SCION INSTRUMENTS
A Techcomp Company

CATALYTIC APPLICATIONS

ENHANCING CATALYTIC APPLICATIONS
WITH GAS CHROMATOGRAPHY

INTRODUCTION

IN THE RAPIDLY ADVANCING FIELD OF CHEMISTRY, CATALYSTS PLAY A PIVOTAL ROLE IN ACCELERATING CHEMICAL REACTIONS, THEREBY MAKING PROCESSES MORE EFFICIENT AND ENVIRONMENTALLY FRIENDLY.

Gas Chromatography (GC) is emerging as a critical analytical tool that significantly enhances the study and application of catalytic processes.

CATALYTIC APPLICATIONS

CATALYSTS ARE INDISPENSABLE IN VARIOUS INDUSTRIAL APPLICATIONS, INCLUDING PETROCHEMICALS, PHARMACEUTICALS, AND ENVIRONMENTAL MANAGEMENT.

Their ability to increase reaction rates without being consumed in the process makes them invaluable for sustainable and cost-effective production. However, understanding and optimizing catalytic reactions require precise and detailed analysis, where gas chromatography proves to be indispensable.

Gas chromatography allows chemists to separate, identify, and quantify components within a complex mixture, providing unparalleled insights into reaction mechanisms and product distributions. This analytical technique operates by vaporizing a sample and passing it through a chromatographic column, where different compounds are separated based on their interactions with the column's stationary phase.

By coupling GC with detectors such as mass spectrometry (GC-MS), chemists can achieve a high level of specificity and sensitivity in analyzing catalytic reactions.

In this brochure, we will explain the synergistic relationship between gas chromatography and catalytic applications.

Case Studies

Through real-life case studies and practical insights, we will illustrate how Gas Chromatography 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.

Discover the transformative potential of gas chromatography in pushing the boundaries of chemical research and industrial innovation.

KEY BENEFITS

GAS CHROMATOGRAPHY (GC) IS A POWERFUL ANALYTICAL TOOL THAT PROVIDES NUMEROUS BENEFITS WHEN APPLIED TO THE STUDY AND OPTIMIZATION OF CATALYTIC PROCESSES.

Here a some of the key advantages of integrating GC into catalytic applications, demonstrating its value across various industries and research domains:

Precision and Accuracy:

- GC offers exceptional precision and accuracy in separating and quantifying complex mixtures. This capability is crucial for understanding the performance and efficiency of catalysts, allowing for detailed analysis of reaction intermediates and products.

Real-Time Monitoring:

- One of the significant advantages of GC is its ability to provide real-time monitoring of catalytic reactions. This enables researchers and engineers to observe the progress of reactions as they occur, facilitating immediate adjustments and optimizations to improve yield and selectivity.

Enhanced Catalyst Design:

- By using GC to analyze the effects of different catalysts under various conditions, scientists can design catalysts with improved properties. This includes enhancing the activity, selectivity, and stability of catalysts, leading to more efficient and cost-effective chemical processes.

Environmental Benefits:

- GC aids in the development of greener catalytic processes by identifying and quantifying harmful by-products and emissions. This supports the creation of environmentally friendly technologies that reduce the ecological footprint of industrial activities.

Versatility and Adaptability:

- GC is highly versatile and can be adapted to a wide range of applications, from petrochemicals and pharmaceuticals to environmental analysis. This flexibility makes it an indispensable tool for researchers working on diverse catalytic systems.

Detailed Mechanistic Insights:

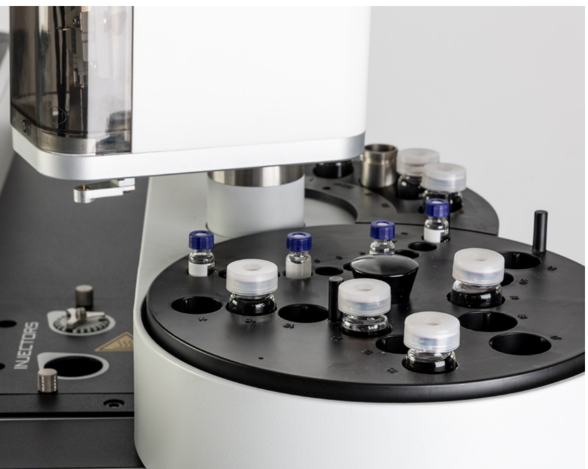
- GC provides detailed mechanistic insights into catalytic processes by identifying reaction pathways and intermediates. This information is vital for understanding how catalysts work at a molecular level and for developing new and improved catalytic materials.

Improved Process Efficiency:

- By enabling precise control and optimization of catalytic reactions, GC helps improve overall process efficiency. This leads to reduced costs and increased productivity in industrial applications, making processes more economically viable.

High Sensitivity and Specificity:

- GC, especially when coupled with mass spectrometry (GC-MS), offers high sensitivity and specificity. This allows for the detection and quantification of trace components, which is essential for fine-tuning catalytic reactions and ensuring product purity.



The integration of gas chromatography in catalytic applications provides a multitude of benefits that enhance research capabilities, environmental sustainability, and industrial efficiency.

This synergy between GC and catalysis paves the way for innovative solutions and advancements in chemical processes.

INDUSTRIES AND APPLICATIONS

GAS CHROMATOGRAPHY (GC) IS AN INVALUABLE TOOL IN ENHANCING THE APPLICATIONS OF CATALYSTS ACROSS VARIOUS INDUSTRIES AND RESEARCH DOMAINS.

Here, we outline key applications where GC plays a pivotal role in optimizing and advancing catalytic processes:

Petrochemical Industry:

- In the petrochemical sector, GC is extensively used to analyze and optimize catalytic cracking and reforming processes. It helps in identifying and quantifying hydrocarbons and other by-products, ensuring that catalysts are performing efficiently and selectively. This leads to improved yields of desired products such as gasoline and other fuels, while minimizing unwanted by-products.

Pharmaceuticals:

- The pharmaceutical industry benefits greatly from the use of GC in the synthesis of active pharmaceutical ingredients (APIs). Catalysts are often used to facilitate complex chemical reactions, and GC allows for precise monitoring of these reactions. This ensures the purity of the final product and helps in the optimization of reaction conditions, reducing costs and improving overall efficiency.

Environmental Analysis:

- GC is crucial in developing catalysts for environmental applications, such as pollution control and the reduction of greenhouse gas emissions. It is used to monitor the effectiveness of catalytic converters in vehicles and industrial processes. By analyzing emissions and by-products, researchers can develop more effective catalysts that reduce harmful pollutants.

Renewable Energy:

- In the field of renewable energy, GC is used to enhance the development of catalysts for processes such as biomass conversion and hydrogen production. For example, GC helps in analyzing the composition of bio-oils and syngas produced from biomass, enabling the optimization of catalysts that convert these materials into renewable fuels and chemicals.

Food and Beverage Industry:

- The food and beverage industry uses GC to ensure the safety and quality of products by analyzing flavor compounds and contaminants. Catalysts are often employed in the production of food additives and preservatives, and GC helps in monitoring these catalytic processes to ensure they are efficient and produce high-quality outcomes.

Materials Science:

- In materials science, GC is used to study and develop catalysts for the synthesis of advanced materials such as polymers and nanomaterials. By analyzing the intermediates and products of catalytic reactions, researchers can fine-tune the properties of materials, leading to innovations in various applications, including electronics, coatings, and biomedical devices.

Academic Research:

- In academic settings, GC is an essential tool for studying fundamental aspects of catalysis. It allows researchers to explore reaction mechanisms, identify transient species, and develop new catalytic materials. This foundational research drives innovations and applications across multiple industries.

By integrating gas chromatography into catalytic applications, researchers and industries can achieve more efficient, sustainable, and cost-effective processes.

The precision, versatility, and real-time monitoring capabilities of GC make it an indispensable tool in advancing the field of catalysis.

CASE STUDIES

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.

Toluene hydrogenation

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 by-products.

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.

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 industrial-scale 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.

Customer Case Example

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.

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 (n-hexane), 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.

System Configuration

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/Na_2SO_4 & Rtx-1 and two FID ➔ hydrocarbons determination

Software:

- CompassCDS

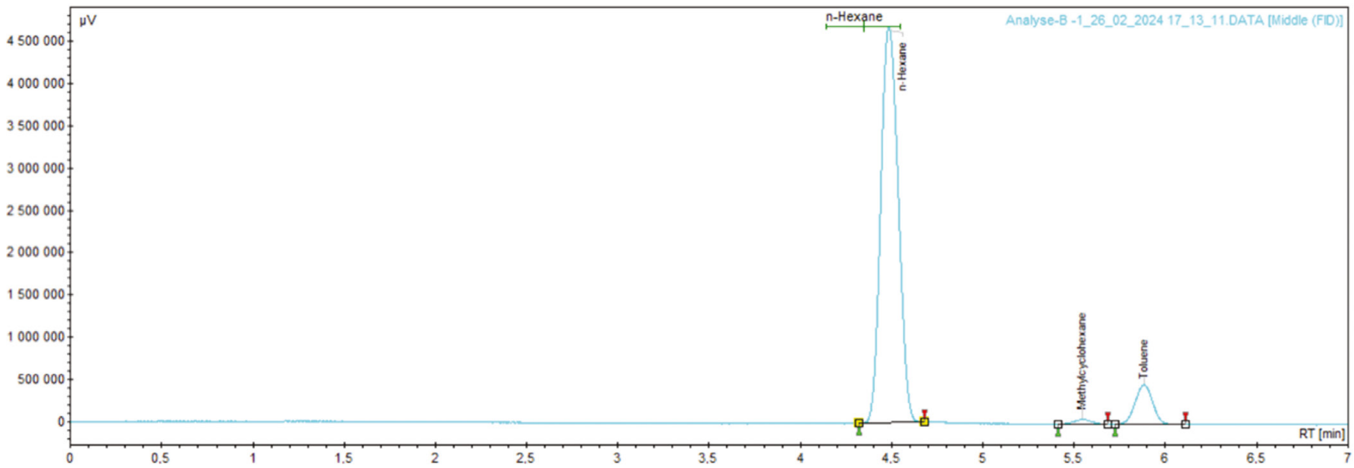


Figure 1: Example chromatogram of an n-hexane, methylcyclohexane and toluene standard

CASE STUDIES

CO_2 Methanation

Carbon dioxide (CO_2) methanation represents a promising approach towards mitigating greenhouse gas emissions by converting CO_2 into methane (CH_4), a valuable energy carrier and precursor for various industrial processes. This chemical transformation involves complex interactions between CO_2, hydrogen (H_2), and catalyst materials under specific temperature and pressure conditions. Monitoring the progress of CO_2 methanation in real-time is critical for optimizing reaction parameters, improving catalyst performance, and maximizing methane production efficiency. Gas Chromatography (GC) has become indispensable in this regard, offering precise and sensitive analysis of gas-phase components present in the reaction mixture.

Online Analysis in CO_2 Methanation

Gas Chromatography can be used for online analysis to continuously monitor the concentrations of CO_2, CH_4, H_2, and potentially other gas-phase species such as water vapor (H_2O) and carbon monoxide (CO). The setup typically involves sampling the reactor effluent at regular intervals using an automated sampling system, followed by injection into the GC system for separation and detection. Advanced techniques such as multi-dimensional GC or GC coupled with mass spectrometry (GC-MS) may also be utilized for enhanced separation and identification of trace components.

Applications and Benefits:

Real-time Monitoring:

- Enables continuous measurement of reaction kinetics and product distributions, facilitating immediate adjustments to reaction conditions.

QuantitativeAnalysis:

- Provides accurate quantification of CO_2 conversion, methane selectivity, and other reaction parameters crucial for process optimization.

Catalyst Evaluation:

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

ProcessControl:

- 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.

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

CO_2 Methanation:

SCION 8500-GC 3 channels

- 1st channel: GSV, two columns Molsieve 5A & Hayesep Q and TCD ➔ H_2 determination
- 2nd channel: GSV, two columns Porapak R and TCD ➔ CO, CH4 and CO2 determination
- 3rd channel: GSV, column apolar SCION-1 and FID ➔ hydrocarbons determination

Software:

- CompassCDS

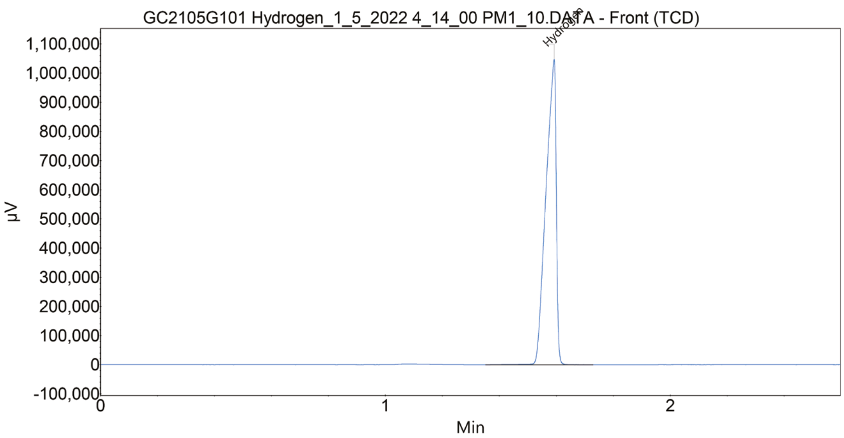


Figure 2: Example chromatogram from the 1st channel (TCD) showing a hydrogen standard

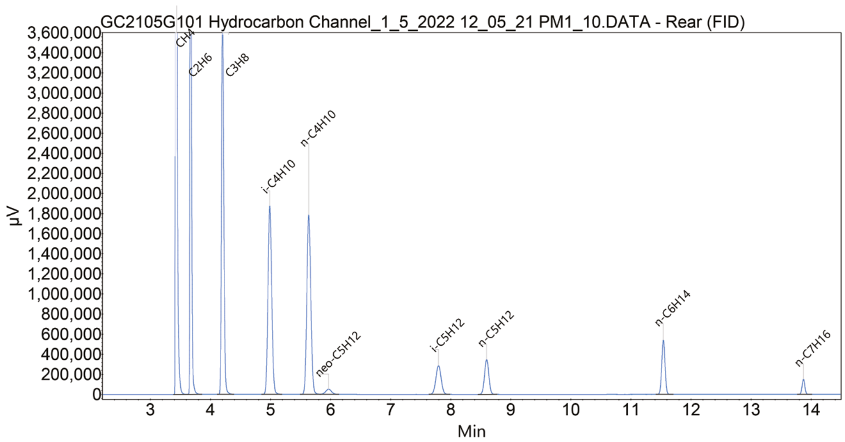


Figure 3: Example chromatogram from the 3rd channel (FID) showing a mixed hydrocarbon standard

CASE STUDIES

Propane Aromatization

Propane aromatization plays a pivotal role in the petrochemical industry by converting light alkanes such as propane into aromatic hydrocarbons like benzene, toluene, and xylenes (BTX). These aromatics are essential precursors for polymers, plastics, and high-octane fuels. The process typically involves heterogeneous catalysis under specific temperature and pressure conditions to achieve high yields of aromatics while minimizing unwanted by-products. Evaluating catalyst performance is critical for enhancing process efficiency and economic viability. Gas Chromatography has emerged as a versatile technique for real-time analysis of reaction products, enabling precise measurement of catalyst effectiveness and product distribution.

Gas Chromatography for Catalyst Evaluation

In propane aromatization studies, Gas Chromatography is employed to analyze the effluent from the reactor where propane is converted into aromatic hydrocarbons. The GC system is equipped with appropriate detectors to monitor the presence and concentration of benzene, toluene, xylenes, and other relevant compounds. Samples are typically collected periodically during the reaction to assess changes in product distribution and catalyst performance over time. Advanced GC techniques such as temperature-programmed desorption (TPD-GC) or GC coupled with mass spectrometry (GC-MS) may be utilized for detailed characterization of reaction intermediates and by-products.

Applications and Benefits

Quantitative Analysis:

- Provides accurate measurement of aromatic hydrocarbon yields and selectivity, essential for comparing catalyst performance.

Reaction Kinetics:

- Enables real-time monitoring of reaction kinetics, identifying optimal reaction conditions for maximizing BTX production.

Catalyst Stability:

- Evaluates catalyst stability and resistance to deactivation mechanisms such as coke formation or metal leaching.

Process Optimization:

- Facilitates adjustments in catalyst design and operating parameters to enhance overall process efficiency and economic viability.

Customer Case Example

In the following example, SCION Instruments worked with our customer to provide a Gas Chromatography based analytical tool for evaluating catalysts in propane aromatization, offering insights into reaction kinetics, product distribution, and catalyst stability. By leveraging the SCION GC's capabilities, it is possible to optimize catalyst design and reaction conditions to achieve higher yields of aromatic hydrocarbons while minimizing energy consumption and environmental impact.

Method

The reactor effluent is collected and sampled at 1, 4, 8, 12, 16, 20, 30, 40, 50 and 60 minutes, using a multi-position Valco valve and then is analyzed into GC-FID. During sampling in the 10-port valve loops, the TCD continuously analyzes the quantities of hydrogen and methane.

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 (propane) with those of the desired product (benzene, toluene) 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

Propane Aromatization:

SCION 8500-GC 2 channels

- 1st channel: GSV, two columns Shincarbon ST & Hayesep Q (backflush) and TCD ➔ H2 & methane determination
- 2nd channel: 10 loops selecting valve, GSV, S/SL injector, column SCION-DHA and FID ➔ hydrocarbons determination

Software:

- CompassCDS

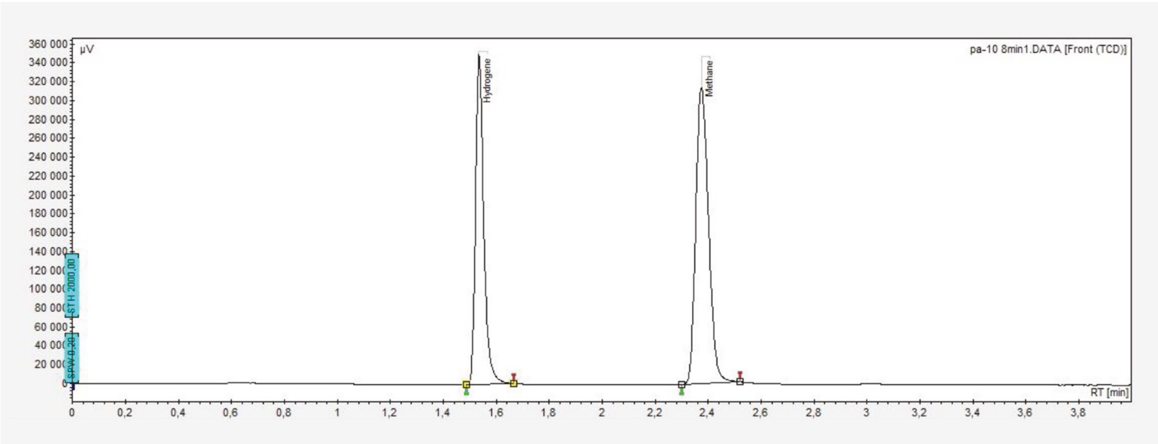


Figure 4: Example chromatogram from the 1st channel (TCD) showing a hydrogen and methane standard

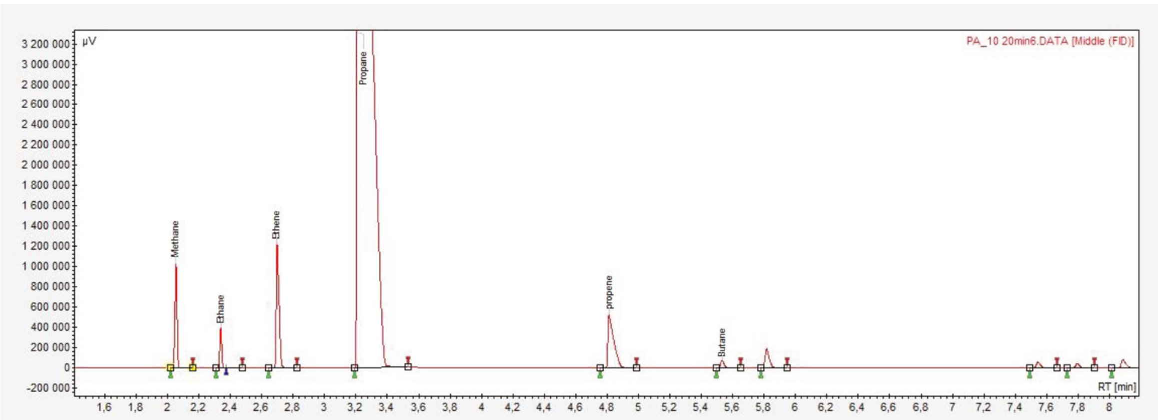


Figure 5: Example chromatogram from the 2nd channel (FID) showing a mixed hydrocarbon standard

CASE STUDIES

Ammonia Synthesis

Ammonia synthesis, discovered by Fritz Haber and Carl Bosch in the early 20th century, revolutionized agricultural productivity and industrial chemistry. The process involves the reaction of nitrogen (N_2) and hydrogen (H_2) over an iron-based catalyst at high temperature and pressure conditions. Continuous monitoring of ammonia synthesis is crucial for maintaining optimal reaction conditions, maximizing yield, and minimizing energy consumption. Gas Chromatography has emerged as a versatile analytical technique for real-time analysis of reaction products and by-products, offering insights into catalyst performance and process efficiency.

Online Analysis in Ammonia Synthesis

Gas Chromatography can be used for online analysis to continuously monitor the concentrations of ammonia, nitrogen, hydrogen, and potentially other gas-phase species such as nitrogen oxides (NOx) and methane (CH_4). Samples are typically withdrawn from the reactor effluent at regular intervals using an automated sampling system and injected into the GC system for separation and detection. Advanced techniques like GC coupled with mass spectrometry (GC-MS) may be employed for enhanced specificity and identification of trace components.

Applications and Benefits

Real-time Monitoring:

- Enables continuous measurement of reaction kinetics and product distributions, facilitating immediate adjustments to reaction conditions for optimal performance.

Quantitative Analysis:

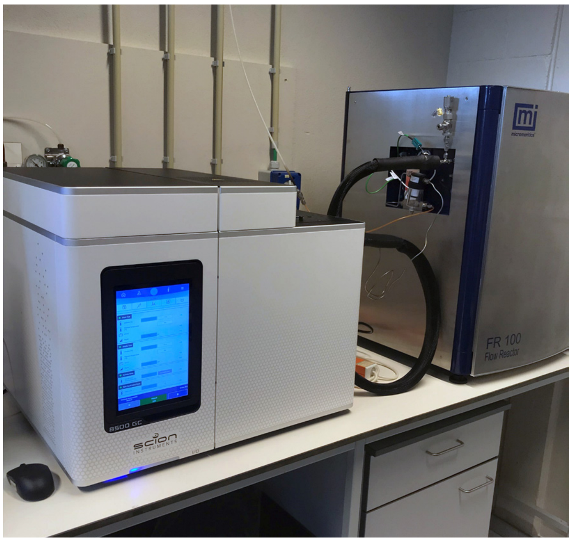
- Provides accurate quantification of ammonia yield, nitrogen conversion, and hydrogen utilization efficiency, essential for process optimization.

Catalyst Evaluation:

- Evaluates catalyst activity, selectivity, and stability under dynamic reaction conditions, aiding in the development of robust catalyst systems.

Process Control:

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



Customer Case Example

In the following example, SCION Instruments worked with our customer to provide a Gas Chromatography based analytical tool for online analysis during ammonia synthesis, offering real-time insights into reaction kinetics, product distribution, and catalyst performance.

By leveraging the SCION GC's capabilities, it is possible to optimize catalyst design, improve reaction efficiency, and advance sustainable practices in ammonia production.

Method

The SCION GC is used to perform online analysis of the ammonia synthesis. The quantification of H_2, N_2 will be done on a first TCD and ammonia on a second TCD.

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 (N_2 and H_2) with those of the desired product (NH_3) 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

Ammonia Synthesis:

SCION 8500-GC 2 channels

- 1st channel : GSV, two columns Molsieve 5A & Hayesep Q and TCD ➔ H_2 & N_2 determination
- 2nd channel : GSV, column Hayesep Q and TCD ➔ NH_3 determination

Software:

- CompassCDS

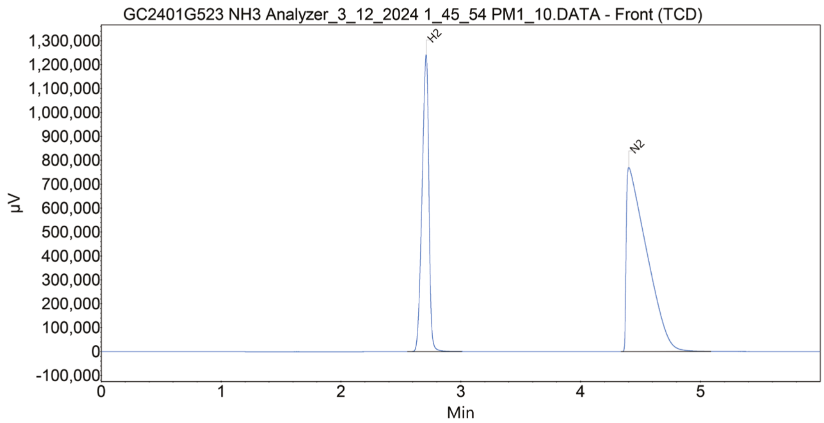


Figure 6: Example chromatogram from the 1st channel (TCD) showing a hydrogen and nitrogen standard

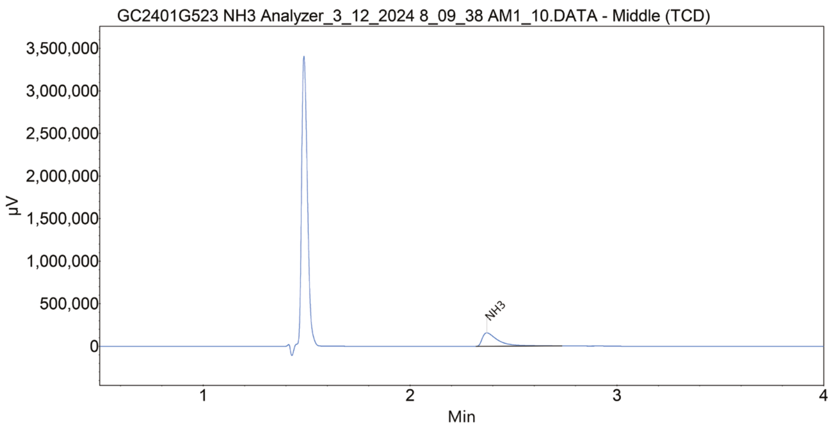


Figure 7: Example chromatogram from the 2nd channel (TCD) showing an ammonia standard

CASE STUDIES

Toluene Methanolation

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:

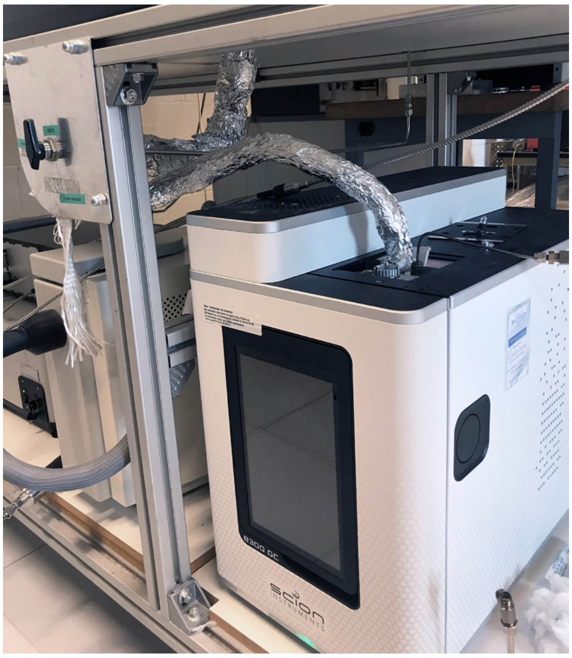
- Provides accurate quantification of methylbenzene yield, toluene conversion efficiency, and methanol utilization, crucial for optimizing catalyst design and process conditions.

Catalyst Evaluation:

- Evaluates catalyst activity, selectivity towards desired products, and resistance to deactivation mechanisms, supporting the development of efficient catalytic systems.

Process Optimization:

- Facilitates fine-tuning of operational variables such as temperature, pressure, and catalyst composition to maximize methylbenzene production while minimizing environmental impact and 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 analysis during the toluene methanolation processes, offering real-time insights into reaction dynamics, product distribution, and catalyst performance.

By leveraging the SCION GC's capabilities, it is possible to optimize reaction conditions, enhance catalyst efficiency, and advance sustainable practices in chemical synthesis.

Method

The SCION GC is used to perform online analysis of the toluene methanolation. The quantification of toluene, methanol and xylene isomers will be done on a FID.

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 (toluene and methanol) with those of the desired product (xylene isomers) 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

Toluene Methanolation:

SCION 8300-GC

- GSV, S/SL injector, column S-WAX and FID ➔ methanol, toluene & xylenes determination

Software:

- CompassCDS

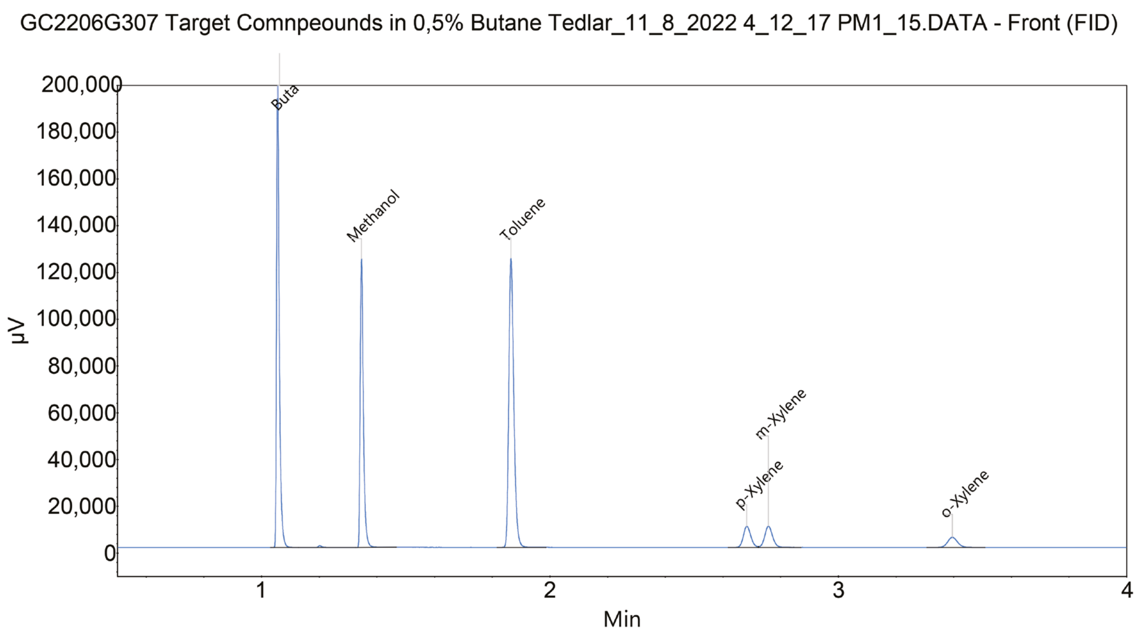


Figure 8: Example chromatogram (FID) showing a mixed standard containing butane, methanol, toluene and xylenes

CONTACT OUR TEAM

Explore the limitless possibilities of Gas Chromatography in catalytic applications.

Contact us to learn more about how Gas Instruments can revolutionize your processes and accelerate innovation in your industry.

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