DOI: 10.34854/ICPAF.51.2024.1.1.130

MODELING OF ACETYLENE AND HYDROGEN FORMATION DURING PLASMA JET PYROLYSIS OF METHANE *)

Bilera I.V, Lebedev Yu.A., Titov A.Yu., Epstein I.L.

Institute of Petrochemical Synthesis named after. A.V. Topchiev RAS, 119991, Moscow, Leninsky Prospekt, 29, batukaevtimur95@gmail.com

The purpose of this work is to conduct a numerical simulation of the reaction of methane conversion into acetylene under plasma jet pyrolysis conditions and compare the results obtained with the available experimental data [1, 2]. In a plasmatron operating on methane or hydrogen, a reached temperature is about 3000-8000 K. Then a stream of high-enthalpy gas enters the second chamber (reactor), where it meets streams of “cold” methane. The composition of the hot gas leaving the plasmatron was determined from a thermodynamic calculation for p = 1 atm. The mixing of gas flows from the plasmatron and supplied to the reactor occurs at the beginning of the reactor and is considered instantaneous. To determine the parameters of the resulting mixture, a system equations of mass and energy conservation equations was used. Quenching the reaction products effectively cools the reaction mixture to temperatures at which chemical reactions can be neglected. The calculation used a model of a plug-flow reactor, which included mass balance equations for all components and an energy balance equation. We took the mechanism of acetylene pyrolysis by Wang and Frenklach as the basis for the kinetic scheme [3]. Along with processes with neutral particles, processes with charged particles were included in the kinetic scheme. The processes of ionization and dissociation by direct electron impact and ion exchange reactions were taken into account. In addition, based on the model developed in [4], soot formation was taken into account. This model includes the processes of nucleation, surface growth of solid particles and their coagulation. A polyaromatic model was used for the formation and surface growth of nuclei.

In the calculations, the values of the weight flows of cold and hot gas were varied. The results of calculations of the main products of methane decomposition (hydrogen and acetylene) are in good agreement with experimental data. For methane dissociation products, the amount of which is insignificant and methane itself, there is a discrepancy between the calculated and experimental results at a small flow rate of cold methane. Our estimates show that this difference may be due to the assumption of instantaneous mixing of the plasma flow and cold methane. An analysis of the main processes of methane decomposition and acetylene formation was carried out in cases where hydrogen was used as a plasma-forming gas and when methane was used. In addition to gas products, the soot yield was calculated. The lowest soot yield is obtained when the ratio of the weight flows of cold and hot gas is equal to unity. The maximum yield of acetylene was observed when the ratio of the weight flows of cold and hot gas was equal to 1.2 at times of about 10^{-3} s.

The work was carried out within the framework of the state program of the Institute of TIPS RAS

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*) abstracts of this report in Russian