Dispersion and Simulation of Bhopal Gas Disaster as Case of Applied Chemical Science

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Abstract - **The Bhopal Gas Disaster, of 2nd-3rd December, 1984, caused by a "run-away chemical reaction" of Methyl IsoCyanate stored in a Stainless Steel Tank, of UCIL (Union Carbide of India Ltd) Factory, is undoubtedly the worst chemical disaster of the world. The sheer magnitude of the industrial catastrophe has aroused the conscience of the world. The incriminated Tank 610 E of the 'Pesticide Plant' of Union Carbide Corporation (UCC) in Bhopal was maintained by its Indian counterpart, Union Carbide India Limited (UCIL). Unlike minor accidents in their US Plants, immediately following the chemical run-away reaction of Methyl IsoCyanate (MIC) in Bhopal, there was a massive release of toxic gases into the atmosphere which spread rapidly over a densely populated area of Bhopal City, the capital of Madhya Pradesh, India. In this paper, we present and analyse various aspects of the leak of toxic gas from the Union Carbide Plant at Bhopal, India in December 1984. The physicochemical properties of the deadly methyl isocyanate (MIC) and its biological activity, as well as the probable causes of the accident, are discussed. The role of meteorology and topography with regard to the dispersion process is also documented. The Mechanical and Human both errors considered in these study. By the Toxic simulation study rectify the results. For the Simulation ALOHA (AREAL LOCATIONS OF HAZARDOUS ATMOSPHERES,5.4.4) software is used, developed by National Oceanic and Atmospheric Administration, USA which is available on the respected sites. The model output gives an estimate of the ground level concentration and the approximate time of arrival of the plume front in the various affected localities.**

Dry deposition and the aqueous phase conversion of MIC with the humid atmosphere were also featured in the model. The model results seem to be fairly well correlated with the scantily available mortality distribution records. The Bhopal Gas Leak shows us the complexity of the chemical society we live in today. The fact is, that we do not know which compounds we might be exposed to from chemical plants, and we do not know in what way and to which degree these compounds are harmful to us, in the short-term and in the long-term. The NGOs and trade unions usually fight for what is best for human beings. But we must realise that this is not the primary goal of a company. What is good for a company is not always good for the people. For the people, and for public health, it is good with small income differences, strong working rights legislation, protection of water and ground, manpower-rich companies and the making of strong demands on the company concerning the work environment and the environment as a whole. For the companies it is good to have few employees, ease in exchanging the labourers, an unsafe labour market which leads to the employed working hard and keeping silent and low demands on the work environment and environment.

I. INTRODUCTION

The atmosphere, which makes up the largest fraction of the biosphere, is a dynamic system that continuously absorbs a wide range of ***solids***, ***liquids***, and ***gases*** from both natural and man-made sources. These substances travel through air, disperse, and react with one another and with other substances both physically and chemically. Most of these constituents, eventually find their way into a depository such as the ocean, or to a receptor such as man. Some substances such as helium, however, escape from the biosphere. Others such as carbon dioxide may enter the atmosphere faster than they enter a reservoir and thus gradually accumulate in the air.

UCIL (Union Carbide India Limited) was incorporated in India in 1934. In 1969, the Bhopal Plant begun operations as a pesticide formulations plant on land leased from the Indian State of Madhya Pradesh. As a formulations plant, UCIL imported the chemical components of pesticide products and mixed the final product, such as the "Sevin" pesticide, in India. At that time, UCC owned 60% of UCIL. In the latter half of the 1970s, the Bhopal Plant was back-integrated into a facility capable of manufacturing the pesticides itself; in connection with this project, UCC's (Union Carbide Company) ownership interest in UCIL was reduced to 50.9%. The Bhopal Plant operated as a manufacturing facility for only a few years. In the normal course of operations, the Bhopal Plant generated wastes; generally, solid wastes were disposed in on-site tanks and pits, while wastewater was treated and then pumped to three solar evaporation ponds lined with low density black polyethylene sheets. Plaintiffs allege that toxic substances seeped into a ground aquifer, polluting the soil and drinking water supply in residential communities surrounding the former Bhopal Plant site. In 1984, after a catastrophic gas leak claimed thousands of lives, the Government of India closed the Bhopal Plant. In 1994, UCC sold its stake in UCIL; UCIL subsequently changed its name to EIIL. In 1998, EIIL terminated its lease of the Bhopal Plant site and surrendered the property to the state government of M.P.

Fig. 1: The GPS location of Bhopal City (Capital of M.P.)

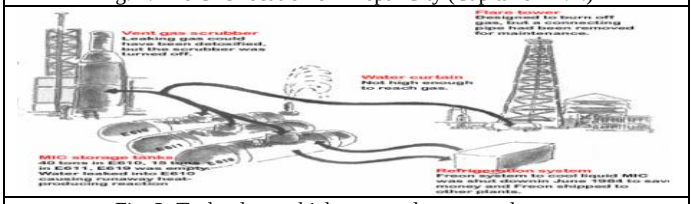


Fig. 2: Technology which was used was not adequate.

The Bhopal gas tragedy is one of the worst industrial air pollution disasters that has ever occurred in the world. The count down for the disaster started around 0030 IST when untreated vapors of methyl isocyanate (MIC) were seen escaping through a nozzle of 33 m high atmospheric vent-line, from the Union Carbide (UC) plant located at Bhopal (India), in the early hours of Monday~ 3 December 1984. During the night Dec 2-3, 1984, large amounts of water entered a tank containing 43 tonnes of Methyl isocyanate (MIC) in Union Carbide's plant in Bhopal, India [3 & 4]. A strong chemical reaction started and a big cloud of toxic gases spread over the sleeping town. 500,000 people were exposed to the gases. 8,000 died within the first week, and 8,000 since. 100,000 have permanent injuries. Today, Dow Chemical has taken over Union Carbide Corporation. The survivors fight for their right to full economic compensation and medical care. Together with other residents, they fight for Dow and the Government of India to clean up the polluted area and the ground water. Fig. (1) Shows the Global Positioning of the Bhopal City with the details of the disaster and Fig. (2) Shows basic locations of all the production, storage and distribution unit operations.

Methyl isocyanate (**MIC**) is an organic compound with the molecular formula CH_3NCO. Synonyms are isocyanatomethane, methyl carbylamine, and MIC. Methyl isocyanate, as shown in Fig. (3), is an intermediate chemical in the production of carbamatepesticides pesticides (such as carbaryl, carbofuran, methomyl, and aldicarb). It has also been used in the production of rubbers and adhesives. As a highly toxic and irritating material, it is extremely hazardous to human health [1 & 2].

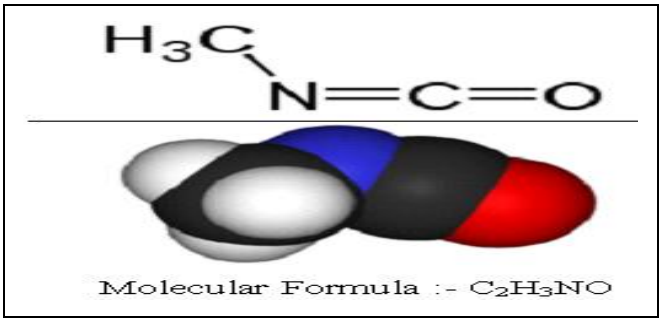


Fig. 3: Methyl-Isocynate.

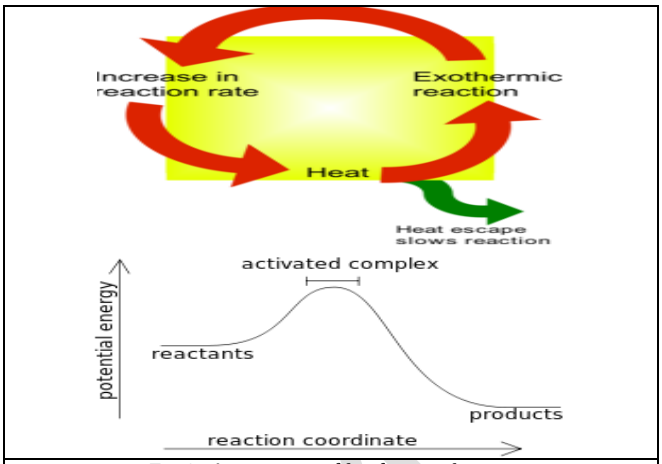


Fig 4.: An energy profile of an exothermic

It was the principal toxicant involved in the Bhopal disaster, which killed nearly 8,000 people initially and approximately 20,000 to 30,000 people in total. Methyl isocyanate (MIC) is extremely toxic as represented in Fig. (4). The threshold limit value set by the American Conference on Government Industrial Hygienists is 0.02 ppm. MIC is toxic by inhalation, ingestion and contact in quantities as low as 0.4 ppm. Exposure symptoms includes coughing, chest pain, dyspnea, asthma, irritation of the eyes, nose and throat, as well as skin damage. Higher levels of exposure, over 21 ppm, can result in pulmonary or lung edema, emphysema and hemorrhages, bronchialpneumonia and death. Although the odor of methyl isocyanate cannot be detected at 5 ppm by most people, its potentlachrymal properties provide an excellent warning of its presence (at a concentration of 2–4 parts per million (ppm) subject's eyes are irritated, while at 21 ppm, subjects could not tolerate the presence of methyl isocyanate in air). Proper care must be taken to store methyl isocyanate because of its ease of exothermically polymerizing (see Reactions in Fig. (5), and its similar sensitivity to water. MIC must be stored at temperatures below 40°C (104°F) & preferably at 4°C (39°F).

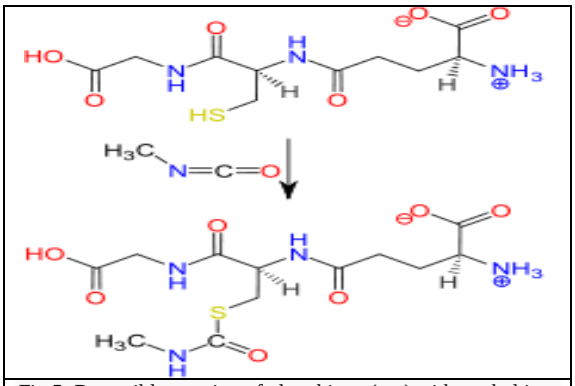
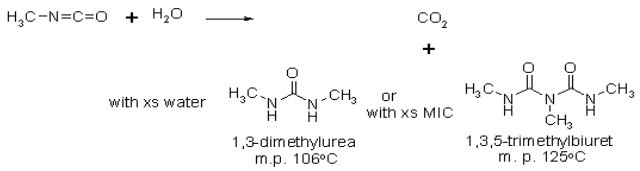
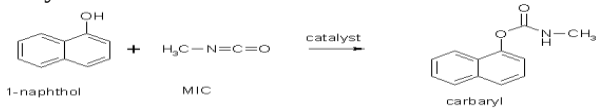


Fig 5: Reversible reaction of glutathione (top) with methyl isocynate (MIC, middle) allows the MIC to be transported into the body.

Methyl isocyanate reacts readily with many substances that contain N-H or O-H groups. With water, it forms 1,3-dimethylurea and carbon dioxide with the evolution of heat (325 calories per gram of MIC).

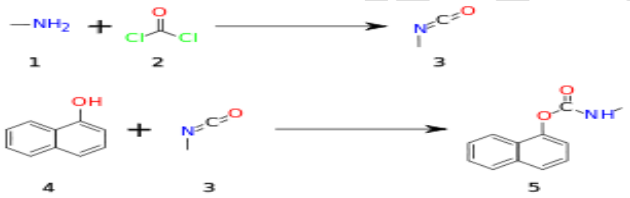


At 25 °C, in excess water, half of the MIC is consumed in 9 min.; if the heat is not efficiently removed from the mixture, the rate of the reaction will increase and rapidly cause the MIC to boil. If MIC is in excess, 1,3,5-trimethylbiuret is formed along with carbon dioxide. Alcohols and phenols, which contain an O-H group, react slowly with MIC, but the reaction can be catalyzed by trialkylamines or dialkyltin dicarboxylate. Oximes, hydroxylamines, and enols also react with MIC to form methylcarbamates.



Carbaryl (1-naphthyl methylcarbamate) is a chemical in the carbamate family used chiefly as an insecticide. It is a white crystalline solid commonly sold under the brand name **Sevin**, a trademark of the Bayer Company. Union Carbide discovered carbaryl and introduced it commercially in 1958.

Bayer purchased Aventis CropScience in 2002, a company that included Union Carbide pesticide operations. It remains the third-most-used insecticide in the United States for home gardens, commercial agriculture, and forestry and rangeland protection. About 11 million kilograms were applied to U.S. farm crops in 1976.[1] As a veterinary drug, it is known as **carbaril**. Carbaryl is produced by treating methyl isocyanate (**3**) with 1-naphthol (**4**).



Alternatively, 1-naphthol (**1**) is first converted to its (2) chloroformate (**3**) which is then treated with methylamine to give the desired product (**4**).

In November 1984, most of the safety systems were not functioning and many valves and lines were in poor condition. In addition, several vent gas scrubbers had been out of service as well as the steam boiler, intended to clean the pipes. Another issue was that Tank 610 contained 42 tons of MIC, more than safety rules allowed for. During the night of 2–3 December 1984, water entered a side pipe that was missing its slip-blind plate and entered Tank E610 which contained 42 tons of MIC. A runaway reaction started, which was accelerated by contaminants, high temperatures and other factors. The reaction was sped up by the presence of iron from corroding non-stainless steel pipelines. The resulting exothermic reaction increased the temperature inside the tank to over 200 C (392 F) and raised the pressure. This forced the emergency venting of pressure from the MIC holding tank, releasing a large volume of toxic gases. About 30 metric tons of methyl isocyanate (MIC) escaped from the tank into the atmosphere in 45 to 60 minutes. The initial effects of exposure were coughing, severe eye irritation and a feeling of suffocation, burning in the respiratory tract, blepharospasm, breathlessness, and stomach pains and vomiting. People awakened by these symptoms fled away from the plant. Those who ran inhaled more than those who had a vehicle to ride. Owing to their height, children and other people of shorter stature inhaled higher concentrations. **The gas cloud,** The gases were blown in southeastern direction over Bhopal. As of 2008, UCC had not released information about the possible composition of the cloud. Apart from MIC, the gas cloud may have contained phosgene, hydrogen cyanide, carbon monoxide, hydrogen chloride, oxides of nitrogen, mono-methyl amine (MMA) and carbon dioxide, either produced in the storage tank or in the atmosphere. As the gas cloud was composed mainly of materials denser than surrounding air, it stayed close to ground and spread outwards through surrounding community. **Thermal runaway** by definition the enthalpy change has a negative value: $\Delta H < 0$ in an exothermic reaction, gives a negative value for ΔH, since a larger value (the energy released in the reaction) is subtracted from a smaller value (the energy used for the reaction). For example, when hydrogen burns: $2H_2$ (g) + O_2 (g) → $2H_2O$ (g), $\Delta H = -483.6$ kJ/mol of O_2. An **exothermic reaction** is a chemical reaction that releases energy in the form of light or heat. It is the opposite of an endothermic reaction. Expressed in a chemical equation: reactants → products + energy.

Table (1) :- Chemicals dumped by Union Carbide management in and around the factory from 1969 to 1984.

S.No.	Chemicals	Amount	Use in	Pollution
1.	Methylene Chloride	100 MT	Solvent	Air
2.	Methanol	50 MT	Solvent	Air
3.	Ortho-idichlorobenzene	500 MT	Solvent	Air, Water, Soil
4.	Carbon tetrachloride	500 MT	Solvent	Air
5.	Chloroform	300 MT	Solvent	Air
6.	Tri methylamine	50 MT	Catalyst	Air
7.	Chloro benzyl chloride	10 MT	Ingredient	Air, Water, Soil
8.	Mono chloro toluene	10 MT	Ingredient	Air, Water, Soil
9.	Toluene	20 MT	Ingredient	Air, Water, Soil
10.	Aldicarb	2 MT	Product	Air, Water, Soil
11.	Carbaryl	50 MT	Product	Air, Water, Soil
12	Benzene Hexachloride	5 MT	Ingredient	Air, Water, Soil
13	Mercury	1 MT		Water, Soil
14	Mono methyl amine	25 MT	Ingredient	Air
15	Chlorine	20 MT	Ingredient	Air
16	Phosgene	5 MT	Ingredient	Air
17	Hydro chloric acid	50 MT	Ingredient	Air, Soil
18	Chloro sulphonic acid	50 MT	Ingredient	Air, Soil
19	Alpha Naphthol *	50 MT	Ingredient	Air, Soil
20	Napthalin	50 MT	Ingredient	Air
21	Chemical waste Tar	50 MT	Waste	Water, Soil
22	Methyl Isocyanate	5 MT	Ingredient	Air, Water, Soil

Sodium methoxide, triethyl phosphine, ferric chloride and certain other metal compounds catalyze the formation of the MIC-trimer, while the high-molecular-weight polymer formation is catalyzed by certain trialkylamines. Since the formation of the MIC trimer is exothermic (298 calories per gram of MIC), the reaction can lead to violent boiling of the MIC. The high-molecular-weight polymer hydrolyzes in hot water to form the trimethyl isocyanurate. Since catalytic metal salts can be formed from impurities in commercial grade MIC and steel, this product must not be stored in steel drums or tanks. The MIC must be stored at temperatures below 40^0C (104^0F) and preferably at 4^0 (39^0F). The toxic effect of the compound was apparent in the Bhopal disaster, when around 42,000 kilograms (93,000 ^{0} lb) of methyl isocyanate and other gases were released from the underground reservoirs of Union Carbide India Limited (UCIL) factory, detailed chemicals was present at time of disaster is listed in Table [1].

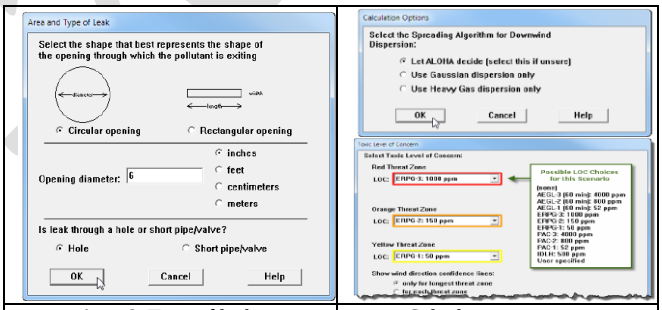
Installing safety devices can cost between 15-30 % of outlay at a plant's inception. In light of UCC's $20 million investment in Bhopal, this amounts to $3-6 million. Carbide's own documents show that the company trimmed $8 million off their initial cost estimates, the plant was supposed to cost a total of $28 million. In 2002, secret Union Carbide documents obtained by "***discovery***" during a class action lawsuit brought by survivors against UCC, revealed for the first time that the technology used at the fatal Bhopal factory including the crucial units manufacturing carbon monoxide and MIC was "***unproven***," meaning the company knew it could pose unknown risks. This is how they had saved so much money they didn't install safety mechanisms that had been tried and tested and known to be effective. When managers make a deliberate decision to stop an activity, they usually let it quietly lapse and do not draw attention to the **CHANGE**. However one report frankly stated, "The data collection system was run for a period of about 3 years. The system is now no longer running not because it was unsuccessful, but because the management emphasis on the works has changed. The emphasis is now on the reduction of unnecessary work, not on the reductions of breakdowns [7 & 8]

II. METHODOLOGY

A chemical vapor cloud is composed of a pollutant chemical and air in a ratio that changes with time and location. Clouds containing chemicals with high molecular weight, or aerosols, can be sufficiently dense that gravity has a significant effect on their movements. These dense gas clouds are modeled differently in ALOHA than clouds that are not directly affected by gravity. ALOHA incorporates two semi-empirical air dispersion models:

- The Gaussian model is appropriate for pollutants clouds that are not directly affected by gravity;
- The Heavy Gas model is appropriate for pollutant clouds with densities greater than the ambient air and affected in a significant way by gravity.

These air dispersion models used for neutral and dense pollutant plumes in ALOHA can account for vertical gradients in wind speed and atmospheric turbulence, but do not account for topographic steering or winds that vary with time. Guidance on when to model and how to interpret modelling results, in terms of evaluating the potential effects of the discharge on the environment, will be contained in a separate document currently being prepared by the Ministry entitled the Good Practice Guide for Assessing Discharges to Air. Although these two areas are integrally linked they have been separated to avoid excessive complexity in one document. Modelling the gas leak. The existing models for the dispersion of air pollutants may be broadly classified into two groups: analytical models such as Gaussian plume/puff and numerical models. The Gaussian type of dispersion models which assumes that the winds are constant in space and time may fail in an urban environment. Most of the modifications to incorporate the changes in wind speed and direction with height, are based on at/hoc assumptions.



Area & Type of leak. | Calculations options.

Fig. 6 :Area and type of leak & calculations options.

Limitations

- ALOHA does not account for the effects of fires or chemical reactions.
- ALOHA does not account for terrain steering effects.
- ALOHA does not model dispersion effects associated with building wakes.

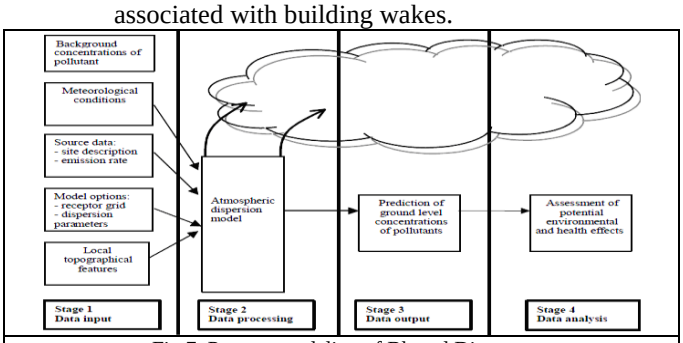


Fig 7: Process modeling of Bhopal Disaster.

The accuracy and uncertainty of each stage must be known and evaluated to ensure a reliable assessment of the significance of any potential adverse effects. A model is a simplified picture of reality [9].

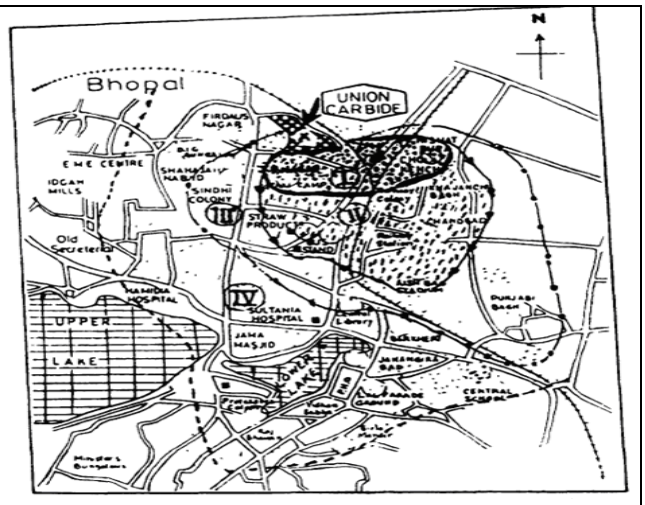
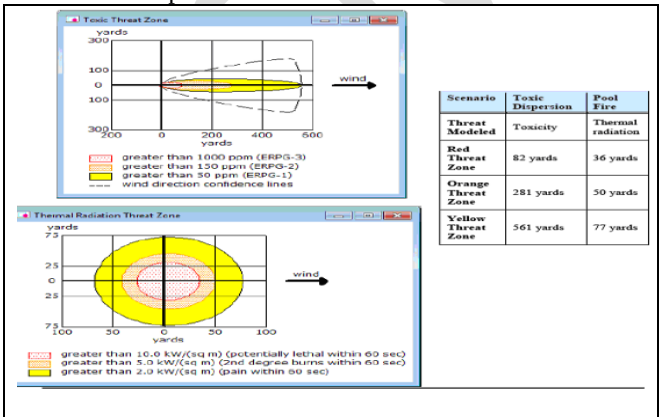


Fig [8]: The gas affected areas determined on the basis of mortahty state stacs are indicated by dots and the concentration of dots approximately represents the extent of the effect. Contours in & cate the parts per million isopleths are classified as follows: Zone I, 50 ppm; Zone II, 15 ppm, Zone III, 1.5 ppm and Zone IV, < 1 0 ppm.

It doesn't contain all the features of the real system but contains the features of interest for the management issue or scientific problem we wish to solve by its use. Models are widely used in science to make predictions and/or to solve problems, and are often used to identify the best solutions for the management of specific environmental problems. An atmospheric dispersion model is a:

- Mathematical simulation of the physics and chemistry governing the transport, dispersion and transformation of pollutants in the atmosphere.
- Means of estimating downwind air pollution concentrations given information about the pollutant emissions and nature of the atmosphere.

Dispersion models can take many forms. The simplest are provided in the form of graphs, tables or formulae on paper. Today dispersion models more commonly take the form of computer programs, with user-friendly interfaces and online help facilities.



Scenario	Toxic Dispersion	Pool Fire
Threat Modeled	Toxicity	Thermal radiation
Red Threat Zone	82 yards	36 yards
Orange Threat Zone	281 yards	50 yards
Yellow Threat Zone	561 yards	77 yards

Fig [9]: This is a footprint plot generated by ALOHA. The footprint represents an overhead view of the area where the concentration of the chemical released is predicted to exceed the LOC at some time during the hour after the release begins. How to interpret a footprint depends on what level of concern is being used.

III. CONCLUSIONS

ALOHA Software are widely used, well understood, easy to apply, and until more recently have received international approval. Even today, from a regulatory point of view ease of application and consistency between applications is important [5 & 6]. Also, the assumptions, errors and uncertainties of these models are generally well understood, although they still suffer from misuse. ALOHA software used Gaussian-plume models for the dispersion Modelling. Gaussian-plume models play a major role in the regulatory arena. The Gaussian-plume formula is derived assuming 'steady-state' conditions. That is, the Gaussian-plume dispersion formulae do not depend on time, although they do represent an ensemble time average. The meteorological conditions are assumed to remain constant during the dispersion from source to receptor, which is effectively instantaneous. Emissions and meteorological conditions can vary from hour to hour but the model calculations in each hour are independent of those in other hours. Due to this mathematical derivation, it is common to refer to Gaussian-plume models as steady-state dispersion models. In practice, however, the plume characteristics do change over time, because they depend on changing emissions and meteorological conditions. One consequence of the plume formulation is that each hour the plume extends instantaneously out to infinity. Concentrations may then be found at points too distant for emitted pollutants to have reached them in an hour.

On the night of Dec. 2nd and 3rd, 1984, a Union Carbide plant in Bhopal, began leaking. due to run-away reactions, temperature and pressure rise and the safety valve lifted to the atmosphere. About 25-27 tons of the deadly gas methyl isocynate spread through the city of Bhopal. Half a million people were exposed to the gas. Protective systems that should have prevented or minimized discharge were out of service. Refrigeration system to cool the reactor was down. Scrubbing system to absorb the released vapour was not immediately available. Flare system to burn vapours getting past the scrubber was out of service.Lessons we learned form Bhopal Tragedy; (1) Reduce inventory of hazardous material (MIC), (2) Keep all the safety related equipment in order (3) Keep residential areas away from the plant, (4) Proper Management. The Logical Framework Approach (LFA) seems more complete and useful for a complex situation like the Bhopal gas leak. The problem and objectives trees look like a chain of events from where there are branches and roots. The matrix makes it possible to clarify what processes/changes from other instances are needed if the project is to succeed. As this is an analysis of an accident that has already happened, the matrix deals with both prevention and management. The results of the overall investigation are discussed and it is demonstrated that the commonly held view that water-washing of a certain header caused the disaster is physically impossible. Evidence is presented which indicates that direct water entry into the methyl isocyanate storage tank was the likely initiating cause of the Bhopal disaster. [8]

The Bhopal gas leak clearly illustrates the threat to public health posed by the chemical industry: (a) A hazardous work environment. (b) The risk of exposure for the host population. (c) Direct damage to the environment during the production process, which creates hazards to human health. (d) Production of substances, in this case pesticides, that are toxic to human beings when used, and are the cause of many deaths in large parts of the world. (e) Production of substances that have long-term toxic effects on the environment, and which may lead to contaminated food and water as well as to decreased food production in the long run.

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