

Mechanism of Methyl Methacrylate Polymerization in the presence of the initiating system "azobisisobutyronitrile-ferrocene"

Sultanova A.A.¹, Yanborisov V.M.²

¹ Academy of Sciences of the Republic of Bashkortostan

² Ufa State Petroleum Technological University

E-mail: A.A.Sultanova@yandex.ru

In order to suppress the gel effect in the radical polymerization of methyl methacrylate (MMA), experimental studies on the use of metallocenes (MC) are being intensively carried out. However, the mechanism of the polymerization reactions in the presence of an initiator and a real MC is not set, as well as the kinetic parameters of these reactions. A scheme of radical coordination polymerization (RCP) [1] is proposed, and the process proceeds by the reactions of Organometallic Mediated Radical Polymerization (OMRP) [2]. In [3], an algorithm for simulating the process of radical polymerization of MMA in the presence of real initiators by the Monte Carlo method was developed and programmed.

The purpose of this work was to determine the mechanism of polymerization of MMA in the presence of azobisisobutyronitrile (AIBN) and ferrocene (FC).

The results of modeling the polymerization of MMA in the presence of the initiator of AIBN and FC according to the schemes of RCP and RCP-OMRP coincided, it was impossible to select with certainty the type of MMA polymerization mechanism. Therefore, in order to identify the mechanism of the process, experimental data on the polymerization of MMA in the presence of a macroinitiator were additionally used [4]. In this case, when solving the inverse problem, it was possible to adequately describe the conversion of the monomer in the simulation of the process according to the RCP-OMRP scheme.

Thus, by simulation by the Monte Carlo method, it has been shown that in the polymerization of MMA in the presence of the initiating system of AIBN-FC, both RCP and OMRP reactions occur.

References

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