Let's Take A PEEK at the PEAC Software

PEAC Example –Methyl Isocyanate

by S. Bruce King

This month our example is Methyl Isocyanate, which has a chemical formula of (CH_3NCO). Methyl Isocyanate is listed under the UN # (United Nations Number) by the US Department of Transportation: UN 2480. Methyl Isocyanate CAS# is: 624-83-9.

Many may remember the 1984 where a nighttime accidental release of this chemical had a tragic impact on the residents living nearby. In Bhopal, India, accidental acute inhalation exposure to Methyl Isocyanate resulted in the deaths of about 3,800 people and adverse health effects experienced by many of the 170,000 or more survivors. Pulmonary edema was the probable cause of death in most cases, with many deaths resulting from secondary respiratory infections. Survivors continue to exhibit damage to the lungs and eyes. Reproductive effects and increased number of stillbirths and spontaneous abortions were noted in the survivors of the Bhopal, India accident.

Persons exposed only to Methyl Isocyanate gas pose no risk of secondary contamination. Persons whose skin or clothing is contaminated with liquid Methyl Isocyanate can secondarily contaminate rescuers by direct contact or through offgassing of vapor.

At temperatures below 39 °C (102 °F), Methyl Isocyanate is a very flammable colorless liquid that readily evaporates when exposed to air. Gaseous Methyl Isocyanate is slightly heavier than air.

Although Methyl Isocyanate has a pungent odor, adverse health effects have been reported at or below the human odor threshold; therefore, odor detection is not a reliable indicator of exposure.

Methyl Isocyanate is readily absorbed through the upper respiratory tract. Methyl Isocyanate can also be absorbed through the digestive tract or skin.

Description At temperatures below 39 °C (102 °F), Methyl Isocyanate is a very flammable liquid that readily evaporates when exposed to air. Methyl Isocyanate liquid is colorless with a pungent odor. Most people can smell Methyl Isocyanate vapors at levels as low as 2 to 5 ppm. Methyl Isocyanate is handled and transported as a very flammable and explosive liquid.

Sources/Uses Methyl Isocyanate is made by reacting methylamine with phosgene. The primary use of Methyl Isocyanate is as a chemical intermediate in the production of pesticides (carbamates). It is also used to produce polyurethane foams and plastics.

Physical Properties:

Description: Colorless liquid at room temperature; volatile, flammable, explosive in air

Warning properties: Pungent odor of Methyl Isocyanate may not be adequate to warn of acute exposure. Most people can detect Methyl Isocyanate at levels of 2 to 5 ppm (1 ppm is equivalent to 2.35 mg/m3)

Molecular weight: 57.05 daltons

Boiling point (760 mm Hg): 102 °F (39.1 °C)

Freezing point: -49 °F (-45 °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 and the NIOSH Pocket Guide as shown above, is –49°F. Yet in the PEAC-WMD database the value is listed and displayed as –112°F. The lower value –112°F is found in other references (e.g., the USCG Chris Manual 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.*

Vapor pressure: 348 mm Hg at 68 °F (20 °C)

Water solubility: 6.7% at 68 °F (20 °C)

Flammability: highly flammable

Flammable Range: 5.3 % to 26 % (concentration in air)

Synonyms: Isocyanomethane, Isocyanatomethane, Methylcarbylamine, and MIC.

Standards and Guidelines:

OSHA PEL (permissible exposure limit) = 0.02 ppm (averaged over an 8-hour workshift) with a skin notation

NIOSH IDLH (immediately dangerous to life or health) = 3 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: Methyl Isocyanate reacts violently with water. Methyl Isocyanate is incompatible with oxidizers, acids, alkalis, amines, iron, tin, and copper.

Routes of Exposure:

Inhalation Inhalation is the major route of exposure to Methyl Isocyanate. The vapors are readily absorbed through the lungs. The odor threshold is

approximately 100 to 250 times higher than the OSHA PEL TWA (Permissible Exposure Limit Time Weighted Average of 0.02 ppm). Significant exposures to Methyl Isocyanate occur primarily in occupational settings. Acute exposure to Methyl Isocyanate vapors below the odor threshold can be irritating to the eye and respiratory epithelium. Acute exposure to higher vapor concentrations may cause severe pulmonary edema and injury to the alveolar walls of the lung and death. Survivors of acute exposures may exhibit long-term respiratory effects. **Odors of Methyl Isocyanate may not provide adequate warning of hazardous concentrations** because the Immediately Dangerous to Life or Health (IDLH) limit is only 3 ppm and the threshold for detection of Methyl Isocyanate vapors ranges from 2 to 5 ppm in humans. Significant exposure to Methyl Isocyanate vapors would most likely be the result of accidental release of Methyl Isocyanate to the air such as occurred in Bhopal, India in 1984, where the primary effect was pulmonary edema with some alveolar wall destruction. Methyl Isocyanate is heavier than air; therefore, exposure in poorly ventilated, enclosed, or low-lying areas could result in asphyxiation.

Children exposed to the same levels of Methyl Isocyanate as adults may receive larger doses because they have relatively 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 Methyl Isocyanate found nearer to the ground. Children may be more vulnerable to corrosive agents than adults because of the smaller diameter of their airways.

Skin/Eye Contact Direct contact with liquid or concentrated vapors of Methyl Isocyanate may cause irritation of the skin or eyes and severe ocular damage. Direct skin contact may result in dermal absorption. Significant dermal exposure to Methyl Isocyanate would not likely occur outside an occupational environment in which Methyl Isocyanate is stored or used.

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

Ingestion Although ingestion is unlikely, ingestion of liquid Methyl Isocyanate could produce severe gastrointestinal irritation.

Health Effects

Methyl Isocyanate is irritating and corrosive to the eyes, respiratory tract, and skin. Acute exposure to high vapor concentrations may cause severe pulmonary edema and injury to the alveolar walls of the lung, severe corneal damage, and death. Survivors of acute exposures may exhibit long-term respiratory and ocular effects. Methyl Isocyanate may be a dermal and respiratory sensitizer.

Mechanisms of Methyl Isocyanate-induced toxicity are not known. Persistent respiratory and ocular effects may reflect Methyl Isocyanate-induced immunologic effects. Methyl Isocyanate may cross the placenta and enter a developing fetus. Individuals especially susceptible to the toxic effects of Methyl Isocyanate include those with existing disorders of the respiratory system or eyes.

Acute Exposure

Mechanisms of toxicity have not been clearly elucidated for Methyl Isocyanate; however, carbamylation of globin and blood proteins may play a role. Persistent respiratory and ocular effects may reflect Methyl Isocyanate-induced immunologic effects since antibodies specific to Methyl Isocyanate have been demonstrated in the blood of exposed patients. Methyl Isocyanate is highly reactive; therefore, it is not metabolized in the classical sense. The onset of respiratory effects following acute exposure to Methyl Isocyanate can be immediate in some cases. In others, respiratory injury can evolve over periods of hours or days. Exposure-related deaths sometimes can occur as late as 30 or more days post-exposure, due in part to the development of pneumonia.

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

Respiratory Methyl Isocyanate vapors are severely irritating and corrosive to the respiratory tract. Symptoms may include cough, chest pain, dyspnea, coma, and death. Irritative respiratory symptoms such as pulmonary edema and bronchial spasms may occur in immediate response to exposure. Methyl Isocyanate-induced pulmonary edema may progress to effects such as alveolar wall destruction and pneumonia, which may ultimately lead to respiratory failure and death. Some respiratory effects may progress in severity over a period of hours to days post-exposure. Asthmatic reactions and long-term respiratory effects have been reported.

Children may be more vulnerable to corrosive agents than adults because of the smaller diameter of their airways. Children also may be more vulnerable to gas exposure because of relatively higher minute ventilation per kg and failure to evacuate an area promptly when exposed.

Ocular/Ophthalmic Severe eye irritation can result from exposure to Methyl Isocyanate vapors or direct contact with the liquid. Symptoms may include immediate eye pain, lacrimation, photophobia, profuse lid edema, and corneal ulcerations. Ocular exposure may result in long-term or permanent eye damage.

Dermal Methyl Isocyanate is a skin irritant and may cause chemical burns upon dermal contact at high exposure levels. Because of their relatively larger surface area: body weight ratio, children are more vulnerable to toxicants that affect the skin.

Gastrointestinal Nausea, vomiting, abdominal pain, and defecation have been reported after acute exposure to Methyl Isocyanate vapors.

Potential Sequelae Initial irritative symptoms of the respiratory tract may progress to more serious respiratory injury over a period of hours to days following exposure to Methyl Isocyanate vapors. Compromised lung tissue may be susceptible to bacterial pneumonias. Exposure may result in permanent eye damage. Methyl Isocyanate may also be a respiratory and dermal sensitizer.

Renal tubular necrosis, reduced liver function, and miscarriage were associated with Methyl Isocyanate exposure in the Bhopal, India incident.

Chronic Exposure

Chronic exposure to Methyl Isocyanate may result in chronic obstructive lung disease.

Carcinogenicity Methyl Isocyanate has not been classified for carcinogenicity.

Reproductive and Developmental Effects Methyl Isocyanate is not included in the list of *Reproductive and Developmental Toxicants*, a 1991 report published by the U.S. General Accounting Office that lists 30 chemicals of concern because of widely acknowledged reproductive and developmental consequences. Increased rates of spontaneous abortions and neonatal deaths among victims of the Bhopal accident were observed for months following exposure. However, the precise role of Methyl Isocyanate in developmental toxicity is difficult to determine. Poor oxygenation resulting from compromised lung function may be involved. Animal studies indicate that inhalation exposure during gestation may result in decreased numbers of live births and decreased survival during lactation. There was no evidence of a dominant lethal effect in exposed male mice. Genotoxicity testing in animals indicates that Methyl Isocyanate may have the capacity to affect chromosome structure, but it apparently does not induce gene mutations.

In using the PEAC application we access information for the chemical by first locating Methyl Isocyanate 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.

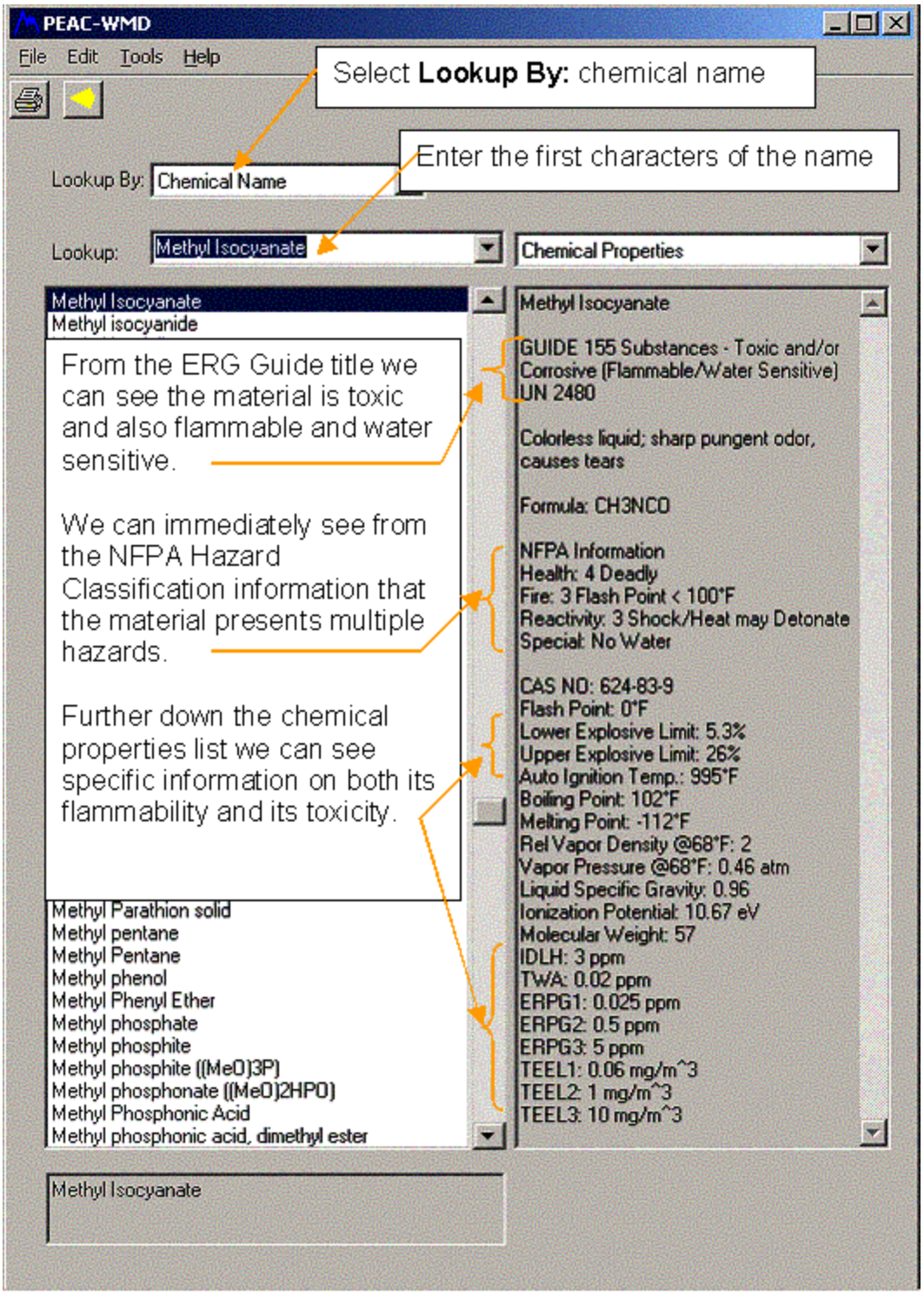


Figure 1 – Using the Lookup By: Name for Methyl Isocyanate using the PEAC-WMD for Windows application

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.

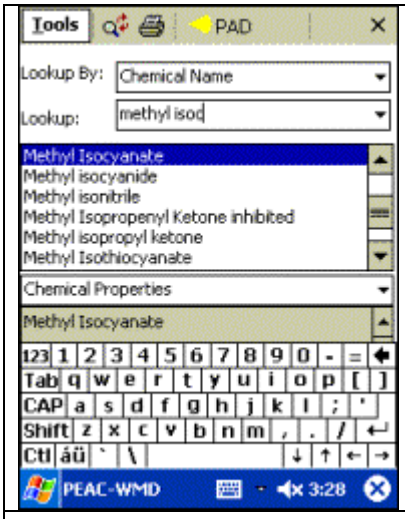


Figure 2 – Selecting Methyl Isocyanate using the PEAC-WMD for Pocket PC application

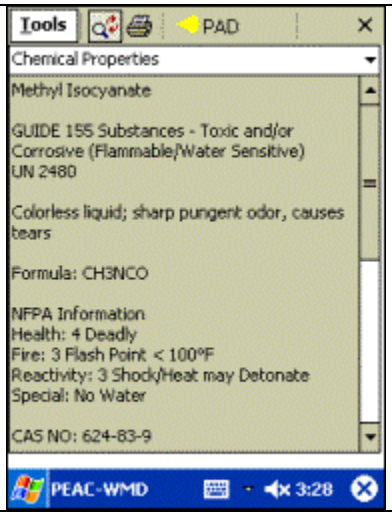


Figure 3 – The top portion of the Chemical Properties Data Display Screen

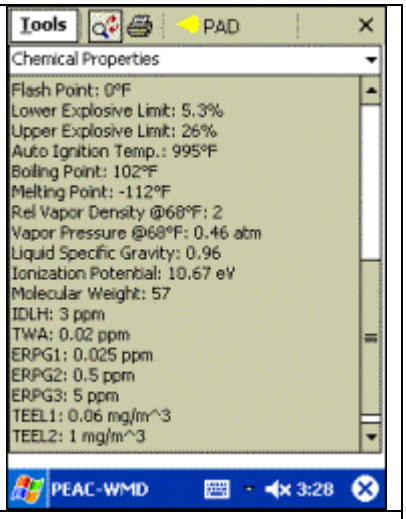


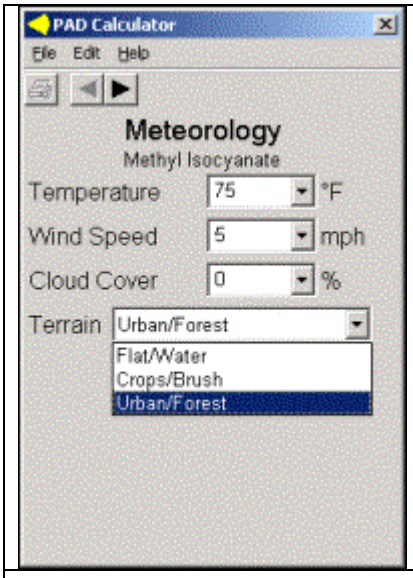
Figure 4– The bottom portion of the Chemical Properties Data Display Screen

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 Methyl Isocyanate as the involved chemical we'll set the location to be pesticide manufacturing facility located just outside Baton Rouge, LA. The date is February 9, 2004, about 4:00 PM with a temperature of 75°F, a wind speed of 5 mph with a clear sky. The hypothetical release involves a storage tank (8' in diameter and 30' tall) that contains Methyl Isocyanate that has a valve knocked off the bottom of the tank. The contents have created a liquid pool that is about 150' in diameter. The PEAC tool can provide guidance with regards to toxic vapor cloud that is released.

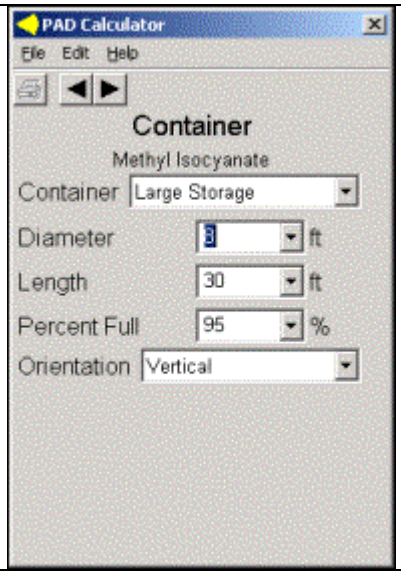
If you decide to follow along as we proceed through these examples, remember to set the location to Baton Rouge and set the date and time to the proper values, otherwise you'll compute different values. We'll use a terrain type of urban/forest since this is a manufacturing facility and has buildings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



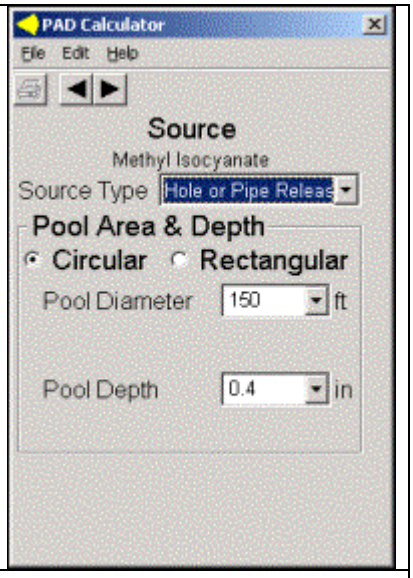
Meteorology

It's Baton Rouge in February and the temperature about 75°, wind is set for 5 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 an 8' diameter and a 30' 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 102°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 January 14th

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 3 ppm. This evacuation or standoff distance is based on the toxicity of Methyl Isocyanate, **not** the flammability.

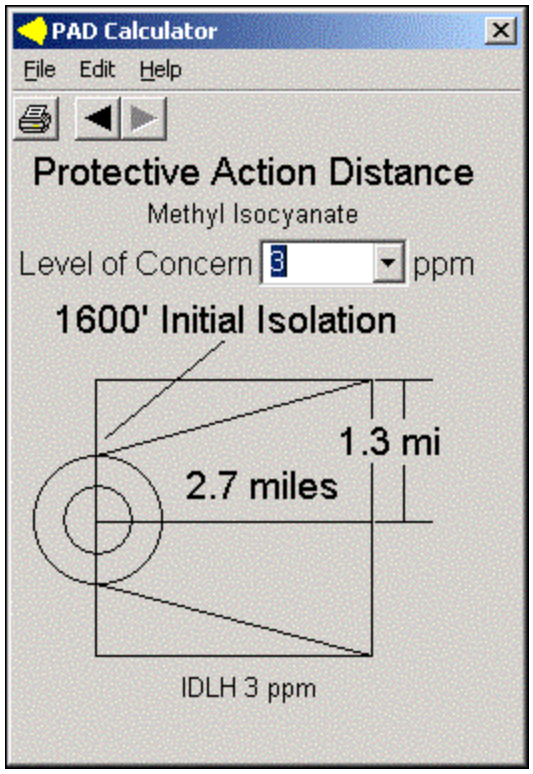


Figure 6 – Default PAD for Methyl Isocyanate using the IDLH of 3 ppm

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 0.5 ppm.

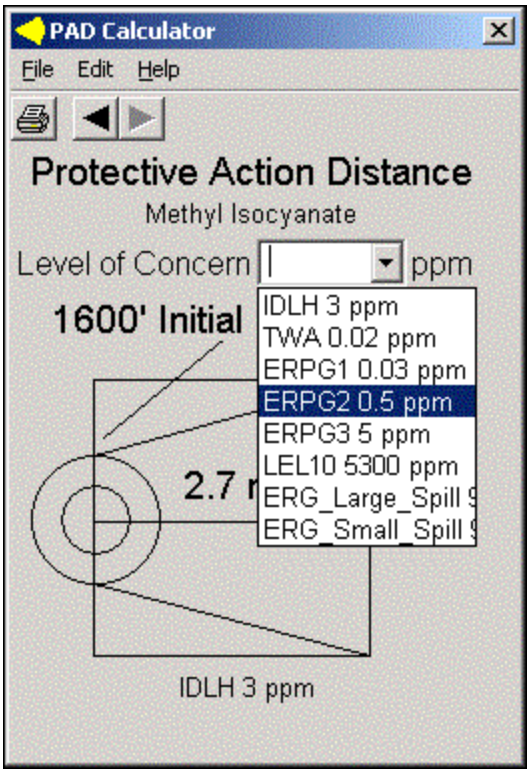


Figure 7 – Selecting another Level of Concern

A warning screen will be displayed as shown in Figure 8, this just notifies the user that the calculated PAD is greater than 7 miles and meteorology and surface conditions can change over these long distances and change the results of the predictions.

Figure 8 – Warning message displayed if the PAD is greater than 7 miles

Once the warning message has been acknowledged, the calculated PAD will be displayed, Figure 9.

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

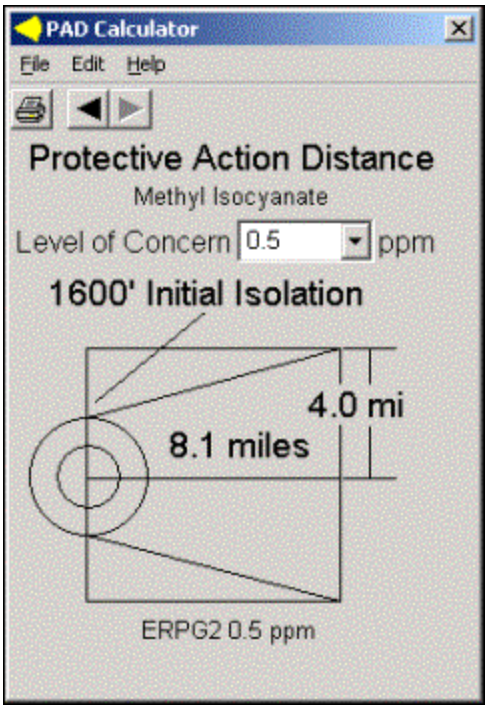


Figure 9 – Calculated PAD using the EPRG-2 Level of Concern

Portions of this discussion were adapted from the US EPA web site at: http://www.epa.gov/ttn/atw/hlthef/methylis.html. 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/.