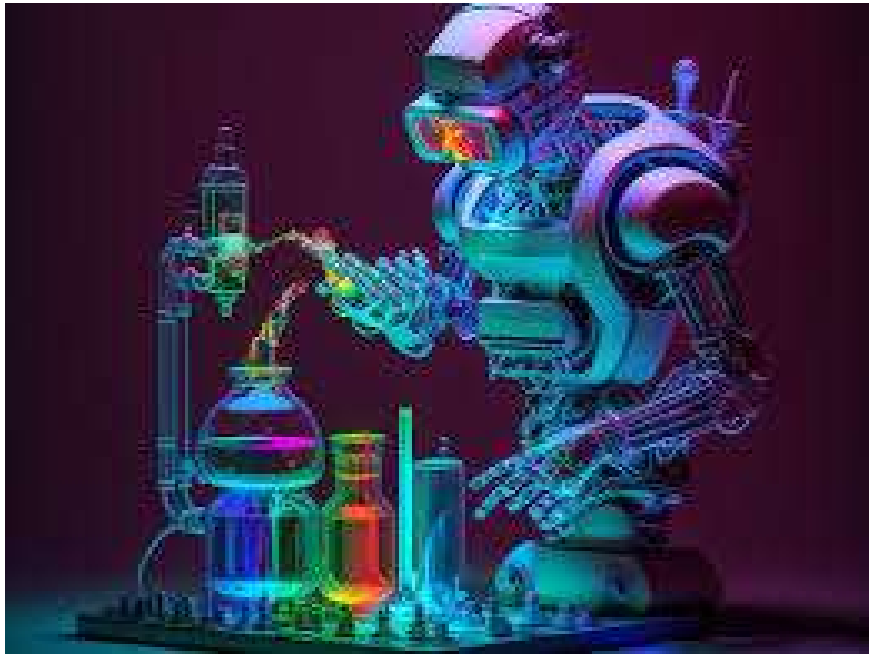
The SCC,DCC and AI

Seminar- Fall 2023



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Advanced Materials and Chemical Technology

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Current world trend

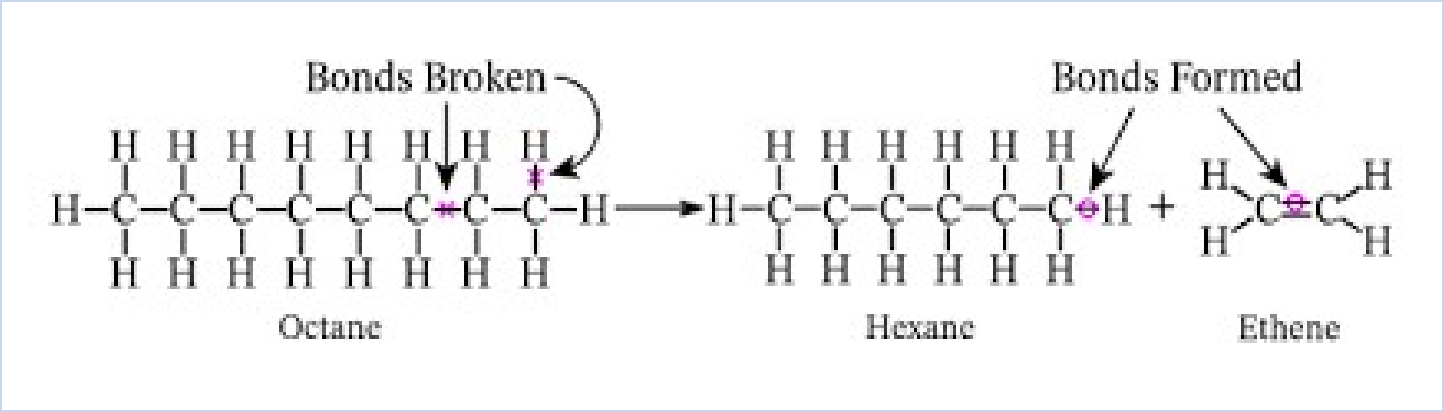
World is electrolyzing. Cars run by electricity because it is clean energy. However we have still huge amount of fossil fuels. Our research plan is to find the more effective and cheap substance that can help to produce a fuel can release more energy and less waste. So that we can use rest of the oil resources more efficiently.

•What is SCC and DCC?

WHAT IS CRACKING?

Cracking is a technique used in oil refineries whereby large and complex hydrocarbon molecules are broken down into smaller and lighter components that are more useful for commercial or consumer use. Cracking is a critical stage in the process of refining crude oil

Creaking means getting substances from crude oil step by step. Firstly we get gasoline because its weight is light. Then we started to get the fuels that are heavier e.g. kerosene, diesel etc.



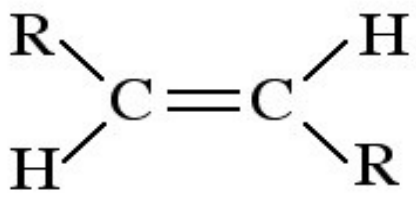
- *SCC- Steam Creaking Catalysis*
  We creak the crude oil with water without air and under pressure (I creak dodecane mixture of oil mostly olefins looks like yellowish liquid)

- *DCC- Dodecane Creaking Catalysis*
  We creak the crude oil without water (it helps us to not spend time to clean up the olefins from water)

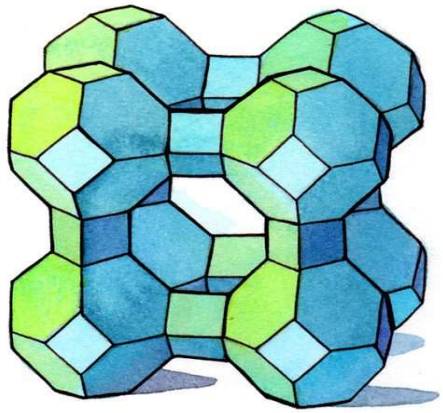
SCC experiment

My research work is olefin production by using zeolites

Olefins are a class of chemicals made up of hydrogen and carbon with one or more pairs of carbon atoms linked by a double bond.



Zeolites are minerals that contain mainly aluminum and silicon compounds. Zeolites are microporous, crystalline aluminosilicate materials commonly used as commercial adsorbents and catalysts.



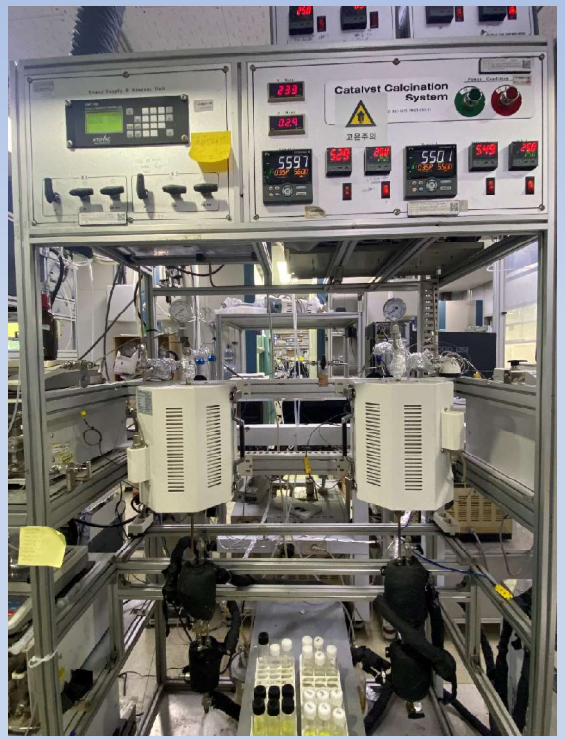
What is catalysts- a substance that increases the rate of a chemical reaction without itself witness any permanent chemical change

- We have two machines.

  DCC- Dodecane Creaking Catalysis

  SCC- Steam Creaking Catalysis

We use a machine can create the condition that keep the substances under 600 C^0



My current research is SCC

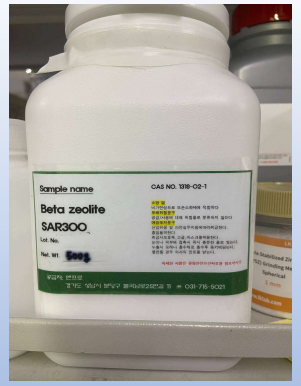
- Normal SCC reaction

- 1. Sample loading in reactor
- 2. Pretreatment- giving 550 C temperature to the catalysis to make it ready for experiment (It takes 12 hours)
- 3. SCC reaction (it lasts 6 hours. Every one hour we monitor the temperature in the oven and collect sample from machine)
- 4. Puna analysis (this analysis can show us what gases and liquids we get from creaking)

Working process

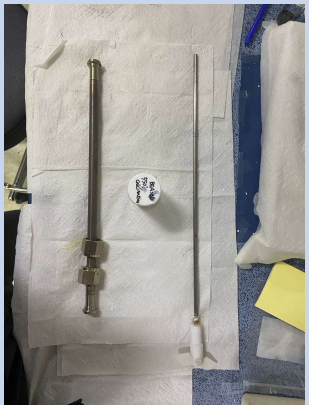
- 1. Sample loading reactor

- We prepare the catalysis BEA 360, 25,100, 83 (zeolites). I put zeolites under pressure within 1 min then I grind. After that I sift the material with sieve that has 150nm holes. I get 0.675 gr zeolites one experiment.
- I need a tube that can be tightened top and bottom. I will put in the tube glass cotton to hold the zeolites. I clean inner thermocouple with wipes until there is not any powder left. (Tube should be cleaned with ethanol C2H5OH).
- After that I tighten the tube inside the oven then I open the air and N2 and heating band and set the temperature. Then I will add dodecane and water to the cycle system so dodecane can be decompositioned into small molecular organic substances.



BAE360

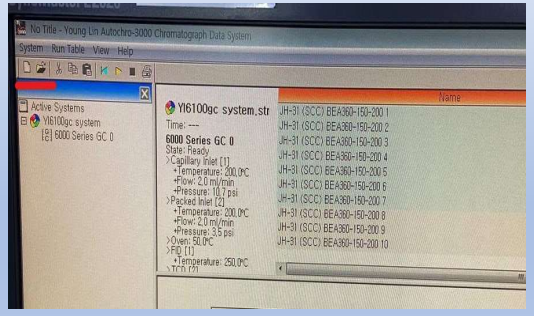
Hydrolic Press

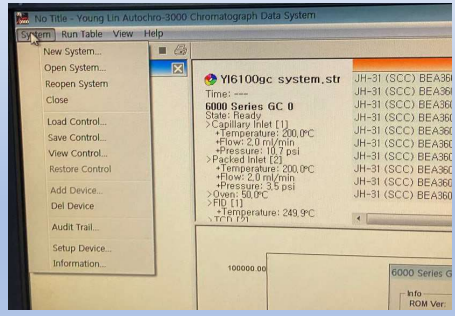


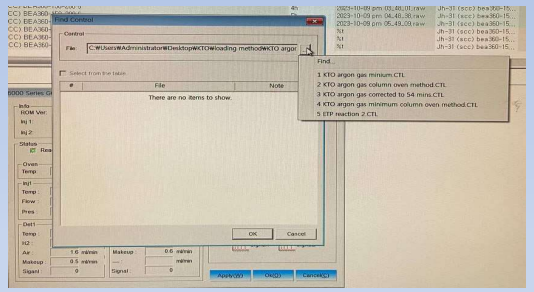
Inner thermocouple (Tube)

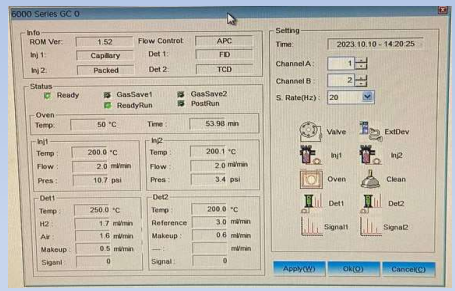
Working with program Autochro-3000 (chromatograph data system)

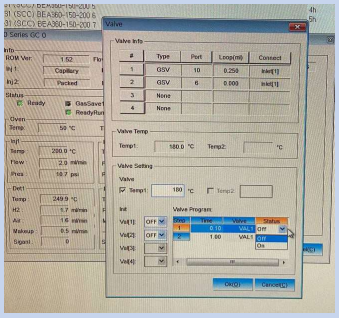
- System → Load control → Oven method →OK Apply that process. We check the H2 and Air
- Starting the oven(heating and process cycle, Autoignition and Electrometer are automatically turned on)
- Valve → Off →On Flament-Off → On
- We open the N2 flow so it adsorb into dodecane and catalysis
- When experiment starts I run the program that record all the data

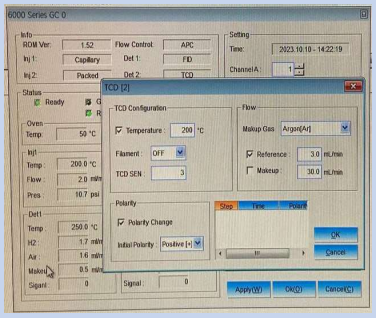


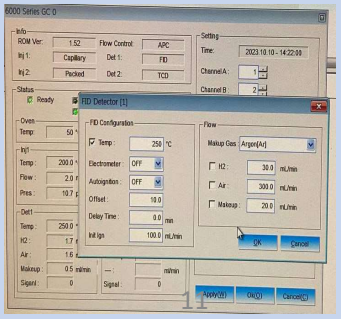












Importance of AI in my work

The AI role in my research work

- Generally I spend 3 days, 2 days to make experiment and 1 day to check the final materials. I use 3 programs in my research work.

Autochro-3000	(chromatograph data system)
AND	(to monitor weight change)
Puna	(Analysing the cracked molecules)

It is essential that I must write down all the details from the machine (e.g. the temperature and the weights of substances at the exact time).

If I make a mistake like to be late even 1 min can affect the final result and we may not know the exact process.

Why we should use AI more in chemical chromatography

- AI reduces huge amount of time and money related to problem.
- Powerful computing hardware can give us huge opportunity to learn and monitor multiple experiments at the same time thanks to AI.
- Another area where AI can be beneficial in chromatography analysis is in the development of automated systems that can optimise the chromatography process. AI can also be used to monitor and control the chromatography process in real-time, making adjustments to the conditions as needed to ensure optimal performance.
- It reduces the risk of human error

Future work

According to reduce the time and money for that experiment we have to make the program can do experiment.

- In our chemical experiment we do only 40% work by hand other 60% of it is done by computer programs and chromatography machines. However even that 40% work takes significantly more time and effort and it is not safe too.

- Solution
- Chemical Simulation Software- it is based on **prediction of materials properties.** It can support **chemical reaction optimization too.**

THANK YOU FOR LISTENING