Using a Powerful Computer for Acquiring and Processing Chromatographic and Other Analytical Data

Die Verwendung eines Groß-Computers für die Erfassung und Verarbeitung chromatographischer und anderer analytischer Daten

Acquisition et traitements de données chromatographiques par un ordinateur puissant

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Summary: The I. F. P. System is able to perform quantitative gas chromatographic analysis and also to process other analytical data such as those of x-ray fluorescence, mass spectrometry, nuclear magnetic resonance and pilot plant sensors. Off-line calculations may be handled simultaneously like scientific computations and management. The system configuration is such that every computer with 16 bits words and sufficient memory size can be used. The principal characteristics are given on hardware and software developed by I. F. P. services. More details are given for gas chromatographic data processing especially for the computer-dialog, which is done by a sophisticated control panel. Some specified methods are illustrated by examples.


Résumé: Le système développé par l’Institut Français du Pétrole permet de traiter en ligne les analyses quantitatives de chromatographie gazeuse et les données d'autres appareils d'analyses tels que fluorescence X, spectrométrie de masse, résonance magnétique nucléaire et capteurs d'unités pilotes. Des calculs scientifiques et de gestion peuvent être effectués en même temps que l'exploitation en temps-réel. La configuration du système est telle que tout ordinateur à mot de 16 bits et de taille mémoire suffisante peut être utilisé. Les principales caractéristiques des appareillages employés et des calculs développés sont exposées dans ce rapport. L'acquisition et le traitement des données chromatographiques sont repris plus en détail, un pupitre de dialogue très spécialisé a été développé pour cette technique. Quelques méthodes spécifiques sont illustrées par des exemples.

Introduction

Once the principle of computer data acquisition has been admitted, the problem of choosing computer size must be tackled. In every case this problem must be considered in the light of the data to be processed and the financial and technical means available.

The problem of the Institut Français du Pétrole was as follows: drawing up a general automation system for all modern analysis and control techniques for pilot plants. In 1969 the purchasing of several specialized computers had to be planned. This was a fairly costly solution and proved much less efficient in many cases (especially for gas chromatography and mass spectrometry) [2].

Since the Institute was in possession of sufficient technical and financial means in May 1969, decided to develope its own hardware and software for operating analytic equipment.

This system is the result of close collaboration between several divisions, i.e. the Geophysics Division for the hard-ware and Engineering and Analytic Physics Divisions for the software.

The system is conceived so as to be adaptable to any type of computer provided it is sufficiently powerful. Our system operates with an IRIS 50 computer manufactured by the Compagnie Internationale d’Informatique (C. I. I.). It began operating in August 1970, the chromatography section was hooked up in January 1970, then during 1971 the following sections were successively added: mass spectrometry (slow), nuclear magnetic resonance, x-ray fluorescence and pilot-plant sensors.
Table I shows the leading technical features of the computer as well as of its standard peripheral hardware.

The standard computer operating system has been modified only slightly for real-time use. It includes the following processors:
- teletypewriter handler
- ASSIRIS
- FORTRAN
- link editor
- loader
- librarian
- JOB DISQ

### Table I: Computer characteristics

**C.I.I. IRIS 50 Computer**
- 64K octets memory size
- 16 bit words
- Control unit:
  - simple operations are wired
  - floating options and decimal computing are not wired
  - 0.95 μsec basic cycle

**Standard peripheral hardware**
- a DIAM disc unit with 6 million octets and 115 msec mean access time
- a 800 lines/minute printer
- a 800 cards/minute reader
- a card punch

The system works on a time-sharing principle including, besides the real-time, the capability of scientific calculating, compiling and management. The capacity of the system is sufficient to:
- simultaneously process these problems
- store all these data on disc:
  1) - data acquired for different apparatus
  2) - operational data such as qualitative and quantitative identification tables
  3) - teletypewriter dialog programs for mass spectrometry gas chromatography and x-ray fluorescence
  4) - programs:
    - for using computed data
    - for printing the results (mass spectrometry, gas chromatography)

### I. F. P. Automation System

Actually, the computer system is connected to:
- A group of 8 research gas chromatographs connected to a control panel and a typewriter for dialoguing with the computer
- A slow scanning mass spectrometer (peak duration about 1 second) connected to a typewriter
- A nuclear magnetic resonance apparatus
- Two x-ray fluorescence instruments connected to a typewriter

These instruments are located adjacent to the computer.

**II** - A group of 20 routine gas chromatographs located in buildings about 350 meters from the computer

**III** - Pilot-unit sensors located about 100 meters from the computer

Whereas data acquisition is done simultaneously, the data processing is done sequentially job by job and printed out on the fast printer making up part of the computer.

The extension project now being carried out calls for:
- 32 additional gas chromatographs
- fast-scanning mass spectrometry
- x-ray diffraction
- liquid chromatography
- infrared spectrometry

The general organization of the system is very homogeneous and, in most of the cases we are concerned with in this discussion, includes:
- the analyser
- a local station with the multiple role of:
  - amplification
  - filtering
  - elementary dialog with the computer (READY – START – STOP)
  - multiplexer input by specific channel number
  - digital-analog converter

For fast-scanning mass spectrometry (1 peak ≈ 5 x 10⁻³ sec) the scanning speed is too great to be handled by the multiplexer. This analysis device will be equipped with a faster digital-analog converter (16 000 points/second). The numerical data obtained will be stored in a buffer memory and computer processed in delayed time. The digitalized data are then processed in the central computer which gives the results of the operation requested. In most cases this is an analysis bulletin containing the identified constituents and their amounts. In some cases such as x-ray diffraction or mass spectrometry, the computer supplies a series of punched cards. These cards are used as variable data in too bulky computing programs currently processed with our CDC computer or are used in sorting operations requiring a large library existing on the CDC.

Dialoguing with the computer is done via several typewriters. These are distributed so as to be near the analysis equipment. Considering the number of instruments of the same type connected to the computer as well as the great number of computing methods used in gas chromatography, it was necessary to develop a more sophisticated dialoguing system. Therefore, we built a very complete control panel which will be described below.

### Hardware Configuration

The system is quite extensive and details of its concept cannot be given here.