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FAULT DETECTION IN GAS CHROMATOGRAPH DURING CONCURRENT ANALYSIS

Mr. Jayachandran Chekkala and Dr. P. B. Kumbharkar.

JSPM's Rajarshi Shahu College of Engineering (An Autonomous institute affiliated to SPPU), Pune.

ABSTRACT

Process Industries comprises of many complex instruments for the correct and synchronized operations. Gas chromatograph (GC) is one of such complex instruments, used to control quality. Injector, column, detector and recorder are critical parts of GC functionality. During Concurrent Analysis, single GC will be able to analyse multiple input samples at simultaneously using multiple Detectors/Columns. GC outputs the separated measured components through chromatogram consists of series of peaks. Peak height, width, shape depends upon component concentration/retention time and health of critical parts of GC. The tendency of slight changes of peaks in chromatograms over time will be of use in predicting the fault at earlier stages, as how an expert predicts the possibility of fault. This paper proposes how the fault is detected during concurrent analysis in GC using multiple columns and detectors, further, how to confirm the fault with additional check. When a fault is identified as per exhibited symptoms in one detector among multiple detectors in concurrent analysis GC, the fault can be confirmed by analysing the same sample through another Detector.

1. INTRODUCTION

Gas chromatography is very popular and reliable method to separate, identify and measure components from an input gas mixture. The components in an input gas mixture gets separated by distributing between a stationary phase which remains fixed in a place and a mobile phase which carries the components of given mixture through the medium being used. Gas chromatography is widely used to analyse volatile materials in industries related to petroleum products, food & beverages and pharmaceuticals.

During Concurrent Analysis in GC, multiple samples from various input gas streams will be separated and measured. Concurrent Analysis uses a greater number of columns and detectors for analysis various components. In case of some gas mixtures, sample will be passed through multiple columns and detectors for separating, detecting and measuring various categories of components.

Major functional parts of Chromatography are sample injection, components separation from input sample gas mixture, identification of individual components (elements & compounds) and measurement of separated components. Gas chromatography analyse gases. Solids and Liquids gets analysed in their respective vapour phase. The gas samples should be ensured in their pure state without any moisture and impurities for correct analysis.

During Concurrent Analysis which component alarming out pattern indicating fault in which column and/or which detector need to correctly matched. It will help in replacing the defective component.

Basic block diagram of GC during concurrent analysis is depicted in Fig. 1.1, followed by details of each of the functional part.

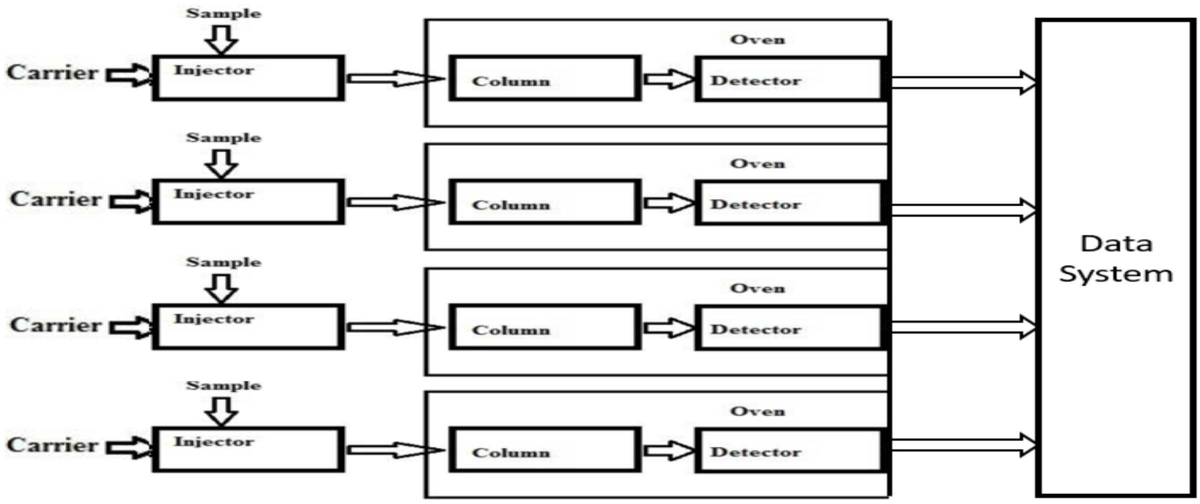

Fig. 1.1:**Basic block diagram of GC during Concurrent Analysis**

Carrier: Continuous flow of an inactive gas, which carries sample from injector through columns and Detectors till Vent.
Sample: Small quantity of a gas mixture, which need to be separated and measured.
Injector: Ensures injection of input gas sample and carrier gas into columns.
Column: Long chemical coated tube, which can influence the pace of molecules of each component differently, so that they get separated during flow.
Detector: Eluted components through column gets detected with quantity details.
Oven: It maintains required temperature of column for separation and detector for detection.
Multiple sets of above parts are used in Concurrent Analysis to facilitate separation and measurement of multiple gas samples simultaneously. Concurrent Analysis GC employs multiple Injectors, Columns, Detectors and Ovens in a single GC.

The distribution of a solute between the mobile and stationary phases in chromatography is described by k, the partition coefficient, defined by:

In chromatography the partition coefficient (k) describes the solute distribution between stationary phase and mobile phase. Equation 1.1 defines the partition coefficient (k) as

$$k = \frac{C_s}{C_m} \qquad \text{..... 1.1}$$

Cs: Stationary phase Solute Concentration
Cm: Mobile phase Solute Concentration

The input gas mixture sample molecules get carried through chromatographic column by mobile phase. Each component of gas mixture (analyte) will have specific characteristic affinity for the stationary phase during transportation, which influences the time to get retained in the column. The time taken by the analyte starting from sample injection till the respective peak maximum is known as retention time of the component. Equation 1.2 defines the retention time (t_r) as

$$t_R = t_S + t_M \qquad \text{.....} \qquad 1.2$$

t_S: Time spent by analyte in stationary phase
t_M: Time spent by analyte in mobile phase

The amount of each component in gas mixture is proportional to the area underneath respective peak in the chromatogram.

GC is capable of correctly compute quality of gas with high repeatability, by identifying and measuring components of composition. Hence, GC is highly preferred to control quality by ensuring the desired quantity of each component. GC measurement accuracy enabled its application in many industries like pharmaceutical: drug-testing, oil & gas: refining and custody transfer, food: quality control.
Principle components/parts are bound to failures and faults can be occurred during their operation. There is probability of occurrence of faults in various principle components of GC. GC analysing many samples

simultaneously will use greater number of principle components, the possibility of faults will be more. It is more important to correctly identify faulty component and fix for desired GC output quality. Fault would be not tolerated because it directly affects on cost, productivity and efficiency. Concurrent Analysis GC has more dependency to ensure quality of a greater number of samples, hence in case of fault more loss. Usually following faults can occur in GC critical parts: injector, chromatographic column or detector.

- Injector: Contaminated Injector, Injector Leak, Injector volume is too large, Syringe worn
- Column: Improper Connection/Column Installation, Column Bleed, Column Contamination, Column Deteriorating, Damaged Stationary Phase, Column Overload, Loss of Stationary Phase, Bleed at high temperature and Normal Degradation of Column with Use.
- Detector: Detector contamination, Detector Filament Out of Balance, Dirty or Defective Detector, Defective detector filaments, Detector Overload and Normal Degradation of Detector with Use

2. RELATED WORK

Most samples that chemists want to analyse are mixtures. Chemists use chromatograph as an analytical tool because it aids to correctly separate components in a mixture for subsequent use or quantification. The gas chromatograph makes it possible to separate the volatile components of a very small sample and to determine the amount of each component present. In case of complex gas mixture multiple chromatographs need to be employed to separate and measure all the components. Alternately, the GC capable of performing concurrent analysis can be used for analysing complex mixtures as it consists of multiple columns and detectors.

GC during concurrent analysis, results are shown in form of multiple chromatograms (one per each sample) which are graphical representations of analysis. Peaks in chromatograms are get changed due to faults, which leads to incorrect result and they will not be useful to decide quality of the input samples.

Functionality of GC gets greatly affected by various faults in one or more its parts. There is a definite need to detect faults, faulty parts and fix as early as possible. It will ensure to maintain quality analysis results of all concurrent input gas mixture samples. Gas chromatograph overall health need to be ensured by ensuring good health of all parts like Injectors, Columns and Detectors required for concurrent analysis.

3. SUMMARY OF RELATED WORK

N. V. Mahajan, A. S. Deshpande and S. S. Satpute specified the use of Convolutional neural network(CNN) to predict the faults by irregularities in pattern of gas chromatogram. Faults like shoulder peak, negative peak and good peak has identified. Inception Network architecture of neural network is used for the prediction of these faults [1].
Ms. S. S. Patil, Prof. S. K. Pathan proposed a system or method to predict the fault using the combination of statistical methods, artificial neural network (ANN) and fuzzy logic [2].
K. A. Vidhya, R. Soorya, N. Saranavan, T. V. Geetha and M. Singaravelan specified an efficient entity resolution technique in biomedical records, symptom vs. disease where a particular symptom, subjected to ambiguity and recommended top-k treatments for the disease to the health care professionals [3]
Shafqat M. Virk; Aslam Muhammad; A. M. Martinez-Enriquez proposed findings in study of different vehicle fault prediction techniques, using artificial neural network and fuzzy logic-based model[4]
K.V. Shihabudheen, G.N. Pillai gave a general overview of the state-of-the-arts of neuro-fuzzy systems and easily refer suitable methods according to their research interests. Different neuro-fuzzy models are compared and a table is presented summarizing the different learning structures and learning criteria with their applications [5]
Gayathri M, A. Sudha explored an enhanced Multilayer Perceptron Neural Network based machine learning technique and a comparative analysis is performed for the modelling of fault-proneness prediction in software systems [6]
ZeFeng Wang and Zarader, Argentieri, S. proposed system to detect fault in aircraft by using artificial neural network for decision making system in aircraft. They designed fault diagnosis system for same which will be useful for pilots and central system to control. They have also suggested that for better and accurate results ann can be paired with any other intelligence system like genetic algorithm, fuzzy logic [7]
Chafaa, K., Slimane, N. , Boutarfa, develop scheme based on the artificial neural network and fuzzy logic as a extension of previous or existed fault detection and diagnosis system. They used robot and sensors and actuator and implemented in matlab. There results showing the faults of sensors and actuators detected and classified very efficiently and accurately. In this they focus on the parameters changes due to fault in sensors and actuators [8]
Yimin Shao, K. Nezu proposed concept of the degree of creditability of parameter value variations (DCPV factor) to solve problem that on-line monitoring and failure diagnosis of rolling element bearings are affected by monitoring parameter value variations caused by the intrusive vibration signals [9]

Zhongdi Liu; Xiang'Ao Meng; Jiajia Cui; Zhipei Huang; Jiankang Wu proposed an algorithm to classify 12-lead ECGs into 9 categories, which extracts expert features including generic features and specific features with statistics and physiology significance [10]

Du Z, Tsow F, Wang D, Tao N enabled the study of chemical separation processes in real-time by miniaturizing and integrating the Micro-GC separation and detection units[11]

S.L. Rivera E.J. Klein Developed an intelligent algorithm to automatically categorize chromatographic peaks resulting from the separation of protein mixtures using ion exchange chromatography. A vector quantizing neural network (VQN) was trained and used to classify peaks into six distinct categories based on peak geometry: Gaussian, fronted, tailed, leading shoulder, trailing shoulder, and overlapping and the VQN correctly classified 90% of the test peaks[12]

Sunghun Kim; Hongyu Zhang; Rongxin Wu; Liang Gong proposed after eliminating the noises using a noise detection and elimination algorithm, defect prediction accuracy is improved[13]

Meisamshabanpoor and Mehregan Mahdavi presented an implementation of recommendation system and its algorithm considering recommendation concept and its definition[14]

Lingli Li; Jianzhong Li; Hong Gao evaluated their rule-based ER algorithm on real data sets and showing both their rule discovery algorithm and rule-based ER algorithm can achieve high performance through experimental results[15]

Tim Menzies; Jeremy Greenwald; Art Frank showed that defect predictors are demonstrably useful and, on the data studied, yield predictors with a mean probability of detection of 71 percent and mean false alarms rates of 25 percent[16]

T. Menzies; J.S. Di Stefano

Presented defect detectors yield results that are stable across many applications and are inexpensive to use and can be tuned to the specifics of the current business situations[17]

N.E. Fenton; N. Ohlsson

confirmed that the number of faults discovered in pre-release testing is an order of magnitude greater than the number discovered in 12 months of operational use and important result was strong evidence of a counter-intuitive relationship between pre- and post-release faults [18]

T.-J. Yu; V.Y. Shen; H.E. Dunsmore

Presented a mathematical model to estimate the number of defects remaining in software, which may also be used to guide software developers in evaluating the effectiveness of the software development and testing processes[19]

Bonnie MacKellar; Christina Schweikert; Soon Ae Chun presented a semantic integration approach using RDF triples to develop an integrated clinical trial knowledge representation, by linking different Linked Open Data such as clinical trials provided by NIH as well as the drug side effects dataset SIDER[20]

3. OBSERVATION ON SURVEY

#	Fault Detection from Symptoms & Expert Data	Related to Gas Chromatograph	Fault/Disease Other Field	Fault detection from other sources	Confirmation with additional check
Ref.1	✓	✓	x	x	x
Ref.2	✓	✓	x	x	x
Ref.3	✓	x	✓	x	✓
Ref.4	✓	x	✓	x	x
Ref.5	x	x	x	x	x
Ref.6	x	x	✓	✓	x
Ref.7	x	x	✓	✓	✓
Ref.8	x	x	✓	✓	x
Ref.9	✓	x	✓	x	✓
Ref.10	✓	x	✓	x	x
Ref.11	x	✓	x	x	x
Ref.12	x	✓	x	x	x
Ref.13	✓	x	✓	x	✓
Ref.14	x	x	✓	✓	x
Ref.15	x	x	✓	✓	✓
Ref.16	✓	x	✓	✓	x
Ref.17	✓	x	✓	✓	x
Ref.18	✓	x	✓	✓	x
Ref.19	✓	x	✓	✓	✓
Ref.20	x	x	✓	✓	x

Accurate analysis results are possible in case of all critical parts are functioning without any fault. The health of the GC instrument needs to ensure considering all faults. Prediction of fault is very much possible from symptoms exhibited like how a disease gets identified using export doctor knowledge. GC Expert knowledge rules repository will be of great aid of predicting fault correctly.

CHALLENGES:

In case of concurrent analysis multiple injectors, columns and detectors are used in GC. The concentration changes in input gas sample will cause variations in output chromatogram peaks from which symptoms are to be identified.

1. How to identify faulty part from symptoms observed in multiple chromatograms?
2. In case of any fault gets identified through exhibited symptoms referred from expert knowledge, How to confirm the reason for symptoms indicating faulty part are not because of the variations in input sample gas?

4. PROPOSED WORK

In medical field, Doctors can identify early symptoms of patients and suggest medications to avoid complicated diseases. Doctors use already published expert knowledge and own expertise acquired over the time to correctly predict the disease from symptoms. There are such automated telemedicine systems available, where symptoms vs expert knowledge repository used to identify and suggest correct medicines to patients.

In the similar line, by developing a system of GC expert knowledge rules of symptoms vs faults repository it will be possible to identify various faults in GC parts. The expert would be able make an almost correct fault from the observed symptoms. By analysing the parameters of chromatograms like Retention time, Peak shape, Area under peak, Peak height, Peak width, Resolution, there can be a possibility to detect GC faults.

Table 4.1: **Component wise Column and Detector Details**

#	Component	Eluting from Column	Detector Used
1	carbon dioxide (CO_2)	1	TCD – 1
2	carbon monoxide (CO)	1	TCD – 1
3	sulphur dioxide (SO_2)	2	TCD – 2
4	nitrous oxide (NO)	2	TCD – 2
5	nitrogen dioxide (NO_2)	2	TCD – 2
6	carbon (C)	3	FID – 1
7	Sulfur	4	FPD - 1

Table 4.2: **GC Expert knowledge Rules of Symptoms Causing Possibility of Faults**

#	Symptom	Fault causing Symptom as per Expert
1	Increase in Retention Time	Detector Contamination
2	Decrease in retention time	Column deteriorating
3	Irregular baseline drift when operated isothermally	Column Contamination or Major Leakage
4	Loss of resolution	Major Leakage
5	No peak	Major Leak
6	Only one peak present	Detector Contamination
7	Peaks less than standard number	Column deteriorating or Major Leakage
8	Increase in peak width	Column Contamination
9	Increase in peak area	Column Contamination

Following conclusions can be draws referring above table:

- Column Contamination might result into Increase in Peak width or Increase in Peak area.
- Deteriorating Column might result in to Decrease in Retention Time or missing Peaks
- Detector Contamination might result in to missing peaks
- Major Leak can cause no peaks
- Minor Leak can cause missing peaks

Detecting fault in GC during concurrent analysis by developing algorithms to

i. Read symptoms (generated from previous work)
ii. Read data tables consisting information of which component getting eluted from which column and which detector (Table: 4.1)
iii. Read expert knowledge rules (Table: 4.2) to detect possible fault.

When a sample was getting analysed expecting three peaks, but the chromatogram shows only one peak and two peaks are missing, as shown in figure: 4.1: the sample 1 getting analysed through column 1 and detector 1. The expert knowledge rules repository as per Table: 4.2, indicates the reason for the missing peaks symptom could be the detector 1 got contaminated.

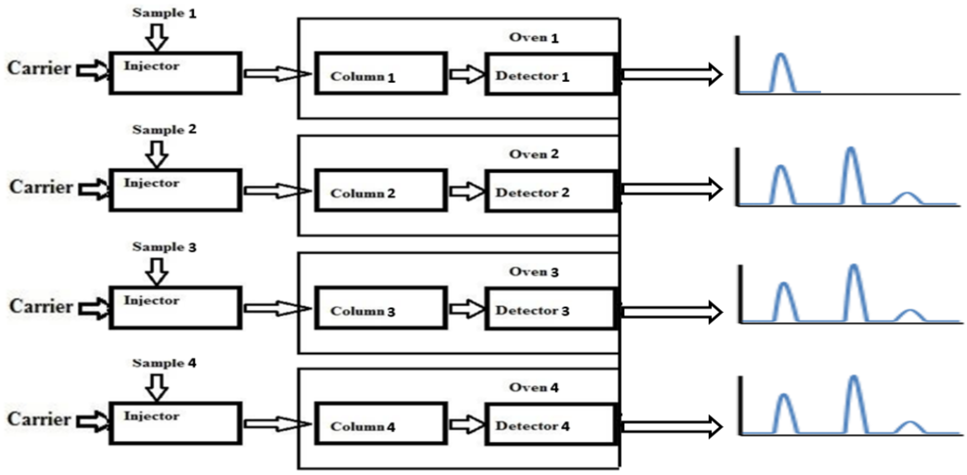

Fig. 4.1: **Missing Peaks Symptom observed through Column1 and Detector 1 during Concurrent Analysis**

Proposed fault confirmation by passing the same sample1 through one/two different sets of column and detector simultaneously as shown in figure 4.2. The same sample getting analysed through column 1+detector 1, column 2+detector 2 and column 3+detector 3.

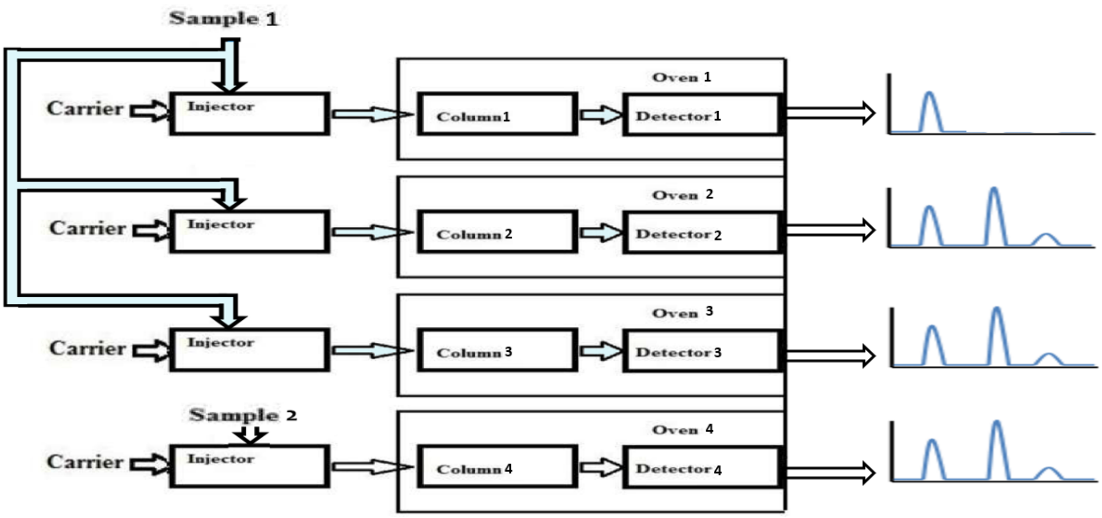

Fig. 4.2: **Proposed missing Peaks Symptom Confirms Detector 1 Contaminated as same Sample1 results all three peaks correctly through other sets of Column and Detector**

The faulty detector 1 analysis results only one peak but other two detector 2 and detector 3 analysis results all three peaks correctly. This confirms that the input Sample1 is reliable and Detector 1 Contaminated whereas Detector 2 and Detector 3 are not contaminated.

5. CONCLUSION AND FUTURE WORK

In case of faults in parts of Gas Chromatograph, the results will be incorrect and mis guide the dependent decisions in conducting the operations. Faults in GC will lead to poor quality control, which can degrade the performance of the industry, can cause accidents and will greatly impact the business. It is very momentous to detect faults in gas chromatography efficiently and in early stages. It is possible to detect faults from symptoms in GC results patters using expert knowledge repository. In future the systems can be optimized towards predicting faults with more accuracy and very well in advance. The prognosis would be possible in case of more complex GC configurations.

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