MECHANISM OF HYDROCARBON PRODUCTION FROM SYNTHESIS GAS ON THE SURFACE OF A HIGHLY DISPERSED IRON CATALYST

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Abstract. This article studies the mechanism of hydrocarbon production from synthesis gas in the presence of a highly dispersed iron catalyst. The study analyzes the main stages of Fischer-Tropsch synthesis, the activity of the iron catalyst, the influence of carbonyl and carbide phases. Experimental and theoretical results allow us to explain the mechanism of the process of formation of high molecular weight hydrocarbons from synthesis gas. The results of the study are important for creating effective catalysts in the production of alternative fuels and chemical raw materials.

Keywords: synthesis gas, highly dispersed iron catalyst, Fischer-Tropsch synthesis, hydrocarbons, catalytic activity, carbide phase, reaction mechanism.

Synthesis gas ($CO + H_2$) is an important raw material in the chemical and energy sectors, from which hydrocarbons, liquid fuels and other chemical products are obtained. Fischer-Tropsch synthesis (FTS) is one of the main technologies of this process and places high demands on catalysts. Iron-based catalysts are particularly relevant due to their low cost and flexibility. This article will examine in detail the role of highly dispersed iron catalysts in the FTS process and the mechanism of hydrocarbon formation.

Disperse systems are heterogeneous systems consisting of widely distributed small particles of two or more phases. Typically, one of the phases forms a continuous dispersion medium, and the other phases are evenly distributed in this medium in the form of small crystals, solid amorphous particles, droplets or bubbles. A disperse can also have a complex structure, an example of which is a system consisting of two phases that are absorbed into each other's volume, which can form a continuous dispersion medium.

Disperses are divided into two groups depending on the size of the particles:

1) coarse, with dispersed phase particles 1 μm and larger;

2) colloidal systems with dispersed phase particles from 1 nm to 1 μm. Systems consisting of particles of the dispersed phase with a size equal to atoms and small molecules up to 1 nm constitute true solutions. The physicochemical properties of the disperse depend on the intermolecular bonds between the dispersed phase and the dispersion medium and the surface area formed between them. The properties of the dispersion are studied in colloidal chemistry.

Iron oxide is the raw material for active iron metal catalysts. Usually, metals and their oxides can catalyze the reaction, but metals have higher activity and selectivity. To prevent iron oxide from becoming an intermediate product that is unsuitable as a catalyst at high temperatures or in the presence of H2, it can be converted into iron by pre-treatment before thermal reduction.

Iron oxide catalysts have a sufficient selectivity. In order to effectively change the direction of the reaction, many companies have developed mixed catalysts. For example, the catalyst for the gas-phase oxidation of alcohols to aldehydes and ketones is a mixed catalyst of iron oxides.

Evaluation of iron oxide catalyst: testing its macroscopic physical properties and microstructure. Macroscopic physical properties include catalyst density, geometric shape and size, mechanical strength, etc. Microstructure and physicochemical properties mainly include the chemical composition, phase structure, dispersion, valence, and oxidation-reduction properties of the catalyst body and surface.

Iron catalysts play an important role in the conversion of synthesis gas into hydrocarbons. The activity and selectivity of these catalysts depend on the following:

- Dispersion level - highly dispersed iron particles have a large surface area, creating favorable conditions for the reaction.
- Carbide phases - phases such as Fe_5C_2 and Fe_3C are actively involved in the formation of hydrocarbons.
- Auxiliary components - the addition of substances such as K, Cu, SiO_2 increases the activity of the catalyst.

Synthesis gas is converted into hydrocarbons on the surface of the iron catalyst through the following stages:

- Adsorption - CO and H_2 are adsorbed on the catalyst surface.
- Activation and dissociation - the CO molecule dissociates on the iron surface and breaks down into C and O atoms.
- Carbonyl and carbide formation – Carbide phase is formed, which is the main component of the FTS reaction.
- Chain growth and hydrocarbon formation – C and H atoms polymerize to form products such as methane, olefins, paraffins.

In addition, dual-functional catalysts containing active metal (metal carbide) nanoparticles for CO hydrogenation and acid sites for hydrocracking/isomerization are very promising for the selective production of gasoline or diesel fuel. Controlling secondary reactions using new solid acid materials such as mesoporous zeolites leads to excellent product selectivity.

Studies have shown that using a highly dispersed iron catalyst:

- Increased production of C_2-C_4 olefins,
- Reduced production of CH_4,
- Stable carbide phase, ensuring long-term catalyst activity.
- The changes on the catalyst surface were studied by infrared spectroscopy (FTIR), X-ray diffraction (XRD) and electron microscopy.

FTIR- Fourier Transform Infrared Spectroscopy (FTIR) analyzer is used in the semiconductor manufacturing industry FTIR is a spectral analysis tool that uses infrared spectroscopy to analyze impurity concentrations through Fourier transform.

The spectrometer mainly consists of a light source, a Michelson interferometer, a detector and an interferometer.[1]

In conclusion, the highly dispersed iron catalyst has high efficiency in producing hydrocarbons from synthesis gas, which greatly contributes to the development of Fischer-Tropsch synthesis. The stability of the carbide phase ensures long-term operation of the catalyst and increases the possibility of obtaining target fractions of hydrocarbons.

References

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