Case Study

Toluene hydrogenation

Version 1, June 2024, SCION Instruments



Toluene hydrogenation - Catalytic Applications with Gas Chromatography

Toluene hydrogenation is pivotal for producing methylcyclohexane ($C_6H_{11}CH_3$), which serves as a hydrogen carrier and precursor in various industrial applications. The process involves reacting toluene ($C_6H_5CH_3$) with hydrogen over a suitable catalyst under specific temperature and pressure conditions. Continuous monitoring of toluene hydrogenation is essential for optimizing catalyst performance, maximizing product yield, and minimizing energy consumption. Gas Chromatography (GC) has emerged as a reliable technique for real-time analysis, offering precise measurement of reaction intermediates and byproducts.

Online Analysis in Toluene Hydrogenation:

Gas Chromatography can be used for online analysis to continuously monitor concentrations of toluene, methylcyclohexane, hydrogen, and potentially other gas-phase species such as methane and ethane. Automated sampling systems collect reactor effluent samples at regular intervals, which are then injected into the GC system for separation and detection. Advanced techniques like GC-MS may be utilized for enhanced specificity and identification of trace components, supporting comprehensive analysis of reaction kinetics and catalyst performance.

Toluene Hydrogenation Applications and Benefits:

Real-time Monitoring:

• Enables continuous tracking of reaction progress and product distribution, facilitating prompt adjustments to reaction conditions for optimal performance.

Quantitative Analysis:

• Provides accurate measurement of toluene conversion, methylcyclohexane yield, and hydrogen utilization efficiency, crucial for optimizing catalyst activity and selectivity. Catalyst Evaluation:

• Evaluates catalyst stability and effectiveness under dynamic reaction conditions, supporting the development of robust catalyst systems for industrialscale applications.

Process Optimization:

• Facilitates fine-tuning of operational parameters such as temperature, pressure, and feed composition to maximize methylcyclohexane production while minimizing environmental impact and energy consumption.

Toluene Hydrogenation Customer Case Example

The following real-life case studies and practical insights illustrate how Gas Chromatography solutions from SCION Instruments can be leveraged to enhance the efficiency, selectivity, and sustainability of catalytic processes. Whether you are a researcher, a process engineer, or an industry professional, you will gain valuable knowledge to advance your understanding and application of catalysts using gas chromatography.

In the following example, SCION Instruments worked with our customer to provide a Gas Chromatography solution to improve the efficiency and effectiveness of the toluene hydrogenation processes through real-time monitoring and analysis. By leveraging the SCION GC's capabilities, it is possible to optimize catalyst design, improve process efficiency, and advance sustainable practices in chemical synthesis and energy storage.



Case Study

Toluene hydrogenation

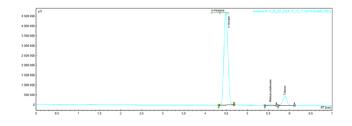
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Method

During the reaction period lasting from 1 to 3 minutes, the reactor effluent is sampled every 30 seconds using a multi-position Valco valve and then subjected to analysis by a SCION GC equipped with an FID detector. The GC analysis yields total area values for each constituent present in the reactor effluent, including toluene, methylcyclohexane, and n-hexane. These total areas serve as quantitative measures indicating the quantities of each compound generated during the reaction.

By comparing the total areas of the initial substance (toluene) with those of the desired product (methylcyclohexane) and any unwanted by-products (nhexane), researchers subsequently calculate the conversion rate, selectivity, and turnover frequency of the reaction. These calculations offer valuable insights into the efficiency and performance of the catalyst system, enabling the optimization of reaction conditions to enhance both product yield and selectivity.



Toluene hydrogenation method

System Configuration

During the reaction period

Toluene hydrogenation :

SCION 8500-GC 2 channels

10 loops selecting valve, GSV, S/SL injector, column Rtx-1 (equivalent to SCION-1), selecting valve GSV, two columns Alumina/Na2SO4 & Rtx-1 and two FID à hydrocarbons determination

Software : CompassCDS