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Treatment of BTEX from Water Produced with a SCWR using UniSim Design
Overview

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Introduction

• This research aims to treat contaminated water with BTEX, reacting hydrocarbons with oxygen present in abundance in the atmospheric air, it will occur the conversion of these compounds into carbon dioxide and water, through a reactor SCWR(Supercritical Water Reactor).
• To accomplish this aim it will be done a steady state simulation and a dynamic simulation using the tool UniSim Design R430.
• And besides treating the water it is possible to generate energy and heat to feed the process itself.
• To improve and study the performance of the plant it will be used a PID controller.
Summary

- Poluted Water Produced of Petroleum with BTEX
- Larger quantity produced

Problem

Proposed Solution

- Reaction of BTEX with oxygen from atmospheric air in a SCWR

Simulation

- Steady state simulation
- Dynamic simulation (using PID regulators)

Conclusion

- Reclyce of energy
- Treated and clean water
Produced Water of Petroleum

• Formation water
  – Naturally present in water geological oil reservoir and in injected water;

• Comes from the injection of water into the reservoir in order to increase the production;

Its production is inevitable!
Produced Water of Petroleum

• There are many different levels of pollution and toxicity, it depends of the geography and the location soil;

• The global production onshore and offshore of water is about 290 million barrels per day, compared to approximately 90 million barrels of oil. These values represent a ratio of 3:1 or nearly 70% in volume of water produced.

A serious concern!
The BTEX compounds

• The compounds that causes more concern regarding its disposal in the environment are benzene, toluene, ethylbenzene and xylenes (BTEX);
• They are often the most abundant in the produced water;
• The water when contaminated by BTEX compounds are extremely toxic to the environment and to humans.
• Although through the use of the right technology, it is possible to treat the water produced for different reuses, including for human consumption.

A global environmental concern!
Brazilian context

• In Brazil there are many petroleum exploration fields (onshore and offshore), with a total oil supply of 2.7 million barrels per day, nearly 3% of the global oil production;

• It is of great importance the treatment of produced water, given that the oil sector tends to grow in the country, as well as oil production and water produced.

A global environmental concern!
Supercritical Water Reactor (SCWR)

Generation of energy for the process itself!
Supercritical Water Reactor (SCWR)

Minimal operating conditions of the SCWR:

- Supercritical Temperature of water = 374 °C
- Supercritical Pressure of water = 22 MPa

Operating conditions of the SCWR (in Steady State Simulation):

- Temperature before the reactor = 1200 °C
- Temperature in and after the reactor = 1500 °C
- Pressure = 22 MPa
The following reactions occur in the SCWR:

- **Benzene**: \( 2 \text{C}_6\text{H}_6 + 15 \text{O}_2 \rightarrow 12 \text{CO}_2 + 6 \text{H}_2\text{O} \)

- **Toluene**: \( \text{C}_7\text{H}_8 + 9 \text{O}_2 \rightarrow 7 \text{CO}_2 + 4 \text{H}_2\text{O} \)

- **Etil-benzene**: \( 2 \text{C}_8\text{H}_{10} + 21 \text{O}_2 \rightarrow 16 \text{CO}_2 + 10 \text{H}_2\text{O} \)

- **Xilene**: \( 2 \text{C}_8\text{H}_{10} + 21 \text{O}_2 \rightarrow 16 \text{CO}_2 + 10 \text{H}_2\text{O} \)
Simulation components

- The flowsheet is composed of the following components:
Simulation components

- Compressor
  - PW2
  - PW3
  - K-100
  - WC1
  - Air1
  - Air2
  - WC2
  - K-101

- Product
  - VLV-Product
  - Product-1

- TIC-100
- XIC-100

- SET-1
- ADJ-1
- V1
- VLV-V1
- V1-1
Steady State Simulation

Diagram showing flow between various components labeled as E-101, K-100, K-102, V2, V1, V3, V4, PW1, PW2, PW3, Q2, WC1, WC2, SET-1, ADJ-1, WT, and GBR-100, with arrows indicating the direction of flow.

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Dynamic State Simulation

PID Regulation
Stripchart (PID regulation)

Temperature in the reactor

OP : bleu
SP : red
PV : green
PID Regulation

Measure the temperature in the reactor outlet flow

NO

Temperature > 1550 °C

YES

Increase the withdrawal of energy in the reactor

Decrease the temperature in the reactor

Decrease the withdrawal of energy in the reactor

Increase the temperature in the reactor

Temperature in the reactor
Stripchart (PID regulation)

Conversion of oxygen in the reactor

OP : bleu
SP : red
PV : green
Measure the concentration of oxygen in the reactor outlet

- **NO**
  - Decrease the air flow at the entrance of the reactor
  - Decrease the conversion of oxygen in the reactor

- **YES**
  - Increase the air flow at the entrance of the reactor
  - Increase the conversion of oxygen in the reactor

**Conversion of oxygen in the reactor**
Results and Discussion

• It was possible to convert all the BTEX compounds;
• We can generate energy with the turbine to feed the process itself, by feeding one of the compressors;
• The temperature reached in the reactor is high, but it is possible to decrease it using a heat exchanger after the two compressors and at the same time it is possible to use this heat for another industrial process;
• It is a clean process, as it is used the oxygen present in the air atmospheric as reagent and we do not generate pollutants;
• The water produced of petroleum can now be discarded into the sea without causing any damage to the environment or to humans.
References

• U.S. Energy Information Administration (US EIA)


• https://www.gen-4.org/gif/jcms/c_9360/scwr

• http://www.sci-news.com/