A. Nesterov, M. Pojarskii, O. Posudiievska

MODELLING OF CHEMICAL AND TECHNOLOGICAL PRODUCTION PROCESS OF FERROCENE CARBOXYLIC ACID

Ferrocene and its derivatives improve energy characteristics of solid rocket propellants. This work presents the created computer model of industrial production of ferrocene carboxylic acid, based on the laboratory method of synthesis of ferrocene carboxylic acid from ferrocene and carbon dioxide gas, employing ChemCAD software, version 7.1.2 [2].

The process of synthesis starts with the preparation of the solution of benzene, ferrocene, and aluminium chloride [2]. Solution is mixed and heated to 40℃. Carbon dioxide gas is added to the solution, the reaction proceeds with the temperature of50℃. After the reaction is completed, the solution is cooled to 6℃. Then, cold 12% aqueous solution of tin dichloride is added to the cooled solution after the synthesis for decomposition of aluminium chloride. The heterogeneous mixture is filtrated from the precipitate. The mixture of benzene and water is separated. After filtration the precipitate is dissolved in 20% aqueous solution of sodium hydroxide and is filtrated from the precipitate of undissolved ferrocene. 0.1 M HCl is added for acidification of alkalic solution to precipitation of ferrocene carboxylic acid. The precipitate is washed with clean water and dried in the air. Determined that10.28 g of ferrocene carboxylic acid is obtained from 16 g of ferrocene with the output of 52%.

Each technological operation is modelled by the corresponding UnitOp from the ChemCAD program [1]. Modelling of the processes of mixing of benzene, aluminium chloride and ferrocene, as well as modelling of the reaction of ferrocene with CO_2,aremodelled by the Stoichiometric reactor module. The process of cooling of the reaction mass after the action of the reactor is simulated using the Heat Exchanger module. Two heat exchange flows are supplied to the Heat Exchanger module, the mass flow of which is calculated in accordance with the heat balance of

cooling process. Decomposition of the catalyst is modelled by the Stoichiometric reactor module. Filtration of the suspension is modelled by the Centrifugal filtration module. Separation of water and benzene is modelled by the Component separator module. Dissolution of crystalline sodium hydroxide and washing of the sediment after filtering the suspension with an alkalic solution are modelled by the Stoichiometric reactor module. Filtration of the ferrocene sediment from an alkalic aqueous solution is modelled by the Centrifugal filtration module. The process of acidification of an alkalic solution of ferrocene carboxylic acid is modelled by the Stoichiometric reactor module. Filtration of the sediment of ferrocene carboxylic acid from an aqueous solution is modelled by the Centrifugal filtration module. Washing of ferrocene carboxylic acid with water is modelled by the Solids washer module. Drying of ferrocene carboxylic acid is modelled by the Dryer module.

The resulting model allows us to analyse the consumption of substances and energy, to choose the optimal mode of operation of the technological scheme and to project real productions when required. Optimization of the model shows the feasibility of separating the processes of mixing of the components and carrying out the reaction with carbon dioxide gas, the need for cooling the reaction mixture exactly to6℃ in order to reduce the influence of heat of the reaction of aluminium chloride with water, the possibility of drying the product in a conventional oven at a temperature of 100℃.

REFERENCES

1. ChemCAD version 7. User guide – Houston, Texas: Chemstetions Inc, 2016. – 154 p.
2. Neto, A. F. New Synthesis of Ferrocene Monocarboxylic Acid and Systematic Studies on the Preparation of Related Key-Intermediates / A. F. Neto, J. Miller, V. Faria de Andrade, S. Y. Fujimoto // Z. Anorg. Allg. Chem. –2017. –Vol. 628. – № 1. –P.209–216.