Case Study

Toluene Methanolation

Version 1, July 2024, SCION Instruments

Toluene Methanolation - Catalytic Applications with Gas Chromatography

Toluene methanolation is a catalytic process aimed at transforming toluene ($C_6H_5CH_3$) into methylbenzene ($C_6H_4CH_3OH$) by adding methanol (CH_3OH). This reaction holds industrial significance due to methylbenzene's versatility as a chemical intermediate in the production of solvents, adhesives, and pharmaceuticals. Continuous monitoring and optimization of toluene methanolation are crucial for maximizing product yield and minimizing energy consumption. Gas Chromatography is an effective analytical technique for online analysis, enabling real-time measurement of reaction dynamics and product formation.

Online Analysis in Toluene Methanolation

Gas Chromatography can be used for online analysis to continuously monitor concentrations of toluene, methylbenzene, methanol, and other gas-phase species present in the reactor effluent. Automated sampling systems collect periodic samples from the reaction mixture, which are then injected into the GC system for separation and detection. Advanced techniques such as GC-MS may be employed for enhanced specificity and identification of trace components, aiding in comprehensive analysis of reaction intermediates and by-products.

Applications and Benefits:

Real-time Monitoring:

- Enables continuous tracking of reaction kinetics and product distributions, facilitating rapid adjustment of reaction parameters for optimal performance.

Quantitative Analysis:

- Provides accurate quantification of methylbenzene yield, toluene conversion efficiency, and methanol utilization, crucial for optimizing catalyst design and process conditions.

Catalyst Evaluation:

- Evaluates catalyst stability and performance under dynamic reaction conditions, aiding in the development of efficient CO_2 methanation catalysts.

Process Control:

- Facilitates fine-tuning of operational parameters such as temperature, pressure, and feed composition to maximize methane yield and minimize energy consumption.

Customer Case Example

In the following example, SCION Instruments worked with our customer to provide a Gas Chromatography based analytical tool for online monitoring and analysis of CO_2 methanation processes. By leveraging the SCION GC's capabilities, it is possible to optimize reaction conditions, enhance catalyst performance, and improve overall process efficiency.

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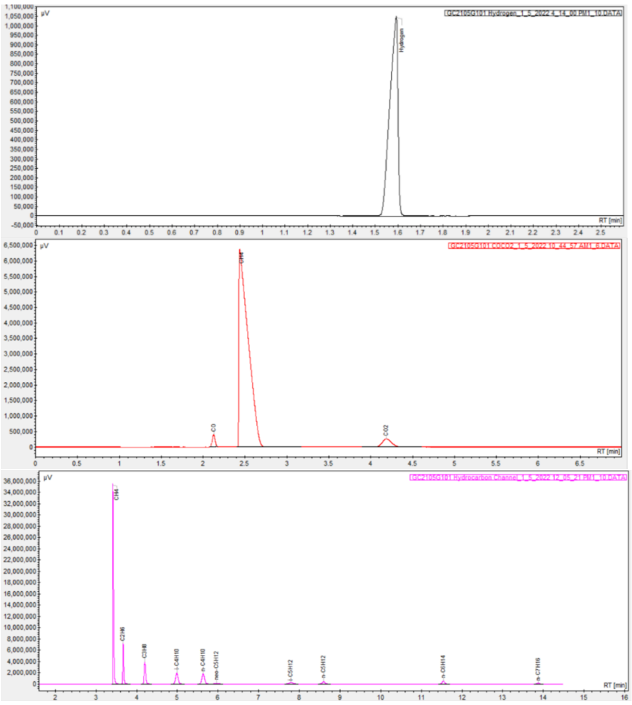
Method

The SCION GC is used to perform online analysis of the methanation reaction. The quantification of H_2 will be done on a first TCD. A second TCD will be dedicated to the reaction gases (CO_2, CO, CH_4). An FID will be used for the analysis of organic products from potential side reactions (light hydrocarbon, light alcohol, formic acid).

The results obtained from the SCION GC analysis provide the total areas of each constituent. These total areas serve as quantitative measures of the amounts of each compound produced during the reaction.

By comparing the total areas of the starting material (CO_2 and H_2) with those of the desired product (CH_4) and any undesired by-products, they can calculate subsequently the conversion, selectivity, and turnover frequency of the reaction.

These calculations provide valuable insights into the efficiency and performance of the catalyst system, allowing for optimization and improvement of the reaction conditions to enhance product yield and selectivity.



System Configuration

CO2 Methanation :

SCION 8500-GC 3 channels

1st channel : GSV, two columns Molsieve 5A & Hayesep Q and TCD à H2 determination

2nd channel : GSV, two columns Porapak R and TCD à CO, CH4 and CO2 determination

3rd channel : GSV, column apolar SCION-1 and FID à hydrocarbons determination

Software : CompassCDS