NASA TECH BRIEF

Goddard Space Flight Center

Analysis of Low Resolution Mass Spectra

The problem:

To precisely determine gas constituents from measurements of the mass/peak-height spectrum from a residual gas analyzer (a low resolution mass spectrometer).

The solution:

A computer program that applies a recently developed spectral-analysis technique to the analysis of low-resolution mass spectra. Applications of this program include residual gas analysis for work in space environmental simulators, space environment contamination, and air pollution monitoring.

How it's done:

A pre-elimination process is used to compare the unknown sample spectrum with a reference library of standard spectra. A resulting running library is then utilized in a linear least-squares regression analysis of the unknown sample spectrum. A reference library of an unlimited number of standard spectra may either be formed from tables of mass spectra or other literature values, or generated by the user. A preprocessing section in the program screens out those reference library spectra whose base-peaks cannot contribute more than a specified minimum amount to the unknown sample spectrum. The remaining library spectra form the running library for the analysis.

A "best-fit" of the running library spectra to the unknown sample spectrum is calculated using a linear least-squares regression technique. The amounts of those spectra contributing to the "best-fit" are the results of the analysis.

Notes:

1. This program was written in FORTRAN IV for use on an IBM-360/91 with a level 18 compiler.
2. Requests for further information may be directed to:

    COSMIC
    University of Georgia
    112 Barrow Hall
    Athens, Georgia 30601
    Reference: B71-10267

Patent status:

No patent action is contemplated by NASA.

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