Let's Take A PEEK at the PEAC Software

PEAC Example–Crotonaldehyde

by S. Bruce King

This month our example is Crotonaldehyde, which has a chemical formula of (C_4H_6O). Crotonaldehyde is listed under the UN # (United Nations Number) by the US Department of Transportation: UN 1143. Crotonaldehyde exists as one of two isomers; the *trans* isomer is listed as CAS# (Chemical Abstract Service Number) 4170-30-3 and CAS 123-73-9, while the *cis* isomer is listed as CAS# 15798-64-8.

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

At room temperature, Crotonaldehyde is a clear, colorless to straw-colored liquid with a pungent, suffocating odor. It is highly flammable and burns to produce carbon dioxide and some toxic gas carbon monoxide. It is volatile, producing toxic concentrations at room temperature. Vapors may travel to a source of ignition and flash back. The odor of Crotonaldehyde provides adequate warning of hazardous concentrations.

Crotonaldehyde is highly toxic by all routes. Exposure causes inflammation and irritation of the skin, respiratory tract, and mucous membranes. Delayed pulmonary edema may occur after inhalation. Systemic effects occur in animals after oral exposure, but have not been reported in humans.

Description Crotonaldehyde exists in two isomeric forms (*cis* and *trans*) that have similar properties and effects. Crotonaldehyde is produced commercially as a mixture of the two isomers (>95% *trans* and <5% *cis*). At room temperature, the mixture is a clear, colorless liquid that turns yellow upon contact with air or exposure to light. It has a pungent, suffocating odor. Crotonaldehyde should be stored in a cool, dry, well-ventilated area in tightly sealed containers. It is very flammable and may polymerize violently. Crotonaldehyde should be stored separately from alkaline materials such as caustics, ammonia, organic amines, or mineral acids, strong oxidizers, and oxygen. Crotonaldehyde is soluble in water, alcohol, ether, acetone, and benzene.

Sources/Uses Crotonaldehyde is generally produced by aldol condensation of acetaldehyde, followed by dehydration. A process involving direct oxidation of 1,3-butadiene to Crotonaldehyde with palladium catalysis has also been reported. Crotonaldehyde is produced during the combustion of paper, cotton, and plastics, and is a component of cigarette smoke.

Crotonaldehyde was formerly used in the manufacture of n-butanol, but currently, the most extensive use of Crotonaldehyde is in the manufacture of sorbic acid. Crotonaldehyde has also been used as a warning agent in fuel gases, in the preparation of rubber accelerators, in leather tanning, as an alcohol denaturant, and as a stabilizer for tetraethyl-lead.

Physical Properties:

Description: Clear, colorless liquid that becomes yellow with exposure to light or air.

Warning properties: Sharp, pungent odor at 0.035 to 0.12 ppm; adequate warning of acute or chronic exposures.

Molecular weight: 70.09 daltons

Boiling point (760 mm Hg): 215.6 °F (102 °C)

Freezing point: -105.7 °F (-76.5 °C)

Vapor pressure: 19 mm Hg at 68 °F (20 °C)

Gas density: 2.41 (air = 1)

Specific gravity: 0.85 (water = 1)

Water solubility: 181 g/L at 20 °C

Flammability: 55 °F (13 °C)

Flammable range: 2.1% to 15.5% (concentration in air)

Synonyms: beta-methylacrolein; propylene aldehyde; ethylene propionate; crotonic aldehyde; but-2-enal; 2-butenal; crotonal; topanel; methyl acrolein; butenal; crotonaldehyde inhibited; (E)-crotonaldehyde; (E)-2-butenal; trans-2-butenal.

Standards and Guidelines:

OSHA PEL (permissible exposure limit) = 2 ppm.

NIOSH IDLH (immediately dangerous to life or health) = 50 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) = 10 ppm.

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

Routes of Exposure:

Inhalation Inhaled Crotonaldeyhyde is highly toxic. Crotonaldehyde is irritating to the upper respiratory tract even at low concentrations. Its odor threshold of 0.035 to 0.12 ppm is lower than the OSHA permissible exposure limit (2 ppm); thus, odor may provide an adequate warning of potentially hazardous concentrations. Crotonaldehyde 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 Crotonaldehyde vapor as adults may receive a larger dose because they have greater lung surface area:body weight ratios and higher minute volume: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 Crotonaldehyde vapor found nearer to the ground.

Skin/Eye Contact Crotonaldehyde is highly toxic by the dermal route. Direct contact with liquid Crotonaldehyde 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 No information was located pertaining to ingestion of Crotonaldehyde by humans. Crotonaldehyde is very irritating; thus, ingestion would probably produce chemical burns of the lips, mouth, throat, esophagus, and stomach. In animal studies, ingestion has led to systemic toxicity.

Health Effects

Crotonaldehyde is severely irritating to skin, eyes, and mucous membranes. Inhalation of Crotonaldehyde 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 Crotonaldehyde produces toxic symptoms is not known, but the compound is highly reactive. No information was found as to whether the health effects of Crotonaldehyde in children are different than in adults. Exposure to Crotonaldehyde 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 Crotonaldehyde produces toxic symptoms is not known, but the compound is highly reactive, cross-links DNA, and inhibits the activities of some enzymes *in vitro*, including cytochrome P450 and aldehyde dehydrogenase. *In vitro* treatment of human polymorphonuclear leukocytes with Crotonaldehyde produced a dose-related decrease in surface sulfhydryl and soluble sulfhydryl groups and inhibition of superoxide production. Onset of irritation is immediate, but pulmonary edema may be delayed.

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

Respiratory Crotonaldehyde produces irritation of the respiratory-tract. Relatively high-concentration inhalation can lead to pulmonary edema. Clinical cases of sensitization have been reported.

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

Dermal Crotonaldehyde is a skin irritant. Contact with the liquid may cause second- and third-degree skin burns. Skin contact may also result in allergic contact dermatitis.

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

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

Gastrointestinal No cases involving ingestion were located. Because Crotonaldehyde is a known irritant, it is likely to cause burns of the lips, mouth, throat, esophagus, and stomach.

Potential Sequelae After an acute, relatively high-concentration exposure, persons may become sensitized to Crotonaldehyde.

Chronic Exposure Apart from rare cases of sensitization, no adverse effects in humans chronically exposed to relatively low concentrations of Crotonaldehyde 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 Crotonaldehyde may possibly be a human carcinogen. The International Agency for Research on Cancer has determined that Crotonaldehyde is not classifiable as to its carcinogenicity to humans.

Reproductive and Developmental Effects No studies were located that address reproductive or developmental effects of Crotonaldehyde in humans. Crotonaldehyde can cause degeneration of spermatocytes in mice. No information was found as to whether Crotonaldehyde crosses the placenta, but it has been measured in breast milk. Crotonaldehyde 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. No teratogenic effects from acute exposure have been reported.

In using the PEAC application we access information for the chemical by first locating Crotonaldehyde in the database. The following figures show the screens displayed for chemical properties, Figure 1 for the *PEAC-WMD for Windows* application and Figure 2-4 for the *PEAC-WMD for the Pocket PC* application.

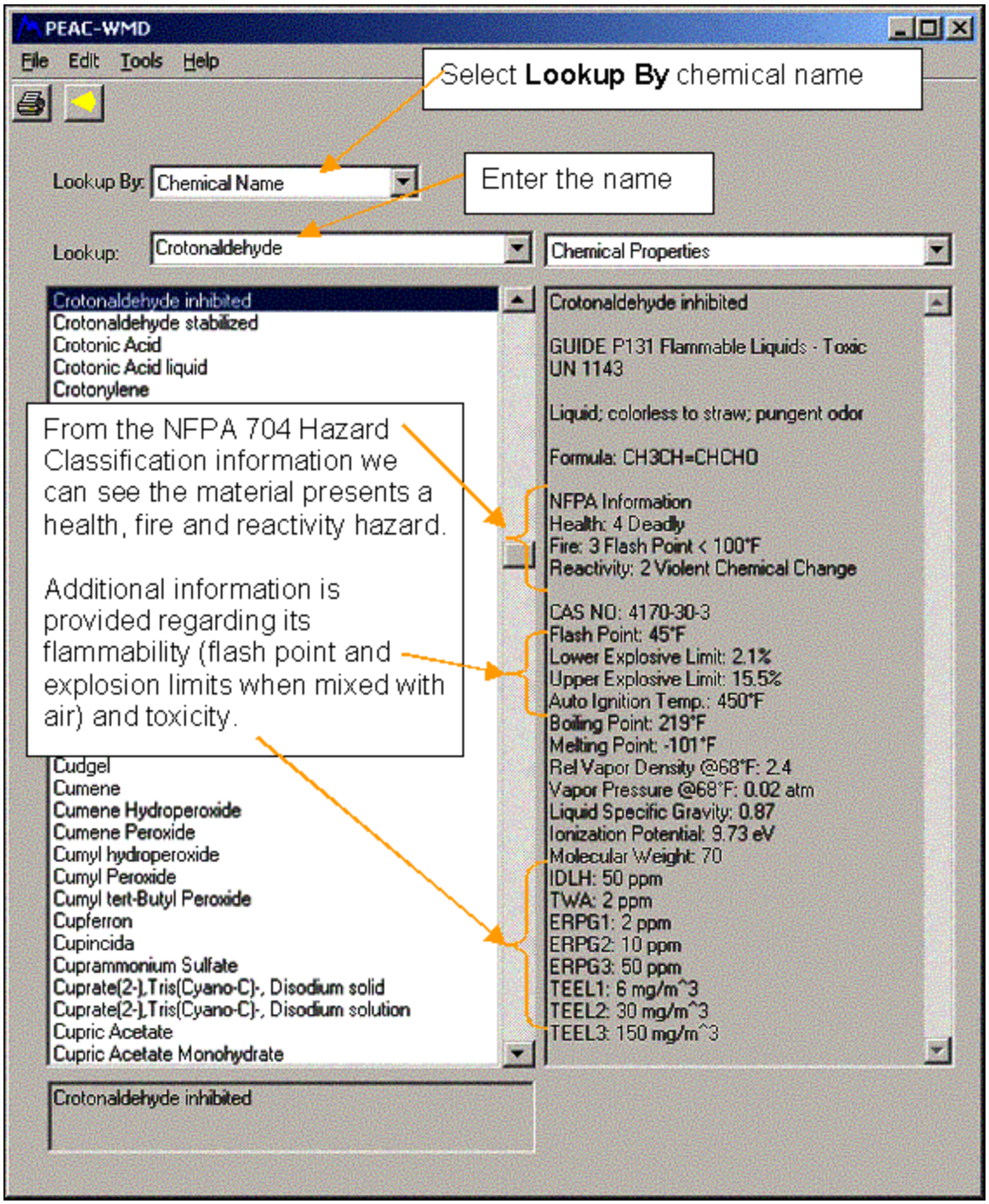


Figure 1 - Using the Lookup By: Name for Crotonaldehyde using the PEAC-WMD for Windows application

Review of the information displayed in the chemical properties screen whether in Figure 1 (above) or Figures 2-4 (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, ERPGs, 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.

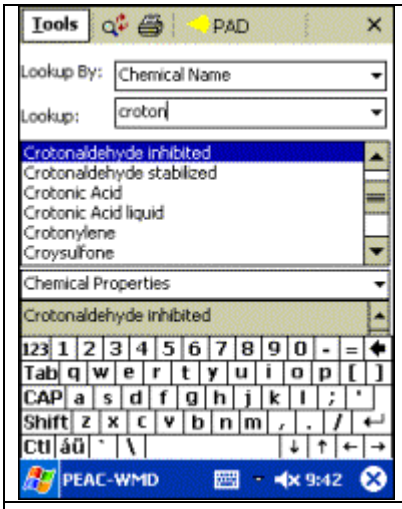


Figure 2 – Selecting Crotonaldehyde using the PEAC-WMD for Pocket PC application

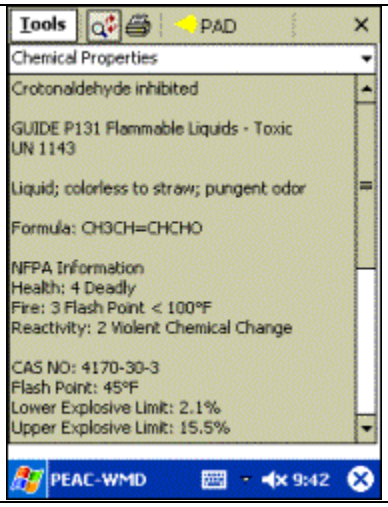


Figure 3 – The top portion of the Chemical Properties Data Display Screen

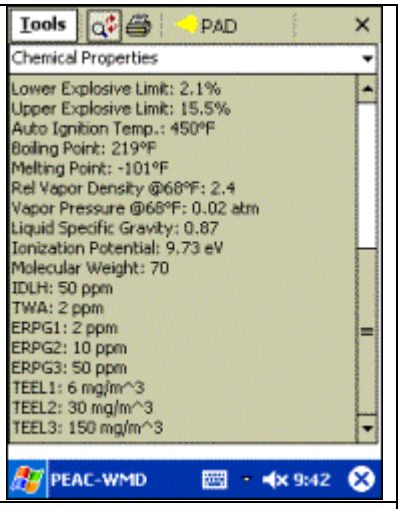


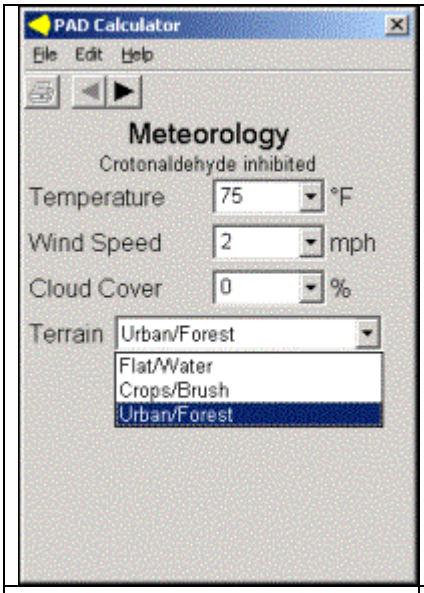
Figure 4– The bottom portion of the Chemical Properties Data Display Screen

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 Crotonaldehyde as the involved chemical we'll set the location to be plastics manufacturing facility located just outside Houston, TX. The date is March 11, 2004, about 10:00 AM with a temperature of 75°F, wind speed of 2 mph and a clear sky. The hypothetical release involves a storage tank (15' in diameter and 50' high) that contains Crotonaldehyde and a valve has been knocked off the bottom of the tank. The contents have created a liquid pool that is about 200' in diameter. The PEAC tool can provide guidance with regards to toxic vapor cloud that is released.

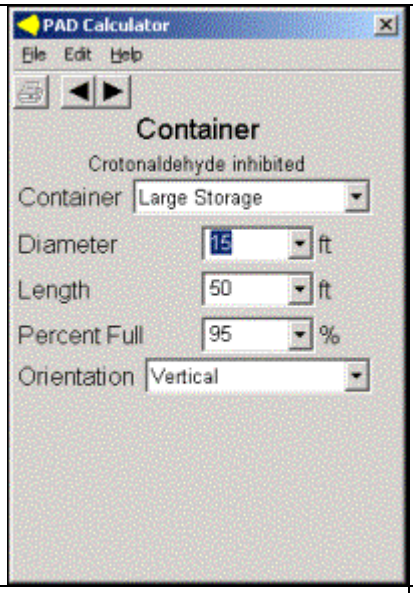
If you decide to follow along as we proceed through these examples, remember to set the location to Houston and set the date and time to the proper values, otherwise you'll compute different values. We'll use a terrain type of urban/forest since this is a manufacturing facility and has buildings and 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 5. 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.



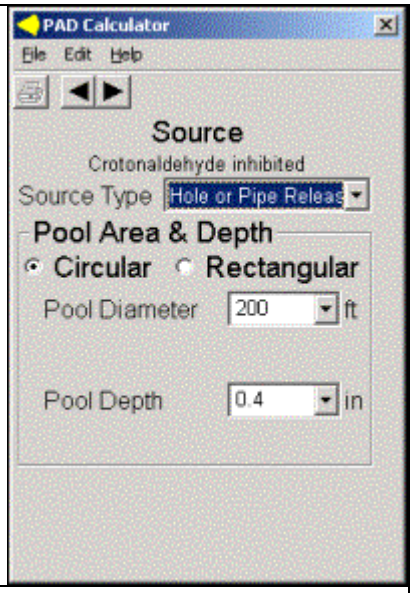
Meteorology

It's Houston in March and the temperature about 75°, wind is set for 2 mph, clear skies and the terrain is **Urban/Forest** since it's a processing facility setting.



Container

We have selected from our list of container sizes the **Large Storage** selection with a 15' diameter and a 50' tall. This gets us a quick estimate of how much material might be involved.



Source

We have selected a **Hole or Pipe Release**, and since the liquid boils at 219°F it will form a liquid pool. So the application asks for a pool depth and diameter.

Figure 5 – 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 6. This calculates a **PAD** (Protective Action Distance) based on the default **Level of Concern** the IDLH of 50 ppm. This evacuation or standoff distance is based on the toxicity of Crotonaldehyde, **not** the flammability.

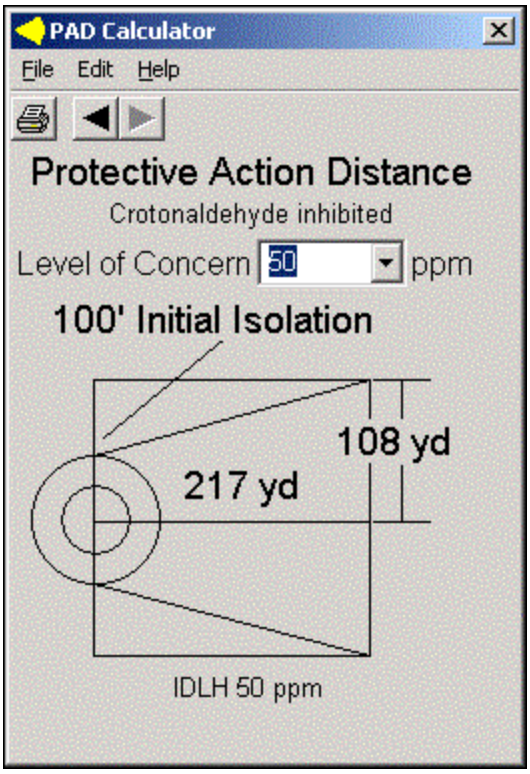


Figure 6 – Default PAD for Crotonaldehyde using the IDLH of 50 ppm

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 7. In this figure we select the ERPG-2 value or 10 ppm.

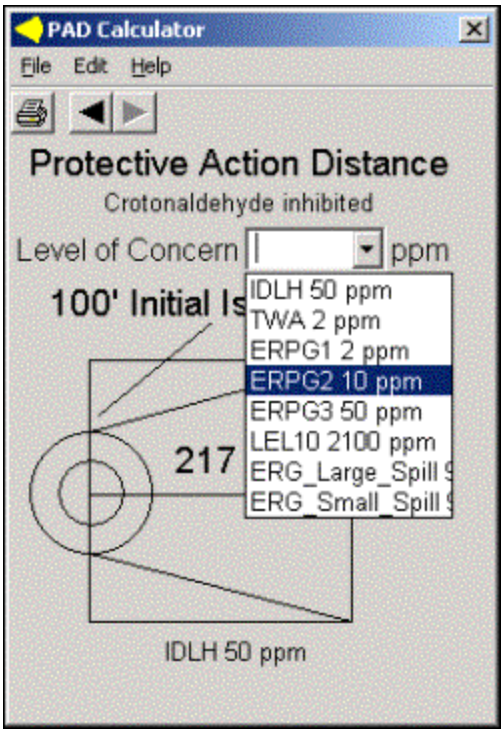


Figure 7 – Selecting another Level of Concern

The calculated PAD will be displayed, see Figure 8.

Figure 8 –Calculated PAD using the EPRG-2 Level of Concern

In addition to the toxicity of the released material, the user should also remember the flammability issue with Crotonaldehyde 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/.