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Linear and non-linear methods applied to fitting non-isothermal kinetic curves of dehydration of PAAG hydrogel swollen to equilibrium and non-equilibrium state

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Hydrogels are three-dimensional cross-linked structures capable of absorbing significant amounts of water, water solutions, and biological liquids without dissolving or losing their structural integrity. The main goal of this work was to describe the kinetics of non-isothermal dehydration of poly(acrylic acid)-g-gelatin (PAAG) hydrogel, swollen in distilled water to different swelling degrees, by using the Weibull distribution function of reaction times. The comparative analyses of linear and non-linear methods of fitting non-isothermal kinetic curves of dehydration of PAAG hydrogel were performed and the influence of linear and non-linear fitting methods on the value of the parameters determined by the Weibull distribution of reaction times and the quality of fitting was investigated. The non-isothermal thermogravimetric curves were recorded at different heating rates (5 K min-1 to 20 K min-1) from 290 K to 460 K at the same conditions. The quality of the fit in the case of the linear regression method was evaluated using error functions (the coefficient of determination, 〖(R〗 ^2) and chi-square test (χ^2)), while the quality of the fit using non-linear regression method was evaluated using five different error functions (the sum square of errors (ERRSQ), the hybrid fractional error function (HYBRID), the average relative error (ARE), the Marquardt's percent standard deviation (MPSD) and the sum of absolute errors (EABS)). For all the examined swelling degrees and heating rates, the quality of non-linear fitting was higher than that of the linear method fitting. The lower quality of fitting in the case of applying the linear regression method is a consequence of the double logarithm applied in this method, which results in an unrealistic increase in the value of the Weibull function parameters. Changes in the values of the Weibull parameters with the degree of swelling of the hydrogel and the rate of heating during dehydration indicate a change in the state of absorbed water when the degree of swelling changes. Based on the obtained results, we have shown that both examined ways of fitting non-isothermal conversion curves allow the fitting of experimental conversion curves of dehydration of PAAG hydrogel.

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