EXPLORATORY ANALYSIS OF COAL TAR USING NON-TARGETED ANALYSIS TECHNIQUES

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Abstract: This study explored coal tar samples obtained from an underground coal gasification (UCG) trial that got terminated due to exposure of the reactor. The tar samples were investigated using Non-Targeted Analysis (NTA) techniques. The analysis of the tar data led to a possible list of compounds that can be monitored to indicate the exposure of a reactor during the underground coal gasification process.

Introduction

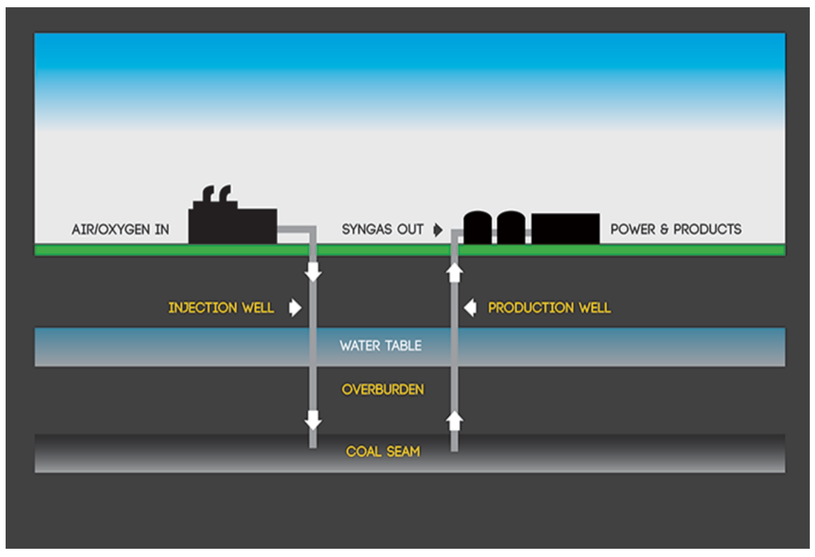

Fig 1. Schematic diagram of UCG showing the injection of air or oxygen to produce syngas and coal tar through chemical reactions in the coal seam [1]

UCG → Direct mining of coal in coal seam

Benefits:

- Access deep, thin to mine coal seams
- Reduces greenhouse gas emission and has potential for CO_2 capture
- Decreases the dangerous effects of mining on miners.

Problem statement and aim

•Interest in clean energy sources to generate power has led to worldwide UCG research and trials.

•Six days trial in Barbara mine in Mikolow, Poland carried out in August, 2013. The underground reactor was exposed which led to an unstable operation in the UCG process and eventual trial termination.

•Samples of the coal tar were collected throughout the trial in order to investigate their possible usage or disposal[2,3]. Part of the tar samples were observed to have undergone chemical changes due to the exposure.

•This study aims to perform an exploratory data analysis on the tar samples to discover any chemical trends in the tar that can help in monitoring the UCG process to determine exposure of the reactor. Although UCG has many benefits, it has not been commercially adopted, and one of the reasons is due to the lack of set parameters to monitor the UCG process

Methodology

NTA with Two-dimensional gas chromatography and time of flight mass spectrometry (GCxGC-TOFMS)

ChromaTOF Tile and Microsoft Excel:
Fisher ratio (F-ratio) and Principal component analysis (PCA)

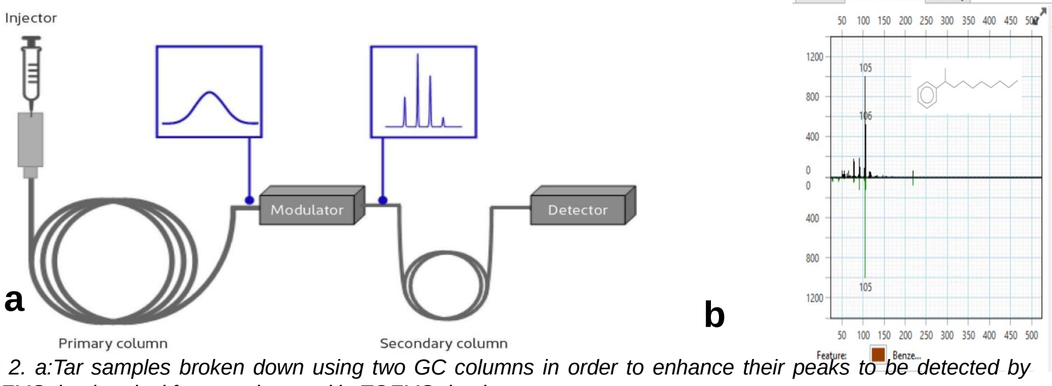

Fig 2. a:Tar samples broken down using two GC columns in order to enhance their peaks to be detected by TOFMS. b: chemical feature observed in TOFMS database

Non targeted GCxGC-TOFMS analysis was combined with statistical techniques to identify unknown compounds in the tar.

F-ratio was used to find compounds that differs between two different classes of samples by comparing the class-class variance by the within class variance. Then PCA was used to group the samples into clusters and find out what compounds were responsible for the grouping.

Results

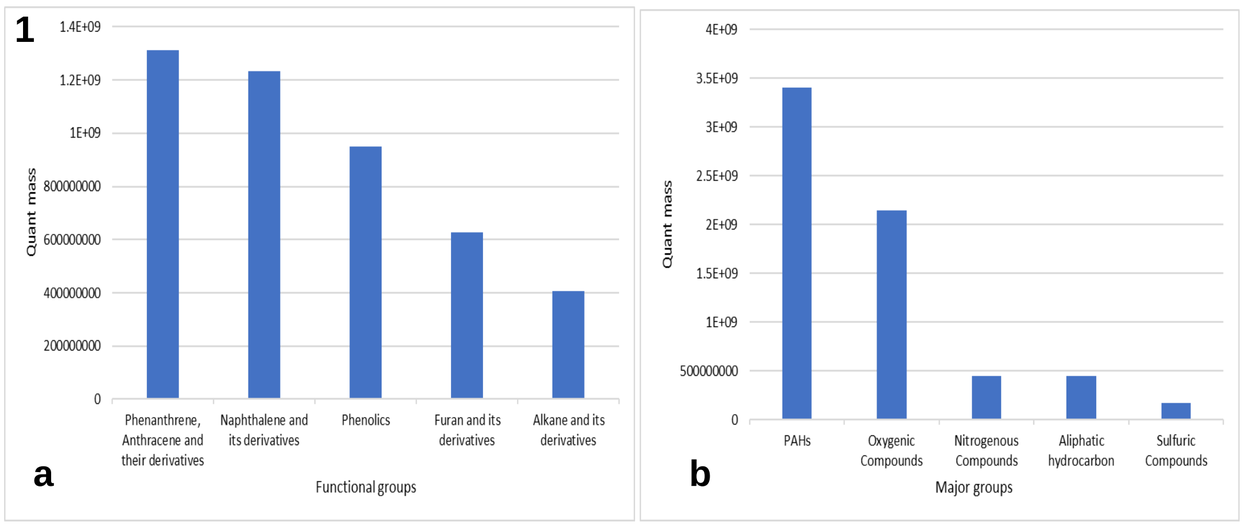

Fig 3. a: Top five functional groups of compounds that distinguish the samples the most, b: Top major groups of compounds that distinguish the samples the most

Table 1. Top five compounds with largest positive and negative change between stable and unstable operation of the UCG process

Negative change		
Name	Functional group	Major group
Anthracene, 1,8-diethynyl-	Phenanthrene, Anthracene and their derivatives	PAHs
2-Oxo-6-phenyl-4-(4-hydroxyphenyl)-1,2-dihydropyrimidine	Alcohol, Ketone, and Imidazole	Alcohol, Ketone and Imidazole
Indeno[1,2,3-cd]pyrene	Pyrene and its derivatives	PAHs
Benzo[ghi]fluoranthene	Fluoranthene	PAHs
9H-Cyclopenta[a]pyrene	Pyrene and its derivatives	PAHs
Positive change		
Name	Functional group	Major group
o-Cyanobenzoic acid	Acid, Ester	Oxygenic Compounds
1,5-Hexadiene, 2,5-dipropyl-	Hexadiene	Oxygenic Compounds
Pyridine, 2,3,5-trimethyl-	Pyridine, Pyrimidine and its derivatives	Nitrogenous Compounds
Benzene, octyl-	Benzene and its derivatives	PAHs
Benzene, (1-methylheptyl)-	Benzene and its derivatives	PAHs

315 unique compounds were found

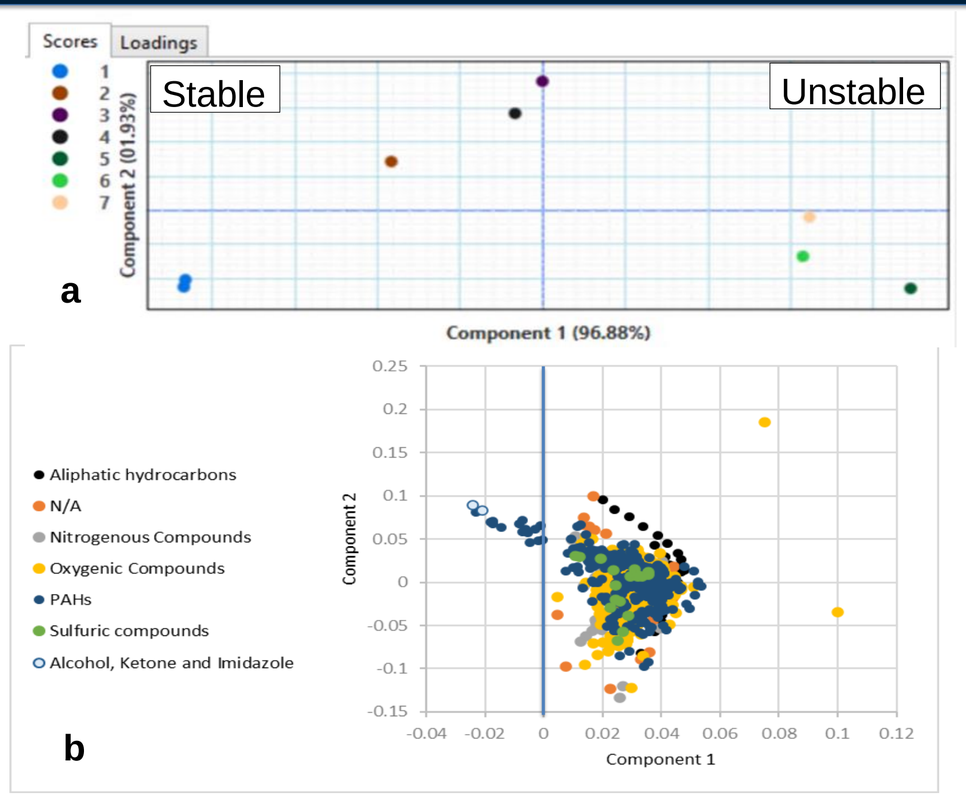

Fig 4. a: Samples clustered by PCA . b: Compounds causing the clustering during the stable and unstable operation of the UCG

Conclusion

- ChromaTOF Tile worked as a very useful tool to perform F ratio and PCA to find compounds that differentiate between both gasification stages
- Discovered a possible list of compounds that could be monitored during the UCG process to determine exposure of an underground reactor.

Further research: Explore individual compounds that should be monitored

References

1. UCG Process – Oxeye Energy [Internet]. [cited 2021 Aug 12]. Available from: https://www.oxeyeenergy.com/ucg-process/
2. Sampsonidis Ioannis. Semi-volatile organic compounds in underground coal gasification effluents: from sample preparation to data analysis. 2019.
3. Wiatowski M, Muzyka R, Kapusta K, Chrubasik M. Changes in properties of tar obtained during underground coal gasification process. International Journal of Coal Science and Technology. 2021;

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