Let's Take a PEEK at the PEAC Software

An Example from the PEAC software by S. Bruce King

This month our example is Ethylene Oxide, which has a chemical formula of C_2H_4O . Ethylene Oxide is a colorless gas or liquid with ether odor. It is a health hazard because of its toxicity and it is extremely flammable forming mixtures with air that are flammable or explosive. It is shipped as a liquefied, compressed gas. Both the gas and liquid are potential fire and explosion hazards. Ethylene oxide has a sweet, ether-like odor at air concentrations above 500 ppm. Ethylene oxide is soluble in water and organic solvents. It is highly flammable and, in vapor form, is subject to explosive decomposition. The liquid is stable to common detonating agents, but polymerization may be violent after initiation by acids, bases, or heat. Polymerization is catalyzed by certain metal chlorides and hydroxides. Both liquid and gaseous ethylene oxide are very reactive. It is relatively stable in aqueous solution, or when diluted with carbon dioxide or halocarbons.

Ethylene oxide reacts with water, strong acids, alkalies, and oxidizers; chlorides of iron, tin, and aluminum; and oxides of iron and aluminum.

Ethylene oxide is produced by catalytically reacting ethylene and oxygen. Ethylene oxide ranks 26th in volume among the major industrial chemicals produced in the United States. About 65% of ethylene oxide is used for synthesis of ethylene glycol, an antifreeze product. A mixture of 88% Freon and 12% ethylene oxide is used as a cold sterilizing agent for foods and medical equipment and supplies. Ethylene oxide is also used as a fumigant and fungicide in the manufacture of medical products and spices, and as a chemical intermediate.

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

OSHA STEL (short-term exposure limit) = 5 ppm (15 minute exposure)

NIOSH IDLH (immediately dangerous to life or health) = 800 ppm

AIHA ERPG-2 (emergency response planning guideline) (maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to 1 hour without experiencing or developing irreversible or other serious health effects or symptoms which could impair an individual's ability to take protective action) = 50 ppm

Ethylene oxide is a highly reactive alkylating agent that reacts with many constituents of tissue resulting in cellular and tissue dysfunction and destruction. Evidence for human exposure to this chemical is the presence of ethylene oxide adducts of DNA and hemoglobin. Direct contact with liquid ethylene oxide or solutions of ethylene oxide produces immediate local irritation of skin and mucous membranes. Inhalation of high concentrations of ethylene oxide can cause CNS depression or pulmonary edema. The onset of symptoms may be delayed for up to 72 hours.

Ethylene Oxide has a melting point of -171°F and a boiling point of 51°F. Its molecular weight is 44.1, and has a relative vapor density is 1.49 (compared to air), so it will seek low

areas. It has a vapor pressure of 1,110 mm Hg at 68°F (1.46 atmosphere). The lower Explosive Limit (LEL) is 3%; the Upper Explosive Limit (UEL) is 100%.

The important thing to remember when dealing with Ethylene Oxide 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 -** Store in a cool, dry place. Keep container closed when not in use.
- **Handling** Wash thoroughly after handling. Remove contaminated clothing and wash before reuse. Avoid contact with eyes, skin, and clothing. Avoid ingestion and inhalation.
- **Protection -** Wear appropriate protective gloves, clothing and goggles -- as recommended by the manufacturer. Always wear thermal protective clothing when handling refrigerated/cryogenic liquids.
- **Respirators -** A respiratory protection program that meets OSHA's 29 CFR 1910.134 and ANSI Z88.2 requirements or European Standard EN 149 must be followed whenever workplace conditions warrant a respirator's use.
- **Small spills or leaks -** Clean up spills immediately, using the appropriate protective equipment.
- **Incompatibilities -** Reacts violently with many compounds. Avoid metal fittings containing copper, silver, mercury or magnesium; ammonia, oxidizing agents; acids, organic bases; amines; certain salts; alcohols; mercaptans, ferric chloride; magnesium perchlorate; m-nitroaniline; trimethylamine, potassium, tin chlorides; alkanethiols; bromoethane; aluminum chloride; aluminum oxide; iron chlorides; and iron oxides. Avoid air, heat, acids and bases, metal or metal chloride catalysts. Hazardous polymerization may occur. Avoid acids; covalent halides such as chlorides of aluminum, iron (III), tin (IV); basic materials like alkali hydrides, ammonia, amines, and potassium; catalytically active solids such as aluminum or iron oxides or rust, chlorides of boron, aluminum, tin, and iron; some carbonates; and metals such as copper and copper alloys.

Hazardous Decomposition - Irritating and toxic fumes and gases.

Other hazards - The gas is heavier than air and may travel along the ground; distant ignition possible.

Health related information

Exposure effects

Pulmonary irritation is likely after inhalation; dyspnea may occur. Convulsive movements, twitching, malaise, lethargy, headache, seizures and dizziness have been reported. Serious exposure may result in coma. Chronic exposure may result in peripheral and central

nervous system effects, including neuropsychiatric symptoms, cognitive dysfunction and polyneuropathies. Ethylene oxide has been fetotoxic and teratogenic in experimental animals.

- **Ingestion -** Nausea, vomiting and diarrhea may occur.
- **Inhalation -** Pulmonary irritation is a common symptom after inhalation. Pulmonary edema may be seen with acute exposures. Pneumonia may be a complication of ethylene oxide exposure. A rare report of asthma has also been reported.
- **Skin** May be toxic/fatal if absorbed through skin. Contact may cause burns, severe injury and/or frostbite.
- **Eyes -** Contact may cause burns, severe injury and/or frostbite.

<u>First aid</u>

- **Ingestion -** If victim is conscious and alert, give 2-4 cupfuls of milk or water. Get medical aid immediately.
- **Inhalation -** Get medical aid immediately. Remove from exposure to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen.
- **Skin** Get medical aid. Flush skin with plenty of soap and water for at least 15 minutes while removing contaminated clothing and shoes. Remove contaminated clothing and shoes.
- **Eyes -** Irrigate exposed eyes with copious amounts of tepid water for at least 15 minutes. If irritation, pain, swelling, lacrimation, or photophobia (light sensitivity) persist, the patient should be seen in a health care facility.

In using the PEAC application we access information for the chemical by first locating Ethylene Oxide 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.

| M PEAC-WMD | | | | |
|--|---|--|--|--|
| Elle Edit Iools Help | | | | |
| <u> </u> | | | | |
| Enter the chemical name Ethylene Oxide. | | | | |
| Lookup By. Chemical Name | | | | |
| Lookup: Ethylene Oxide | Chemical Properties | | | |
| Ethylene monochloride | Ethylene Oxide | | | |
| Ethylene Nitrate Ethylene Oxide | GUIDE P119 Gases - Toxic - Flammable | | | |
| Ethylene Oxide and Carbon Dioxide Mixture with more than 6 | n 6% (UN 1040 | | | |
| E Very quickly we can see from | 9% t Colorless gas or liquid with ether odor | | | |
| Classification that the material is | han : Formula: C2H4O | | | |
| toxic and flammable. | Not my Shipped as liquefied gas under its own vapor pressure. | | | |
| Et This is also indicated by the | NFPA Information | | | |
| Elash Point, LEL, and published | re that Fire: 4 Flash Point < 73* | | | |
| toxicity values seen below. 🛌 | Heactivity: 3 Shock/Heat may Detonate | | | |
| Ethylene Thiourea | Known Larcinogen | | | |
| Ethylene trichloride Ethylenebis9Dithiocarbamato)Manganese | CAS NO: 75-21-8 Flash Point -20*F | | | |
| Ethylenebis[Dithiocarbamic Acid] Manganese Salt ethylenecarboxylic acid | Lower Explosive Limit: 3% Upper Explosive Limit: 100% | | | |
| Ethylenediamine Ethylenediamine (anhydrous) | Auto Ignition Temp.: 804°F Boiling Point: 51°F | | | |
| Ethylenediamine Tetracetic Acid | Melting Point: -171°F Bel Vanor Density @68°E: 1.5 | | | |
| Ethylenedisininetetraacetic acid, disodium salt Vapor Pressure @68*F: 1.46 atm | | | | |
| Ethyleneimine Ionization Potential: 10.57 eV | | | | |
| Ethylenimine | Molecular Weight: 44 | | | |
| Ethylfluorophosphonic acid, isopropyl ester Ethylformic acid | IDLH: 800 ppm TWA: 0.1 ppm | | | |
| Ethylhexaldehydes 2-Ethylhexyl Acrylate | ERPG2: 50 ppm ERPG3: 500 ppm | | | |
| 2-Ethylhexyl Chloroformate Di-(2-Ethylhexyl)Peroxydicarbonate (<=77% in Solution) | TEEL1: 5 mg/m^3 | | | |
| Di-(2-Ethylhexyl)Peroxydicarbonate (Technically Pure) | | | | |
| Ethylene Oxide | | | | |
| | | | | |
| | | | | |

Figure 2-Using the Lookup By: Name for Ethylene Oxide 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, the published toxicity values, e.g., IDLH, and ERPGs (Emergency Response Protection Guidelines) published by American Industrial Hygiene Association are provided. We will use the IDLH as the Level of Concern when we develop the PAD a little later.



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. Ethylene Oxide has a very high vapor pressure (1,110 mm Hg) at room temperature, so if the chemical is released from a container it will exit as a gas. 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 Ethylene Oxide as the spilled chemical we'll set the location to be Ft. Lauderdale, FL and the time as 11:00 PM on April 15th. A railcar of Ethylene Oxide has been involved in an accident just off US Highway 1. There is a 2-3" hole in the railcar, venting vapor very rapidly. The temperature is about 80°F, the winds are about 2 mph, and it's a clear night (no clouds).

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 7. 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 Ft. Lauderdale and the time to 11:00 PM, April 15th.

| PAD Calculator Ele Edit Help Meteorology Ethylene Oxide Temperature 80 ● °F Wind Speed 2 ● mph Cloud Cover 0 ● % Terrain Urban/Forest | PAD Ealculator Ele Edit Help Container Ethylene Oxide Container Failcar Diameter B tt Length 33 tt Percent Full 95 % Orientation Horizontal T | PAD Calculator Ele Edit Help Source Ethylene Oxide Source Type Hole or Pipe Releas Release Hole Hole Diameter Hole Height 0 ft |
|---|---|--|
| Meteorology | Container | Source |
| It's Ft. Lauderdale in April and the temperature about 80°, 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. | 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. | Since the scenario has a 2-3" hole so we've assumed a worst-case scenario and used a 3" hole, we've selected a Hole or Pipe Release as the Source type of release. |

Figure 7– Calculating a PAD using the PEAC System

By pressing the right arrow at the top of the screen, the PEAC system will display a screen as shown in Figure 8. This calculates a **PAD** (Protective Action Distance) based on the default **Level of Concern** the IDLH of 800 ppm. This evacuation or standoff distance is based on the toxicity of Ethylene Oxide, not its flammability. Since it is so flammable, extreme care needs to be given to ignition sources in the immediate vicinity of the release.

Clicking or tapping on the pop up list for the **Level of Concern** a list of published toxicity values for Ethylene Oxide is displayed. Clicking or tapping on the ERPG-2 value of 50 ppm (Figure 9) and will allow the PEAC tool to recalculate a PAD for the 50 ppm concentration **Level of Concern**. In our example a warning screen appears as shown in Figure 10, that the calculated PAD is greater than 7 miles and conditions can change substantially over long distances. After acknowledging the warning message, the PAD for the 50 ppm concentration is displayed (Figure 11).



Figure 8– Default PAD for Ethylene Oxide

| PAD Calculator | × | | | |
|-------------------------------|--|--|--|--|
| <u>File</u> Edit <u>H</u> elp | | | | |
| | | | | |
| Protective Action Distance | | | | |
| Ethylene Oxide | | | | |
| Level of Concern | ✓ ppm | | | |
| 200' Initial Is | IDLH 800 ppm TVVA 0.1 ppm | | | |
| | ERPG2 50 ppm | | | |
| | LEL 10 3000 ppm | | | |
| 1.8 r | ERG_Large_Spill 9 ERG_Small_Spill 9 | | | |
| (Ψ) | | | | |
| | | | | |
| IDLH 80 | D ppm | | | |
| | | | | |

Using the IDLH of 800 ppm

Figure 9– Selecting another Level of Concern

| PEAC-WMD | | × |
|---|--|---------------------------------------|
| The PAD is in excess of 7 miles substantially. Use the results | (11.3 km). Be aware that wind speed & terrain withi with caution. | in the predicted PAD will likely vary |
| | OK | |

Figure 10- Warning that calculations for PAD exceed 7 miles

| AD Calculator |
|----------------------------|
| Eile Edit Help |
| |
| Protective Action Distance |
| Ethylene Oxide |
| Level of Concern 50 - ppm |
| 200' Initial Isolation |
| |
| |
| 4.3 mi |
| 8.6 miles |
| |
| |
| |
| ERPG2 50 ppm |
| |

Figure 11- PAD for ERPG-2 (50 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: <u>http://www.inchem.org/</u>. Additional information was also adapted from the National Occupational Health & Safety Commission web site: <u>http://www.nohsc.gov.au/</u>, provided by the Commonwealth of Australia. Additional information was also adapted from the Agency for Toxic Substances and Disease Registry (ATSDR) Web site for Medical Management Guidelines at: <u>http://www.atsdr.cdc.gov/</u>. Additional information was adapted from the Ethylene Oxide User's Guide developed by a collaborative effort of Hoechst Celanese Polyester Intermediates, Occidental Chemical Corporation, Shell Chemical Company and SunCompany, Inc. (1999, August) found

at: <u>http://www.ethyleneoxide.com/html/introduction.html</u>.