THE AGRICULTURAL CHEMICALS COMPUTERIZED INFORMATION SYSTEM (ACCIS) AT ROHM AND HAAS COMPANY

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ABSTRACT:
The ACCIS computer system at Rohm and Haas Company is an integrated information system used by the Agricultural Chemicals Group. It consists of many computer programs, files, and databases spanning three computer environments designed to provide the user, either biologist, chemist, or manager, with information on the biological activity of queried chemical compounds.

INTRODUCTION:
Rohm and Haas Company is a producer of a wide range of high quality specialty chemicals. One of the major divisions within Rohm and Haas Company is the Agricultural Chemicals Division, a producer of fungicides, insecticides and herbicides for the world markets. Their Agricultural Chemicals Computerized Information System (ACCIS) which operates on personal computers, an IBM 3084 running MVS/TSO, and a VAX 8700 running VMS, is used over 400 times per week by more than 100 users. The role of ACCIS in the discovery of new agricultural chemicals begins with the entry of either purchased or in-house synthesized chemical compounds into ACCIS. Once entered or registered into ACCIS, biologists screen these compounds for fungicidal, insecticidal, and herbicidal activity and enter their findings into ACCIS. Reports combining chemical structures and biology are generated as the result of either sub-structure or formula searching or interactive queries.

ROLE OF SAS® BASED SOFTWARE IN ACCIS:

Biological Entry:
Users within each of the major screening groups, fungicides, insecticides and herbicides enter biological information into ACCIS using SAS/AF® applications called from CLISTS on the IBM mainframe. Figure 1 illustrates a 'typical' SAS/AF application for biological entry. Users are presented with a number of options that either call SAS programs or additional menu screens. Some of these options include entering information using customized PROC FSEDIT screens, creating specialized reports, branching to ISPF, and transferring data to System 2000 databases. Data transfer is accomplished by writing selected information from SAS data libraries to sequential files that are later used as input in COBOL programs that validate the data, produce error reports and update System 2000. Users are notified on their custom FSEDIT screen when experiments have been registered into the database. Another useful option is HELP, which serves two purposes. One, it instructs the user how to use the application. Second, it helps to serve as documentation. Approximately eight versions of this SAS/AF scheme are used by the various screening groups at Rohm and Haas Company.

Chemical Entry:
Users enter chemical structures and other chemical information into an MS-DOS based personal computer program using CHEMBASE, a software package from Molecular Design Ltd. Worksheets containing other information are also imported into CHEMBASE after they have been manipulated using PC SAS programs. Daily, the information in CHEMBASE databases is exported to a central database on the VAX using a software package called MACCS from Molecular Design Ltd. The database package, MACCS, is a chemical structure database package that also provides excellent utilities for substructure and data searching. Because Agricultural Chemical's Biology and major report writing capabilities are located on the IBM mainframe, structure and data are exported from MACCS to the IBM mainframe nightly for update into SAS's System 2000 databases and sequential files.

Reporting of Biology and Chemistry:
On the IBM mainframe, users are presented with a CLIST driven menu that allows them to choose a number of query options. An integral part of these queries are PROC FSEDIT screens which allow the user to enter query information. Once entered, the query information is included within COBOL generated reports. Options are provided to print these reports using either a Xerox 8700 printer or Apple LaserWriters.

REASONS FOR THE SUCCESS OF ACCIS:

1. ACCIS is menu-driven.
2. Custom SAS/AF and SAS FSEDIT screens are easy to use and customize.
3. Interactive queries are easy to perform.
4. Several report formats are available including those that combine structure and biology.
5. The updating of databases is performed nightly with minimal support from computer personnel.
6. Because ACCIS is not confined to any one computer environment, ACCIS can take advantage of strengths of each computer system.

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FIGURE 1. BIOLOGICAL INPUT

SAS/AF

ENTER → CURRENT

BROWSE → ARCHIVED

REPORTS

ARCHIVED → CURRENT

TRANSFER

CHECK

EXP #

ISPF

FLOWCHART

HELP

DIRECTIONS

SYSTEM 2000
FIGURE 2. CHEMICAL ENTRY

PC

WORKSHEETS

CHEMBASE*

STRUCTURE ENTRY

VAX

DATA SEARCH

MACCS*

SSS SEARCH

IBM

SYSTEM 2000

SEQUENTIAL FILES

PC-SAS
FIGURE 3. ACCIS REPORTS

IBM

QUERY OPTIONS
FORMULA
SUBSTRUCTURE
BIOLOGICAL QUERIES

SCREENING LEVEL
FUNGICIDE
INSECTICIDE
HERBICIDE

SYSTEM 2000 DBS & BINARY FILES

BIOLOGY
CHEMISTRY
BIO. & CHEM.

REPORTS

FILE
XEROX 8700
LASER WRITERS

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