CHEMICAL WARFARE OPERATIONS

ABSTRACT:

In 1915 the first Chemical warfare operation in modern history, most of the research is done based on experimental chemistry and the animal science laboratory for testing and measurement of toxicity dose and lethal dose. The aim of this chapter is laid a stable foundation for design of chemical warfare agents and design principle for chemical warfare operations .from theoretical physical chemistry, fluid flow mechanics and theoretical thermodynamics.To develop very efficient chemical warfare gas agent, the Optimum a gas chemical warfare agents are defined as having colorless, odorless and lethal concentrations at very low concentrations. Very low hydrolysis in water, high stability and high solubility in water.The first stage of development, in any chemical warfare agent, is selection of the method of exposure and the harm mechanisms. The main elements and groups are used for the development of gas-chemical warfare agents. , these elements and groups are classified based on harm mechanisms. The first group of halogens is Cl, F, Br, and I. The second group is unsaturated oxides: carbon monoxide and sulfur oxides. The third group is Toxic elements such as cyanide, sulfur, and arsenic. The Fourth group is organic phosphorus. These elements and groups are combined with phenyl, benzyl, Xylyl, Methyl, Ethyl, and vinyl groups Such as Halogens Methyl. There are several kinds of calculations and experimental testing to be carried out, such as thermodynamics calculations(Gibbs free energy calculations, enthalpy formation and analysis, entropy analysis), reaction kinetics, reaction rates for any chemical agents with target compounds, and then experimental studies for the effect of gas nerve agents on animals.Design chemical warfare operation has many process parameters to study, for developing the desired chemical cloud for the volume occupying 3 meters above ground for the battlefield area by multiplying three meters in the area. Meteorological are very important parameters for atmospheric fluid flow in design chemical warfare operation. Chemical warfare gas agent at lethal requirement concentration for producing the highest lethality rate. This is a combined process of convective mass transfer and diffusion mass transfer. Producing chemical cloud with lethal concentration and time of operations, meteorological parameters

Keywords: chemical warfare agent, reaction kinetic, reaction rate, Meteorological , chemical cloud, Optimum a gas chemical warfare,

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1. INTRODUCTION :

Chemical weapons are defined as chemical substances that have the ability to react with the human body if exposed to them, destroying the human body and generating death. These chemical substances are classified based on their presence phase. Gas chemical warfare agents, liquid chemical warfare agents, and solid chemical warfare agents.The purpose of using chemical weapons is to generate a high lethality rate in enemy troops units and generate uninhabitable areas and buffer zones in the war field. As well as destroy food production areas, food and feedstock, livestock or cropland.The harm mechanisms of chemical warfare agents are based on chemical reactions between human body parts and chemical warfare agents.Gas chemical warfare agents are classified as choking agents, blister agents, nerve agents, and blood agents.Choking agents react with molecules of biological fluids and the skin of the respiratory system inside the lining of the airways, such as the nose, throat, and lungs, and cause irreversible biochemical changes.Blood agents release cyanide ions. Hemoglobin is bound with cyanide, stopping it from using oxygen in red blood cells.Blistering agents are used for alkylating human body molecules such as proteins, cellular membranes, and nucleic acids Which leads to cancer.Nerve agents inhibit acetylcholine, producing an excess of acetylcholine, overstimulating the neuromuscular junction,Disrupt neurotransmission, leading to neurological damage and death.

2.DESIGN PRINCIPLES OF CHEMICAL WARFARE AGENTS:

Chemical warfare agents are used against enemy troops, causing mass killings. The killing mechanisms are due to the reaction between the human body and chemical warfare agents.There are four ways to expose chemical warfare agents: by eye, inhalation, dermal and ingestion.Optimum a gas chemical warfare agents are defined as having colorless, odorless and lethal concentrations very low concentrations.Very low hydrolysis in water, high stability and high solubility in water.Human body tissues are classified into four kinds:connective tissue, epithelial tissue, muscle tissue, and nervous tissue.Connective tissues are bound, moved and supported by other types of tissues, such as blood, bone and lymph tissues.Epithelial tissues provide cover and protection for other tissues inside the body or outside the body, such as skin, the lining of the lung, and the lining of the various passages inside the body Epithelial tissue contains proteins, water, lipids, and carbohydrates.Muscle tissue is a soft tissue such as cardiac tissue or muscles around the stomach.Muscle tissue contains mitochondria, Myoglobin, water, lipids, proteins, ATP, ADP, nucleic acid,cytochrome oxidase, hexokinase, phosphofructokinase, and Carbohydrates. .Nerve tissue contains nerve cells to carry electrical signals to and from various parts of the body.Nerve tissue is contained in water, lipids, proteins,Carbohydrates, and nucleic acids.For designing gas chemical warfare agents, the first step is to select the method of exposure. There are three methods of exposure: inhalation of vapors, dermal contact or eye contact.The second step in designing a gas chemical warfare agent is to choose the locally poisons or systemic poisons.There are several toxic elements groups used in gas chemical warfare agents :The main elements and groups are used for the development of gas-chemical warfare agents. , these elements and groups are classified based on harm mechanisms. The first group of halogens is Cl, F, Br, and I. The second group is unsaturated oxides: carbon monoxide and sulfur oxides. The third group is Toxic elements such as cyanide, sulfur, and arsenic. The Fourth group is organic phosphorus.These elements and groups are combined with phenyl, benzyl, Xylyl, Methyl, Ethyl, and vinyl groups Such as Halogens Methyl.There is a strong connection between chemical composition,

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toxic effects, and harm mechanisms. Such as local poisoning harm mechanisms, generally chemical reactions between strong oxidative agents such as phosgene.Choking agents are classified as local poisoning type This choking agent reacts instantly with biological tissue, such as lung lining tissues and skin tissues.Choking agents are oxidized biological molecules such as nucleic acids and proteins in the lining of the lungs and respiratory tract. The oxidization process for biological molecules by hydrochloric acid (HCL) and hypochlorous acid (HClO). HClO penetrates cells and reacts with proteins to degrade cellular structures.

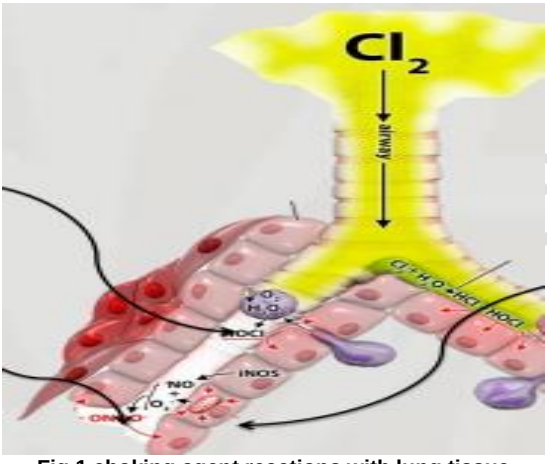


Fig.1 choking agent reactions with lung tissue

Lethal reaction for a choking agent:

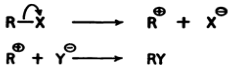
$$Cl_2+H_2O \rightarrow HCl+HOCl$$

$$COCl_2+ H_2O \rightarrow 2HCl+CO_2$$

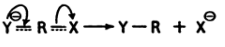
Hydrochloric acid reacts with DNA, proteins, and DNA enzymes; this is the so-called denaturation reaction between hydrochloric acid and respiratory system lining, such as lung lining tissues (proteins, carbohydrates, DNA, and DNA repair enzymes). The oxidation reaction between Hydrochloric acid and respiratory lining tissues changes the nature of those tissues.

Blistering agents are classified as local poisoning type. Blistering agents have harm mechanisms by alkylating biological molecules such as nucleic acids, DNA, proteins, and cellular membranes components. Alkylating is the replacement of an active hydrogen in biological molecules with an alkyl group, an aliphatic group, or an aliphatic-aromatic (e.g., benzyl) group.An alkylation reaction is a type of chemical reaction that introduces an alkyl group into other molecules.Alkylating process is affected by DNA replication and causes cells to die.Vesicants (blistering agents) are chemical warfare agents that cause blistering lesions in the skin, respiratory tracts, lungs and mucous membranes.Alkylating process is a chemical reaction attached of alkyl group to an organic molecule of skin tissue through substitution.Alkylation is the reaction of electrophilic chemical compounds or alkylating agents with the nucleophilic centers in organic macromolecules(Nucleophiles are chemical substances that can donate electrons. Electrophiles are substances that can accept electrons).Blistering agents are generated in huge inflammatory reaction, with poisoning by blistering agents and the destruction of exposing tissues.Blistering Chemical warfare agents are alkylating agents, which are capable of replacing a hydrogen atom in another molecule by an alkyl radical group, generating massive

inflammatory reactions in tissues of skin.This including electrophilic attack by the alkylating agent, such as reactions of replacing radical group to a molecule containing an atom in a lower valency state.There are two types of alkylating process, first-order nucleophilic substitution and second-order nucleophilic substitution .



Alkylation First order



alkylation second-order

Blistering agents are very reactive chemicals with protein, DNA and other skin tissues, causing blisters or vesicles on skin,other epithelial tissues and mucous membrane upon exposing blistering agents.

Lethal reaction for a blistering agent: sulfur mustard alkylation of DNA

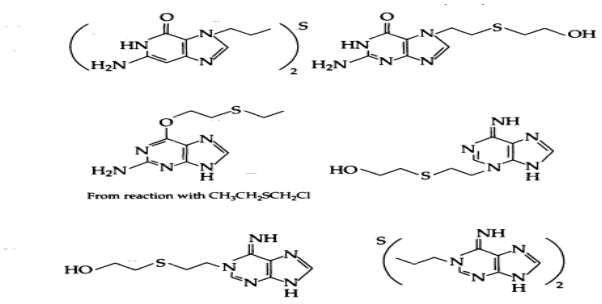


Fig.2

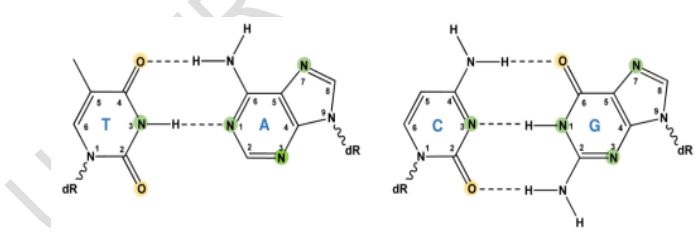


Fig.3 DNA Alkylation

Alkylation process causes DNA damage. Due to transfer alkyl groups to the nitrogenous bases.Causing by blistering agents such as sulphur mustard. Alkyl groups are caused in cross-linking in DNA, RNA.

For the design and development of any gas blistering agents, there are several kinds of calculations and experimental testing to be carried out, such as thermodynamics calculations(Gibbs free energy calculations, enthalpy formation and analysis, entropy analysis), reaction kinetics, reaction rates for blistering agents with target compounds, and then experimental studies for the effect of gas blistering agents on animals.

Blood agents are classified as systemic poisons type. These blood agents are inhaled to release cyanide ions in the blood and bind with hemoglobin. This

prevents cells from using oxygen. Cyanide ions are distributed via the bloodstream and bind to the metabolic enzyme cytochrome oxidase , generally enters the body via inhalation. They inhibit the ability of blood cells to utilize and transfer oxygen.There are two types of blood agents: cyanide-based agents and arsine-based agents.The cyanide ions interrupt electron transfer in the mitochondria, stopping oxygen utilization in cells,The cyanide ion is bonded with hemoglobin to produce cyanhemoglobin.Hydrogen cyanide is absorbed through respiratory by inhalation. Then release the cyanide ions into the bloodstream of the human body.The arsine ions are destroying the red blood cells.Thus blood agents are poisons that effectively cause the body to suffocate.Inhibiting oxygen consumption strategy for the development and design of gas-chemical warfare blood agents, by using mitochondrial cytochrome oxidase.Cytochrome c oxidase is the terminal electron acceptor of the mitochondrial electron transport chain, catalyzing the oxidation of ferrocytochrome c by oxygen.HCN binds tightly to the binuclear center of oxidized cytochrome oxidase.The inhibition process is done by binding cyanide with methemoglobin. The toxicity of the body is a process of inhibition of the catalytic function of cytochrome oxidase enzymes due to the failure of hemoglobin to carry oxygen due to binding cyanide with methemoglobin.the formation of cyanide methemoglobin

Lethal reaction for a blood agent:

$$Hb^{+}\ OH_2+HCN \rightarrow HbCN+H_3O^{+}$$

$$Hb^{+}\ OH_2+CN \rightarrow HbCN+H_2O$$

$$HbOH+HCN \rightarrow HbCN+H_2O$$

$$HbOH+CN^{-} \rightarrow HbCN+OH^{-}$$

For the design and development of any gas blood agents, there are several kinds of calculations and experimental testing to be carried out, such as thermodynamics calculations(Gibbs free energy calculations, enthalpy formation and analysis, entropy analysis), reaction kinetics, reaction rates for blood agents with target compounds, and then experimental studies for the effect of gas blood agents on animals. Nerve agents are classified as systemic poisons type.as nerve agents are inhaled by the respiratory system. The lining of the respiratory system absorbs nerve agents and transports them to the bloodstream. The harm mechanism for nerve agents is based on blockage of impulses between nerve cells or across synapses.The nerve agents have a harm mechanism based on the inhibition of Acetylcholinesterase (AchE).Sarin(GB, O-isopropyl methylphosphonofluoridate) is inhabited acetylcholinesterase by combining a covalent bond with the serine residue at the active site. Releasing Fluoride from the group and producing organ-phosphoester is robust and biologically inactive.The AChE enzyme is a cholinergic enzyme located between nerve cells and in the synapse between animal nerve and muscle cells. This enzyme decomposes acetylcholine into acetic acid and choline the AChE enzyme.AChE is a cholinergic enzyme, this enzyme is converted by hydrolysis ACh to choline and acetate.Acetylcholinesterase catalyzes the hydrolysis of acetylcholine to acetate and choline. And hydrolyze acetic acid esters and can catalyze transacetylations.Nerve agents are defined as acetylcholinesterase irreversible inhibitors.The major mechanism of acute toxicity is the irreversible inhibition of acetylcholinesterase (AchE).Nerve agents have main toxicological effects through Irreversible phosphorylation of esterases in the central nervous system ,have The acute toxic effects are irreversible inactivation of AChE.

Lethal reaction for a nerve agent:

$$E + PX \rightleftarrows E * PX \xrightarrow{k_3} EP + X$$

where, E–enzyme, PX–OP, E* PX–reversible enzyme-OP complex, EP–phosphorylated enzyme, X–OP leaving group. The irreversible inhibition process

has two steps:the first step, enzyme inactivation, which occurs very quickly, and the inhibition influences dominant behavior. The second step generates a stable enzyme complex, phosphorylated enzyme. Inhibitor covalently bonded to the enzyme, which is irreversible inhibition.irreversible inhibition process is a time dependent process is given by this formula

$$\ln \frac{E}{E_o} = -\frac{k_3 t}{1 + K_I / (I)}$$

where, E/Eo–remaining enzyme activity related to initial enzyme activity (control) (Eo), KI–dissociation constant for enzyme-inhibitor complex E* PX, k3–the first rate constant for the conversion of the reversible enzyme-inhibitor complex to phosphorylated enzyme, EP, (I)–inhibitor (OP) concentration, t–time interval after the enzyme and inhibitor mixing. If (I) » (Eo), the reciprocal slope value of linear dependence ln(E/Eo) - t from graph ,the formula below:

$$\frac{1}{k_{app}} = \frac{1}{k_3} + \frac{K_I}{k_3} \cdot \frac{1}{(I)}$$

The values of inhibition parameters, KI and k3, are calculated from the slope and intersection of 1/kapp - 1/(I) linear dependence graph Kapp vs $C_{inhibitor}$. Effective OPs have the following structural features: a terminal oxygen connected to phosphorus by a double bond (oxo form), two lipophilic groups (–R1, –R2) bonded to the phosphorus, and a good leaving group (–X) bonded to the phosphorus.For the design and development of any gas nerve agents, there are several kinds of calculations and experimental testing to be carried out, such as thermodynamics calculations(Gibbs free energy calculations, enthalpy formation and analysis, entropy analysis), reaction kinetics, reaction rates for nerve agents with target compounds, and then experimental studies for the effect of gas nerve agents on animals.

There are four main types of gas chemical warfare agents: blistering agents, choking agents, blood agents and nerves agents.The first step in designing a gas chemical warfare agent is to define the method of exposure: skin dermal or inhalation, or eye or ingestion. The second step in designing a gas-chemical warfare agent is selecting the harm mechanisms by selecting target tissue for damage.Choking agents are mainly affected by the respiratory tract, throat and lungs tissues by oxidation by gas chemical warfare agents such as chlorine and phosgene.A choking agent is an oxidizing agent that reacts with water to form hydrochloric acid, hypochlorous acid and oxygen-free radicals, which directly damage lung tissue and cause pulmonary edema.Blistering agents are oily substances that act as irritants and then as cell poisons on the skin or, when inhaled, cause life-threatening blisters. Such as sulfur mustard, and lewisiteBlistering agents are used for rapid covalent binding with biological tissues such as proteins, DNA, and amino acids and alkylating biological tissues. Cyclic ethylene sulphonium ions, which alkylate amino and sulfhydryl groups in nucleic acids and peptides. Leading to enzyme inactivation, loss of calcium homeostasis, lipid peroxidation, cellular membrane disruption and death.Blood agents inhabit the cell to use oxygen, generally entering the body through inhalation distributed through the blood, such as hydrogen cyanide.The blood agent is used in the cyanide element to inhibition of cytochrome oxidase enzymes and transfer electrons by binding to the trivalent ion in the porphyrin moiety of cytochrome and then interrupting mitochondrial function and oxygen utilization, causing histotoxic hypoxia.Nerve agents are affected by the nervous systems, leading to hyperstimulation of muscles. Such as sarin, soman, tabun and VX.Nerve agents are acted upon by absorption through the skin or through the lungs.Nerve agents contain amides or ester derivatives of phosphoric acid, mainly organophosphate compounds. These compounds inhibit acetylcholinesterase (AChE) and are classified as G or V agents.The first step in the toxicity of nerve agents is the inhibition of AChE. ACHE has two active sites: anionic and esteratic.Nerve agents are inactivated AChE by alkyl

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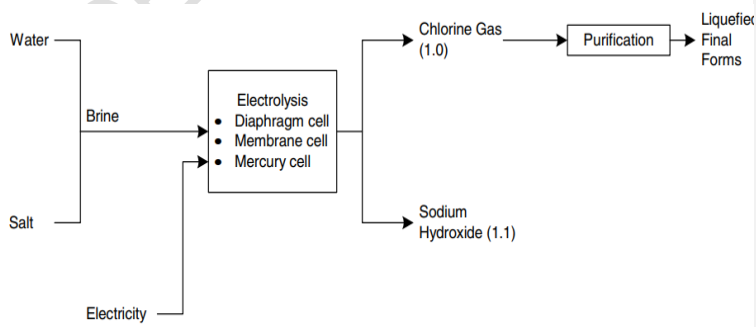
phosphorylation of a serine hydroxyl group at the esteratic site of the enzyme.In the second step ACh accumulates at nicotine, muscarinic and central nervous synapses. The nerve agent eventually loses (nonenzymatically) an alkyl side chain and the stability of the enzyme–nerve agent complex is enhanced,Enzyme inactivation is irreversible, and irrecoverable.

CHOKING AGENTS:

Choking agents are chemicals that can cause swelling of the respiratory tract, disrupt breathing.Choking agents are locally poisons and potentially cause permanent lung damage due to oxidation agents such as hydrochloric acid (HCL) and hypochlorous acid (HClO). HClO penetrates cells and reacts with proteins to degrade cellular structures.these oxidants agents are released due to dissolving or decomposing gas chemical warfare agents such as chlorine and Phosgene.

Chlorine Cl_2:

It is a yellow-green gas at normal temperature.Atomic Symbol Cl Atomic Number 17 ,Atomic Weight: 35.453 , there are three chlorine isotopes ^{35}Cl (75.76 %) and ^{37}Cl (24.24 %) and radioactive ^{36}Cl ($t_{0.5}$ = 301.3 ka) .Chlorine is considered a very strong oxidizing agent and a very reactive element. It has high electron affinity and S^2 P^5 outer electron configuration, highly electronegativity.Chlorine as a gas heavier than air and sparingly soluble in water, it is an oxidative agent for any combustible materials.Chlorine was first separated and produced by the the Swedish scientist Carl Wilhelm Scheele in 1774.Chlorine is very reactive element with many elements, organic and inorganic, and it has hazardous to the aquatic environment.The first gas was used as chemical warfare agent in World War I. Chlorine has a common form, chloride, with a valence of -1. There are other different valence states. Chloride is combined with strong ionic bonds in salts.Chlorine reacts with hydrogen, forming a very corrosive gas called hydrogen chloride. This gas is dissolved in water and forming hydrochloric acid HCl.Chlorine is a part of halogens group in the periodic table (fluorine,chlorine,bromine, and the radioactive elements astatine and tennessin).Halogen means salt maker, which means it reacts with metals and combines many salts.Most of the chlorine on the market is produced by the chlor-alkali method. This method utilizes the electrolysis process for sodium chloride solution. Electricity is used to separate sodium ions and chloride ions in solution by electrolytic cells.The chlorine production process is a second to the aluminum



production process as a consumer of electricity among the electrolytic processes.

Fig.4 chlorine production

The electrolytic cell converts sodium chloride brine tochlorine, and sodium hydroxide can take place in one of three types of electrolytic cells(the diaphragm

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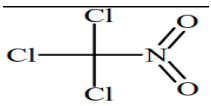
cell, the membrane cell, or the mercury cell).Chlorine is used as a chemical warfare agent. The harm mechanism throughout inhalation by oxidizing biological tissues due to hydrochloric acid (HCL) and hypochlorous acid (HClO). HClO penetrates cells and reacts with proteins to degrade cellular structures.

Chloropicrin(PS):

CCl_3NO_2



Chloropicrin is called PS, or nitrochloroform. Chloropicrin (trichloronitromethane) was patented for use as an insecticide in 1908, found to have lung damage effects, and then used as a chemical warfare agent during World War I. This chemical compound is used as a chemical warfare agent, a fungicide, a herbicide and insecticide. During World War I was used by Russia. Chloropicrin was prepared by reaction between picric acid and sodium hypochlorite, by Scottish chemist John Stenhouse in 1848.Until now, some countries have used chloropicrin as a chemical warfare agent. Chloropicrin has the following physical properties: its molecular weight is 164.38 grams/mol; chloropicrin is a colorless liquid with a boiling point of 112 °C, Chloropicrin is sparingly soluble in water,

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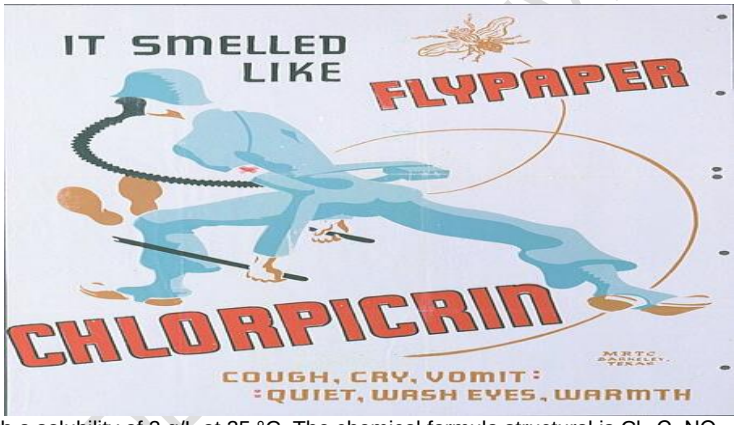

with a solubility of 2 g/L at 25 °C. The chemical formula structural is Cl_3 C−NO_2 .

Fig 5. Identification of chloropicrin

Chloropicrin was called a lung-damaging Agent, a chemical warfare during World War I. For the first time, Chloropicrin was synthesized by,the reaction between sodium hypochlorite and picric acid.

$HOC6H2(NO2)3+ 11\ NaOCl \rightarrow 3\ Cl3CNO2+ 3Na2CO3+ 3NaOH+ 2NaCl$

On an industrial scale, chloropicrin is manufactured by the reaction between nitromethane and sodium hypochlorite.

$H3CNO2+ 3\ NaOCl \rightarrow Cl3CNO2+ 3\ NaOH$

chloropicrin is produced by using the reaction between chloroform and nitric acid.

$Cl3CH + HONO2 \rightarrow Cl3CNO+ H2O$

Inhalation of chloropicrin causes damage to the respiratory system and edema. The harm mechanism is based on oxidizing lung lining tissue (proteins, DNA, RNA,skin, mucosal membranes etc.) in the respiratory system.Chloropicrin reacts with sulfhydryl in hemoglobin, declining oxygen transport.chloropicrin is very harmful for inhalation by human epithelial and lung epithelial cells. Chloropicrin is released in large amounts of reactive oxygen species in an epithelial cell line, and lung epithelial cells revealed massive vacuolization and the number of apoptotic cells. As increasing the chloropicrin concentration. chloropicrin is denatured protein,DNA,etc.chloropicrin toxicity is generated due to the denaturation reactions of lung lining tissues. Causing coughing, bronchitis, and pulmonary edema in humans.

Phosgene CG:

PhosgeneCOCl2 is a chemical warfare gas classified as choking agents.The meaning of Phosgene from Greek phos is light and gene is born. The agent has physical properties a planar molecule, toxic, colorless, musty odor, The C=O distance is 1.18 Å, the C−Cl distance is 1.74 Å and the Cl−C−Cl angle is 111.8°,and nonflammable gas.phosgene is a poisonous gas and, under certain conditions of cooling and pressure, converted to liquid.Phosgene (Carbonyl dichloride) was patented in 1812 by the British chemist John Davy.The First synthesis reaction for phosgene preparation, was by mixingof carbon monoxide and chlorine into sunlight.Phosgene is produced by combining carbon monoxide and chlorine with a catalyst activated carbon .

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$$CO + Cl_2 \rightarrow COCl_2 + Heat$$

The reaction is exothermic, as the reactor that is used must be provided by a heat exchanger for removing heat from the reaction.Inhalation phosgene is oxidized lung lining in the respiratory tracts. Parts of Phosgene are formed with water in mucous membranes in hydrochloric acid, which is oxidized lung lining, and other parts of phosgene are used in the carbonyl group to damage alveolar-capillary membranes, producing non-cardiogenic pulmonary edema. Potentially life-threatening lung injury even after an initial inhalation.Pulmonary edema is the most common lung lining injury due to choking agents.Denaturation disrupts protein structure, to damage biological function for proteins by chemical agents.

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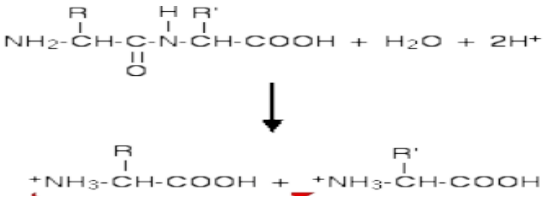

Fig.6 Denaturation protein by acid

Denaturation process for a protein molecule, it is broken chemical bonds to unravel the tight bundle of amino acids. Causing the protein molecule to unfold. Losses of biological functions and changes of shape. Phosgene is rapidly hydrolyzed; the reaction is hydrolysis by water, yielding carbon dioxide and hydrochloric acid in aqueous solution to CO2 and HCl. Phosgene is electrophilic and undergoes attack by a variety of nucleophiles. Phosgene reacts with different types of nucleophiles, such as primary and secondary amines, hydroxyl groups, and thiols. In addition, it also reacts with macromolecules, such as enzymes, proteins, or other polar phospholipids. Formation of covalent bonds, disrupting molecular functions of these molecules.

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Diphosgene(DP):

Diphosgene has the formula ClCO2CCl3,Diphosgene is an organic synthesis chemical compound. Diphosgene are highly toxic compounds due to inhalation. Oxidizing respiratory tracts resulting in pulmonary edema, pulmonary emphysema, and death.In May 1916, it was recorded as diphosgene as a chemical compound and as a chemical warfare agent in the world during World War I.Diphosgene is manufactured by using radical chlorination of methyl chloroformate by using UV light.

$Cl\text{-}CO\text{-}OCH_3 + 3\ Cl_2 \xrightarrow{(hv)} Cl\text{-}CO\text{-}OCCl_3 + 3\ HCl$

$H\text{-}CO\text{-}OCH_3 + 4\ Cl_2 \xrightarrow{(hv)} Cl\text{-}CO\text{-}OCCl_3 + 4\ HCl$

Diphosgene has physical properties: a colorless liquid with an odor similar to that of musty hay, high vapor pressure,Molar mass197.82 g/mol,liquid at room temperature, Density 1.65 g/cm3,melting point −57 °C (−71 °F; 216 K), boilingpoint 128 °C (262 °F; 401 K)Solubility in water insoluble.Diphosgene vapors are destroyed in the gas masks in 1916.Diphosgene is converted to phosgene due to heating or catalysis with charcoal, and is a valuable reagent in the synthesis of organic compounds.

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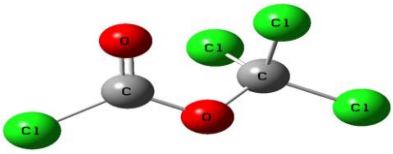
Fig.7 Diphosgene Chemical structure



Diphosgene is behaved in the same manner as phosgene. Diphosgene is formed with water in mucous membranes in hydrochloric acid, which is oxidized lung lining, and other parts of Diphosgene are used in the functional group to damage alveolar-capillary membranes, producing non-cardiogenic pulmonary edema. Potentially life-threatening lung injury even after an initial inhalation. Pulmonary

edema is the most common lung lining injury due to choking agents. Denaturation disrupts protein structure, to damage biological function for proteins by chemical agents.

Disulfur decafluoride:

Disulfur decafluoride is also called as sulfur pentafluoride or sulfur(V) fluoride , a chemical compound with the formula S_2F_{10}.Disulfur decafluoride has physical properties as a colorless, volatile liquid with a smell similar to sulfur dioxide. molecular weight 254.1 ,boiling point 29 C, melting point -92 C.Disulfur decafluoride is a highly toxic gas, Disulfur decafluoride is manufactured by using electrical discharges in SF_6.disulfur decafluoride is a strong oxidation agent compared to phosgene.disulfur decafluoride reacts with water in mucous membranes, forming sulfurous acid and hydrofluoric acid.These acids are oxidized lung lining tissues (protein, DNA, etc.).Disulfur decafluoride is manufactured by photolysis of this compound.

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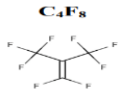
$$\mathbf{2\ SF_5Br \rightarrow S_2\ F_{10} + Br_2}$$

Disulfur decafluoride is a colorless gas or liquid and sulfur dioxide odor. Stronger, higher than phosgene, four times as poison. Due to Denaturation process in the lungs into SF_6.

Perfluoroisobutene:



Perfluoroisobutene (PFIB) is a colorless toxic gas,high electrophilic properties, odorless, hydrophobic reactive gas with boiling point 7 °C, melting point -130 °C and density 1.592 g/litre.Exposing by inhalation into the human body, the harm mechanism is based on oxidizing the lung lining tissues and denaturing respiratory system tissues. Causing pulmonary edema associated with problems in breathing.PFIB is decomposed to a radical anion, fluorophosgene, and hydrogen fluoride.PFIB reacts with water in mucous membranes, forming acids.These acids are oxidized lung lining tissues (protein, DNA, etc.),The higher the ractivity, the higher the toxicity.The high electrophilicity natural of PFIB due to the strong electron-attracting effects of the fluorine atoms of the trifluoromethyl groups and the conjugation of the fluorine's p electrons with the double bond of the vinyl group.PFIB reacts with nucleophilic reagents, to producing radical byproducts.PFIB is manufactured by pyrolysis of perfluoropropylene and also by thermal decomposition of polytetrafluoroethylene.

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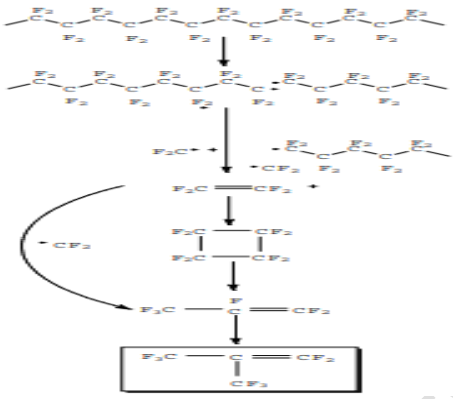

Fig.8 Preparation Perfluoroisobutene

PFIB is a highly toxic gas, stronger than phosgene by ten times to the lungs.The pulmonary epithelium signs due to damaging pulmonary by PFIB highly hydrophobic gases are reacted with lung tissue.

Acrolein(CH2=CHCHO):

acrolein or propenal is an α,β-unsaturated aldehyde,volatile flammable,Empirical formula C3H4O ,Structure C=C-C=O ,Molecular weight 56.06 g/mol,Vapor pressure 274 mm Hg 25°C, Vapor density1.94 (Air = 1), Specific gravity 0.8389 20°C ,Boiling point 52.5°C at 760 mm Hg,Melting point 88°C,Water solubility 208 g/L 20°C. very toxic gas was discovered in 1839 by the Swedish chemist Jöns Jacob Berzelius.Acrolein is manufactured by oxidizing of propene by air in presence of metal oxides as catalyst.Acrolein is a clear or yellow liquid with a burned, sweet, choking odor.

$CH3CH=CH2+ O2\rightarrow CH2=CHCHO + H2O$

Exposing Acrolein through dermal and inhalation to human body. Acrolein has high electrophilic and reactive with different lung lining tissue such as DNA, Protein, due to its nature of bifunctional electrophile, acrolein−DNA adducts show a tendency to cyclization.Producing permanent damage in lung due to exposing several times small amount. Producing permanent damage in lung due to exposing several times small amount.The polarization of the double bond of the aldehyde group in acrolein is increased reactivity, and nucleophilic. acrolein reacts with sulfhydryl and amino groups on proteins,DNA.

Diphenylcyanoarsine($C_{13}H_{10}AsN$):

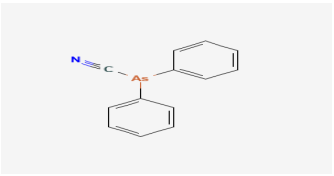

Fig.9

Diphenylcyanoarsine is called Clark 2 , in 1918 was discovered by Sturniolo and Bellinzon.Diphenylcyanoarsine is a chemical compound.Inhalation of this chemical substance is caused the Pulmonary edema in lungs. Diphenylchloroarsine is manufactured by oxidation of phenyl-hydrazine with arsenic acid in presence of a suitable catalyst, then by hydrochloric acid. Another

way Diphenylchloroarsine is manufactured by reaction of the chloro-compound with potassium cyanide or the intermediate diphenylarsenoxide with hydrocyanic acid.Arsenical compounds are weaponized during world wars I and II.the synthesis of Clark II for used as a highly powerful vesicant weapon in a range of climatic conditions, including those with very low temperatures

BLISTERING AGENTS:

Blistering agents are highly reactive oxidative chemicals that cause cellular-level changes by oxidizing cellular membranes, carbohydrates and proteins.Blistering agents are compounds that react with electron-rich atoms in biologic molecules to form covalent bonds, such as DNA alkylating.Blistering agents are locally poison swhich cause serious inflammation of the skin and the breathing system .

Sulfur mustard ($C_4H_8Cl_2S$):

Sulfur mustard, is a highly toxic chemical warfare agent and called the king of war gas. Sulfur mustard at room temperature has a viscous liquid, garlic odor. Sulfur mustard gas has powerful blistering effects and alkylating effects on human body tissue.Sulfur mustard has the following physical properties: molecular mass 159.07 g·MOL−1, appearance colorless if pure, Normally ranges from pale yellow to dark brown. Slight garlic or horseradish type odor, Density 1.27 g/mL, liquid, Melting point 14.45 °C (58.01 °F; 287.60 K), boiling point 217 °C, begins to decompose at 217 °C and boiling at 218 °C, Solubility in water 7.6 mg/L at 20°C.Exposing sulfur gas is generated by damaging at different parts on the human body, such as the dermal and respiratory tract.Sulfur mustard gas is a very reactive gas due to the polar carbon-chlorine bonds and the ability of the sulfur atom to stabilize a reactive episulfonium ion. This is a very effective electrophile and reacts with nucleophiles.Molecular Orbital Theory: the Highest Occupied Molecular Orbital of the nucleophile is reacted with the Lowest Unoccupied Molecular Orbital of the electrophile.Sulfur mustard is responsible for skin burn, eye burn,eyelids swell,and blisters.Causing coughing, bronchitis, and long-term respiratory disease. Exposing a large amount of sulfur mustard causes death.The first time was used at Ypres in September 1917 by the German army.Sulfur Mustard is reacted with proteins, RNA, and phospholipids, by cytotoxic to forming DNA alkylating and cross-linking.In 1822, depretz is synthesized sulfur mustard by the reaction between ethene and sulfur dichloride.

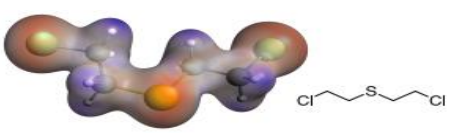

Fig.10

$SCl_2 + 2\ CH_2 = CH_2 \rightarrow (\ Cl\text{-}CH_2\ CH_2\ )_2S$

Synthesis of sulfur mustard in a two-step process by Meyer and Richardson.

$$2\,(HO\text{-}CH_2CH_2\text{-}Cl) + \underset{K_2S}{} \rightarrow (HO\text{-}CH_2CH_2)_2S + 2KCl$$

$$3\,(HO\text{-}CH_2CH_2)_2S + \underset{2PCl_3}{} \rightarrow 3(Cl\text{-}CH_2CH_2)_2S + 2H_3PO_3$$

$$(HO\text{-}CH_2CH_2)_2S + \underset{2HCl}{} \rightarrow (Cl\text{-}CH_2CH_2)_2S + 2H_2O$$

alkylation and cross-linking for DNA, proteins, and phospholipids due to reaction with sulphur mustard.The mustrads are the cyclization of an ethylene group to generate a highly reactive sulfonium or immonium electrophilic center. This reactive electrophile is combined with nucleophilic sites in the macromolecules of cells.These reactions produced modified functional groups of these macromolecules, DNA, RNA and membrane components.

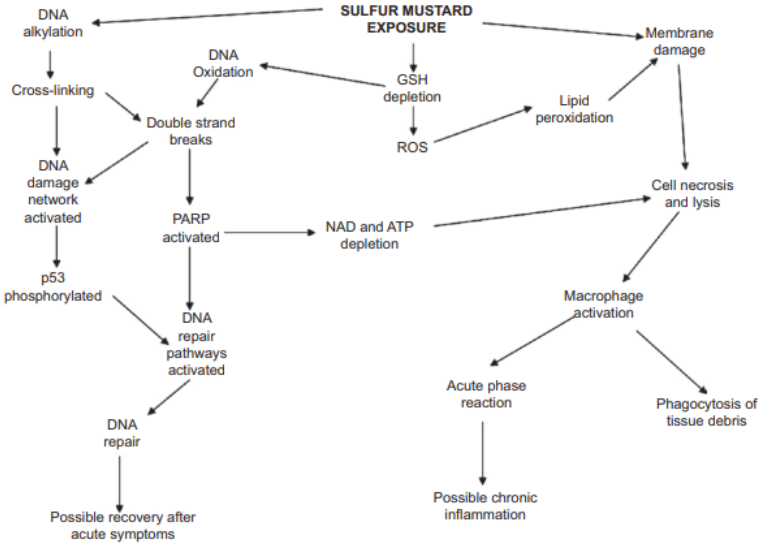

Fig.11

Nitrogen-mustard(HN-1(C6H13Cl2N),HN-2(C5H11Cl2N), HN-3(C6H12Cl3N)): Nitrogen mustards are tertiary bis(β-chloroethyl)amines with vesicant activity. All are active as alkylating agents.Nitrogen mustard has different end uses, from chemical warfare agent to as anticancer agent. Nitrogen mustard is a very effective chemical warfare agent until now still in use. It is in storage by several countries from the time of World War II.A nitrogen mustard agent is synthesized utilizing nicotinic acid as the carrier of the alkylating substituent that forms an ester group on a heterocyclic ring.

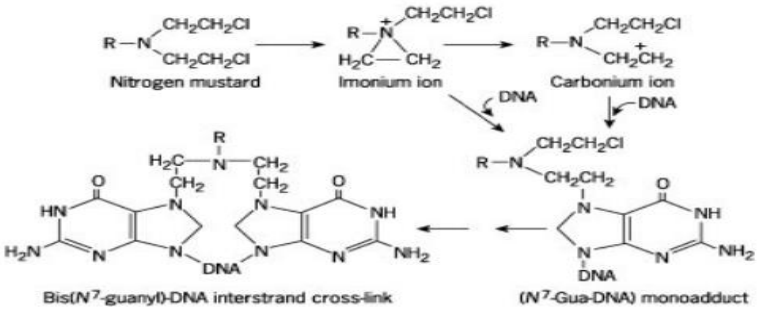

Fig.12

The Harm mechanism of nitrogen mustrads is based on alkylation reaction for human body tissues in contact with nitrogen mustrads.The harm mechanism of action of nitrogen musturads. Nitrogen mustard exerts their earliest visible effects on the nucleus, causing DNA damage.Nitrogen musturads are associated with decreased DNA synthesis. The decreased DNA synthesis is in turn ascribed to the formation of DNA interstrand cross-links that prevent the DNA from acting as an effective template for DNA replication.HN1has the following physical properties: **$(ClCH_2CH_2)_2NC_2H_5$** ; Molecular weight 170.08; Physical state oily liquid; Solubility in water limited; Miscible in organic solvents; Vapor pressure 0.25 mm Hg at 25C.HN2has the following physical properties:**(ClCH2CH2)2NC2H3,**Molecular weight 156.07 ,Physical state oily liquid, Solubility in water Limited; miscible in organic solvents, Vapor pressure 0.427 mm Hg at 25C, Density liquid: 1.09 at 20C vapor 5.9.HN3has the following physical properties:**$N(CH_2CH_2Cl)_3$**,Molecular weight 204.54,Physical state liquid, Solubility in water: Limited; miscible in organic solvents,Vapor pressure 0.0109 mm Hg at 20C,Density liquid: 1.15.

Phosgene oxime($Cl_2C=N-OH$):

Phosgene oxime is classified as a blistering agent. The method of exposure to this agent by inhalation, ingestion, or skin contact. There is very little biological damage by exposing to this agent at concentrations below 8%.By exposing this agent by skin at a concentration equal to or higher to 25 mg/kg.By exposing by inhalation at 0.2 mg-min/m^3 of air and becoming unbearable at 3 mg-min/m^3Generating local tissue damage and systemic toxicity. Exposing to Phosgene oxime, that causes skin, eye and pulmonary damage.Phosgene oxime is a chemical organic compound. Phosgene oxime was first made in 1929. Phosgene oxime is a colorless solid, often yellowish liquids.Phosgene oxime has the following physical properties, Molar mass 113.93 g·MOL−1,Appearance colorless or white solid, Phosgene oxime has Odor Strong disagreeable and irritating, melting point 35 to 40 °C (95 to 104 °F; 308 to 313 K), boiling point 128 °C (262 °F; 401 K), Solubility in water 70%.Phosgene oxime is a manufactured for use in chemical warfare operation as a chemical warfare agent.Exposing occurs by inhalation or ingestion. In 1929, Phosgene Oxime was discovered in Germany as a chemical warfare agent. Phosgene Oxime has a fruity odor. Causing corrosive and tissue oxidation and alkylation. Phosgene oxime is manufactured by the reduction of chloropicrin by a combination of tin metal and hydrochloric acid for producing the active hydrogen. The function of active hydrogen is a reducing agent for chloropicrin.

Cl3CNO2+ 4 [H] → Cl2C=N−OH +HCl+ H2O

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exposure to even low con
damage, particularly in th

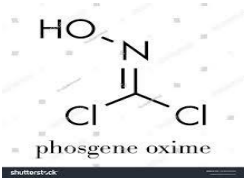

Fig.13

$Cl_2+H_2O \rightarrow HOCl+HCl$
$CH_3COCCl:NOH+HOCl \rightarrow CH_3COOH+Cl_2C:NOH$
Phosgene oxime is manufactured from acetone and aqua regia, is dissolved in water and treatedin the following two steps.

The Phosgene oxime compound is electrophilic and forms bonds with nucleophiles.
Lewisite ($C_2H_2AsCl_3$) :
lewisite has the following physical properties: an oily, colorless liquid with an odor like geraniums.a chemical warfare blister agent. Very toxic. When pure, a colorless oily liquid solidifying at -13 °C. Impurities cause colors ranging from brown to violet,Boiling point at Decomposes at 190 °C, melting point at 0.1°C,Density 1.888 g/cm3 at 20ºC,Vapor pressure 0.58 mmHg at 25°C,Solubility in water 500 mg/L, rapid hydrolysis, Relative vapor density (air = 1) 7.1 Molecular weight 207.3 g/mol. . Faint odor of geranium. .in 1930 lewisite was used by empire of army Japan forces against Chinese forces.in 2007 USA disposal of their own stockpiles. Lewisite was synthesized in 1904 by Julius Arthur Nieuwland during their research.

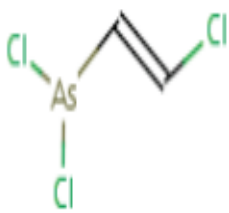

Fig.14 Lewisite structure

Lewisite is synthesized from arsenic trichloride, acetylene, hydrochloric acid, and mercuric chloride.Lewisite has the features of a blistering agent and systemic poison.Lewisite are alkylated biological molecules such as nucleic acids, proteins

and cellular membrane components. The Alkylation and cross-linking of DNA can lead to cancer.Lewisite has harm biochemical mechanisms. It is inhibited in enzymes for thiol groups. pyruvic oxidase, alcohol dehydrogenase, succinic oxidase, hexokinase, and succinic dehydrogenase. The first step is inhabited of carbohydrate metabolism, primarily because of inhibition of the pyruvate dehydrogenase complex.Lewisite is manufactured by the addition of arsenic trichloride to acetylene in the presence of a suitable catalyst.

$$AsCl3 + C2H2 \rightarrow ClCHCHAsCl2$$

Lewisite has the following Properties, Molar mass 207.32 g/MOL, Density 1.89 g/cm3, melting point −18 °C, Boiling point: 190 °C, Solubility in Water Reacts with Water, Solubility Ethers, Hydrocarbons, THF Vapor pressure: 0.58 mmHg at 25 °C.Lewisite is hydrolyzed in water to form chlorovinylarsonous acid.Lewisite is caused tissue damage pain to the respiratory tract at a non-detectable level.Inhibition of hexokinase activity, increased leakage of lactate dehydrogenase, and decreased concentration of adenosine triphosphate (ATP).The absorption of arsine into lungs enters red blood cells, hemolysis occurs; impairment of the transport of Fe(II) to Fe(III). And then an antioxidant system of enzymes, leading to rapid denaturation of proteins.In general, arsenic compounds, Inorganic arsenic is generally considered to be more toxic than organic form .

BLOOD AGENTS:

A blood agent is a toxic chemical compound that contains arsine or cyanide. Entering the human body through inhalation, skin absorbed into the blood. Blood agents are systemic poisons that inhibit the intake of oxygen into the blood and thereby cause the loss of body function.Blood agents are prohibited; the blood and red blood cells of oxygen transport throughout the human body. The blood agents contain arsine and cyanide.Blood agents are chemical weapons that harm the body by preventing cells from using oxygen, by suffocation. The cyanide-based agents block the electron transport chain in the mitochondria, causing stopping cellular respiration. The arsine-based blood agent are damaged red blood cells. Generating hypoxia of the cells and cessation of cellular respiration.

Hydrogen cyanide(HCN):

Fig.15

In 1752, French chemist Pierre Macquer was discovered Hydrogen cyanide.Hydrogen cyanide is a chemical organic compound with the formula HCN and structural formula H−C≡N. It hasMolar mass 27.0253 g/mol ,Colorless liquid or gas,Odor bitter almond-like,Solubility in water Miscible,Hydrogen cyanide is dissolved in water to form hydrocyanic acid , releasing the cyanide anion,CN^- ,Solubility in ethanol Miscible ,Density 0.6876 g/cm^3,Vapor pressure 100 kPa at25 °C,Melting point −13.29 °C,a high toxicity, flammable liquid and boiling point at 25.6°C,Heat of vaporisation210.7 cal/g.Hydrogen cyanide is manufactured by reaction between methane and ammonia in the presence of oxygen at about 1,200 °C over a platinum catalyst.

$$2CH_4 + 2NH_3 + 3O_2 \rightarrow 2HCN + 6H_2O$$

Hydrogen cyanide is manufactured by the reaction of methane and ammonia and platinum catalyst without oxygen.

$$CH_4 + NH_3 \rightarrow HCN + 3H_2$$

HCN is a systemic poison; the harm mechanism is due to inhibition of cytochrome oxidas.The first step is the penetration of cyanide into a protein slot,

then the binding of cyanide to protein, while the second step is the binding of cyanide to heme iron.Cytochrome-C oxidase has a Y-shaped structure. This enzyme is a transmembrane protein inside the mitochondrial membrane. This enzyme has a function, which is to catalyze the transfer of electrons from cytochrome c to oxygen.The binding of cytochrome oxidase, a multimeric iron enzyme complex with cyanide. This chemical reaction is designed based on thermodynamic calculations for Gibbs free energy of chemical reactions and kinetic reaction rate calculations for enzymes.Systemic poisoning is based on releasing heavy cations such as cyanide, arsenic, and organic phosphorus into one of the central circulation systems in the human body, such as the blood circulation system.In the pharmacokinetic studies on cyanide poisoning, the concentration of cyanide in the blood increased relatively slowly as compared to the plasma.Cytochrome oxidase is part of related enzymes, of which several members are found in the cell membrane of aerobic bacteria.

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by 'enzyme complex with
cyanide binding to specifi
oxidase, to inhibit their ac

Cyanogen chloride (CNCl) : Cyanogen chloride has the following properties:a highly toxic chemical organic compound,CNCl, Molar mass 61.470 g MOL−1,Colorless gas, Odor acrid, Density2.7683 mg mL−1 at 0 °C and 101.325kPa,melting point−6.55 °C,boiling point 13 °C,Solubility in water-soluble, Solubility soluble in ethanol or ether, Vapor pressure1.987 MPA at 21.1 °C.Cyanogen chloride is synthesized by oxidation of sodium cyanide with chlorine.Carbon and chlorine are linked by a single bond, and carbon and nitrogen by a triple bond.

$$NaCN+Cl_2 \rightarrow ClCN+NaCl$$

Cyanogen chloride is synthesized by another method by direct chlorination of hydro-cyanic acid, has B.P. 13° C., F.P. - 6° C. During World War I of 1914-18, it was used as a chemical warfare gas (Cyanogen chloride), and until now some countries have stockpiles. Blood particles are converted 30% Cyanogen chloride into hydro-cyanic acid. But Serum are released cyanide ions from Cyanogen chloride. Inhalation CNCl the blood particles are released HCN .HCN is identified directly in liquid blood, lethal effects due to formation of HCN and conversion to HCNS in the human body. The cyanide ion is combined with the iron cytochrome or cytochrome oxidase complex for inhibition of these enzymes.The cyanide is inhibited of certain enzymes by using chemical reactions between cyanide and a Schiff base intermediate, forming cyanohydrin.HCN is used as a pesticide in agricultural against many species. Also, HCN is used in synthesized sodium cyanide and potassium cyanide, which are used mainly in gold and silver mining. Inhalation of hydrogen cyanide is rapidly absorbed in the lungs, then to the blood.

Arsine(SA):

In 1775, chemist Carl Wilhelm Scheele discovered the arsine gas AsH_3 by reacting arsenic trioxide with nitric acid and zinc. Arsine (SA) has the following physical properties: AsH3; Molecular Weight: 77.95 g/MOL; a colourless gas, a garlic odour;Vapor Density: 2.7 ,Boiling Point:-63°C, Density/Specific Gravity: 3.186 g/L ,Vapor Pressure: 11,000 mm Hg at20°C,Freezing Point:-116°C, Aqueous Solubility: Slightly soluble, Volatility: 30,900,000 mg/m3.SA is typically transported as a liquefied compressed gas, highly toxic arsenic compounds; SA is highly flammable.arsine is synthesized by the reaction of arsenic-containing substances with hydrogen in water or acids.Harm Mechanism of Arsine First Step Absorption by the Lung then enters blood and red blood cells.After being absorbed by the lungs, arsine enters red blood reducing oxygen transport by oxidation of Fe(II) to Fe(III). There are two hypotheses: the harm mechanism due to oxidation, and the harm mechanism due to reaction with sulfhydryl groups.

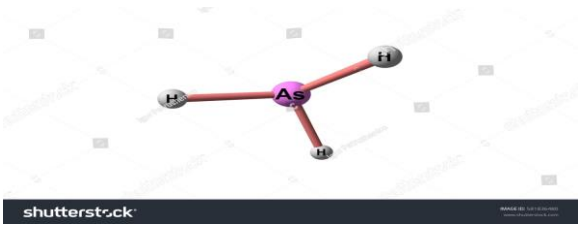

Fig. 16 arsine gas

sources of As3−react with protonic reagents to also produce this gas. Zinc arsenide and sodium arsenide are suitable precursors.

$$Zn_3As_2 + 6\,H^+ \rightarrow 2\,AsH_3 + 3\,Zn_2^+$$

$$Na_3As + 3\,HBr \rightarrow AsH_3 + 3\,NaBr$$

NERVE AGENTS:

Nerve agents are systemic poisons that inhibit neurotransmission, and thereby cause muscle fasciculation and breathing problems.Nerve agents are chemical organophosphates compounds.Nerve agents have a harm mechanism by inhibiting the enzyme acetylcholinesterase (AChE).AchE are classified as the esterase enzymes.The main function of these enzymes is to catalyze the hydrolysis of esters.Esterase enzymes have high affinities for the esters of choline. Several types of choline esters are used as the neurotransmitter of the cholinergic portion of the nervous system.The neurotransmitter, of the cholinergic portion, is a very active nerve agent.At the receptor sites of tissue innervated by the cholinergic nervous system, it hydrolyzes rapidly.Nerve agents have a function, which is inhibition of ChE, then stopping hydrolysis by Ach,Inhibiting the hydrolysis enzyme acetylcholine (AChE) after releasing from neuronsto the synaptic area.The nervous system sends a signal by using neurotransmitters at synapses. The main type of neurotransmitter is acetylcholine. Releases and collects at the receptor site, stimulating the end organ to respond and produce a variety of effects, including muscle contractions.Known as cholinergic nerves and synapses.When A nerve signal is reached the synapse, the nerve releases ACh through the synaptic cleft and combined with receptor sites on the next nerve, muscle, or gland and producing a response.Cholinergic synapses have two types of receptors: muscarinic receptors, nicotinic receptors, or a combination. Blocking the stimulation of the nerve, muscle, or gland, ACh is rapidly broken down by the enzyme acetylcholinesterase (AChE) located in the postsynaptic receptor region, producing.choline, acetic acid, and the regenerated enzyme.nerve agent Chemical, which is provided to biological effects by inhibiting the enzyme AChE, thus allowing the neurotransmitter ACh to accumulate. Then neurotransmitter ACh accumulates and over-stimulates the receptors of the 42 cholinergic nerves and causes hyperactivity of the cholinergic nerves, muscles.

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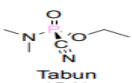
inaccurate phrases, such
no basis in this context.

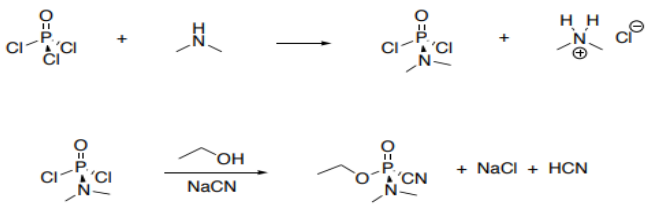
.**Tabun (GA):$C_5H_{11}N_2O_2P$**



Tabun
(GA)

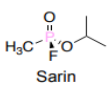
Tabun is a chemical warfare agent from the organophosphatefamily, attacking the nervous system by inhibiting the enzyme of the nervous system for producing high lethality in enemy troops.Tabun has the following: physical properties,Molar

mass162.13g/MOL, Density1.0887 g/cm^3 at 25 °C, Vapor pressure0.07 mmHg,Colorless to brown liquid, boiling point247.5 °C,Solubility in water9.8 g/100 g at 25 °C; 7.2 g/100 g at 20 °C, Tabun is less volatile than Sarin.In 1936, German chemist Gerhard Schrader was discovered synthesis of tabun.tabun is a clear liquid,turning into a yellow or brown liquid withfruity or almond-like odor,slowly volatile and viscous liquid.tabun has a harm mechanism by irreversible phosphorylating the AChE enzyme. As the acetylcholine is phosphorylated, accumulated and not recycled, death due to failure of the respiratory system due to failure of the diaphragm.The first step is the treatment of phosphoryl chloride with gaseous dimethylamine to form dimethylamidophosphoric dichloride and dimethylammonium chloride. the second step Dimethylamidophosphoric dichloride is subsequently treated with excess sodium cyanide to yield the dimethylamidophosphoric dicyanide intermediate, which is treated with ethanol to producing tabun



organophosphorus (OP) nerve agents were banned in 1997, but there are many countries have large stockpiles. Presence would remain a problem as weapons. There are many nerve gas agents (generating blindness and psychological problems…) that are classified in secrete programs, especially in western countries.Exposing organophosphorus compounds (OP) or special types of pesticides produces diverse health problems, such as nervous, endocrine, reproductive, and immune system changes. The main toxicity effects are the inhibition of acetylcholinesterase.The phosphorylation of AChE is the toxicity process for producing lethal effects by resulting in essentially irreversible inactivation of the AChE enzyme.Phosphorylation of AChE in the context of the steric blockade model. Rate constants of phosphorylation are main variables that controlling the time required for inhibition AChE.Structural analysis of acetylcholinesterase (AChE) shows the two sites of ligand interaction in the activesite gorge: an acylation site at the base of the gorge and a peripheral site at its mouth. For ligand binding to the peripheral site alters the reactivity of substrates and organophosphates at the acylation site.Kinetic rate constants for the phosphorylation of AChE reaction are measured based on standard methods. Tabun is a toxic compound used as a chemical warfare agent,not present in nature.

Sarin (GB):$C_4H_{10}FO_2P$


Sarin
(GB)

Sarin's scientifically is called O-isopropyl methylphosphonofluoridate,An extremely toxic organophosphorus compound, A colorless, odorless liquid, known as a chemical weapon as a nerve agent. Exposing at very low concentrations produces high lethal rates. The death can occur within one to ten minutes after direct inhalation of a lethal dose.In 1936, Sarin was discovered by German chemist Gerhard Schrader.Sarin has the following physical properties: molecular mass140.094 g/MOL,clear colorless liquid to brownish, and odorless,

density 1.0887 g/cm3 at 25 °C, meltingpoint−56 °C,boiling point158 °C,Solubility in wate Miscible. The harm mechanism is based on inhibition of the AChE. ACh molecular structure as shown in fig.17 ACh is inactivated by the enzyme AChE, producing choline and acetic acid. Transmission of the impulse ceases, and the membrane repolarizes and is ready to respond again. As a consequence of nerve agent inhibition of AChE, ACh accumulates at synapses.

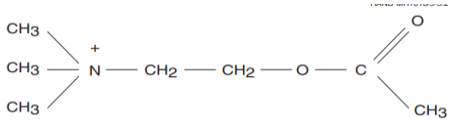


Fig.17

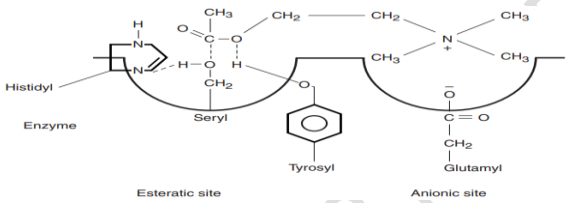


Fig.18

ACh Fig. 18 shows the AChE Active Site, With ACh, nerve agents and organophosphate pesticides bind to the enzyme, first in a reversible way Nerve agent inhibition of AChE, ACh accumulates at synapses, giving rise to uncoordinated bursts of signals,Stimulation function and paralyzing.The phosphorylation of AChE is the toxicity process for producing lethal effects by resulting in essentially irreversible inactivation of the AChE enzyme.Phosphorylation of AChE in the context of the steric blockade model. Rate constants of phosphorylation are main variables that controlling the time required for inhibition AChE.Structural analysis of acetylcholinesterase (AChE) shows the two sites of ligand interaction in the activesite gorge: an acylation site at the base of the gorge and a peripheral site at its mouth. For ligand binding to the peripheral site alters the reactivity of substrates and organophosphates at the acylation site.Kinetic rate constants for the phosphorylation of AChE reaction are measured based on standard methods.there are several kinds of calculations and experimental testing to be carried out, such as thermodynamics calculations(Gibbs free energy calculations, enthalpy formation and analysis, entropy analysis), reaction kinetics, reaction rates for nerve agents with target compounds, and then experimental studies for the effect of gas nerve agents on animals.

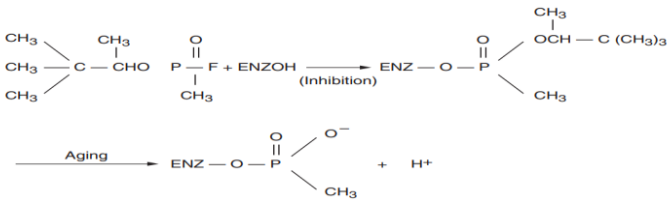


Fig.19 phosphorylation of AChE reaction

Sarin is synthesized by reacting of methylphosphonyl difluoride with isopropyl alcohol and isopropyl amine or alternatively can be prepared by a five-step synthetic route which begins with the treatment of triethyl phosphite with methyl iodide.

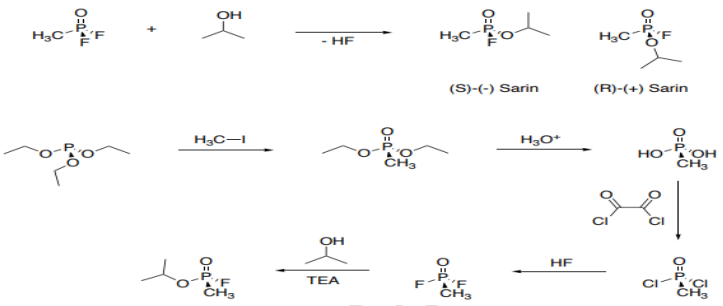
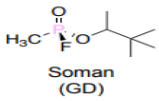


Fig.20 sarin

Soman (GD):$C_7H_{16}FO_2P$



soman is called scientifically O-pinacolyl methylphosphonofluoridate.soman is an extremely toxic chemical gas . It is a nerve agent, casuing high lethal rate by inhibiting the enzyme cholinesterase.Soman has the following physical properties :Mode of action AChE inhibitor,physical state at 20 °CColourless to brown liquid,melting point-42°C,boiling point198 °C, density at 25 °C 1.022gcm-3,vapour pressure at 20 °C 0.40mm Hg, Solubility in water Moderate.The harm mechanism of nerve agent is based on inhibition of acetylcholinesterase, due to the inhibition mechanism is analogous to the hydrolysis of acetylcholine.Soman is synthesized by reacting pinacolylalcohol with methylphosphonyl difluoride.Soman is an organophosphorus nerve agent with a mechanism of action similar to Tabun. Nerve agents inhibit acetylcholine esterase(AChE).First step Acetylcholinesterase is formed covalent bond with organophosphate nerve agents at the active site of the enzyme at the reactive hydroxyl group, this is called phosphorylation.This inhibition is irreversible, resulting in the accumulation of acetylcholine, leading to the continuous stimulation of cholinergic synapses.

The enzyme becomes phosphorylated instead of acetylated.Phosphorylation has a two-step process involving an addition-elimination mechanism.

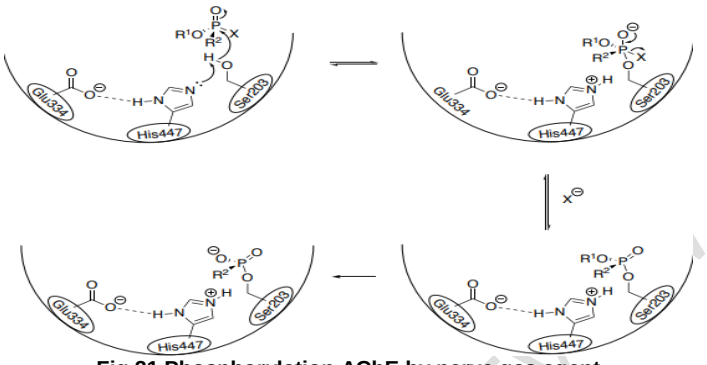
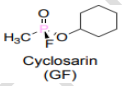


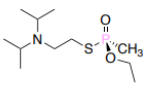
Fig.21 Phosphorylation AChE by nerve gas agent

Cyclosarin (GF): $C_7H_{14}FO_2P$



Cyclosarin is called cyclohexyl methylphosphonofluoridate,a liquid organophosphate nerve agent.Its physical characteristics are Molar mass180.159 g·mol−1,Mode of action AChE inhibitor,Colourless liquid, Density1.1278 g/cm3,melting point−30 °C, Boiling point239 °C, Solubility in water Almost insoluble.In 1938 , Sarin was discovered by German chemist Gerhard Schrader.Cyclosarin is a chemical warfare agent from, organophosphorus compounds family. Organophosphorus compounds are acetylcholinesterase (AChE) inhibitors. The harm mechanism is based on binding to active sites in acetylcholinesterase (AChE), causing phosphorylation of enzyme and accumulation of acetylcholine and failure in diaphragm movement then death.
there are several kinds of calculations and experimental testing to be carried out, such as thermodynamics calculations(Gibbs free energy calculations, enthalpy formation and analysis, entropy analysis), reaction kinetics, reaction rates for nerve agents with target compounds, and then experimental studies for the effect of gas nerve agents on animals.

VX :$C_{11}H_{26}NO_2PS$



VX is a nerve agent toxic chemical compound as part from of the organophosphorus class, subclass thiophosphonate.In 1950 VX was discovered at proton down, England by using the research papers of German chemist Gerhard Schrader.VX is prepared into three steps, The first stage transesterification of methylphosphonothioic dichloride, the second stage

hydrolysis of the formed diester with aqueous sodium hydroxide base.The third stage phosphonothioate sodium salt intermediate is treated with the appropriate aminoethyl chloride to yield the final nerve agent.

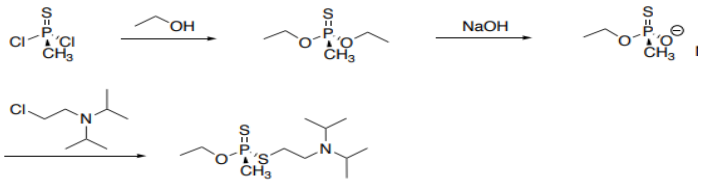


Fig.22 VX Synthesis

VX has the following physical properties :Molar mass 267.37 g·mol−1,Appearance amber liquid, odourless, Density1.0083 g cm−3,melting point −51 °C ,boiling point 300 °C, Vapour pressure0.09 Pa.VX has a harm mechanism based on blocking the enzyme signal for AChE, causing death due to failure of diaphragm for respiratory system.VX are toxic chemical compound, the toxicity of VX is based on increasing the concentrationof synaptic forthe neurotransmitter acetylcholine, by using inhibition reaction of the enzyme acetylcholinesterase by inhibiting the activity of the enzyme acetylcholinesterase. This type of chemical warfare agents belonging to the cholinergic toxidrome are nerve agents, organophosphorus chemicals that act as irreversible inhibitors of acetylcholinesterase.Nerve agents are organophosphorus chemicals that act as irreversible inhibitors of acetylcholinesterase nerve agents are defined as organophosphorus chemicals, producing an irreversible inhibition of acetylcholinesterase.The main catalytic activity of acetylcholinesterase is The serine residue, nerve agents are bound with this part for losing the ability of enzyme and lockdown acetylcholine.To development more efficient chemical warfare agents, integration between systemic poison type and local poison type is produced more lethal rate for chemical warfare agents and also combined arsenic, cyanide, sulphur with organophosphorus compounds for producing chemical warfare agents are acting as blood agent and nerve agent .this is very promote approach.

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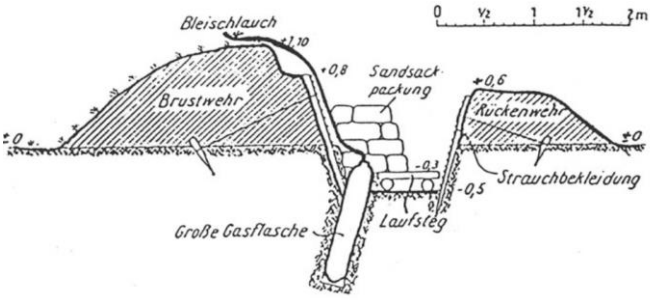
Design principles for Chemical warfare operation:

Any chemical warfare operation has main elements, these elements are defined as chemical warfare agent(nerve agent GB, nerve agent VX, and blister agent HD...), delivery system (artillery and mortar shells, rocket and missile warheads, aircraft bombs, and spray devices...), Meteorological variables, battlefield topography, operation time duration, target size of enemy troops, safety of staff and troops during any chemical warfare operation, clearing and decontamination of the battlefield after the operation.First step in any chemical warfare operation states by defining the target size, by defining the number of enemy troops and occupied land by enemy troops. This is the battlefield.The chemical warfare operation is delivered gas chemical warfare agent at lethal concentration in the air atmosphere at troop's height level. This is done by convective mass transfer of chemical warfare agent.Delivering system for chemical warfare agents is based in open fluid flow over ground level for spraying system such as chlorine delivery system in World War I as shown in fig.23&fig.24.The design, including design process parameters for occupying 3 meters above ground by chemical warfare gas agent at lethal requirement concentration for producing the highest lethality rate. This is a combined process of convective mass transfer and diffusion mass transfer. Producing chemical cloud with lethal concentration and time of operations. The time of operation is defined as the time of chemical cloud at lethal concentration occupying the battlefield at the target area.Around of 188

tons of chlorine gas have been used by the Imperial German Army ,generating



6000-7000 death in French and Canadian troops.

Fig.23

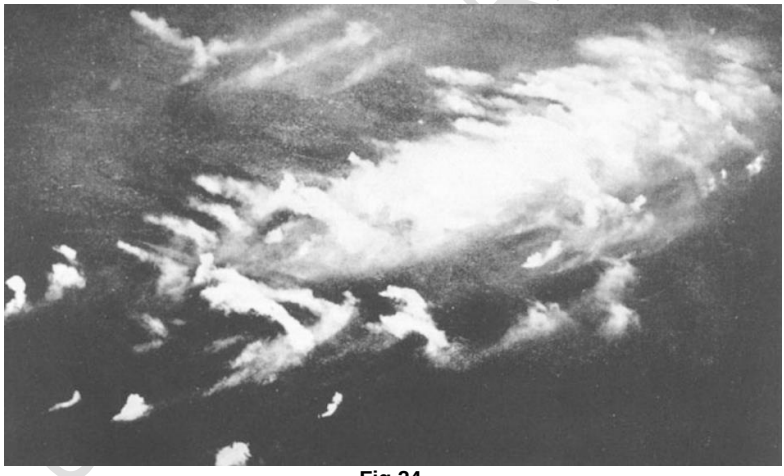


Fig.24

In this battlefield, the imperial German army was used chlorine gas cylinder in trench to releasing gas and producing chemical cloud.Chemical cloud design is based on the volume of air above ground by 3 to 4 meters in the battlefield.The calculations are based battlefield area multiply by elevation 3-4meters.by using gas equation of state calculate other parameters such as temperature ,pressure..

$$P V = m R T$$

where P gas pressure,m gas mass,R gas constant,V gas volume,T temperature.

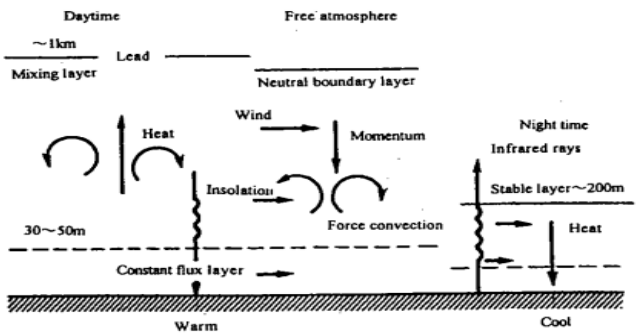


Fig.25 Atmospheric boundary layers

Pressure differences must be created in a force in order to drive the chemical warfare gas, a gent. This force is the pressure gradient Force. The force is from higher chemical warfare gas pressure to lower atmospheric pressure for filling required volume in battlefield special during using spraying system cylinders, artillery shells, mortar shells, missiles chemical warhead.The pressure difference develops over an area, the pressure gradient force begins moving the chemical warfare gas directly across the lines of constant pressure. The closer the spacing of constant pressure, the stronger is the pressure gradient force. The stronger the pressure gradient force, the higher chemical gas mass flow.

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}.(\vec{v}\rho) = 0 \qquad \text{CONTINUITY}$$

$$\frac{D\vec{v}}{Dt} + 2\Omega \times \vec{v} = -\frac{\nabla p}{\rho} - \nabla\Phi - \nu\nabla^2\vec{v} \qquad \text{MOMENTUM}$$

$$\frac{D\theta}{Dt} = 0 \quad or \quad C_p\frac{D\theta}{Dt} = \frac{\theta}{T}\dot{Q} \qquad \text{THERMODYNAMIC}$$

This quantity θ is known as the potential temperature,The Earth rotates with an angular velocity Ω .ν is the kinematic viscosity. V is the velocity is the time,ρ is the density of the fluid,Q is heat transfer. the calculation is based Bernoulli equations for finding process parameters. The case is flow over flat surfaces and calculations based on continuity equation, momentum equations and energy equations. Bernoulli equation also used for more easy calculations.Selection of the suitable chemical warfare agents based on meteorological variables such as wind, temperature, etc. Terrain and vegetation in the target area, Temperature, temperature gradient, wind speed and direction, and precipitation in the target area at the proposed time of employment.

3. RESULTS AND DISCUSSION:

The chemical warfare operations have developed during WWI starting from Ypres battlefield second .the idea using chemicals to creating high lethality in enemy troops.The traditional method for design chemical warfare operation is based on approximation and using rules of thumb .but modern warfare is built on accurate and details calculations. this chapter is introduction to details accurate calculations and mathematical modelling for the process of releasing chemical gas warfare agent and generating desired chemical cloud.

4. CONCLUSION

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The foundation for design of chemical warfare agents and design principle for chemical warfare operations .from theoretical physical chemistry, fluid flow mechanics and theoretical thermodynamics. To develop very efficient chemical warfare gas agent, the Optimum a gas chemical warfare agents are defined as having colorless, odorless and lethal concentrations at very low concentrations. Very low hydrolysis in water, high stability and high solubility in water. The first stage of development, in any chemical warfare agent, is selection of the method of exposure and the harm mechanisms. The main elements and groups are used for the development of gas-chemical warfare agents. , these elements and groups are classified based on harm mechanisms. The first group of halogens is Cl, F, Br, and I. The second group is unsaturated oxides: carbon monoxide and sulfur oxides. The third group is Toxic elements such as cyanide, sulfur, and arsenic. The Fourth group is organic phosphorus. These elements and groups are combined with phenyl, benzyl, Xylyl, Methyl, Ethyl, and vinyl groups Such as Halogens Methyl. There are several kinds of calculations and experimental testing to be carried out, such as thermodynamics calculations(Gibbs free energy calculations, enthalpy formation and analysis, entropy analysis), reaction kinetics, reaction rates for any chemical agents with target compounds, and then experimental studies for the effect of gas nerve agents on animals. Design chemical warfare operation has many process parameters to study, for developing the desired chemical cloud for the volume occupying 3 meters above ground for the battlefield area by multiplying three meters in the area. Meteorological are very important parameters for atmospheric fluid flow in design chemical warfare operation. Chemical warfare gas agent at lethal requirement concentration for producing the highest lethality rate. This is a combined process of convective mass transfer and diffusion mass transfer. Producing chemical cloud with lethal concentration and time of operations, meteorological parameters

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