

Many commercial polymers are currently prepared by free-radical copolymerization of two and more monomers. With increasing number m of their types good prospects appear for imparting to the products of the synthesis a variety of service properties. However, as m grows, the extent of experimental investigations to be performed for revealing optimum conditions for the process of manufacturing of copolymers with desired properties dramatically increases. Establishing the dependence of these latter on initial stoichiometry of monomers and the degree of their conversion by straightforward exhaustive search of possible variants within whole range of initial monomer mixture composition presents rather tedious experimental task even for terpolymerization. In the case of copolymerization of more than three monomers involved the solution of this problem calls for substantially greater amount of time consuming routine experimental work. That is why in designing of processes of synthesis of multicomponent copolymers the mathematical modeling method proves to be of prime importance, which enables a researcher to calculate promptly the values of statistical characteristics of molecular structure of these copolymers as well as to predict some of their performance properties. You could carry out this procedure for the products of free-radical copolymerization of up to $m = 6$ monomers using the other program "Copolymerization Explorer" constituting present package. The program "Copolymerization Kinetics" is intended to find the dependence of the copolymerization rate on time or monomer conversion proceeding from experimental data you obtained by either dilatometry or calorimetry technique.

Mathematical models underlying the programs of present package are commonly recognized in polymer science. The validity of the results, which can be achieved by means of these programs, is ensured by solid physico-chemical experimental verification for great number of real systems. Essential advantage of this package's programs, favoring their ample usage in practice, is the fact that necessary input parameters (such, for instance, as reactivity ratios, the Flory-Huggins parameters, glass transition temperatures) characterize either homopolymers or binary copolymers. The values of these parameters are presently available in literature for many particular polymers which provides you a possibility in many cases to start working with the programs immediately skipping preliminary stage of some additional experiments.

Examining copolymerization of particular monomers you very often face with the necessity to determine the dependence of their overall conversion

p or the rate of its alteration on time t . In order to theoretically find these kinetic curves (integral or differential) you are supposed to have at your disposal a reliable mathematical model of copolymerization properly taking into account all its elementary reactions. Here the situation qualitatively differs from that taking place for the calculations of composition, sequence distribution and composition inhomogeneity of the copolymerization products. All these statistical characteristics are governed at fixed conversion exclusively by the rate constants of chain propagation reactions and can be calculated theoretically provided the values of the reactivity ratios are known. However these characteristics turn out to be insufficient when the necessity arises to calculate the dependence of p or dp/dt on time. The result here depends on the specific features of all elementary reactions including those of initiation and termination of chain. These latter, being diffusion-controlled reactions, were found to be complicated by various physical factors whose accurate account proceeding from current concepts of polymer science constitutes a considerable challenge. No generally recognized kinetic model of chain termination reaction is available so far even for homopolymerization. That is why experimental methods remain as yet the most reliable ones when finding the overall rate of copolymerization.

Among various experimental techniques for the construction of the kinetic curve of copolymerization the gravimetric method is the most straightforward one. However its realization in practice suggests a considerable body of time consuming work. This disadvantage may be successfully obviated by resorting to dilatometric or calorimetric technique which are commonly recognized in investigations of the homopolymerization kinetics. The program in hand will be of assistance to you in performing analogous examination in case of copolymerization of up to six monomers. This program is intended for the construction of an experimental kinetic curve of a copolymerization process on the base of dilatometric and calorimetric data available. Essentially, that no assumptions were made concerning the reactions of chain initiation and termination.

The programs of the package have highly intuitive user-friendly interface. To try the "Copolymerization Kinetics" download the archive, unzip it and run the Setup. To get an idea of the potentialities of the program load one of the predefined base variants (by selecting **Load Base Variant** option in the **File** menu) and perform calculations by clicking on the **Compute!** menu. Many of the special terms encountered in the programs should be readily familiar to those dealing with the free-radical copolymerization. However, an

extensive help is also provided (the help file is located in the same directory with the program).

Here is the list of programs currently present in the “Copolymerization for Windows” software package:

- Copolymerization Explorer
- Copolymerization Kinetics

If you want to get any additional information on the package you may contact Semion Kuchanov at kuchanov@orc.ru.