

Chem-biothreat SAND2013-2700P AWARENESS for law enforcement

Amman, Jordan
5-9 May 2013



CHEMICAL DETECTION AND IDENTIFICATION

SAND No. xxxx-xxxx

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Sandia National Laboratories
International Chemical Threat Reduction
International Biological Threat Reduction

OBJECTIVES

Explain the main tools used for detecting and identifying toxic chemicals

Understand the requirements and limitations of each chemical detection and identification approach

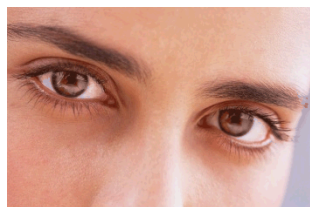
Be able to make appropriate response decisions based on an understanding of the limits of chemical detection and identification



CHEMICAL DETECTION AND IDENTIFICATION

What is the difference between chemical detection and chemical identification?

- Detection will tell you whether a certain chemical is present or not
- Identification will tell you which chemical it is



CHEMICAL DETECTION AND IDENTIFICATION

In what sort of scenarios might one have use for chemical detection and identification?

- Before a release, monitoring for a potential release
 - *Warehouse, factory, chemical storage site*
 - *Important location to protect from a chemical attack*
- During a release or related event
 - *Emergency response to an accidental or intentional release*
 - *Interdiction of suspicious materials, foiling a plot, or a failed attack*
- After a release
 - *Decontamination, cleanup, and recovery*
 - *Investigation*



CHEMICAL DETECTION AND IDENTIFICATION

What would ideal detector characteristics need to be for each of those scenarios?

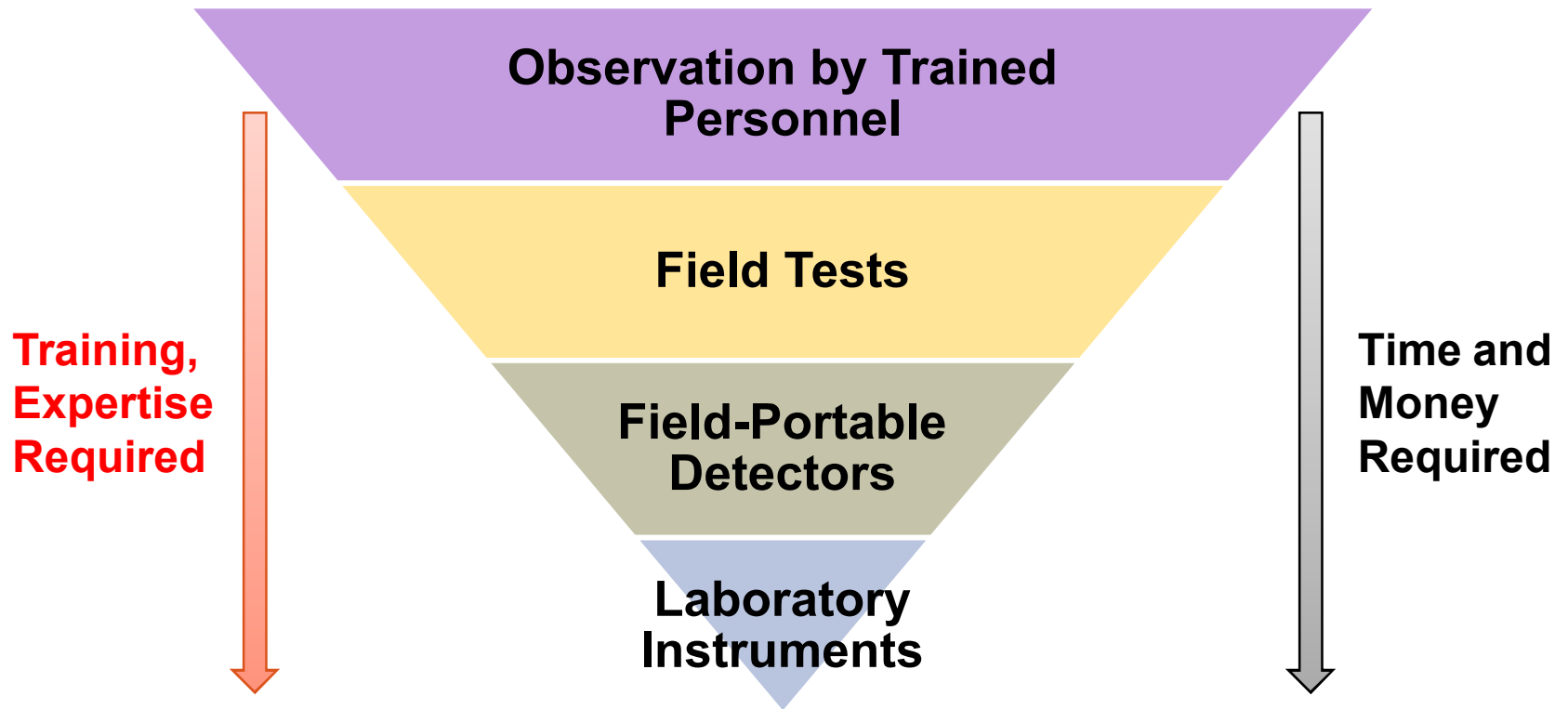
Consider:

- Sensitivity
- Selectivity
- Detection of all or some chemicals/agents
- Presence/absence versus absolute identification, quantitative analysis
- Acquisition time
- Continuous monitoring
- Warm up time
- Calibration requirements
- Reliability/Durability
- Size/portability
- Sampling ability
 - *Solid, liquid, gas*
 - *Handle “real” samples/mixtures versus requiring sample preparation*
- Power requirements
- Consumable/spare parts and maintenance
- Operating conditions
 - *Humidity*
 - *Temperature*
- Ease of use, expertise required

**Each group use these considerations to describe the ideal detector for a different scenario
20 minutes, write down answers**



CHEMICAL DETECTION AND IDENTIFICATION



What kind of information does each level of detection provide?

General information
Detailed information

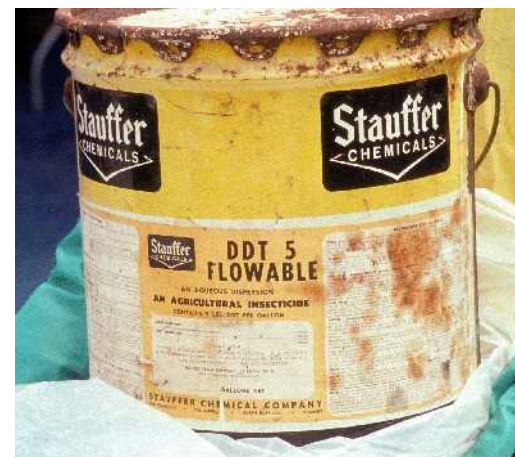


OBSERVATION BY TRAINED PERSONNEL

First line of defense

How?

- Visual observation and odors
 - *Unusual packages or labels*
 - *Leaking containers*
 - *Dead animals*
 - *Many people in the same place with the same signs and symptoms*



Trained
Personnel

GLOBALLY HARMONIZED SYSTEM (GHS) AND OTHER HAZARD LABELS

Corrosive



Irritant



Health Hazard



Acute Toxicity



Flammable



Explosion



Oxidizer



Compressed Gas



Environmental



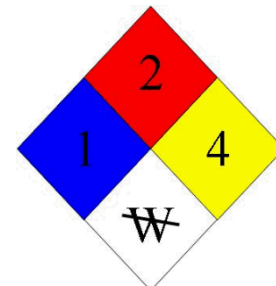
Radioactive



Biohazard



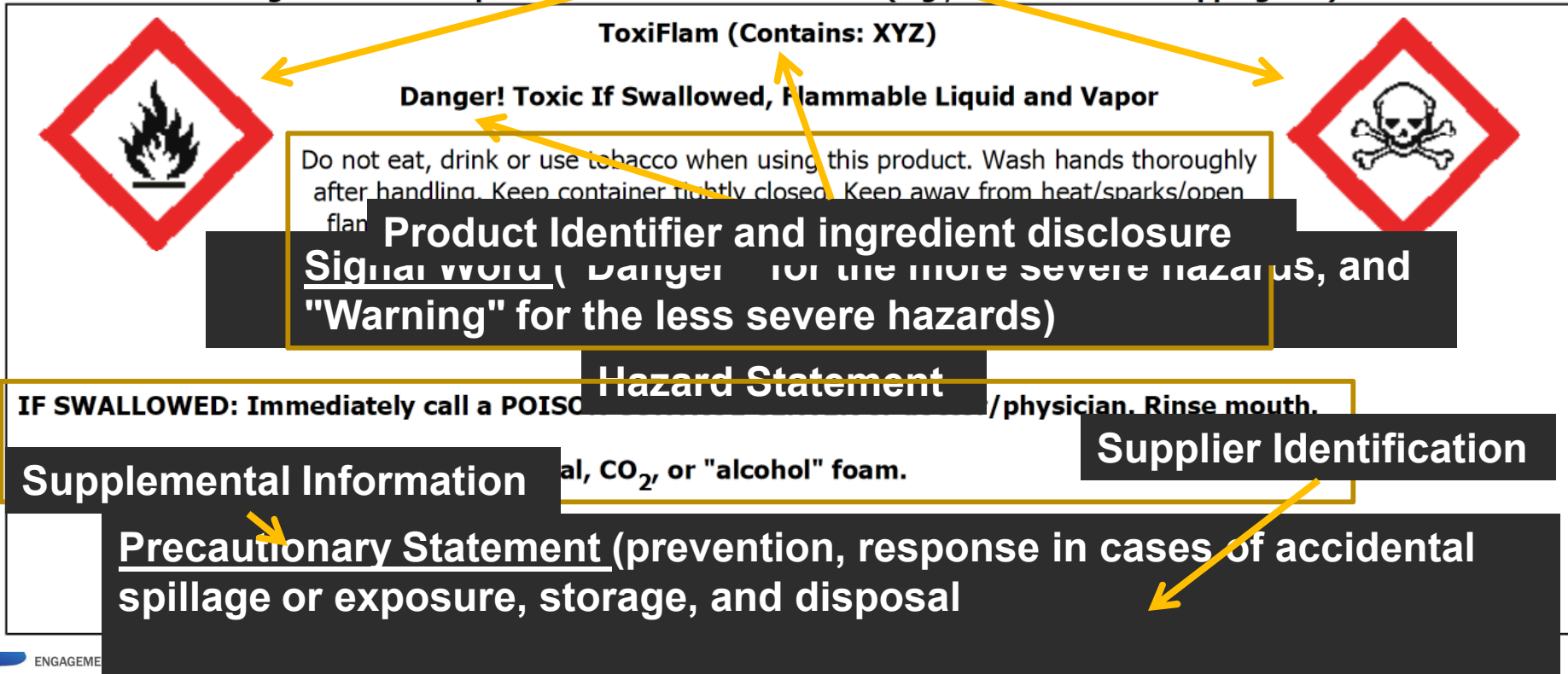
NFPA



**Trained
Personnel**

LABELS

Symbols (Hazard Pictograms)



TRANSPORTATION LABELS

Identify material

- Proper, full chemical name
- ID codes (e.g., UN number)
- Quantities, concentrations, number of containers

Hazard class according to regulations

- Transport symbols

Emergency information

Contact names and phone numbers

Languages



TRANSPORTATION DOCUMENTS

Safety Data Sheets

Shipping order

Bill of lading

Manifest

Full shipper, receiver
addresses

Packing and labeling
certification

Verification of receipt

Follow up documentation

- Incident/accident reports



What about chemical names
on container labels or
transportation documents?

- Over 70 million known substances exist
<http://www.cas.org/>. Accessed March 2013.
- How can you really know what you're dealing with?

CHEMICAL NAMES

Scenario: You are trying to find out more about a suspicious chemical container. The owner says that it is only Kromfax solvent and nothing to worry about.

Do you know what Kromfax solvent is?

Is that a “proper” chemical name or a brand name?

How do you know if its really “nothing to worry about” or not?

How can you find out more?





CHEMICAL NAMES

PURE SUBSTANCES

- Definite and constant composition
- Distinct chemical and physical properties
- Cannot be separated into simpler components by physical means

MIXTURES

- A sample of matter in which two or more pure substances are combined
 - *No chemical reaction*
- Properties depend on the components of the mixture
- Can be separated by physical means

Both **Pure Substances** and **Mixtures** can have many names

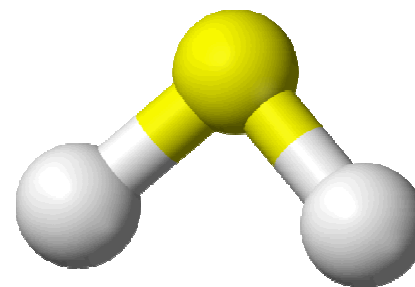
Names of Mixtures may disguise the substances in them



CHEMICAL NAMES

Even pure substances usually have many names

- Hydrogen sulfide (proper chemical name)
- H_2S (chemical formula)
- Hydrosulfuric acid
- Sulfhydic acid
- Sulfur hydride
- Sulfane
- Sewer gas



To deal with this problem, pure substances are given a **unique, internationally standardized identifier**

CAS Registry Number: 7783-06-4

Hydrogen Peroxide 35% FOOD GRADE

DEPOSIT SIGN
\$25.00
CARBOY DEPOSIT
\$15.00

Hydrogen Peroxide
5.1, UN2014, PGII

Danger! STRONG OXIDIZER, Causes eye and skin burns. May cause permanent eye damage. Can react violently with water, acids and other materials.

FIRST AID: Skin-Flush area with water for 15 minutes and remove contaminated clothing and shoes. contact a physician immediately. **EYES**-Flush eyes for 15 minutes contact a physician immediately. **INGESTION**-Do not induce vomiting. Give large quantities of water. contact a physician immediately. **INHALATION**-Remove to fresh air contact a physician immediately.

Fire: Use Dry chemical, Carbon Dioxide, Chemical foam or water fog.

PROTECTIVE EQUIPMENT: Use chemical gloves and clothing to prevent skin contact, safety goggles or full face mask.

SPILL DISPOSAL: Caution: This product may react strong with acids or water. Scoop spilled product into marked disposal containers. Flush spill area with water.

STORAGE/USE/HANDLING: Do not add any other product to this container. Avoid contamination from any source.

Store in original sealed container. Avoid contact with any metals, PVC, wood or any combustibles.

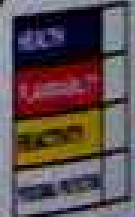
DOT SHIPPING NAME/UN#:

CAS # 7722-84-1
7732-18-5

LOT No. 662531

CODE No. 041

NET WT: 500LBS
145LBS CARBOY



WINDHOIST CHEMICAL CORPORATION
1000 W. 10th Street, St. Louis, MO 63103
TEL: (314) 844-4100

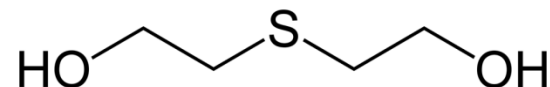
REFER TO MATERIAL SAFETY DATA SHEET
FOR SAFE HANDLING PROCEDURES

FOR CHEMICAL EMERGENCY SPILL, LEAK,
FIRE, EXPOSURE OR ACCIDENT ONLY
CALL: CHEMTREC - DAY OR NIGHT - 1-800-424-9300

CHEMICAL NAMES

Kromfax solvent is also known as:

- 2-(2-hydroxyethylsulfanyl)ethanol (proper chemical name)
- $C_4H_{10}O_2S$ (chemical formula)
- 1,5-Dihydroxy-3-thiapentane
- 2,2'-Dihydroxydiethyl sulfide
- 2,2'-Thiobisethanol
- 2,2'-THIODIAETHANOL
- 3-Thiapentane-1,5-diol
- Bis(2-hydroxyethyl)sulfide
- Bis(2-hydroxyethyl)thioether
- Diethanol sulfide
- ETHANOL, 2,2'-THIOBIS
- Thiodiglycol
- Glyecine A
- NSC 6289
- Tedegyl
- **and many others!**



Dual-use chemical:

- Commercially available, many legitimate uses
- Also a mustard agent precursor

The internet can help find chemical synonyms or connect name to CAS#

www.commonchemistry.org

<http://ccinfoweb.ccohs.ca/chemindex/search.html>

<http://pubchem.ncbi.nlm.nih.gov/>

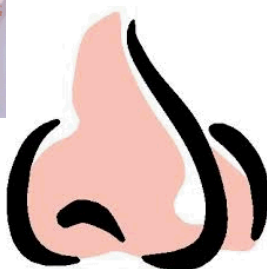
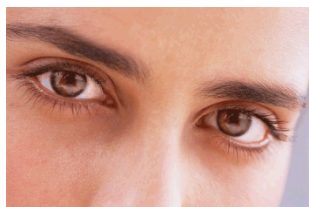


CHEMICAL DETECTION AND IDENTIFICATION

Trained personnel are the first line of defense

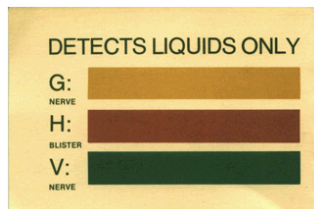
How?

- Visual observation and odors
 - *Unusual packages or labels*
 - CAS Registry Number
 - *Leaking containers*
 - *Dead animals*
 - *Many people in the same place with the same signs and symptoms*



TOOLS FOR CHEMICAL DETECTION

Field Test



- Presence / Absence

Field-Portable Detectors



- Presence / Absence
- Identification
- Semi-quantitative

Laboratory Instruments



- Positive Identification
- Quantitative

Advantages?

- Visual Observation
- Quick results
- Are usually inexpensive
- Less training is needed than other methods
- Are field-deployable

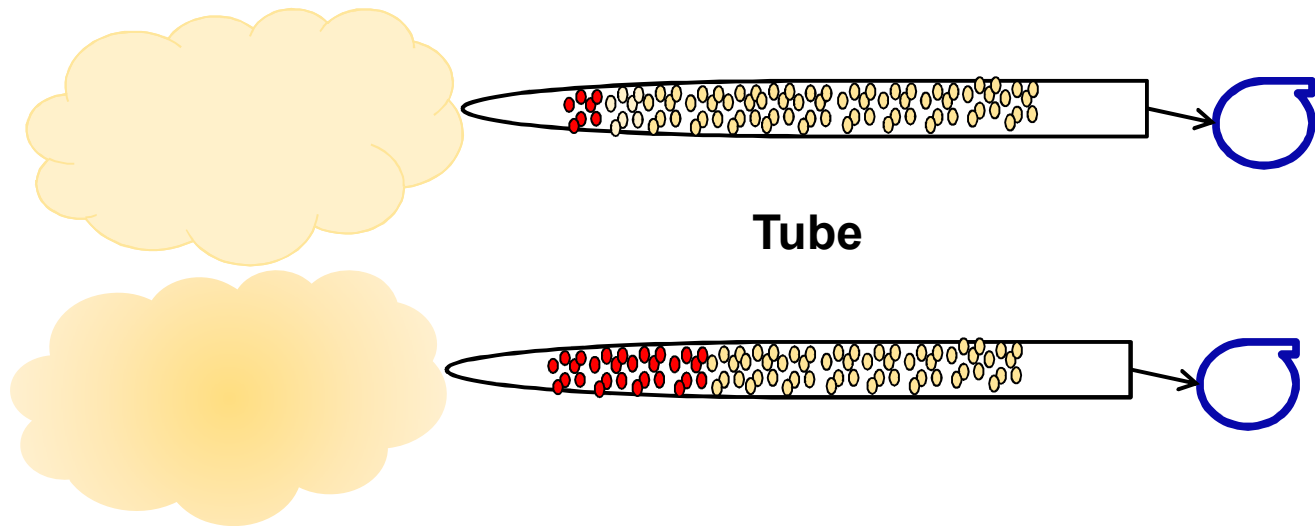
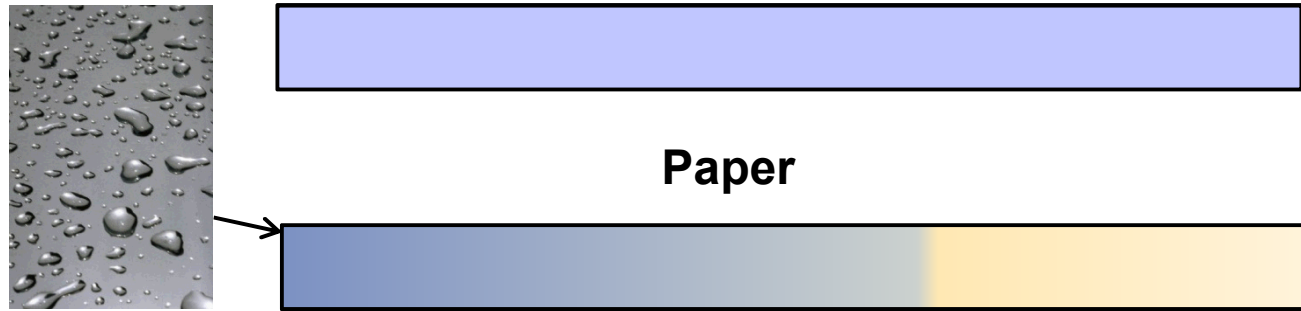
Disadvantages?

- Agent specific
 - *Need the right kit for each possible agent*
- Limited shelf-life
- Interferences
- May be used improperly
- Non-quantitative



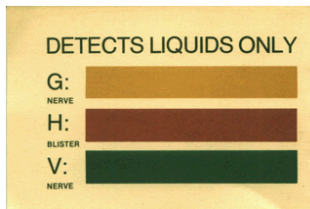
**Field
Test**

Field Tests-Color Tests Paper and Adsorption Tubes



Field Test

Chemical Agent Detector Paper



Color Changes

- Yellow-gold indicates G (nerve) agent
- Red-pink indicates H (blister) agent
- Dark green indicates V (nerve) agent
- If any other color or no color change, liquid cannot be identified



False Negatives

WARNING—When conducting agent tests at night, remove any colored lens because it may provide a false negative response.

False Positives:

A variety of other substances give positive results for CW field tests

Perfume

Cleaners

CW decontaminants

Etc.



FIELD PORTABLE DETECTORS

Field portable detectors are laboratory technologies that have been miniaturized and ruggedized for portable operation

For simple screening:

- Four gas analyzer
- Photoionization detector

For detection (and identification) of CW:

- Ion mobility spectrometer
- Flame photometric detector
- Infrared and Raman spectrometer
- Surface Acoustic Wave Sensor
- Gas Chromatography Mass Spectrometry (GC/MS)



FIELD PORTABLE DETECTORS

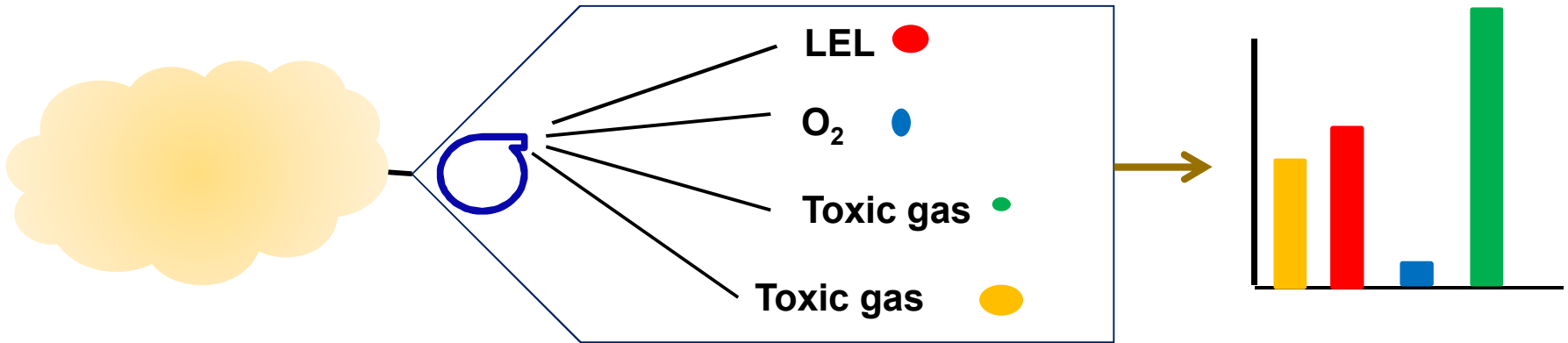
Advantages?

- Are field-deployable
- More sensitive and selective than simple field tests
- May give complimentary data using different technologies
 - *More reliable results than simple field tests*
- May identify agents in addition to giving presence/absence

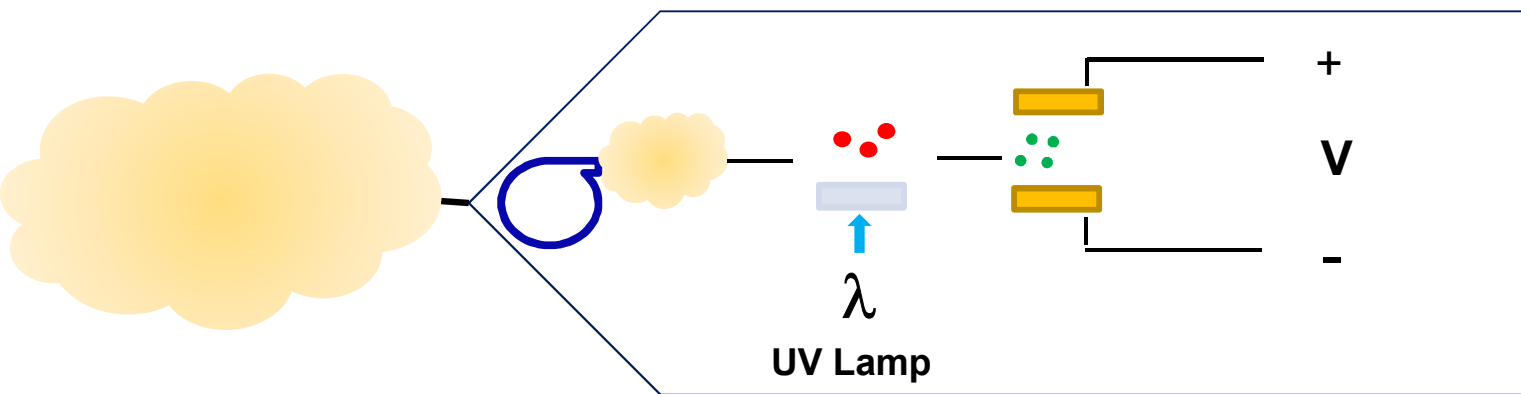
Disadvantages?

- Expensive
- Require consumable parts, spare parts and maintenance
- Require extensive training for proper use, requires calibration
 - *May be used improperly*
- Interferences – prone to giving false positives
- Semi-quantitative at best





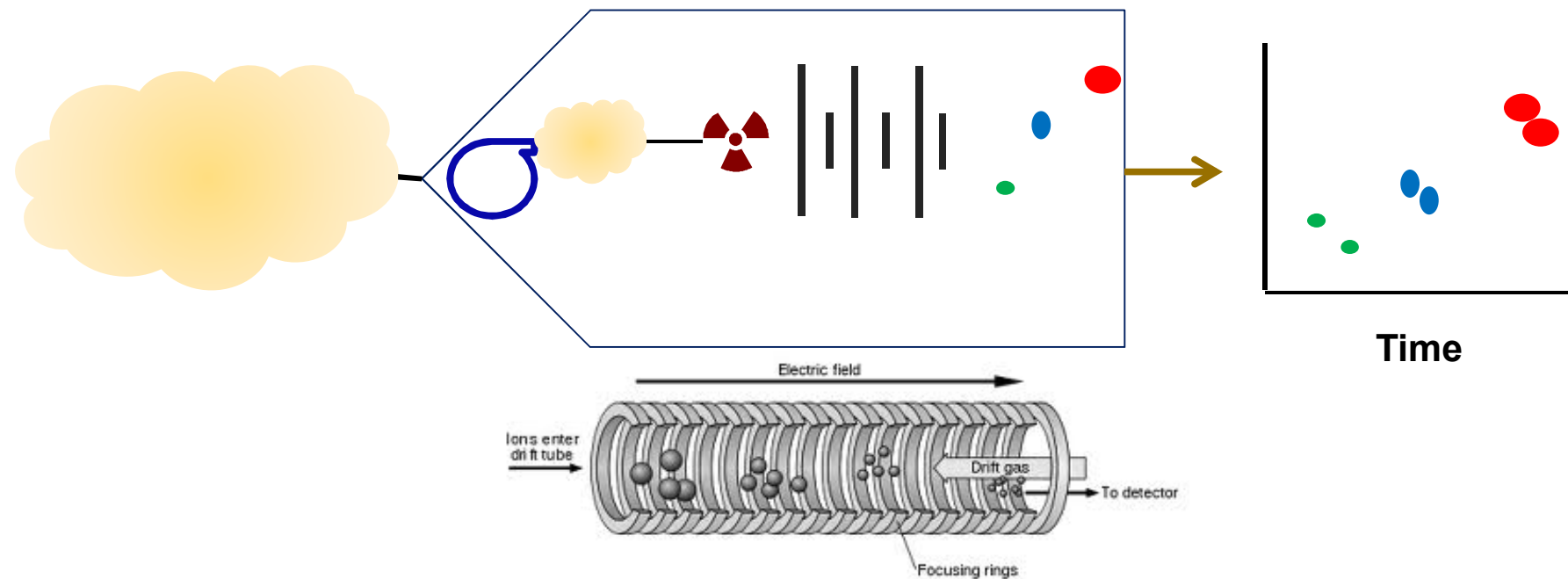
- Sample drawn into instrument and detected by selective detectors
 - Lower explosive limit (LEL) uses catalytic bead sensor or infrared sensor
 - Toxic gases use electrochemical, or metal oxide semiconductor detectors
 - Oxygen detected by electrochemical detector
- Many sources of interference
 - High rates of false positives and false negatives



Changing lamps changes gases detected

- Sample drawn into instrument and ionized by ultraviolet light (UV)
- Gases have their own ionization potential (IP)
- Only gases with an IP below the Lamp Voltage are detected
- Some gases are not detected

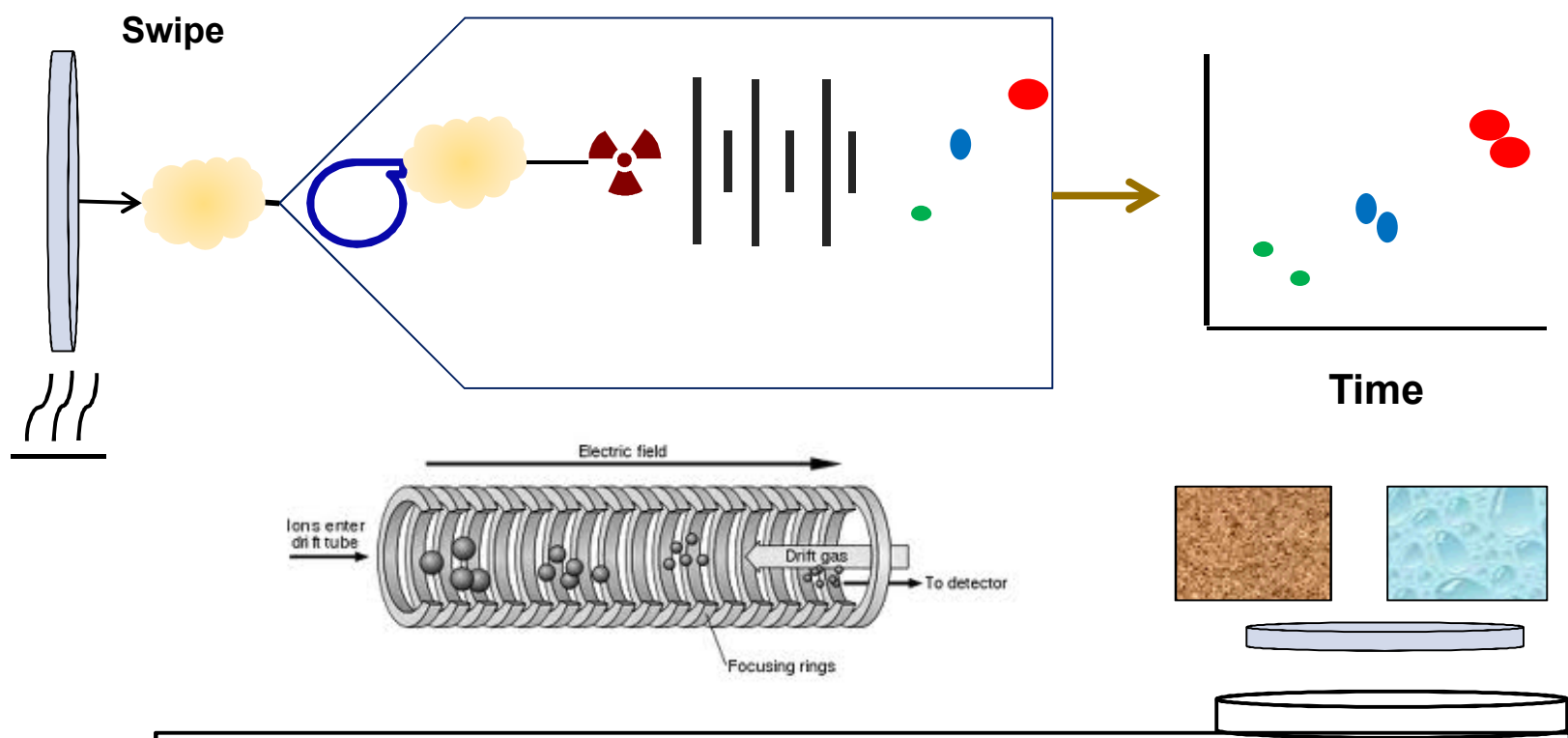
Ion Mobility Spectrometer Vapor Sampling



- Sample drawn into instrument and ionized by radioactive Ni^{63}
- Ions are separated in electric field
- Transit time is characteristic
 - Library/database used as reference for identification
- Many sources of interference
 - High rates of false positives and false negatives

Field-Portable Detectors

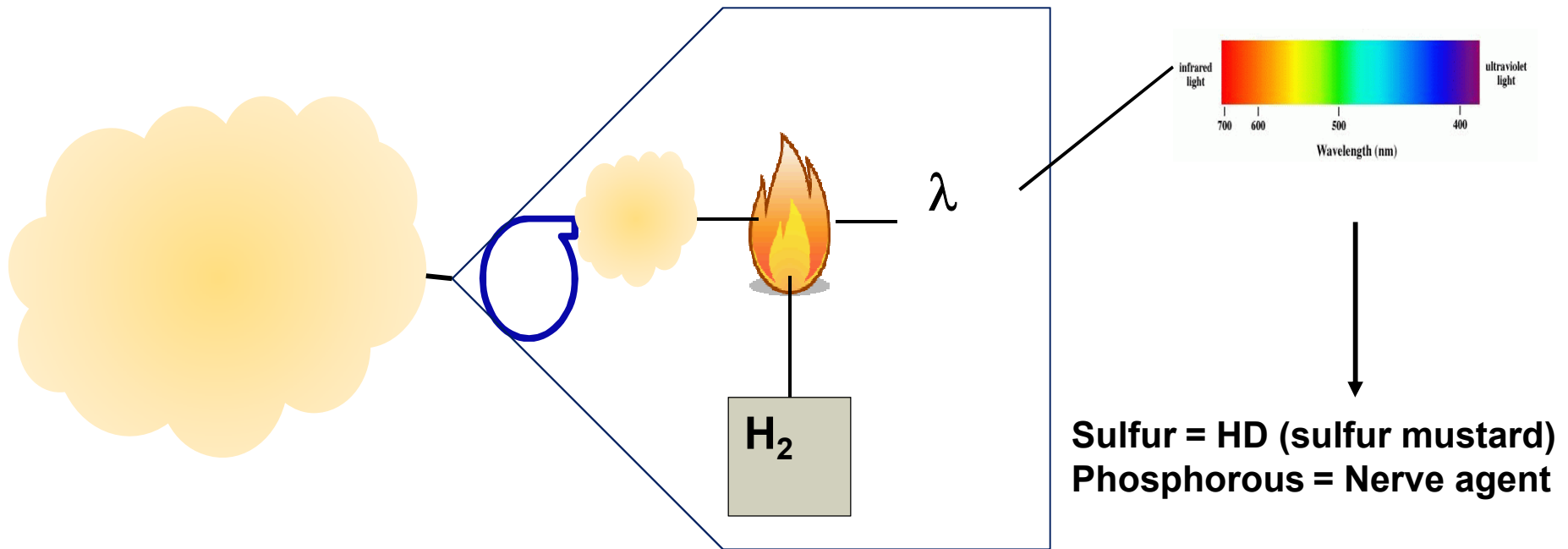
Ion Mobility Spectrometer Solid or Liquid Sampling



- Solid or liquid is collected onto swipes
- Swipes are heated to desorb the sample and create sample vapor
- Many sources of interference
 - High rates of false positives and false negatives

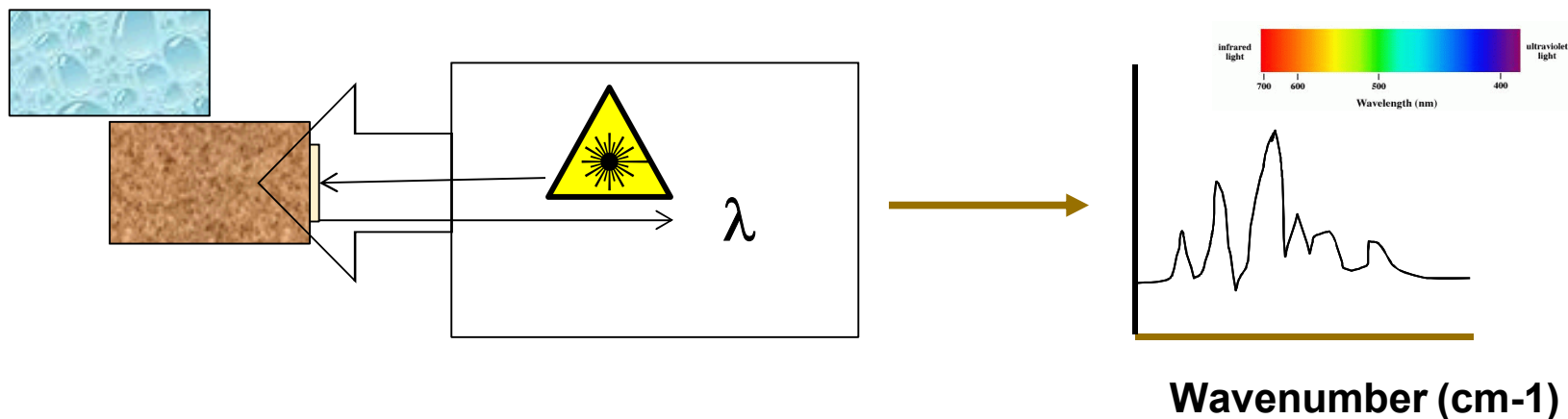


Flame Photometric Detector



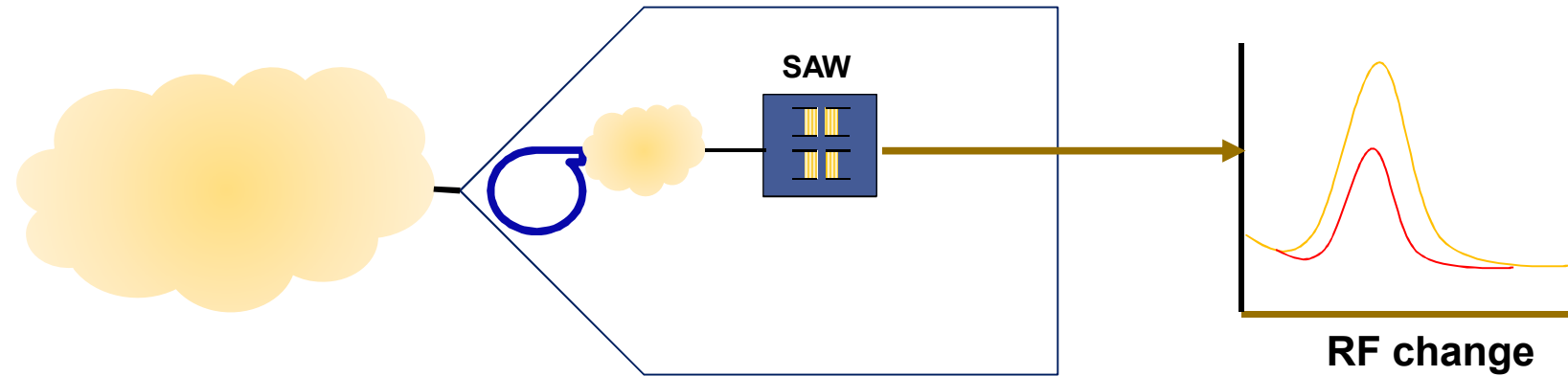
- Vapor is sampled
- Sample is burned in hydrogen flame
- Light is emitted at unique wavelengths for different CW agents
 - Detector is sensitive for nerve agents
- Pesticides especially give false positives

Infrared and Raman Spectrometers

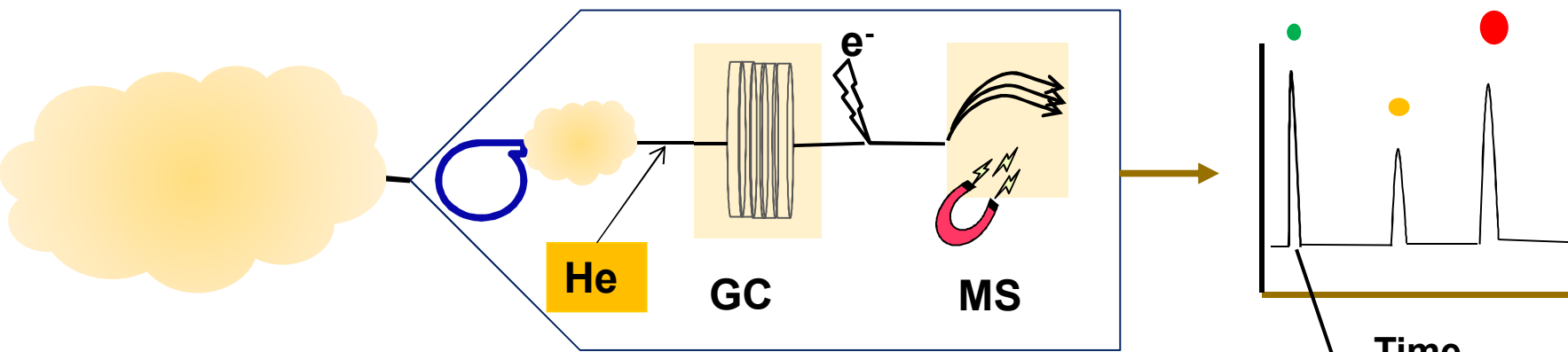


- Solid or liquid samples
- Light hits sample
 - Infrared (FTIR)
 - Laser (Raman)
- Light is collected and measured
 - Absorbed (FTIR)
 - Scattered (Raman)
- Spectra is generated and compared with a library/database
 - “Chemical fingerprint”
- FTIR and Raman are complementary techniques

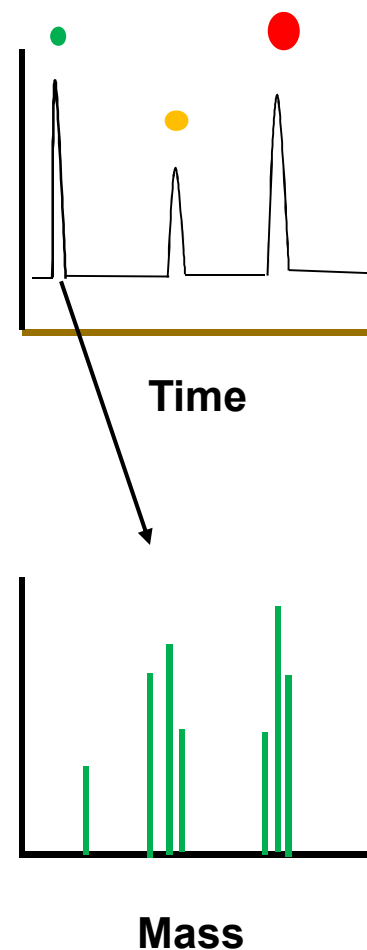
Surface Acoustic Wave Sensor



- Vapor sample absorbed
- Surface wave changes when sample absorbs
- Selective signal for nerve and blister agent
- Interference from pesticides, herbicides, and water (humidity)



- Vapor or liquid sampling
- GC – separation of analytes
 - Differential affinities for mobile versus stationary phases inside a column
- MS – detection and identification
 - Particles of ionized sample are deflected by a magnetic field according to mass
- Spectra are matched to library/database
- Field portable GC/MS requires a carrier gas (He) and consumes a lot of power



LABORATORY INSTRUMENTS

A fully equipped and functional analytical chemistry laboratory

Advantages?

- Precise identification with high degree of confidence is possible
 - *Can confirm analysis by using multiple techniques*
- May be able to handle many different sample types
- Quantitative analysis may be possible

Disadvantages?

- Extremely expensive to set up and maintain
- Slow, real-time analysis is not possible
- Requires trained, experienced chemists and support personnel
 - *May be used improperly by inexperienced or inadequately trained personnel*
- Quality of results are highly dependent on quality of sampling



CHEMICAL ANALYSIS SEQUENCE



**Collect
Sample**



Sample Preparation

- ✓ **Cleanup**
- ✓ **Simple Separation**
- ✓ **Derivatization**



Sample Analysis

Sampling is the most error prone part of the process. Personnel need to know how to collect the right type of sample for lab and field analysis

CHEMICAL DETECTION AND IDENTIFICATION

General information

Observation by Trained Personnel

Field Tests

Field-Portable Detectors

Laboratory Instruments

Detailed information

Training,
Expertise
Required

Time and
Money
Required



CHEMICAL DETECTION AND IDENTIFICATION

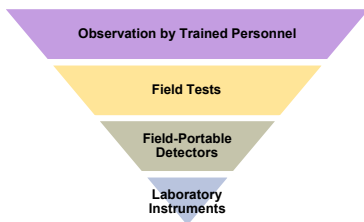
Scenario: A car has crashed into a building in a crowded area. Bystanders not involved in the crash begin complaining of similar symptoms (difficulty breathing and watery eyes). Some people are also reporting a strange odor.

- Does this situation call for chemical detection and identification of some kind?



CHEMICAL DETECTION AND IDENTIFICATION

Discuss the following questions for the **beginning**, **middle**, and **end** stages of this scenario and write down your answers. Time 20 minutes



- What **level of detection** should be used and why? What information will you get? What are the practical considerations and limitations?
- Who is qualified to carry out that detection? What level of training/expertise is required to get reliable/usable information?
- How will the results of detection and identification influence decision making at the scene? How should you deal with uncertainties knowing that detectors are prone to giving false results?
- Any other factors or considerations? What about the safety of the emergency responders?

