Full Paper _Thematic Section:_ Kinetic Research.
Reference Object Identifier – ROI: jbc-02/16-47-9-122 _Subsection:_ Organic Chemistry.
Publication is available for discussion in the framework of the on-line Internet conference "_Butlerov readings_".
http://butlerov.com/readings/
Submitted on December 01, 2016.

Modeling effect of the main synthesis parameters on the properties of carboxymethylcellulose

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Keywords: modeling, carboxymethylation of cellulose, kinetics of carboxymethylation, cellulose, sodium monochloroacetate, sodium hydroxide.

Abstract

Carboxymethyl cellulose is the most widely used and a large-capacity cellulose ether, which is produced on an industrial scale. Carboxymethylcellulose (CMC) has a degree of substitution of 0.6-0.9; polyanionic cellulose (PAC) is a highly substituted CMC with a degree of substitution ≥ 0.9.

Despite the development of numerous studies on the synthesis of CMC in this field we are still particularly relevant when using the new domestic raw materials, in particular pulps prepared from hardwood and softwood trees, flax and other plant crops. Currently, with a comprehensive study of synthesis of CMC at best used experimental design method to the construction of empirical regression equations. The aim of this work is to develop a new approach to research, minimizing the amount of experimental work on the synthesis of CMC using the deterministic model of the kinetics of carboxymethylation of cellulose.

The basis Macrokinetics cellulose carboxymethylation simulation on the following assumptions:

- In the zone of the chemical reactions generated a uniform distribution of the reactants;
- A two-phase system consisting of solid and liquid reactants (cellulose, NaOH, sodium monochloroacetate, H_2O, etc.) is considered as a quasi-homogeneous phase.

The paper considers the model macrokinetic cellulose carboxymethylation. The basic reaction between the hydroxyl groups of cellulose and sodium monochloroacetate flows through the third order (K1 rate constant). Adverse reaction between sodium monochloroacetate and sodium hydroxide proceeds according to second order (rate constant K_2). On the basis of macrokinetic equations obtained theoretical dependence of the degree of substitution of the cellulose OH groups on the initial molar ratios of reactants and the rate constants ratio K_2/K_1.

In processing the experimental data carboxymethylation different pulps for a wide range of molar ratios of reagents the value of K_2/K_1 (relative reactivity) remains constant for the production of pulp and paper mill and certain environmental conditions. Thus, conducting the experiment for a given proportion of reagents and specific K_2/K_1, can be calculated by the theoretical formula for the degree of substitution of any desired ratios of reactants, minimizing the cost of the experimental work.

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