Let's Take A Peek at the PEAC software

PEAC Example – Acrolein

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This month our example is Acrolein, which has a chemical formula of CH_2=CHCHO. Acrolein has a United Nations Shipping# of 1092 and Chemical Abstract Service # of 107-02-8. Acrolein is a clear, colorless, or yellow liquid with a pungent, suffocating odor. It is very flammable and may polymerize violently. Acrolein should be stored in a cool, dry, well-ventilated area in tightly sealed containers separated from alkaline materials such as caustics, ammonia, organic amines, or mineral acids, strong oxidizers, and oxygen. Acrolein is soluble in water, alcohol, ether, and acetone.

Persons exposed only to Acrolein vapor do not pose secondary contamination risks. Persons whose clothing or skin is contaminated with liquid Acrolein can contaminate others by direct contact or off-gassing vapor.

At room temperature, Acrolein is a clear, colorless to straw-colored liquid with a pungent, suffocating odor. It is highly flammable and burns to produce toxic gases (peroxides and oxides of carbon). It is volatile, producing toxic concentrations at room temperature. Vapors may travel to a source of ignition and flash back. The odor of Acrolein may not provide adequate warning of hazardous concentrations.

Acrolein is toxic by all exposure routes. Exposure causes inflammation and irritation of the skin, respiratory tract, and mucous membranes. Delayed pulmonary edema may occur after inhalation. Systemic effects may occur after exposure by any route.

Sources/Uses: Acrolein is produced by oxidation of propylene. Acrolein is principally used as a biocide to control plants, algae, mollusks, fungi, rodents, and microorganisms, for example in recirculation cooling systems. Acrolein has also been used in the manufacture of other chemicals, as a warning agent in gases, as a test gas for gas masks, in military poison gases, in the manufacture of colloidal metals, in leather tanning, and as a fixative in histology.

Synonyms include 2-propenal, 2-propen-1-one, prop-2-en-1-al, acraldehyde, acrylaldehyde, acrylic aldehyde, allyl aldehyde, ethylene aldehyde, aqualine.

Routes of Exposure:

Inhalation Inhaled Acrolein is highly toxic. Acrolein is irritating to the upper respiratory tract even at low concentrations. Its odor threshold of 0.16 ppm is similar to the OSHA permissible exposure limit (0.1 ppm); thus odor may provide an adequate warning of potentially hazardous concentrations. Acrolein vapor is heavier than air, but asphyxiation in enclosed, poorly ventilated, or low-lying areas is unlikely due to its strong odor.

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

Skin/Eye Contact Direct contact with liquid Acrolein causes rapid and severe eye and skin irritation or burns. Exposure to vapor produces inflammation of mucous membranes and it is a potent lacrimator.

Because of their relatively larger surface area:body weight ratio, children are more vulnerable to toxicants affecting the skin.

Ingestion Acrolein produces chemical burns of the lips, mouth, throat, esophagus, and stomach. Nausea, vomiting, and diarrhea also occur.

Physical Properties:

Description: Clear, colorless to yellow liquid.

Warning properties: Suffocating, pungent odor at 0.16 ppm.

Molecular weight: 56.06 daltons

Boiling point (760 mm Hg): 126.5 °F (52.5 °C)

Freezing point: -126 °F (-88.0 °C)

Vapor pressure: 210 mm Hg at 68 °F (20 °C)

Gas density: 1.94 (air = 1)

Specific gravity: 0.84 (water = 1)

Water solubility: 208 g/L at 20 °C

Flash point: -15 °F (-26.1 °C)

Flammable range: 2.8% to 31% (concentration in air)

Standards and Guidelines

OSHA PEL (permissible exposure limit) = 0.1 ppm as an 8-hr

TWA concentration and 0.3 ppm as a 15-minute TWA short-term exposure limit (STEL).

NIOSH IDLH (immediately dangerous to life or health) = 2 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) = 0.5 ppm.

Incompatibilities: Acrolein reacts with caustics, ammonia, organic amines, or mineral acids, strong oxidizers, and oxygen.

Health Effects:

Acrolein is severely irritating to skin, eyes, and mucous membranes. Inhalation of Acrolein may result in respiratory distress and delayed pulmonary edema. Contact with the skin or eyes produces irritation and lacrimation, and can result in chemical burns.

The mechanism by which Acrolein produces toxic symptoms is not known, but the compound is highly reactive. No information was found as to whether the health effects of Acrolein in children are different than in adults. Exposure to Acrolein produces severe respiratory problems and individuals with pre-existing breathing difficulties or skin disease may be more susceptible to its effects.

Acute Exposure: The mechanism by which Acrolein produces toxic symptoms is not known, but the compound is highly reactive, cross-links DNA, and inhibits the activities of some enzymes (including cytochrome P450 and glutathione-S-transferase) *in vitro* by reacting with sulfhydryl groups at the active sites. It has also been shown to suppress pulmonary antibacterial defenses, to release oxygen radicals, and to react with proteins. Onset of irritation is immediate, but pulmonary edema may be delayed and respiratory insufficiency may persist for up to 18 months after exposure.

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

Respiratory Acrolein produces irritation of the respiratory tract, increases airway resistance and tidal volume, and decreases respiratory frequency. It is also ciliastatic. Exposure to Acrolein vapor concentrations as low as 10 ppm can lead to pulmonary edema and death. Inhalation may also cause an asthmatic reaction in sensitized individuals.

Acrolein is a weak sensitizer.

Children may be more vulnerable because of higher minute ventilation per kg of body weight and failure to evacuate an area promptly when exposed.

Dermal Acrolein is a skin irritant. Contact with the liquid may cause skin burns, erythema, and edema.

Because of their relatively larger surface area:body weight ratio, children are more vulnerable to toxicants affecting the skin.

Ocular/Ophthalmic Acrolein liquid or vapor can cause eye irritation and damage to the cornea.

Gastrointestinal Acrolein causes burns of the lips, mouth, throat, esophagus, and stomach. Nausea, vomiting, and diarrhea have been reported. No data were located as to whether ingestion leads to systemic toxicity in humans.

Cardiovascular Acrolein inhalation may cause hypertension and tachycardia.

CNS Serious poisoning may cause CNS depression.

Immunologic Acrolein may have the potential to be immunotoxic. The immune system in children continues to develop after birth, and thus children may be more susceptible to certain chemicals.

Potential Sequelae Respiratory insufficiency may persist for up to 18 months after exposure.

Chronic Exposure: Apart from rare cases of sensitization, no adverse effects in humans chronically exposed to low concentrations of Acrolein have been reported.

Chronic exposure may be more serious for children because of their potential for a longer latency period.

Carcinogenicity The Department of Health and Human Services has determined that Acrolein may possibly be a human carcinogen. The International Agency for Research on Cancer has determined that Acrolein is not classifiable as to its carcinogenicity to humans.

Reproductive and Developmental Effects No studies were located that address reproductive or developmental effects of Acrolein in humans. Acrolein caused developmental effects when injected into rats, but did not cause developmental effects when ingested by rabbits. No information was found as to whether Acrolein crosses the placenta, but it has been measured in breast milk.

Acrolein 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.

Using the PEAC application

In using the PEAC application we access information for the chemical by first locating Acrolein in the database. The following figures show the screens displayed for chemical properties, Figure 1 for the *PEAC-WMD for Windows* application. Last month we started demonstrating some of the features coming out in the new release. The screens captured from the Windows version are from the new release. The Pocket PC version is not quite finished, so the author has not included figures from that version.

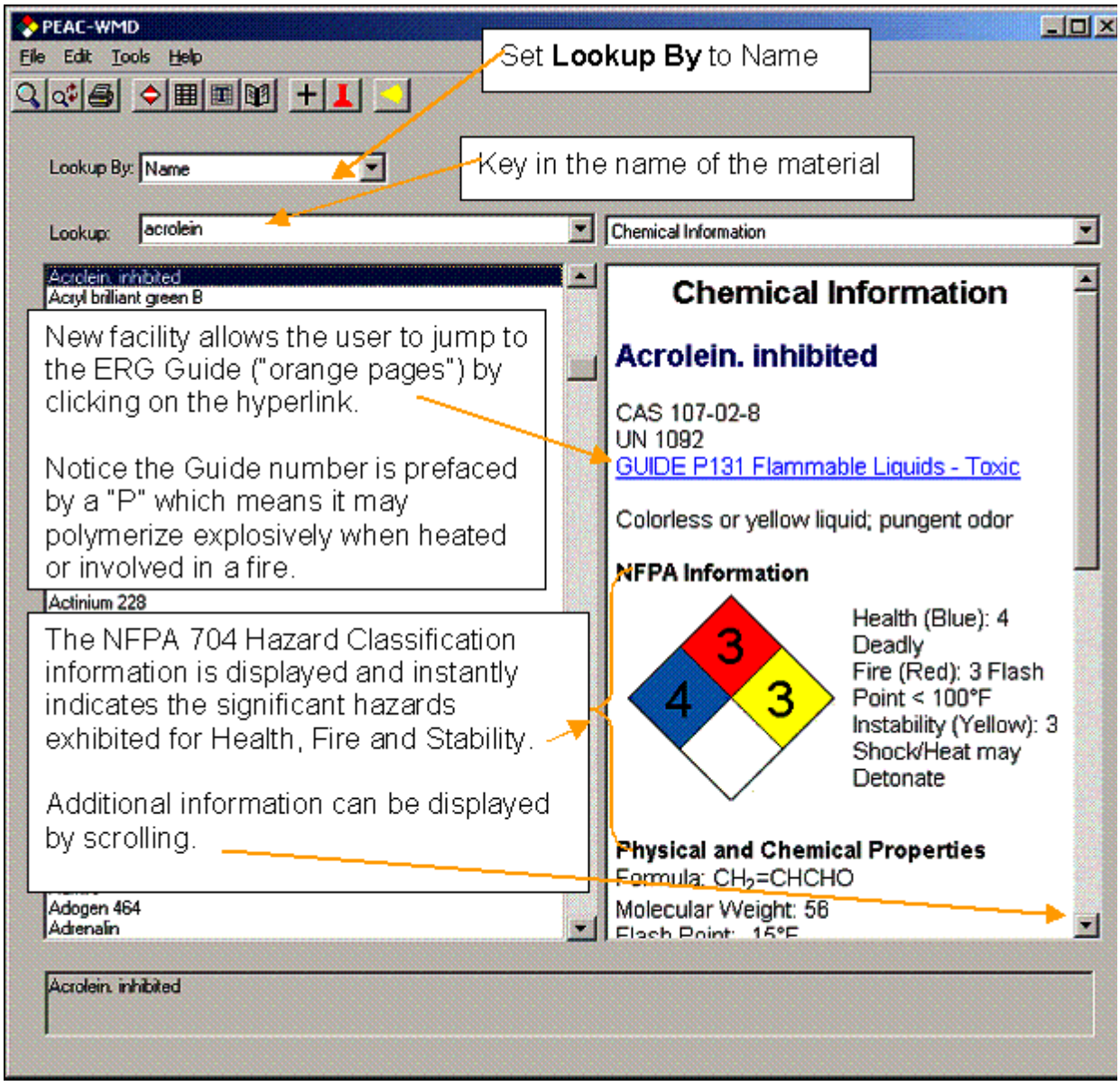


Figure 1 - Using the Lookup By: Name for Acrolein using the PEAC-WMD for Windows application

One of the features of the new release is the inclusion of hyperlinks in the text display fields. In this case the ERG Guide number and name are displayed as a hyperlink. If the user clicks on the hyperlink, the ERG Guide or "orange pages" will be displayed in the **Data Display Box** (Figure 2). If the material has an entry in the "green pages" of the ERG, this will be displayed at the top of the Data Display Box above the "orange pages". Acrolein is an example of such a material as shown in Figure 2. As shown in Figure 1, the Guide number is prefaced by a "P", meaning the material may polymerize explosively when heated or involved in a fire.

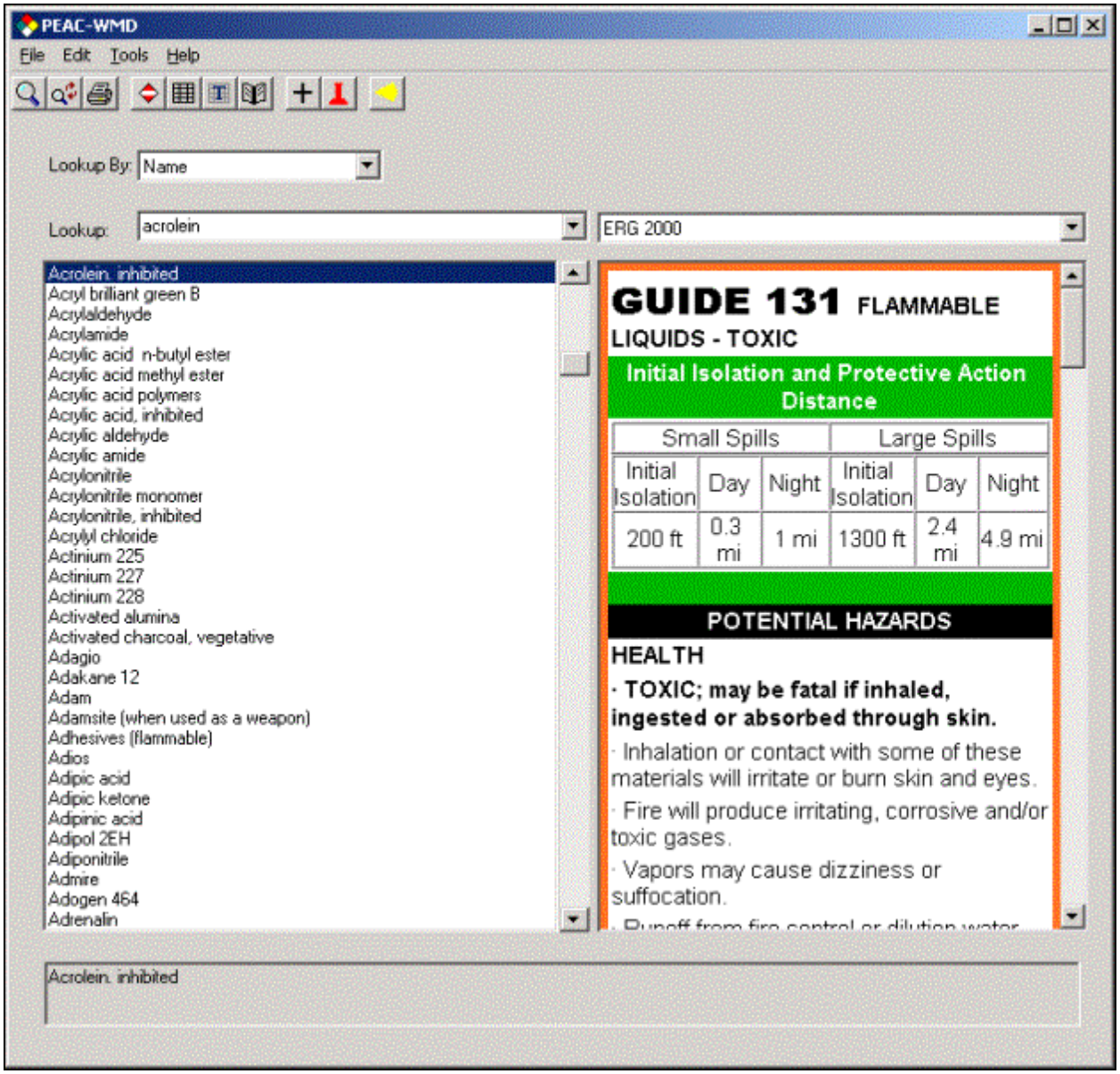
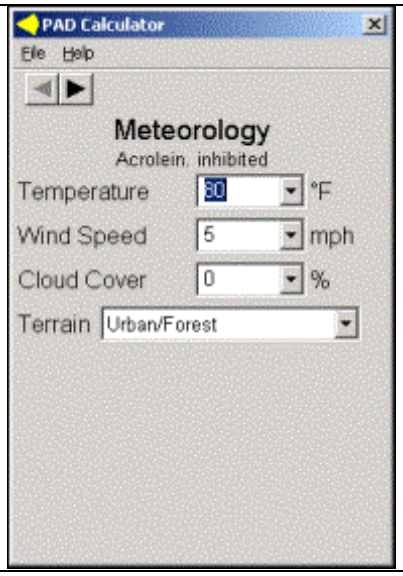


Figure 2 – Displaying the ERG Guide information after clicking on the hyperlink

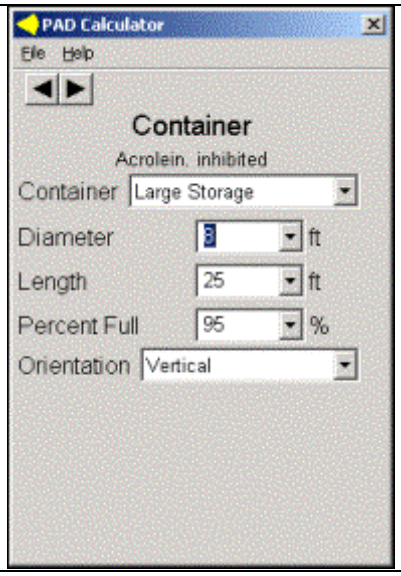
An advantage of using the PEAC tool is assistance in the development of an evacuation zone for those chemicals that produced a toxic vapor cloud. As with all of our examples, AristaTek creates a scenario for a spill or release of the specific chemical and then we work through the development of a PAD (Protective Action Distance) to demonstrate how the PAD calculation portion of the PEAC system works. For our scenario using Acrolein as the spilled chemical we'll use a chemical manufacturing facility in Denver CO. It's 1:40 PM on Sept 10th , the temperature is about 80°F, the winds are 5 mph, and it's a sunny day with no clouds. A storage tank (8' x 25') in the facility that contains Acrolein has lost most of its contents. Fortunately the Acrolein storage the tank and surrounding tanks are contained by a 50' x 50' dike around the tanks that has contained the leaking material. Upon arrival at the scene the HAZMAT response team observes the tank and the liquid pool. A concern is how far to evacuate personnel and the public to prevent inhalation of the toxic material. Another concern is how far to evacuate with regards to the potential flammability of the material.

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 on the PAD icon will display a screen as shown in Figure 3. 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.



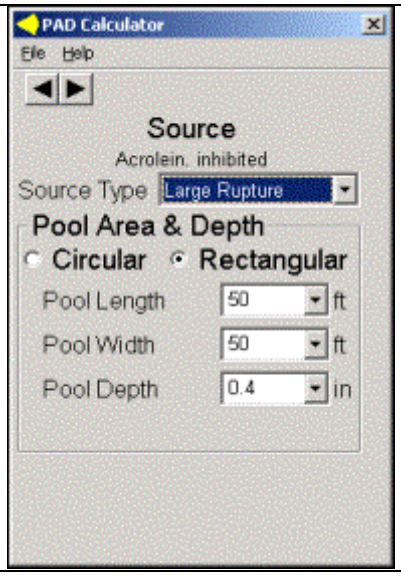
Meteorology

It's Denver in September and the temperature about 80°, wind is set for 5 mph, no clouds and the terrain is Urban/Forest since it's an urban setting (manufacturing facility).



Container

We have selected from our list of container sizes the **Large Storage s**election and filled in the dimensions of the tank.



Source

Since the scenario has most of the contents released we'll use a **Large Rupture** and specify the size of the liquid pool as the size of the dike area around the storage tanks.

Figure 3 – Calculating a PAD using the PEAC System

After specifying the release or source is a **Large Rupture** and specifying the size of the liquid pool (this is because the Acrolein has a boiling point of 127°F and should be a liquid when released from the tank) the user taps the right arrow at the top of the screen and the PAD computation results are displayed, see Figure 4.

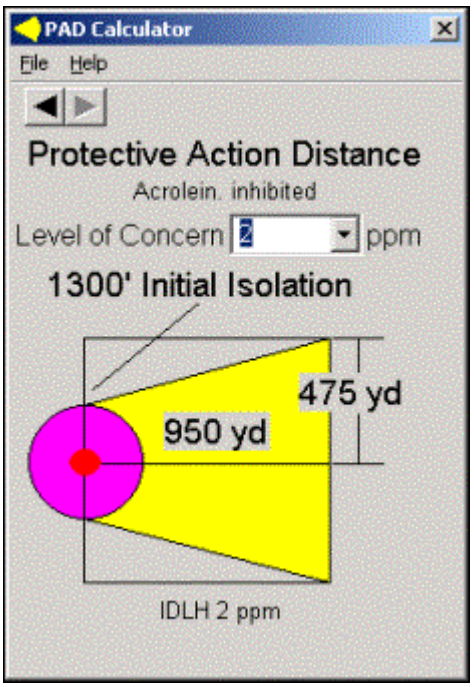


Figure 4 - The PEAC computation for PAD using the IDLH

This PAD (Protective Action Distance) is based on the default **Level of Concern** or the IDLH, which is 2 ppm. The user may want to go with a more conservative value like the ERPG-2, which is 0.5 ppm as shown in Figure 5. The results for this PAD are shown in Figure 6.

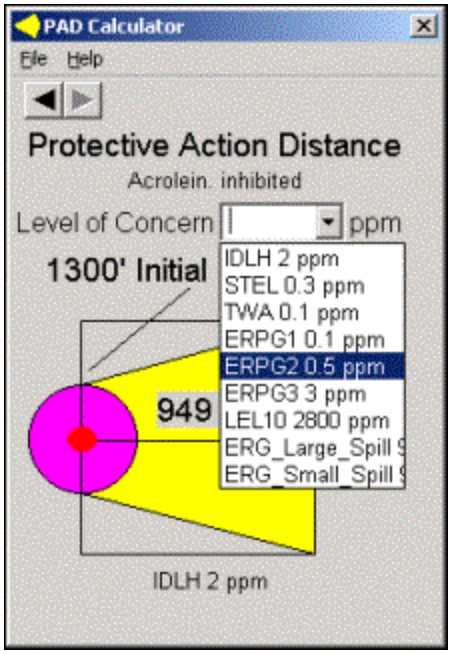


Figure 5 – Selecting a different Level of Concern from the drop-down menu

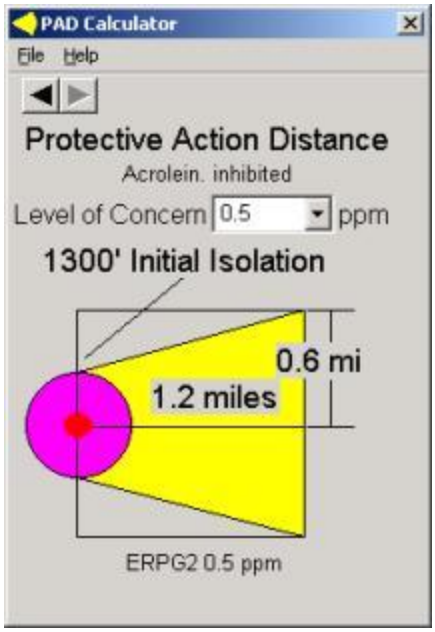


Figure 6 - The PEAC computation for PAD using the ERPG-2

These PADs are only looking at the toxicity aspect and not the flammability issues related to Acrolein. A quick check of the DOT ERG "orange pages" indicates a proper evacuation distance for Guide Number 131 when a fire may be involved is ½ mile if a railcar or tank truck are involved, see Figure 7. While our scenario is not a railcar or tank truck, the volume is close enough that to be safe we would want to move the public back at least that distance in case the vapor cloud was to ignite.

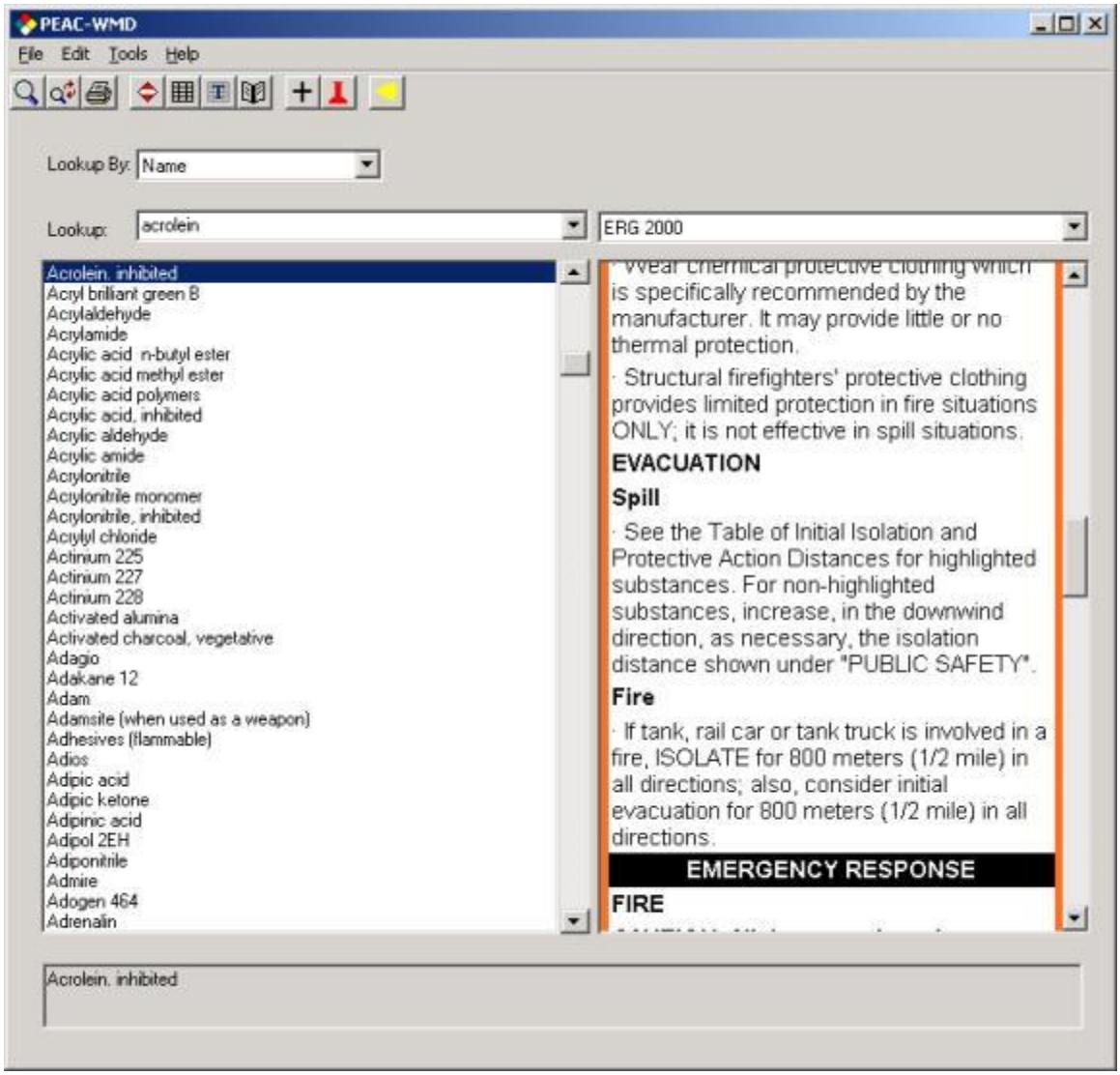


Figure 7 – Additional guidelines if a fire was involved

Portions of this discussion on Acrolein were adapted from the ATSDR Medical Management Guideline document, which can be downloaded from the ADSTR web site at: http://www.atsdr.cdc.gov/mmg.html.