Total Hydrocarbon Analysis by Ion Mobility Spectrometry

John H. Cross
Thomas F. Limero
KRUG Life Sciences
Houston, TX

John T. James
NASA/Johnson Space Center
Houston, TX

Astronauts must be alerted quickly to chemical leaks that compromise their health and the success of their missions. An ideal leak detector would be equally sensitive to all compounds that might constitute a hazard and insensitive to nontoxic compounds. No ideal sensor exists; thus, selection of a methodology is a series of compromises. The commonly used methods are either insensitive at the low exposure levels set by OSHA, NASA, and other organizations or are selectively insensitive to important classes of chemicals such as Freons. After extensive study and experience, the Toxicology Group at Johnson Space Center has selected ion mobility spectrometry (IMS) for development into a broad range, sensitive detector. In addition to the sensing method, signal processing is important in leak detection because a background signal can be expected at all times. The leak-detecting instrument must be programmed to discriminate between authentic leaks and background fluctuations caused by routine operations. A prototype leak detector, called a total hydrocarbon analyzer (THA), based on IMS, has been built to detect many types of compounds known to occur in spacecraft atmospheres. The prototype THA includes four signal-processing algorithms that display the signal as a single value representative of the total hydrocarbon concentration in the air.

The authors of this paper will present the results of an evaluation of the prototype THA in terms related to spacecraft operations. The evaluation included determination of instrumental parameters such as stability and response times. We also included responses to some common components of spacecraft atmospheres in pure form and in binary and ternary mixtures. The output of the four algorithms to the mixtures was found to be noticeably different. These responses will be compared on the basis of their utility for signaling a chemical leak. As a means of evaluating its resistance to a falsely positive response, the THA was challenged with carbon dioxide and methane, compounds whose concentrations normally increase in spacecraft air during human habitation. The instrument showed virtually no response to these interferences. Although the prototype THA is designed for space flight, this detector is expected to be useful for field screening at chemical waste dumps and other environmentally sensitive locations.

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John H. Cross, Ph.D., Thomas F. Limero, Ph.D.
and John T. James, Ph.D.*

*NASA Johnson Space Center

KRUG Life Sciences

Organization

▶ **Background**

▶ **Design Requirements**

▶ **Instrument Selection**

▶ **IMS Design**

▶ **Experiment Discussion**
  – IMS stability
  – Responses to typical contaminants
  – Algorithms

▶ **Conclusions**

Design Requirements

Functional

- Detect Leaks and Spills

- Broad Spectrum Response (ppm)

- Track Decontamination

- No Responses from Major Atmosphere Components (O_2, N_2, CO_2, CH_4, H_2)

Design Requirements (cont'd)

Constraints

- Simple, Fast Operation

- Low Power, Mass, and Size

- Low Maintenance

- Reliable

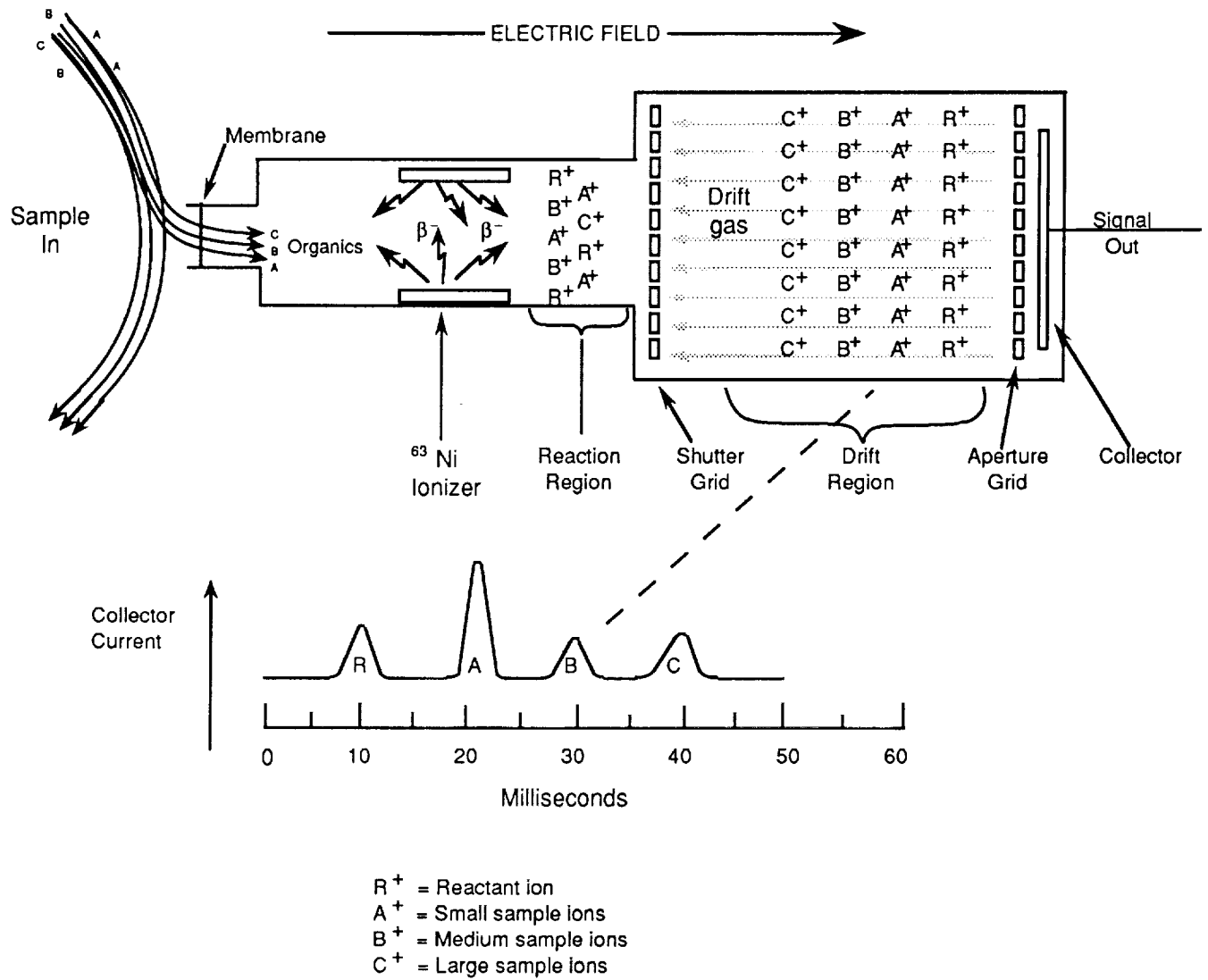- Microgravity Compatible

- Withstand Shock and Vibration of Liftoff

Methodologies

▸ Catalytic Bead

▸ Tin Oxide Ceramic

▸ Photoionization

▸ Ion Mobility Spectrometry (IMS)

Conclusions

▸ Stable Output

▸ High Sensitivity and Precision
   (No response to methane)

▸ Fast Response and Recovery

▸ Complicated Response to Mixtures

▸ Algorithms Trend with Concentration
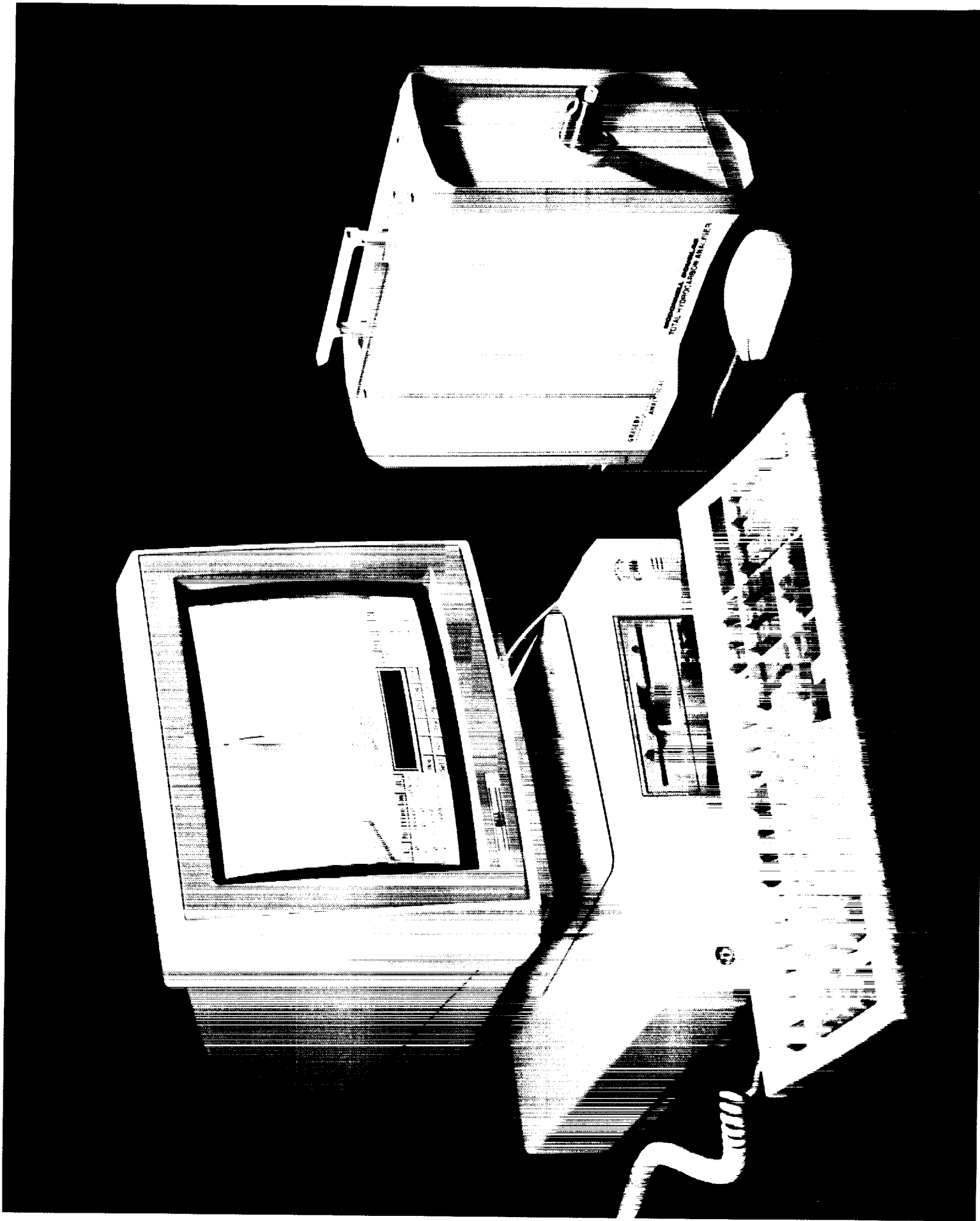
OPERATING PRINCIPLE OF ION MOBILITY SPECTROMETER

Configuration Operation Algorithm Quit

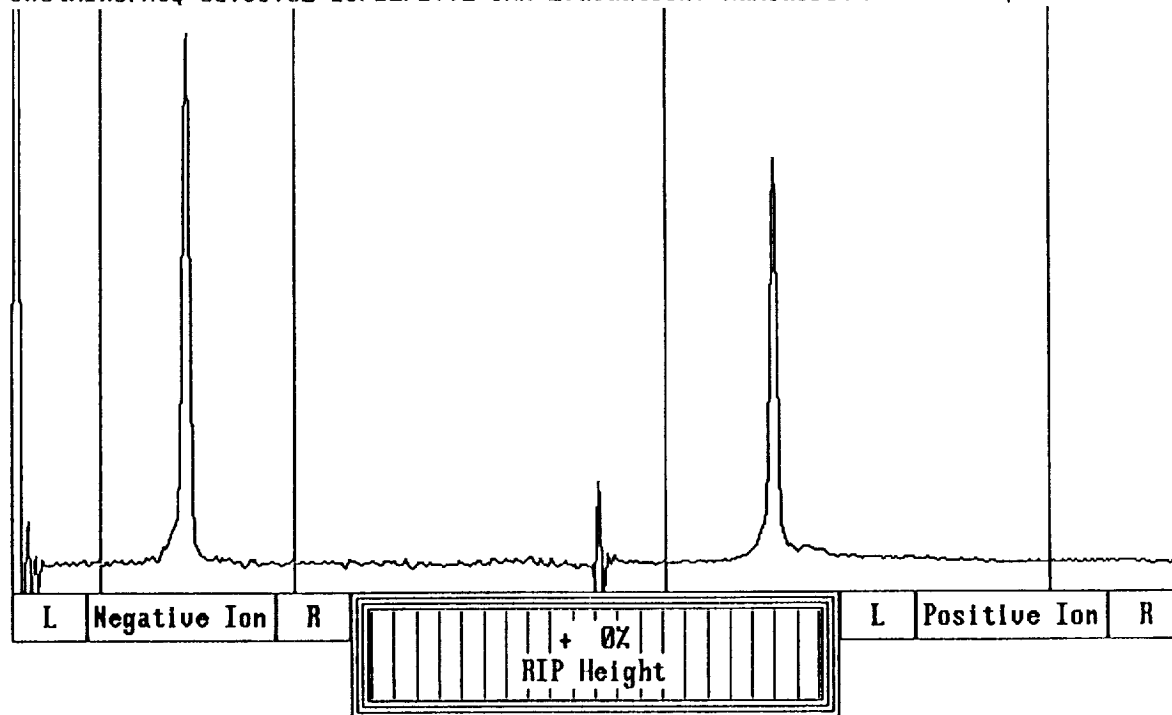JH04nIR0.nCQ 00:55:02 15/12/1992 TIIn Evaluation: Humidified zero air, Jan 4

Table 1: Instrument stability measurements with humidified air.[a]

	Positive Mode			Negative Mode		
Data Set	Baseline (mV)	RIP Height (mV)	RIP Drift time (ms)	Baseline (mV)	RIP Height (mV)	RIP Drift time (ms)
1-5-93	355 ± 4 ± 1	2414 ± 8 ± 0.3	6.40 ± 0 ± 0	354 ± 16 ± 5	3158 ± 16 ± 0.5	6.22 ± 0 ± 0
Average of 10 data sets	359 ± 3 ± .8	2419 ± 39 ± 1.6	6.36 ± .03 ± .5	357 ± 4 ± 1.0	3086 ± 121 ± 3.9	6.19 ± .02 ± 0.3

(a) Average ± Standard Deviation ± Relative Deviation (%).

DC18ACE0.MED 11:17:46 15/12/1992 THA Evaluation. Acetone, 1 ppm, Dec 18, 1992

| L | Negative Ion | R |

+ 45%
RIP Height

| L | Positive Ion | R |
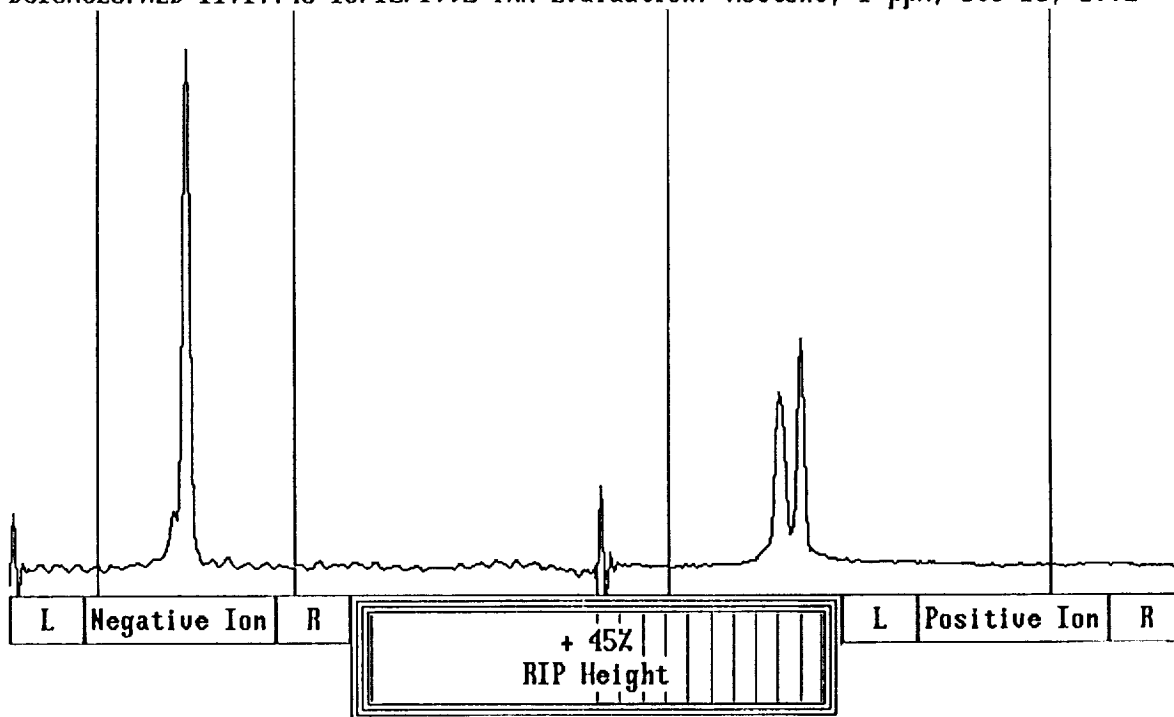
Compound and Concentration	Peak Height (Average ± SD ± Relative Deviation	
	1st Peak	2nd Peak
Acetone 0.4 ppm 1 1.8	644 ± 40mV ± 6.3% 1300 ± 40 ± 3 1701 ± 51 ± 3	-- (a) -- --
MEK 0.1 ppm 0.3 0.9	581 ± 20 ± 6 683 ± 10 ± 1 501 ± 14 ± 3	296 ± 17mV ± 6% 816 ± 19 ± 2 1467 ± 21 ± 1
HCTS 1 ppm 3 ppm 10 ppm	344 ± 49 ± 14 (b), (c) 581 ± 18 ± 3 734 ± 39 ± 5	-- (a) -- --

(a) The acetone spectrum had only one peak.

(b) The larger relative variability was probably partially the result of the method of preparing the sample.

(c) Largest peak in spectrum.

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Configuration Operation Algorithm Quit

L | Negative Ion | R   + 2%   RIP Height   L | Positive Ion | R
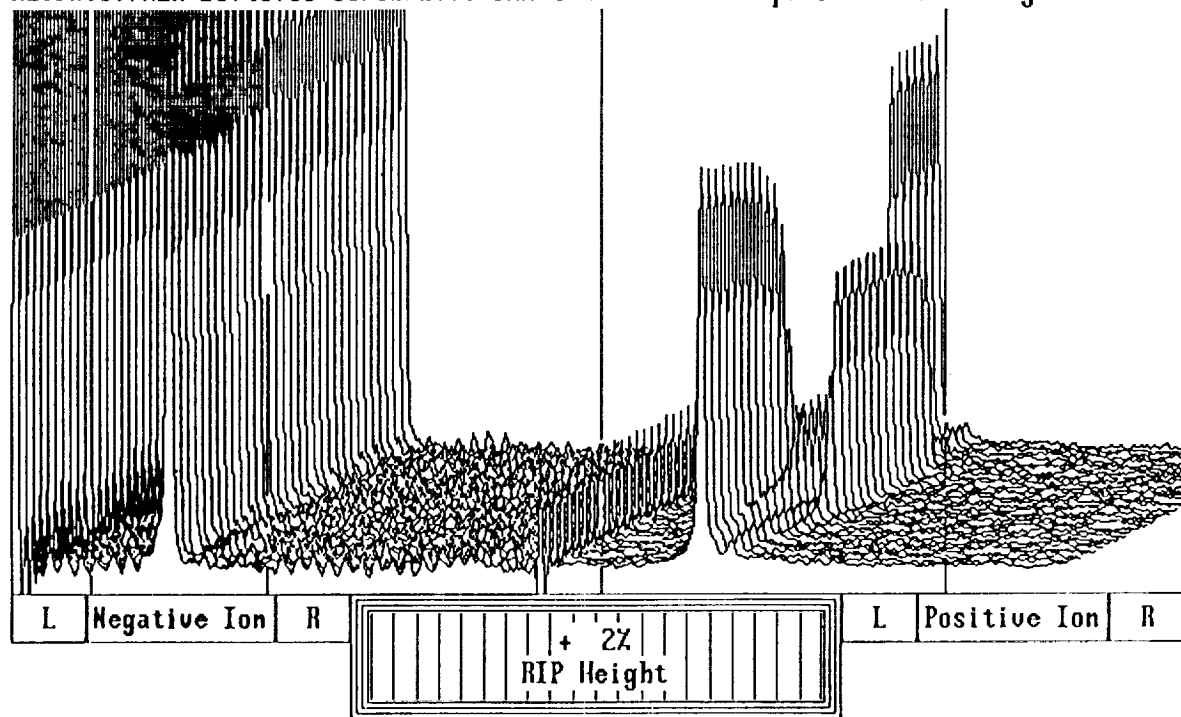
Table 3: Response and recovery times.

Compound	90% Response	90% Recovery
Acetone	3 ± 0 sec	5 ± 1 sec
MEK	3 ± 1	5 ± 1
HCTS	4 ± 1	5 ± 1
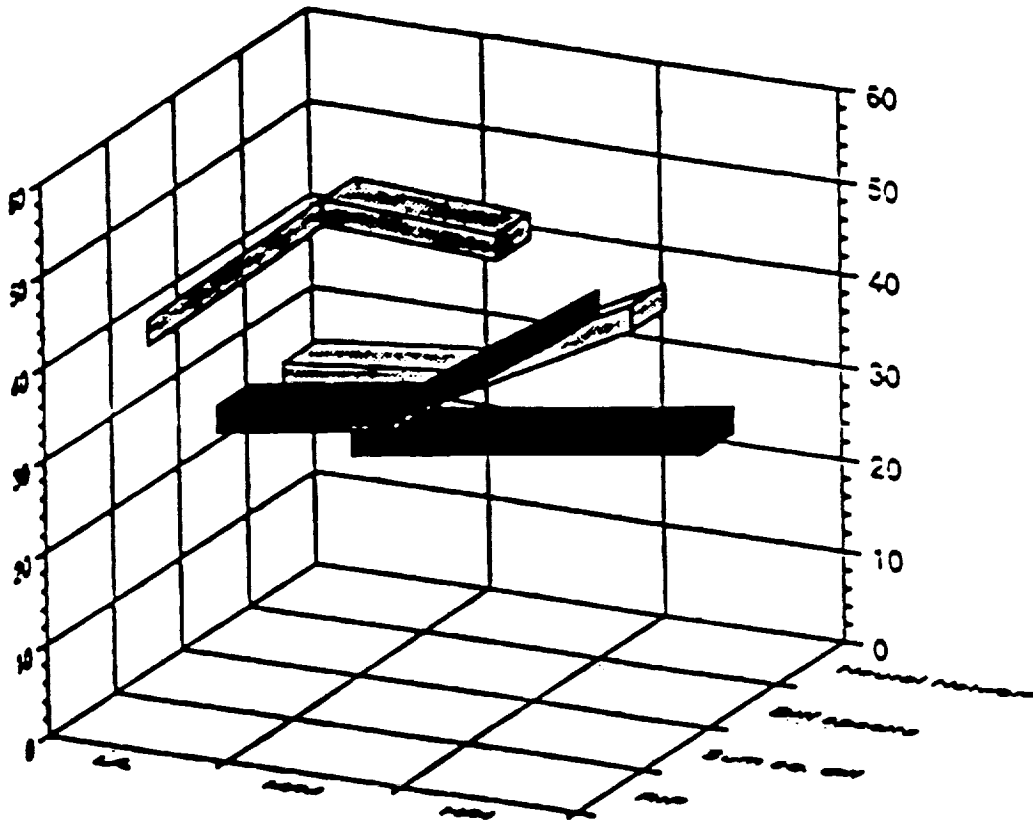
The response of the four algorithms to low, medium, and high concentrations of acetone and MEK.