Methyl Isocyanate Revisited

Methyl isocyanate was used as an example in using the PEAC tool in the February 2004 newsletter. Since then the Fireball calculator tool has been added to the PEAC system. We're revisiting this example using the Fireball calculator feature along with the PAD calculator in order to discover better ways to keep those we are responsible for safe.

The disaster of Bhopal, India in 1984 brings home the constant need for awareness when dealing with hazardous compounds. Around midnight on the night December 2-3, the Union Carbide pesticide plant had a release of 44 tons of methyl isocyanate that dispersed over the city of Bhopal. Rajan Sharma, a lawyer working on the 1984 incident on behalf of the defense, found estimates of 20,000 people who have died as a direct result of the disaster. Mr. Sharman also states that, according to the Indian medical Council for Medical Research, more the 250,000 people still suffer from the exposure to the gas.[1] Recently, studies[2] have shown the powerful adverse health affects that methyl isocyanate can have. Studies done between 2001 and 2005 showed that methyl isocyanate toxicity begins as low as .02 ppm (2.35 mg/m^3) over 8 hours. Eye and respiratory irritation occurs at .05 ppm when exposed for only ten minutes. Even more alarming was the discovery that most people could not detect the odor for concentrations lower than 5 ppm. This means that you are affected before you smell it. A person will experience tearing and shortness of breath only minutes after exposure, even when they haven't ever smelled the compound. By the time a person smells methyl isocyanate, breathing is labored and permanent damage may have been done. At 10 ppm the lungs are damaged in minutes, the human sensory threshold limit is about 21 ppm, and the gas is acutely fatal at 50 ppm. The residents of Bhopal were exposed to concentrations up to 100 ppm. At these levels the residents of Bhopal may have experienced immediate liver failure and lung collapse. Those who did not die in the affected areas in Bhopal were exposed to as little as 13 ppm in Bhopal, but the survivors continue to suffer decreased vital lung capacity (between 25%-75%), permanent disabilities, other chronic ailments and the dramatic increase in miscarriage, infant mortality, and low birth weight reflects the mutagenic effects of the compound.[1, 2]

The tragedy of Bhopal, India is a real world, worst-case scenario that applies directly to all of us. Too many people's lives are at stake if we do not respond appropriately to a disaster like this. Let's recreate a scenario based on the Bhopal incident and walk through it using the PEAC system. In our scenario, the PEAC tools will give accurate information so that the first responder can act responsibly.

The accuracy of the predictions made by the PEAC calculators are dependent in part on the time and day, which is pulled from the settings on the computer, and place of the incident, which is defined within the PEAC tool. As you follow along with your version of the PEAC tool be aware that these results are made on a computer whose time setting are set to December 3, 1984 at 12:00am. In order to get the same results your setting must also be set to these times. You must also set your location in the PEAC tool to match the location of in this simulation. To set the location, open the PEAC tool. In

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[1] Hanna, Bridget , and Ward Morehouse, Satinath Sarangi The Bhopal Reader. New York Apex Press, 2006.

[2] Hazardous Substances Data Bank. "METHYL ISOCYANATE." http://toxnet.nlm.nih.gov. 17 Dec. 2007.

the opening screen click the “Edit” menu at the top of the screen, click on “Location.” The location window includes windows for selecting a city near you, current city, coordinates of the location of the city or incident, and GPS settings. Bhopal, India is not a selection in the select a city drop down menu, so coordinates for the city are imput by hand. The location is typed in under the Current City box. This is the city that will be listed in the final report. The coordinates for the Union Carbide plant in Bhopal, India are 77° 24’ 29” E and 23° 16’ 51”. For this exercise the GPS Setting is “Do not use GPS.” Click OK.

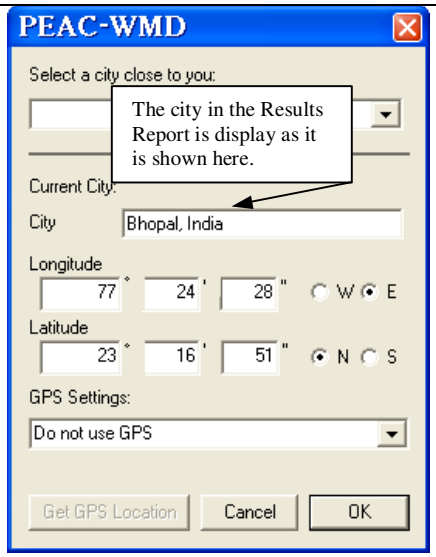

Figure 1

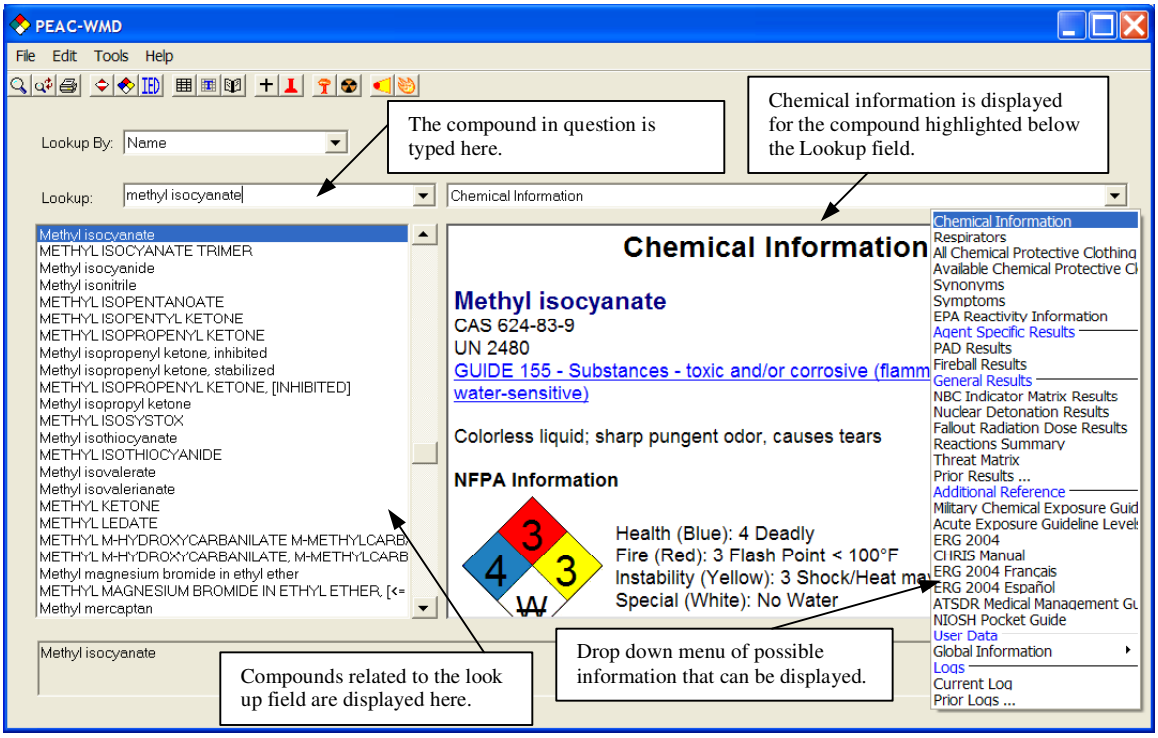

Figure 2 The **opening screen** shows the "lookup" field where the substance entered, the list of selected chemicals along with the current selection (highlighted), and the "Chemical Information" field. By clicking the drop down arrow on the "chemical Information" field, you can browse other information, including previously calculated PAD results, Fireball results, etc.

Upon opening the PEAC tool, "Name" is usually displayed in the "Lookup By" field. If not, select it by clicking on the field, which displays a drop down menu. Just below the "Lookup By" field is the "Lookup" field. Begin to type the compound in this field. As we type the selection, the list of compound below the "Lookup" field narrows until methyl isocyanate is the highlighted entry. The chemical information is display in the adjacent field to the right. By scrolling down in the Chemical Information field we find valuable information in the NFPA 407 Hazard Rating System, or Hazmat Diamond. For methyl isocyanate, the health rating is 4, fire is 3, instability is 3, and it is reactive to water. From our discussion about the Bhopal incident we know about the adverse health affects of the compound, but what about the fire and shock risks. We will assess all of these risks for methyl isocyanate quickly using the tools in the PEAC system.

The PEAC system automatically lets you see only the icons for the calculations that apply to the specific chemical. Press the PAD icon at the top right of the screen. After reading the acknowledgement click "Yes" to continue. Since specific information is limited, in this simulation we will assume that the meteorological conditions of the night of the incident in Bhopal were average for that time of year. The average low temperature for Bhopal in December is 51° F. This should be good estimate for the temperature. The average wind speed is 10 miles per hour coming from the north, or 0°, and 20% cloud cover. The "Terrain" for Bhopal is "Urban/Forest" since the factory is located in the middle of the city. Click the "next" arrow . Again, specific information about the container holding the methyl isocyanate is limited, but a container with dimensions 8 feet in diameter and 30 feet in length will hold about 44 tons of methyl isocyanate so we will assume that this is the size of the tank. In the container screen,

select Large Storage and we will use the dimensions of our simulated tank mentioned above, 8 feet in diameter and 30 feet in length. Leave the default value for "Percent Full" at 95%. The orientation is horizontal. Click the "next" arrow ▶|.

It is believed that the leak in Bhopal was caused by water that that spilled into the storage tank from a ruptured water line. This caused enough pressure to blow a hole in the tank. From this limited information, we will assume that the "Source Type" is a Large Rupture. Although we do not have details on exactly how the storage tank failed, we will assume that the top of the storage tank ruptured for our simulation. Under these simulated circumstances the methyl isocyanate would have evaporated quickly out of the top of the storage tank. If this was the case, for the "Pool Area & Depth" settings we will choose the tank itself and assume it is empty. Therefore we select rectangular and put in our dimensions for the tank, 30 feet for Pool Length and 8 feet for Pool Width. We assume that all of the methyl isocyanate has escaped so the Pool depth will be 0.1 inches. Click the "next" arrow ▶|.

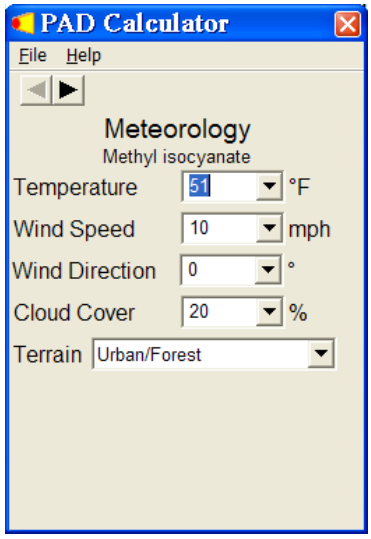

Figure 3 Meteorology: Note that wind direction is in degrees: 0°=wind from the north, 90°=east, 180°=south, 270°=west.

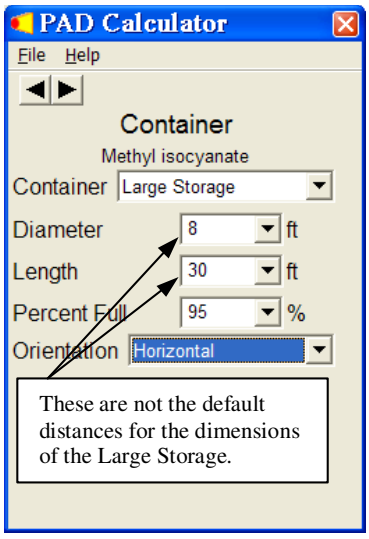

Figure 4 Container: The Dimensions above are not the default distances. Make sure default distances are only used if applicable. If you recalculate your results, the dimensions are returned to the default values.

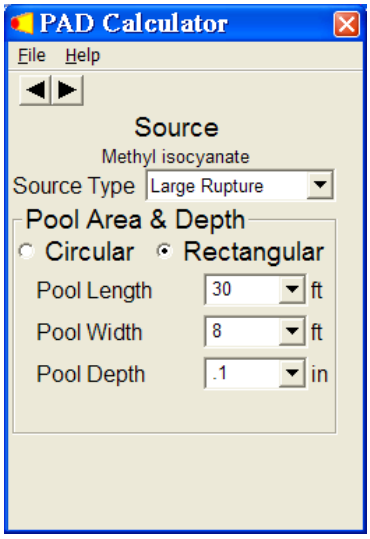

Figure 5 Source

Now we see the PAD calculations. The default Level of Concern (LOC) is the IDLH standard, or 3 ppm. Given what we know about the human toxicity of methyl isocyanate, perhaps a better value for this chemical is the ERPG2 recommendation. Under the "Level of Concern," click the frame to view the drop down menu and select "ERPG2 0.3 ppm."

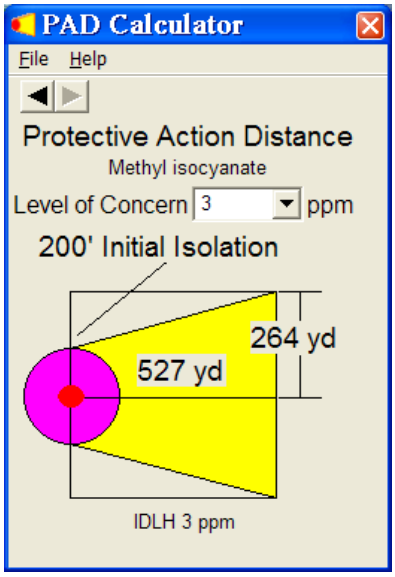

Figure 6 PAD Calculator at the default IDLH Level of Concern, 3 PPM. This Graphic is not to scale.

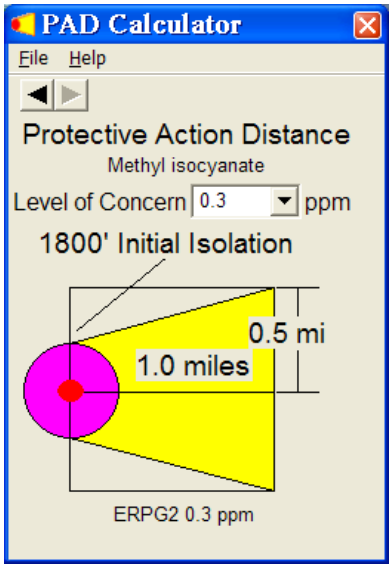

Figure 7 PAD Calculator at the ERPG2 Level of Concern, 0.3 PPM. This Graphic is not to scale.

After selecting methyl isocyanate in the opening screen, the PEAC tool only shows the PAD and Fireball buttons. Although a fireball comes from a vapor cloud explosion, it behaves differently than a chemical that is labeled explosive. Methyl isocyanate is not an explosive, so the explosion calculator is not shown. We will not use the nuclear detonation or nuclear fallout calculators, which are always shown. But we did note the fire hazard in the hazmat diamond, and the fireball calculator button. Methyl isocyanate can be especially dangerous as it evaporates. It's high vapor pressure, 0.46 atm at 68° F, means that it is going to evaporate quickly and have a high concentration as it mixes with air. The concentrations at which the methyl isocyanate/air mixture is the most dangerous are 5.3% to 26% methyl isocyanate by volume, the lower and upper explosive limits. Right above the liquid methyl isocyanate the concentration of the methyl isocyanate is 46%. This far above the upper explosive limit, but the upper explosive limit will be reached as the gas disperses far from the source. This means that there is a greater chance of the gas finding an ignition source because it is spread out over a greater area. Because of this, there is a real danger of the ignited cloud flashing all the way back to the point of origin, burning everything along the way. The methyl isocyanate cloud did not ignite during its release in Bhopal, but the danger was still very real. With the Fireball calculator we will predict the dangers of a fireball that could have happened to the residents of Bhopal. When the PEAC tool calculates a fireball there are a few assumptions. The first assumption is that all of the mass of the compound is in a gaseous form. Second, the distances of the fireball calculation are increased by a safety factor of two to adjust for the asymmetry of the cloud and an amount of drift that the cloud might make due to environmental conditions. These assumptions make for conservative values in order to ensure the safety of those involved. Press the fireball button. Again we choose our hypothetical large storage tank that has dimensions 8'x30' and is 95% full. Click the "next" arrow. We choose the default "Overpressure" setting of 0.5 PSIG and 2nd degree burns for the "Heat" value. Click the next button to view the results.

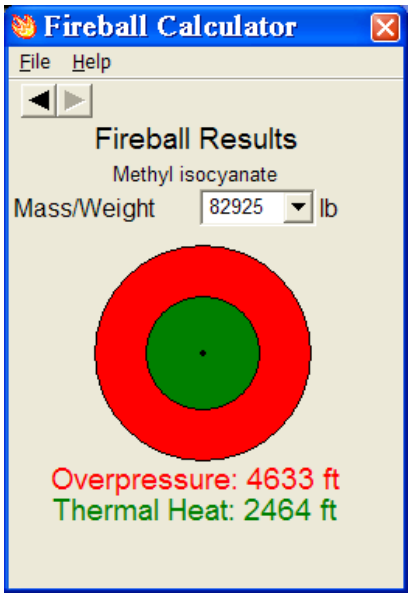

Figure 8 Initial **Fireball Results**. Calculated for the entire volume in gaseous form. Not to scale.

This provides a conservative estimate based on the assumption that all the 83,000 lbs are in the vapor state and applying a safety factor of 2. The gas cloud of isocyanate, if ignited, may impact an area that is larger then the initial isolation distance for health dangers calculated by the PAD. This is an important piece of information. Let's compare the previously calculated PAD to the Fireball data. The PAD Initial Isolation Distance for the spill is 1800 feet. But there is a risk of receiving at least 2nd degree burns within 2074 feet of the source. Beyond that, the Overpressure danger extends out to 4049 feet, wherein one can expect to see at least some broken windows.

Lets go back for a moment and take a look at the Mass/Weight field feature in the Fireball Results. If there was a pool of the compound on the ground or perhaps some is still in the tank, it may not be realistic to assume that the entire compound is in a gaseous form. Therefore the above calculation should be adjusted to accuracy. One feature of the Fireball calculator is the ability to select the amount of gas in the air. Note the "Mass/Weight" field under Fireball Results. The default weight displayed in this field is based on the density of the compound and the volume of the container you specified. Our simulation used an 8'x30' tank that was initially 95% full of methyl isocyanate. For this volume, methyl isocyanate weighs 82,925 pounds. Recall that the initial fireball data is only applicable if the entire mass is in gas form. Alternatively, if you can accurately estimate the mass of the substance in the gaseous state, then you can adjust the "Mass/Weight" field to make the calculation even more accurate. For instance, if the methyl isocyanate storage tank was resealed with half of the compound still inside the tank as a liquid, we know that the other half was released in gas form. Therefore we adjust the "Mass/Weight" field to reflect the amount of methyl isocyanate that was released, or evaporated into the air. If we can accurately determine that half of the compound is still in the container we can make the proper adjustments. The "Percent Full" field is still set to the initial percent full, 95%, and then the "Mass/Weight" field can

be adjusted to half the initial weight, from 82925 lbs to 41463 lbs. This new weight is 50% of the compound that is a gas. The fireball is automatically recalculated. In this way we calculate, for methyl isocyanate, the fireball dangers for a compound in a tank that is initially 95% full and has had 50% of the compound escaped, or evaporated in gaseous form. If you have changed the time and date setting on your computer or the location settings in the PEAC tool, make sure that you revert to your original settings now that we are finished.

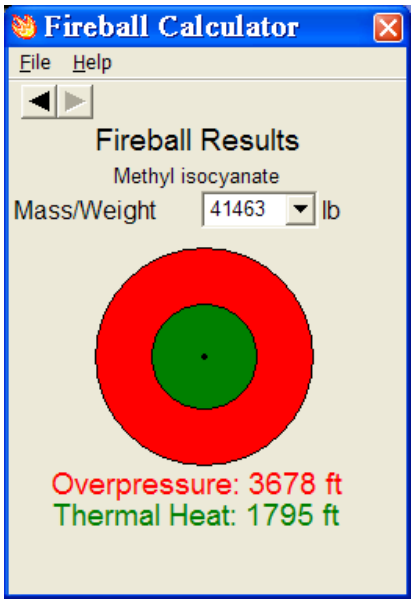

Figure 9 Recalculated **Fireball Results** to account for only a partial release, 50%, of the chemical as a gas.

When acting as a First Responder the user must be aware not only of the toxic health effects of compounds, shown by the PAD, but also of other hazards, a fireball in this case. We are proud to have added the fireball calculator into PEAC version 5.1. If you do not have this calculator and need to update your version of PEAC please contact us. If your license is currently under a Tech Support and Upgrade subscription, this update will be free of charge and can be done over the internet.