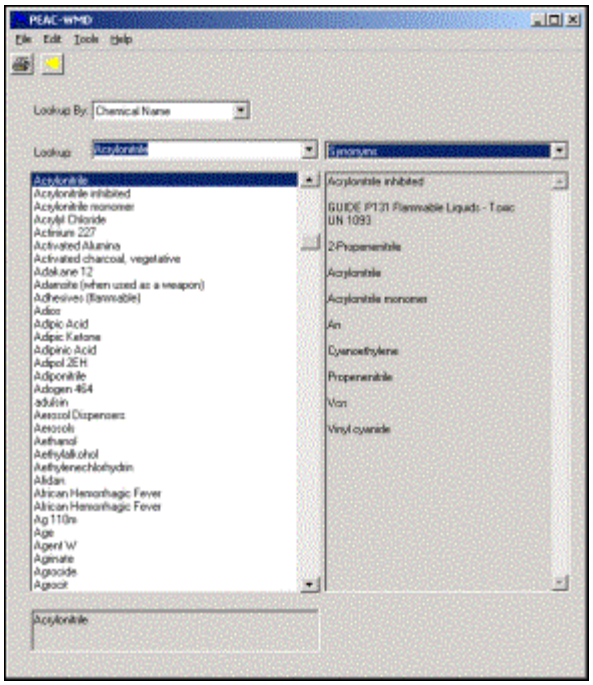


Figure 11 - Synonyms

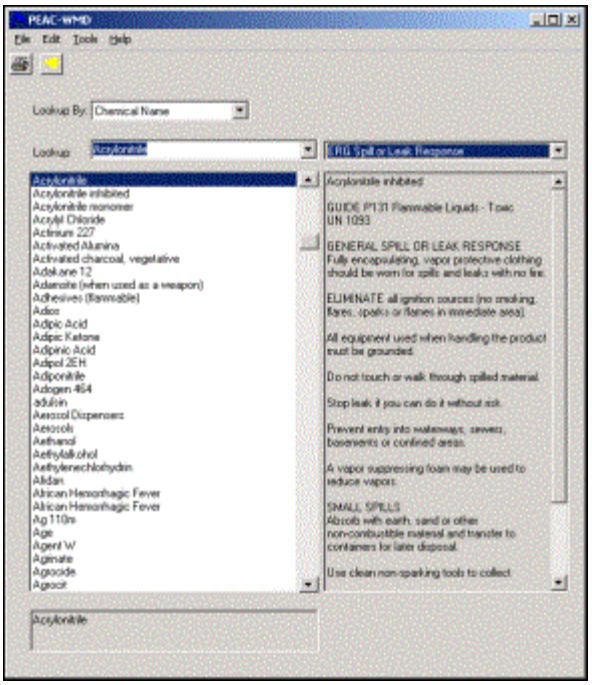
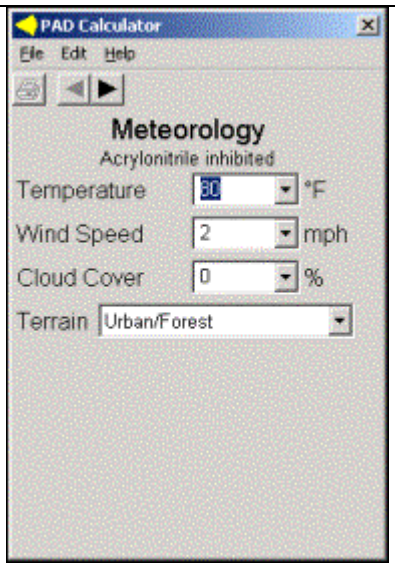


Figure 12 – ERG Spill or Leak Response

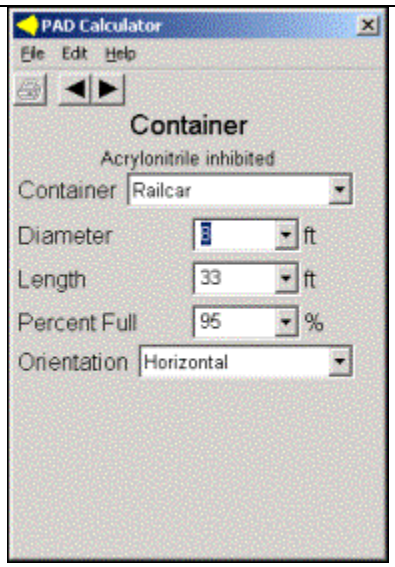
A benefit of using the PEAC tool is assistance in the development of an evacuation zone for those chemicals that produce a toxic vapor cloud. Acrylonitrile will be released from a container as a liquid, but it has a vapor pressure of 83 mm Hg at room temperature and will readily evaporate into the air. 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 Acrylonitrile as the spilled chemical we'll set the location to be on the outskirts of Raleigh, NC and the time as 4:00 AM on May 15th. A railcar of Acrylonitrile on the Norfolk Southern Railroad has been involved in an accident just off US Highway 70 and I-40. There is a 2-3" hole in the railcar, with a liquid pool being formed that is approximately 150' in diameter. The temperature is about 70°F, the winds are about 2 mph, and it's a clear night (no clouds). This is a wooded area with residential and commercial areas nearby and light traffic on the nearby highways.

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 13. 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 Raleigh and the time to 4:00 AM, May 15th.



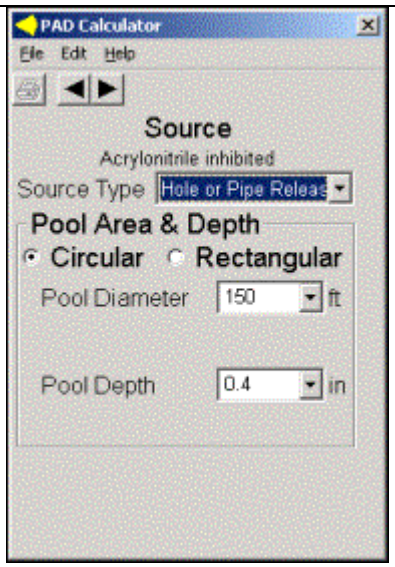
Meteorology

It's Raleigh in May and the temperature about 70°, light wind is set for 2 mph, clear sky so we'll set cloud cover to 0%, and the terrain is Urban/Forest since it's an urban setting.



Container

We have selected from our list of container sizes the **Railcar** selection. This provides us with a default size that should get us pretty close to the actual size.



Source

Since the scenario has a 2-3" hole, we've selected a **Hole or Pipe Release** as the **Source** type of release and specified the size of the liquid pool.

Figure 13 – Calculating a PAD using the PEAC-WMD System

By pressing the right arrow at the top of the screen, the PEAC system will display a screen as shown in Figure 14. This calculates a **PAD** (Protective Action Distance) based on the default **Level of Concern** the IDLH of 85 ppm. This evacuation or standoff distance is based on the toxicity of Acrylonitrile, not its flammability. Since it is flammable, care needs to be given to ignition sources in the immediate vicinity of the release.

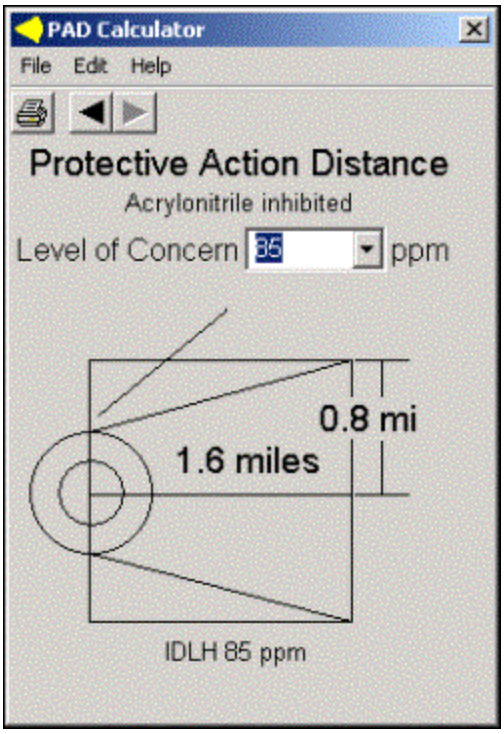


Figure 14 – Default PAD for Acrylonitrile using the IDLH of 85 ppm

Clicking or tapping on the pop up list for the **Level of Concern** a list of published toxicity values for Acrylonitrile is displayed. Clicking or tapping on the ERPG-2 value of 35 ppm (Figure 15) and will allow the PEAC tool to recalculate a PAD for the 35 ppm concentration **Level of Concern**. In our example the PAD for the 35 ppm concentration is displayed (Figure 16).

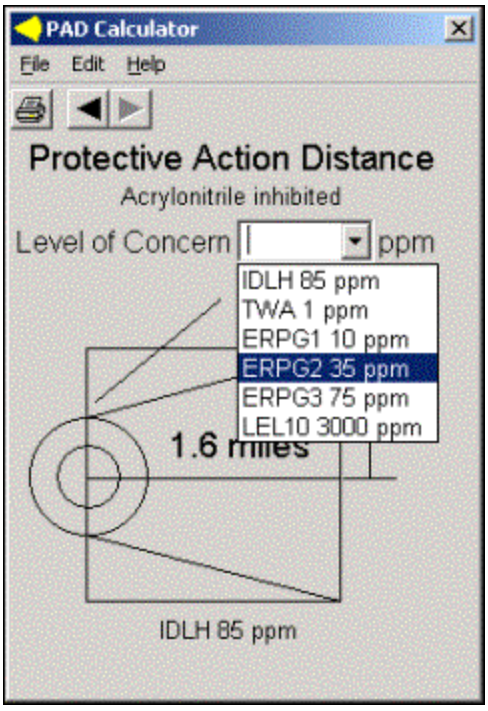


Figure 15– Selecting another Level of Concern

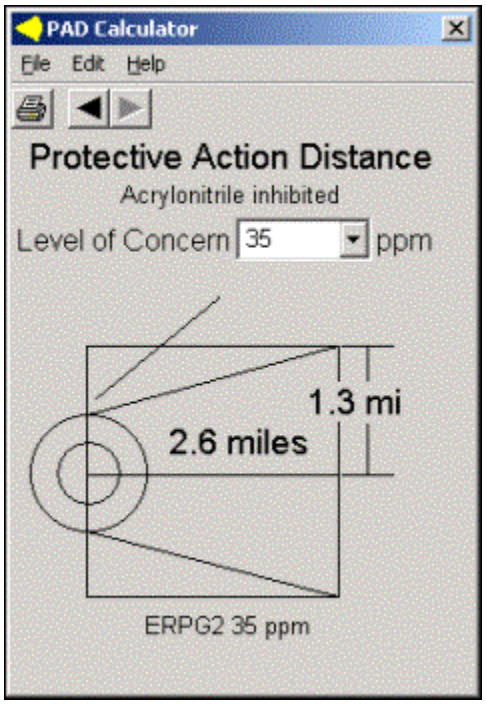


Figure 16 – PAD for ERPG-2 (35 ppm)

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 the web site

provided by International Programme on Chemical Safety (IPCS) INCHEM site located at: http://www.inchem.org/. Additional information was also adapted from the Agency for Toxic Substances and Disease Registry (ATSDR) Web site for Medical Management Guidelines at: http://www.atsdr.cdc.gov/.