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A COMPUTER PROGRAM TO AUTOMATE RESIDUAL GAS ANALYSIS

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About five years ago, a need was foreseen for some system that would automatically determine the gases found in an environmental chamber during spacecraft testing. At that time, this function was performed by a skilled chemist reading the output of a mass spectrometer. At best, this is a time-consuming activity which severely limits the quantity of such scans that the human operator can analyze. Others also foresaw the need for the computer processing of such data, and from time to time the literature would carry a scheme or program to accomplish it. All of these schemes had drawbacks which, when applied to our needs, were insurmountable. For example, one scheme required that a library be built using the exact instrument that would perform the required analysis. Since three different types of mass spectrometer comprising ten individual instruments are in use at GSFC, building such libraries is an impossible task.

In 1968, Trombka and Schmadebeck of GSFC published a least-squares method for resolving complex pulse height spectra which offered a path to a solution to our problem. Using their basic concepts and adding a year's effort, a modification, which is practically a new program, was arrived at. We have a program today, written in Fortran IV and using a matrix inversion method, which successfully analyzes mass spectrometer data. Those aspects of previous programs which were detrimental to our use have been overcome. A library can be built from any published data, such as handbooks, textbooks, compendia, or data generated by other instruments. Results are reasonably good and are understandable in direct proportion to the quality of the library. Thus, data from the user's instrument itself will give nearly perfect answers; from good literature values and a typical mass spectrometer, completely understandable answers; from poor values and poor data, some answers requiring a preknowledge on the part of the user.

Testing the program was done in the most objective manner. Materials were prepared, and mass spectrometric data were taken by one group, and

these raw data were given to a second group who ran the program. Unreasonably difficult mixtures of materials were prepared and run, and the program successfully separated them and printed out a correct analysis each time (see Table 1).

The program is being utilized currently for the solution of experimental spectra, where the spectrometer is being used as a contamination monitor by an untrained spectroscopist.

The ultimate goal is to acquire pushbutton analysis capability. The program is the most difficult link in the chain of steps necessary to achieve this goal. Still required is the electronic hardware for taking the signal from the mass spectrometer, digitizing it, labeling it as to mass number, and putting it on tape in this fashion so that the program can take over. We have begun the work on this last phase and are optimistic that next year all mass spectra can be computer analyzed, and automation will be complete except for the technician who pushes the button.

Table 1—Computer analysis results.

COMPOUND	% RELATIVE ABUNDANCE	
	COMPUTED	ACTUAL
ACETIC ACID	15.3 (±2.0)	15
ACETONE	64.3 (±3.9)	75
CARBON MONOXIDE	3.6 (±2.2)	
ETHANOL	11.3 (±1.8)	10
ETHYL ACETATE	0.8 (±2.0)	
3-ETHYL HEXANE	0.4 (±1.1)	
HYDROGEN CHLORIDE	0.1 (±0.7)	
METHANE	3.3 (±1.1)	