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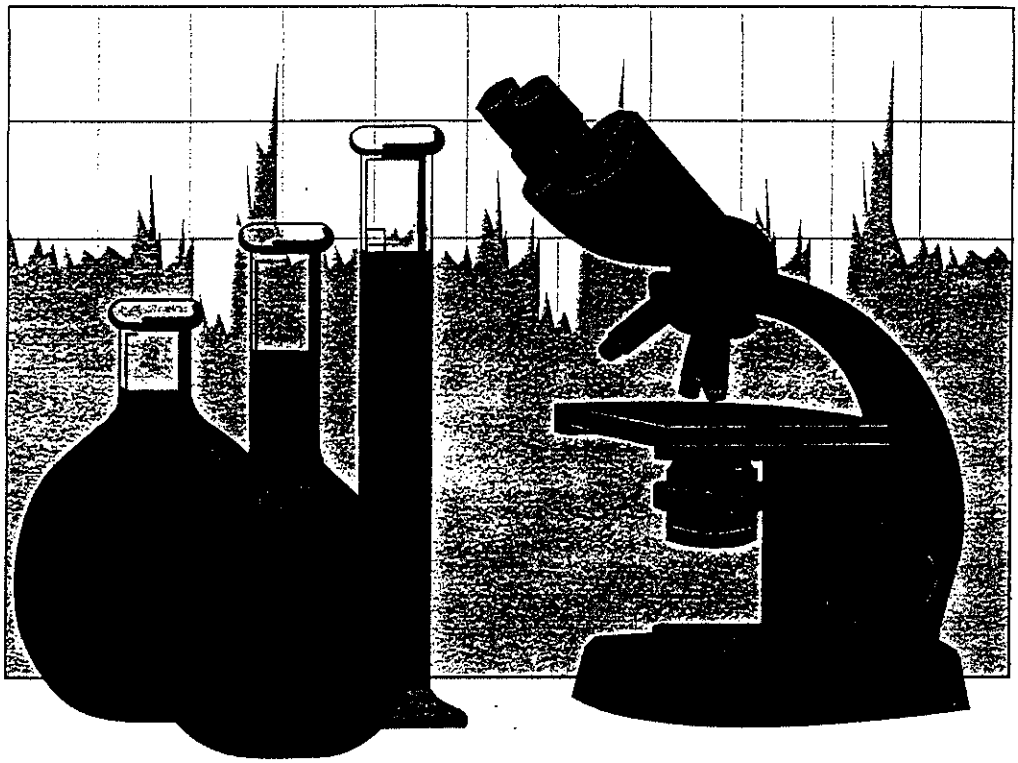

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AN EXPERT SYSTEM CONTROLLER FOR GAS CHROMATOGRAPHY AUTOMATION

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ABSTRACT

We report on the development of an expert system to control the use of a gas chromatograph system in the analysis of hazardous wastes. This automation process allows for analyses to be performed in both a more rigorous and systematic manner, and with an increased rate of throughput. The system includes techniques to monitor the progress of the analyses and determine if any problems or unusual circumstances warrant stopping or changing the process. Our system has been both designed and validated with assistance of analytical chemists.

INTRODUCTION

Hazardous waste sites are inherently dangerous, particularly where there is a lack of detailed knowledge of what is actually present underground. Increasing emphasis is currently placed on the analysis phase of buried waste sites. These wastes must be characterized to determine their elemental, isotopic, and compound content before clean-up can begin. This emphasis on characterization happens early in the process of clean-up and remediation of many such sites. This paper describes the development of software tools for analysis of the contents of buried waste sites, with minimal resulting disturbance or exposure of their underlying contents.

To accomplish this task, our recent research focused on the automation of laboratory analyses, methods, and tools. This automation process allows for analyses to be performed in both a more rigorous, systematic manner, and with an increased

throughput. We present an important example of this approach in the field of gas chromatography. This paper describes a system that is used to perform data assessment on gas chromatography results, and is designed to be fully automated to determine if the data from a gas chromatograph is of acceptable quality. Our software is intended to help meet the growing demand for chemical characterization of soil samples, contents of storage tanks, and water samples.

BACKGROUND, HISTORY, AND GOALS

We created this system as part of the Contaminant Analysis Automation (CAA) project at Los Alamos and Sandia National Laboratories. The CAA program develops an automated environmental analysis system using standardized modules. This allows the chemist to assemble the appropriate test and evaluation modules without any hardware or software incompatibility problems or the neccessity of creating complicated control programs. These systems are designed for use within transportable laboratories at the on-site location. The CAA program is based on the concept of a Standard Analysis Method (SAM), which includes sample preparation, analysis, and data interpretation components. The method accepts samples from the field as input.

After performing automated sample preparation, the samples are then analyzed and passed to an expert system for automatic interpretation and verification of results. The methodology incorporates the use of Standard Laboratory Modules (SLM's), self-contained analysis procedures, combined in an analysis pathway. This involves a series of SLM's which are successively performed on a sample by inserting the sample into each SLM in turn, as needed, and then moving between SLM's with a robot arm. This fully automated process includes data assessment, quality control analysis, and data interpretation components. The work described in this paper is in the data assessment category. The system includes techniques to monitor the progress of the analyses and determine if any problems or unusual circumstances warrant stopping or changing the automated process.

The goal of the system is to take the raw gas chromatographic data directly from the gas chromatography workstation and create a file which is automatically sent to the data assessment system. The data are then analyzed by procedures which are described in detail below. The ultimate goal is to determine if the data are of acceptable quality. If the data are unacceptable, the system determines the problem(s) and recommends solutions to remedy the cause of the problem. Where possible, these solutions will be automatically implemented; otherwise an appropriate operator is notified about the problem and recommended solution. The system stops the automated processing if additional analyses would not be performed properly.

The prototype system demonstrates automated analysis of EPA Method 8080, for organochlorine compounds and poly-chlorinated biphenyls (PCB's). Method 8080 is used to detect Aroclors® (trade name for the mixtures of PCB's sold commercially). We selected this method for automation because of the difficulty in performing analyses of environmental samples of these types of compounds. The complexity of the chromatogram frequently makes the identification and quantification of the components

more difficult. Successful application of this methodology in complex chromatograms tests the methodology and makes future use in less complex chromatograms easier to implement. See reference 1 for further details on CAA.

METHODOLOGY

The approach we currently use involves generating gas chromatograms with vendor equipment and software. We currently use a Varian GC-3400 with Star software on a PC. The reader is referred to reference 2 for general background information on gas chromatography. The Star software outputs the data in one of the industry standardized formats. The data are sent to Matlab on a SUN workstation for signal-to-symptom processing. This processing takes the raw data and, using algorithms developed by Los Alamos National Labs and Sandia National Labs personnel, looks for a series of symptoms for each chromatogram. These symptoms are features of the raw chromatogram data which relate to the peak shape and location of peaks, or to baseline trends and characteristics. Each symptom is assigned a value depending on the presence and relative severity of that symptom. Details of the methodology used in our signal-to-symptom processing are given in references 3 and 4. The calculated values are put into a *symptom file* and sent to the expert system for processing. G2, an expert system software tool from Gensym Corporation,[5] is used to control the process. The entire analysis procedure is:

1. GC gathers and processes raw data with Star software on a PC.

2. Data are transferred to a SUN workstation for input into Matlab.

3. Matlab performs signal-to-symptom processing, using appropriate algorithms.

4. Matlab generates output as a *symptom file* for input into the expert system.

5. Transmit symptom file path to G2 (via message server) and add symptom file to database.

6. Symptom file is imported into the G2 expert system, which determines if data are of acceptable quality or, alternatively, determines problem causes and recommends solution.

7. G2 displays results graphically, and passes problem cause and recommended solution back to operator/user to fix the problem.

Using Expert System Technology

The use of expert system technology in chemical analysis has a long history, beginning in the 1970s with the DENDRAL research.[6,7] Expert systems in chemistry span a broad spectrum, ranging from structure elucidation[6,7,8] to structure and activity

correlation,[9,10] to data interpretation, synthesis planning and experiement design. These systems include analysis of chromatographic behavior.[10,11] An excellent contemporary synopsis of work in expert systems and analytical chemistry may be found in reference 12.

We decided to use artificial intelligence[13] and expert system technology on this project for a number of reasons. First, the AI approach is known for its ability to assist the human expert make intelligent diagnostic decisions. This is usually based on the design in an expert system which uses an explicit set of rules that encode the expert's understanding of a problem, as well as the expert's skills in interpreting signs of faults or breakdown. The system then recommends further tests to confirm these diagnoses.

The second reason for use of the expert system technology is to use the knowledge engineering tools that are readily available. Our system is based on the human expert's analysis of gas chromatographic results. It was necessary to watch experts in this diagnosis, analyze what they were doing and then begin to build up a rule set to reflect their diagnoses. Knowledge acquisition tools, useful in expert system design, assisted in this process. Our validation process included these experts again inspecting our results.

The third reason for employing expert system technology was to use an object-oriented software formulation to describe the test and analysis layout for the gas chromatograph problem-solving process. In an object-oriented expert system, we can define objects to represent each element of the problem-solving process and create methods to describe the functionality of each object/process. Messages are sent between each object to reflect the linkage between that object/process and other components in the problem-solving procedure. Graphic images can represent each object with links reflecting the connection of an object and its related objects/processes. The graphics editor supports easy creation of a schematic to represent each component of the process, as well as the relationships between components. (See Figure 1).

Finally, an object-oriented hybrid software system allows us to link rule-based reasoning to the object-based specification for the components of the gas chromatographic system. This linkage applies the constraints in the expert's analysis of the data processing to the related components of the entire system. The result is an analysis tool that allows human expert reasoning to be automatically applied to the analyses of complex data.

The G2 Expert System Tool

We chose the real-time expert system shell G2 by Gensym Corporation[5] to support the design and structure of our program. Its features include:

1. An object-oriented approach to representing components in a workspace.

2. A graphical user interface with widgets and point-and-click capability.

3. Permission and access levels protected by passwords.

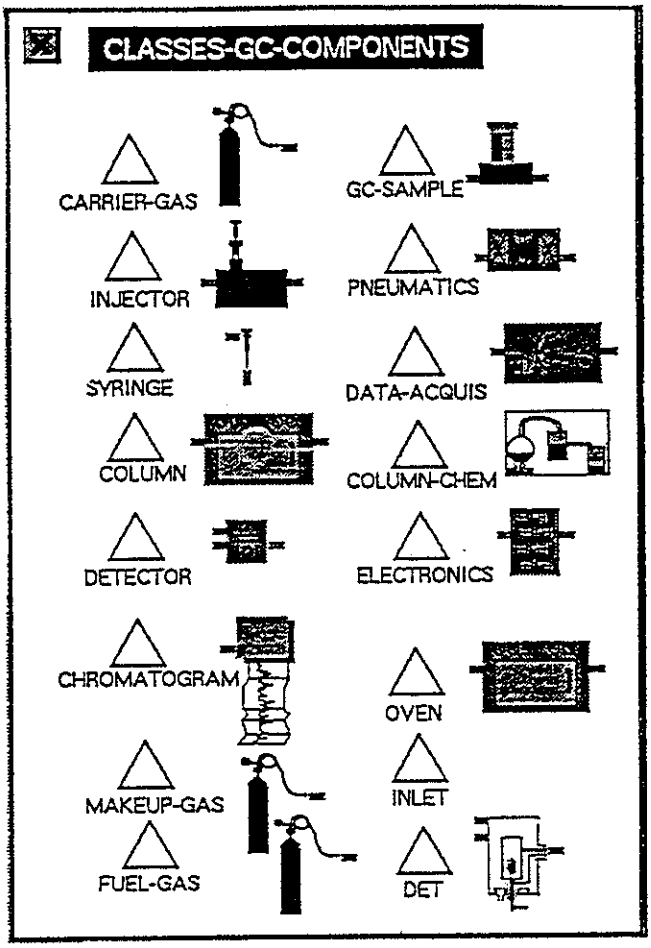

Figure 1. Example objects and their icons from G2. These icons are linked together to reflect the function of each component in the system.

4. A variety of data collection schemes (time and event-based, unsolicited, etc.).

5. A natural language interface for writing rules and procedures. (see examples)

6. A capability for both forward and backward chaining of rules.

The object-oriented user interface enables the user to build applications by developing new objects from old objects by using inheritance and simple *fill-in-the-blank* attribute tables. It also provides a pictorial overview of the process, which can be dynamically updated based on incoming sensor/variable values. The GUI allows the user to view varying levels of detail of components by simply clicking on the component and displaying its table of attributes. New objects may be built and displayed using an icon editor/drawing option to design a specific graphical representations of the object. Figure 1 shows a series of objects that were created using G2's icon editor to represent various objects in the system.

We now take one of the objects of Figure 1, the GC-Sample, and present components of its object definition. The *slot name* for each attribute is in the left

column with its current specification on the right. The *slot* values of the object are currently unbound, *none*, since this object has not yet been linked to a specific system. Modifications and additions to a particular object can be created by the user directly from these attribute tables. The natural language interface is simple enough that domain experts (the analytical chemist) with little programming experience can understand and enter new rules.

Object Name	GC-Sample
User Restrictions	none
Class Name	gc-sample
Superior Class	gc-instrumention
Attributes Specific to Class	none
Class Restrictions	none
Menu Option	a final menu choice
Inherited Attributes	problem cause is "none"
	problem subsystem is "
	gc-manufacture is "none"
	explanation is "
	mode operation is "none"
	carrier gas is "none"
	column diameter is "none"
	column length is "none"
	injector type is "none"
	detector type is "none"
	auto sampler is "none"
	.....
Default Settings	none
Attribute Displays	inherited
.....	

The Expert System Processing

Our current goal is to automate as much processing as possible for all applications. Our ultimate goal is to require no user input. The current method of assessing the data involves starting up the expert system along with a message server system and connecting the communication bridge between them. At this point the expert system is "listening" for messages addressed to it. Whenever a symptom file is generated, a message containing the name and path of the file is sent to the expert system. Rules automatically load this file name into a scrollable menu, which lists all GC symptom files received since the expert system started up. This file may be automatically or manually selected for input into the system and subsequent processing. The actual file is initially added to a database for storage and catalogued for future tracking and any needed auditing.

The symptom file is a specially formatted file (as required by the expert system), which contains a series of attributes and associated fuzzy values corresponding to the

Table 1

Sample Input Symptom File from Program

:SYMPTOM FILE FOR BLEED017.CDF		
13 Apr 1995 17:29:48	the current time	0
:SAMPLE INFO		
0 sample_name	n/a	
0 sample_id	0	
0 sample_type	Calibration	
;FILE INFO		
0 File_source	GCProcCalibration v1.1	
0 Reference_gc_filename	BLEED009.CDF	
0 Retention_time_filename	BLEED_C.RTM	
;INDUCED CAUSE		
0 Induced_cause	ColumnBleed	
0 Severity	0.0	
;SYMPTOMS		
0 ClippedPeaks	0.000	
0 NoPeaks	0.000	
0 RisingBaseline	1.000	
0 IrregularBaseline	0.000	
0 CannotZeroBaseline	-2.000	
0 TailingPeaks	1.000	
0 LeadingPeaks	0.000	
0 UnresolvedPeaks	0.000	
0 GhostPeaks	-2.000	
0 ExtraPeaks	0.000	
0 NegativeDipAfterPeak	0.000	
0 IrregularSpikes	0.000	
0 SensitivityChange	0.670	
0 RetentionTimeShift	1.000	
0 BandBroadening	0.000	
0 SpikePrecision	-2.000	
0 SurrogatePrecision	-2.000	
0 ReplicatePrecision	1.000	
0 HighNoise	0.000	
0 HighBackground	0.000	

presence / absence / severity of each symptom; see, for example, Table 1. Each symptom is a feature related to the chromatogram signal, such as the baseline trend or analyzed shape of the peak. These are compared to expected shape, peak location, etc. Examples of symptoms include tailing peaks or leading peaks, where the shape of the peak deviates from a normal Gaussian distribution and is skewed so that the front or back peak slopes are asymmetrical. Other symptoms include extra peaks (unexpected

peaks) and ghost peaks (where compounds are strongly retained on the column and eluted later with a new injection, resulting in additional peaks). Changes in the expected retention time for a given compound are also compared to a calibration run. Significant changes in peak heights or peak widths are other features that indicate problems in the chromatograph.

Baseline drifting or changes in the baseline trend are also determined. Background *noise* results in features that would also help the chemist determine if a problem is present. Following is a partial list of symptoms that are currently determined by the system:

PEAK'S SHAPE:
- Tailing Peaks
- Leading Peaks
- Unresolved Peaks
- Ghost Peaks
- Rounded Peaks
- Clipped Peaks
- Negative Dip After Peak
- No Peaks
- Irregular Spikes
- Sensitivity Change
- ...and more...

BASE-LINE TREND
- Rising Baseline
- Irregular Baseline
- Cannot Zero Baseline
- High Background Noise
- ...and more...

The symptom file contains either a binary value (0 or 1) or a fuzzy value ranging from 0.00 (completely absent or false symptom) to 1.00 (completely present and true symptom) for each symptom listed above. Binary values are used for those symptoms that are either present or absent, such as clipped peaks. Fuzzy values are used for most of the symptoms where the range reflects the actual severity of the symptom in that chromatogram (i.e., how much tailing is present). The symptom file also includes some general header information identifying the source of the data. Expert chemists have determined that there is a fixed relationship between the presence of particular subsets of these symptoms and particular problems in the gas chromatography instruments, for any given analysis method. The expert system uses this knowledge to determine any problem that might be present. This analysis is based on the suite of symptoms seen in the chromatogram and is reflected in the symptom file.

An input screen allows the user to enter the specific gas chromatograph instrumentation details of his/her specific system. It contains information such as the type of instrument, mode of operation, which carrier gas is being used, column length and diameter, detector type being used, injector type being used, and whether an autosampler is included. For example, if the detector type was not flame ionization (FID), then a rule pertaining to *dust in the flame* would not be applicable, since there is no flame in the detector. Likewise, a setup with a FID would not want to include a rule pertaining to make-up gas, unlike an electron capture detector (ECD) which requires make-up gas. Including information about the instrumentation allows this sort of reasoning.

Whenever the expert system receives notification that a new GC symptom file has been received, it automatically imports the given file, and dynamically creates several objects (GC-chromatogram, GC-peak, and GC-instrumentation) which contain attributes corresponding to the values of the symptoms. A series of rules are in place which link the specific subset of symptoms required for each specific cause to be determined. These rules are activated if the appropriate symptom values are all above the required thresholds for the given rule. These rules associate each subset of symptoms with a given gas chromatogram instrument problem. The expert system has also subdivided the GC instrument into a series of sub-systems. Once the problem(s) is (are) determined, it is isolated to a particular sub-system. This is helpful in correcting the problem. Two examples of problem-determination and symptom rules follow:

```
for any gc-peak GC that is part-of any gc-chromatogram that is generated-by any
    gc-instrumentation GI
if the SensitivityChange of GP >= 0.0 and the ReplicatePrecision of the GC >=
    0.0 and the GhostPeaks of the GC >= 0.0
then conclude that the problem-cause of GI = "Leaking syringe" and
conclude that the problem-sub-system of GI = "syringe"

for any gc-peak GC that is part-of any gc-chromatogram that is generated-by any
    gc-instrumentation GI
if (the value of the SensitivityChange of GP * 1.0) +
    (the value of the GhostPeaks of GP * 0.75) +
    (the value of the NoPeaks of GP * 0.25) +
    (the value of the ReplicatPrecision of GP * 1.0) >= 1.0
then conclude that the problem-cause of GI-14 = "Leaking syringe" and
conclude that the problem-sub-system of GI = "syringe" and
show gc-system-breakdown-causes and
change the arrow icon-color of arrow-syringe to red
```

The last two "ands" of the conclusion of this last rule indicate how partial results of the analysis are reported back to the user. First, the gc-system-breakdown causes are presented to the user in a window and, second, one of the icons (Figure 1) in the sequence of icons that represent the current system changes color (to red) to show the location of the suspected problem. As we will see, justifications for the conclusions as well as recommended fixes for the system are also presented to the user.

But, first we present two more example analysis rules. The first rule shows how the system interates over and anaylzes the peaks within a particular chromatogram.

```
for any gc-chromatogram GC
    for any gc-peak P that is part of GC
        if the highbackgroundnoise of P >= 0.5
           or the cannotzerobaseline of P >= 0.5
           or the irregularbaseline of P >= 0.5
           or the risingbaseline of P >= 0.5
        then conclude that the baseline of GC = "abnormal" and
        conclude that the baseline of P = "abnormal"
```

Table 2

Symptoms vs. Causes for Gas Chromatography - for Capillary ECD System[1,2]

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Retention Time Shift						I	A					A			A
Surrogate Precision	A	U	S	S								S			
Sensitivity Change	A	A	U	A					A	A		A			
Tailing Peaks				S			S	S		S	S				
Unresolved Peaks				S			S	S					S		S
Band Broadening				S				S		S		S	S		
Clipped Peaks										S			A		
Neg Dip After Peak								S	U						
Irregular Baseline								S	U			S			
Rising Baseline					I	A	S	U		S					
Can't Zero Baseline								I	I						
High Noise, electronic						S			U	S	S	S			
High Background, chem'l					I	S		S	U	I	S				
Irregular Spikes															
Ghost Peaks		U	S								I	S	S	I	
Extra Peaks					A			S				I			I
No Peaks	U	I													
Replicate Precision	A	U		S				S				U			
Leading Peaks				S			S								

[1] A = Always; U = Usually; S = Sometimes; I = Infrequently; N = Never.

[2] Column headings:

1 = Mech. Defective Syringe; 2 = Leaking Syringe; 3 = Dirt in Syringe;
4 = Sample Decomposition; 5 = Late Eluting Component; 6 = Column Bleed;
7 = Column Degradation; 8 = Contaminated Column; 9 = Contam. Detector;
10 = Make-up Gas Flow; 11 = Dirt in Injector; 12 = Leaking Septum;
13 = Sample too Conc.; 14 = Sample Size too Large; 15 = Carrier Gas Low.

```
for any gc-peak GC
    whenever symptomfile recieves a value and
    when the sampletype of GC = "unknown"
    then conclude that the ghostpeaks of GC = -1.0
```

We have just presented a small sample of rules from our knowledge base, including one where the problem cause for "leaking syringe" is identified. Our rules are based on a table of symptom/cause relationships which is modified from references 14, 15, and 16 and the knowledge of the chemists mentioned in the acknowledgements of this article. The set of rule relationships is presented in Table 2.

The system uses goal-driven reasoning with a separate rule for each potential problem cause. Rules are written to insure that causes with "Always" symptoms are only indicated if that symptom is present. Similarly, causes with "Never" symptoms will not be indicated if that symptom is present. Each rule includes a confidence factor which is based on the expected, as opposed to actual, presence of each possible symptom for a given cause. For each symptom that is present, if the fuzzy value is above an indicated threshold, (reflecting its presence) then the expert system takes the raw value and then multiplies it by an "expected frequency factor." That expected frequency factor is:

Always = 1.0, Usually = 0.75, Sometimes = 0.5, Infrequently = 0.25, Never = 0.0.

If the value is less than the threshold, then it is set to a value of "0" reflecting its absence. The values are then normalized to the range 0 - 1 to offset the differing number of symptoms present for each cause. Thus, the confidence factor is the observed summed data divided by Total Possible, where

Total Possible = (symptom1 - expected frequency1 + symptom2 - expected frequency2 + ... + symptomn - expected frequencyn).

A graphical schematic of the GC instrument is then displayed, with an arrow indicating the particular subsystem which contains the problem, as well as a list of all specific problems which may be indicated. An additional workspace may be displayed which indicates which symptoms were the ones used to determine the problem, what their observed values were, and the recommended solution. This workspace contains the explanation information commonly requested by the user. If no problems are indicated, then the graphical workspace indicates that the GC is okay or that the expert system could not match the symptoms with any problem cause in the current set of rules. For example, following one problem run, we got the conclusion that the GC system faults were most likely the "sample size" and a "contaminated column." These were presented in prioritized order, and followed by a justification for the conclusions in terms of the rules used:

GC SYSTEMS BREAKDOWN CAUSES: Sample Size
Column

Certainy Factor of Conclucions Contaminated Column: 0.145
Sample Size Too Large: 0.4

Explanation for Sample Size Too Large
Since the RetentionTimeShift of GC = -0.775
and the LeadingPeaks = -0.947
and the BandBroadening = 1.0
then the problem cause is: Sample Size Too Large
and recommendation is: Dilute Sample or Inject Smaller Sample

As may be noted from this explanation, the most likely causes and recommendations for fixing the problem are passed back to the appropriate operator for help in fixing the situation.

CONCLUSIONS AND FUTURE APPLICATIONS

Our system was validated on a rule-by-rule basis by the chemist experts that assisted us in its creation. It has been used extensively in the field to diagnose potential hazardous materials. In each instance the system performed as well as the human expert, but with considerably increased efficiency and speed. Its most important current use, however, is in the research laboratory where its creators continue to add rules that reflect the anamolies they discover in a widening range of diagnoses of gas chromatograph results.

Future applications include automatically fixing the diagnosed problems when possible; however, most of the problems are probably still going to require manual intervention (such as replacing a leaking septum). This methodology assumes that only one problem occurs at a time. This is, in fact, the same assumption used now by Varian in fixing their gas chromatograph instruments.[16] The user would fix the indicated problem, run the next analysis and, if additional problems were indicated, then check and fix the next indicated problem in the instrument.

An additional future application is to incorporate specific instrument histories into the symptom files. This would allow the analyst to track past events such as the number of injections into a particular septum. For example, as the number of injections into a septum increased, the likelihood of a leaking septum would correspondingly increase, and would be reflected in a higher confidence factor in the expert systems diagnosis of "Leaking Septum." Analogous situations include the possibility of column degradation with increased number of analyses using the same column.

The knowledge used in this system is geared towards analysis of a specific EPA method.[1] Additional sets of rules (knowledge bases) may be needed to analyze different EPA methods,[17] or when using radically different instrumentation setups. The development of these additional sets of knowledge, with future incorporation into the control system, would widen the potential applicability of this software.

The control system developed in this project is an example of the type of automated processing that is desirable for future work in the environmental arena. The combination of automated processing, signal-to-symptom processing algorithms, and expert system technology provides a valuable means of improving the quality as well as speeding up gas chromatography analyses. The expert system provides a high level user interface which can be used to automate processes or notify the relevant personnel of the desired corrective action. Additional reasoning can easily be added and the system includes flexibility to allow corrections to the knowledge base to be made fairly simply.

Chromatography is currently used in many different areas besides environmental analyses. These include gas analyses, hydrocarbon analyses, drug and alcohol testing, medical analyses, various applications in the food and beverage industry, and in the chemical process industries. Similar methods could be applied in analyzing chromatography in those other industries. Additional applications for this technology can be developed for other types of chemical analyses as well.

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