

# RAW MATERIALS IN THE POLYMERIZATION REACTION IN THE PRODUCTION OF HIGH-DENSITY POLYETHYLENE, THEIR FUNCTIONS AND PHYSICAL-CHEMICAL PROPERTIES

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## ABSTRACT

This article provides a comprehensive overview of the raw materials used in the production of high-density polyethylene (HDPE), focusing on their functions and physicochemical properties. The roles and significance of ethylene, hydrogen, propylene, butene-1, hexane, catalysts, and co-catalysts in the polymerization reaction of HDPE are analyzed. The chemical and physical characteristics of each substance, as well as their impact on the quality of the polymer, are described. This study aims to improve the HDPE production process and enhance product quality.

## Keywords

(HDPE), High-density polyethylene, Ethylene, Hydrogen, Catalyst, Propylene, Hexane.

## INTRODUCTION

High Density Polyethylene (HDPE) is a strong, tough, easy to clean, chemically resistant, and economically efficient synthetic polymer. It is widely used in almost all branches of modern industry. The chains in its molecular structure are ordered and closely spaced, which increases the density of the polymer and improves its physical properties. Therefore, HDPE serves as the main material in the production of a wide variety of products[1].

High-density polyethylene is used in the following main areas:

- Construction: water pipes, gas pipelines, sewage systems, insulation films, facade panels;
- Agriculture and rural economy: agrofils, water distribution devices, chemical fertilizer packaging;
- Household needs: containers, baskets, toys, mats, household items;
- Automotive: side root tanks, internal plastic parts, safety elements;
- Energy and gas industry: high-pressure pipes;
- Medicine and pharmaceuticals: disposable syringes, containers, storage containers.

The most important step in the production of high-density polyethylene is the polymerization reaction of ethylene, which involves a number of raw materials, reagents and catalysts. Each of them has its own function and determines the properties of the product. Below we will consider these substances in more detail.[2].

1. Ethylene ( $C_2H_4$ ) - The main monomer, molecular weight 28.03.

Function:

Ethylene is a monomer that forms the main links in the polymer chain and is the main building block of HDPE.

Physical properties:

- Colorless gas with a sweet odor;
- Boiling point:  $-103.7^{\circ}C$ ;
- Liquidification point:  $-169.2^{\circ}C$ ;
- Molecular weight: 28.03 g/mol;
- Very slightly soluble in water, soluble in organic solvents;
- Density varies with pressure and temperature.

The obtained ethylene for polymerization must be extremely pure. For this, the ethylene is purified from inert additional nitrogen and impurities. In production, inert compounds are collected during the reductive ethylene, removed from the environment, and new purified ethylene is added to the environment.

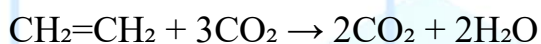
Chemical properties:

Ethylene is an unsaturated hydrocarbon with a double bond, which easily undergoes a number of reactions - addition, hydrogenation, halogenation and hydration reactions. These reactions determine its ability to polymerize.

The most important addition reactions:



Ethylene burns with a flame:



Ethylene undergoes polymerization reactions:



## 2. Hydrogen ( $\text{H}_2$ ) – Chain-controlling substance

Function:

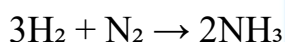
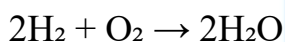
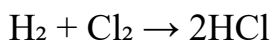
Hydrogen Participates in the synthesis of high-density polyethylene by breaking the chain and controlling the molecular weight of polymer molecules. During the reaction, the active center that grows absorbs  $\text{H}_2$ , and its activity decreases, and the chain stops.

Physical properties:

- Colorless, odorless, light gas;
- Boiling point:  $-252.87^\circ\text{C}$ ;
- Liquefaction point:  $-259.19^\circ\text{C}$ ;
- Density (under normal conditions): 0.0696 g/l.

Chemical properties:

- In the presence of catalysts, it reacts with various elements (halogens, oxygen, nitrogen):



## 3. Propylene ( $\text{CH}_3 - \text{CH} = \text{CH}_2$ )

Function:

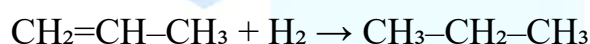
Used to control density and create polymers with specific properties by influencing the polymer structure.

Physical properties:

- Colorless gas with a characteristic odor;
- Molecular mass: 42.08 g/mol;
- Boiling point:  $-47.6^{\circ}\text{C}$ .

Chemical properties:

Since propylene is a compound, it undergoes addition, halogenation, hydrohalogenation, oxidation and other reactions.



4. Butene-1 ( $\text{CH}_3 - \text{CH}_2 - \text{CH} = \text{CH}_2$ )

Function:

Butene-1 is used in technology in very small quantities, it allows you to control the density of the synthesized polymer and create a polymer with a specific target property.

Physical properties:

Butene-1 is a colorless gas with a characteristic odor.

Molar mass 56.11 g/mol

Liquification temperature =  $-185.3^{\circ}\text{C}$ ;

Boiling temperature =  $-6.6^{\circ}\text{C}$

5. Hexane ( $\text{C}_6\text{H}_{12}$ )

Function:

Hexane is used in technology to prepare catalyst suspensions, to control the concentration of polymer suspensions being synthesized in the reactor, and as a substance that transports the suspension to the next process. The reaction in the reactor takes place in a suspension environment.

Physical properties:

- Colorless liquid;
- Molar mass: 86.18 g/mol;



- Melting point =  $-95\text{ }^{\circ}\text{C}$ ;
- Boiling point:  $68^{\circ}\text{C}$ ;
- Slightly soluble in water, soluble in organic solvents.

Chemical properties:

Hexane is a chemically almost inert compound and can undergo decomposition and substitution processes only when appropriate conditions are created. 3500 kJ/mol of energy is required to break the  $\delta$ -bond between C–C. A relatively large energy expenditure of 413 kJ/mol is required to break the bond between C–H. However, despite this, most reactions occur due to the breakage of the bond between C–H, that is, the replacement of hydrogen by other atoms or groups of atoms. It undergoes halogenation, nitration, oxidation, and other reactions.[3,4].

#### 6. Catalyst (HDC/HYC) and cocatalyst (AT)

Function:

Increase the efficiency of the polymerization reaction, attach monomers to the active center and control the reaction.

- HDC/HYC – main catalysts;
- AT  $-(\text{Al}(\text{C}_2\text{H}_5)_3)$  – triethylaluminum – as a cocatalyst;

Physical properties (AT):

- Colorless, self-flammable liquid in air;
- Since this catalyst complex decomposes under the influence of oxygen and moisture in the air, polymerization is carried out in an environment of dehydrated organic solvent (hexane).

- Molar mass: 114.16 g/mol;
- Liquidification temperature =  $-52.5\text{ }^{\circ}\text{C}$ ;
- Boiling point:  $136^{\circ}\text{C}$ .

Chemical properties:

- Reacts vigorously with water, acids, and alcohols;
- The reaction is carried out in an anhydrous, hexane environment under inert nitrogen.

## CONCLUSION

The correct selection and high quality of raw materials and reagents used in the production process of high-density polyethylene ensures the high quality and durability of the product. Ethylene plays an important role as the main monomer, hydrogen controls the chain length, propylene and butene-1 form the special properties of the polymer. Hexane and catalysts play a key role in the efficient conduct of the reaction. Together, these factors ensure the high-tech and economically efficient production of high-density polyethylene.

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