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Optimisation of acrylic fiber temperature regime thermostabilisation with computer modelling

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Abstract

The presence of mineral impurities in acrylic fibers leads to disruption of its structure, additional defectiveness during thermal treatment, reduction of characteristics of carbon fiber produced from it [1,2]. In this paper the issue of acrylic fiber thermal treatment regime optimization involving computer modeling with allowance for density growth kinetics descriptive models and weight loss models, exo-effect and equipment characteristic. The findings are consistent with the data in [3] and confirm the thermal activation capability of thermal stabilization process.

Keywords: PAN- fiber precursor, thermal stabilization, heterogeneous process, quasi-homogeneous process, thermal activation, multi-stage process, process optimization, kinetics models, mathematic modeling, optimal temperature regime.

1. Preface.

The presence of mineral impurities in acrylic fiber in the process of thermal treatment in carbon fiber production leads to the beginning and growth of chemical processes in individual local points of fiber cross-section, which leads to increase of process non-homogeneity by cross-section and degradation of produced carbon fiber parameters [1,2]. In [3,4], it is shown on the basis of influence analysis of impurities mechanisms and initial temperature of acrylic fiber thermal treatment, that it is possible to reduce the impurities influence through the thermal process activation

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by lifting the process on a maximum possible temperature during the early stage, starting the process in maximum possible number of points by cross-section, and to decrease the temperature upon active exoeffect occurrence for conducting the process without thermal stress for acrylic fiber. For implementation of this approach it is necessary to solve the optimization problem of selecting maximum possible treatment temperature in the first area of the process with obtaining the given density on thermostabilisation output and limiting the amount of generated heat because of the exoeffect with thermostabilisation furnace standard means. This paper analyzes the possibility of coordination of these mechanisms of the process and of thermal activation implementation with the method of mathematical modelling on the basis of formal models of density growth kinetics during acryl fiber thermal treatment, mass loss, heat generation with exoeffect.

2. Statement of the PAN-fiber thermal treatment optimization problem.

The process of consecutive acrylic fibers treatment in areas of thermostabilisation oxidation furnace is considered as multi-stage (fig. 1) [5,6].

Every pass of the furnace treatment is a distinct stage and is described with kinetics equations of zero and first

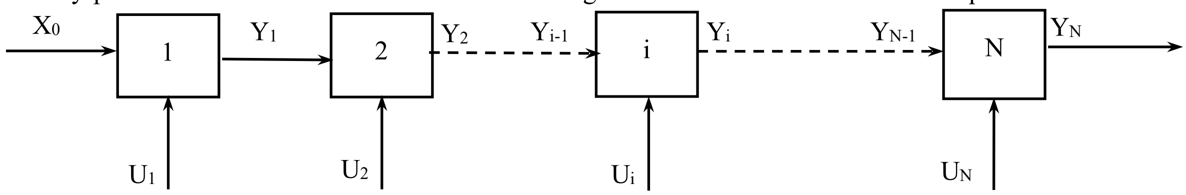

Fig 1. Multistage thermostabilisation process

order by density [7-12]:

$$\frac{d\rho_1}{dt} = \rho_{st} \cdot k_1(T) \cdot e^{-k_1(T)t} \tag{1}$$

$$k_1(T) = k_{01} e^{-\frac{E_1}{RT}} \tag{2}$$

$$\frac{d\rho_0}{dt} = k_0(T) \tag{3}$$

$$k_0(T) = k_{00} e^{-\frac{E_0}{RT}} \tag{4}$$

$$\rho_{st} = b_0^{'} + b_1^{'} T \tag{5}$$

$$\tau = b_0^{''} + b_1^{''} T \tag{6}$$

autocatalytic kinetics equations with nucleation of mass loss mechanisms:

$$\frac{dm_1}{dt} = k_{a1}(T) \cdot m_1 \cdot (M_{01} - m_1) + k_{11}(T) \cdot (M_{01} - m_1) \tag{7}$$

$$m_1^{\gamma}(t) = \begin{cases} 0, & when\ m_1(t) < \gamma_1 \\ m_1^{\gamma}(t) = m_1(t) - \gamma_1, & when\ m_1(t) \geq \gamma_1 \end{cases} \tag{8}$$

$$\frac{dm_2}{dt} = k_{a2}(T) \cdot m_2 \cdot (M_{02} - m_2) + k_{12}(T) \cdot (M_{02} - m_2) \tag{9}$$

$$m_2^{\gamma}(t) = \begin{cases} 0, & when\ m_2(t) < \gamma_2 \\ m_2^{\gamma}(t) = m_2(t) - \gamma_2, & when\ m_2(t) \geq \gamma_2 \end{cases} \quad (10)$$

equations of exoeffect heat flow for two mechanisms of mass loss processes:

$$g = b_1 \cdot \frac{dm_1}{dt} + b_2 \cdot \frac{dm_2}{dt} \quad (11)$$

where $\rho_0, \rho_1, k_0(T), k_1(T)$ - density change, formal equations kinetics constants of zero and first order,

ρ_{st}, τ - steady-state density, process activation time for the current process temperature,

m_1, m_2 - mass loss by the first and second mechanisms,

g - exoeffect heat flow.

These equations link the output parameters of the stage Y_i with the output parameters of the previous stage Y_{i-1} and control inputs on the stage U_i. Output parameters of the stages are acrylic fiber density, amount of heat emitted because of exoeffect, control inputs - fiber pass rate, defining the duration of the chemical process on every stage, and thermal treatment temperature.

Object state variables and control inputs have restrictions, defining possible variation range for them (maximum velocity of rollers and others). Fiber density on the last stage output must be established on set value, and exoeffect heat flow on every stage should not exceed the set value, which is equal to heat flow, that can be evacuated with the furnace fan system.

Obtaining of maximum oxidation uniformity by fiber cross-section corresponds to the maximum possible temperature value, which corresponds to the maximum fiber pass rate on input rollers. This allows to use as the criterion maximum input rollers velocity with equality of output density to the set value and exoeffect heat flows with furnace fan areas feasibility to evacuate the flow.

3. Algorithm of PAN-fiber thermal treatment optimization.

For the problem solution an algorithm is developed, searching the maximum temperature and fiber processing rate through mathematical modeling of the oxidation process. The inputs of the algorithm are: initial acrylic fiber pass rate, initial fiber treatment temperature, set density on the process output, limitations on amount of heat emitted during oxidation process with exoeffect in each area, oxidation process model parameters.

Algorithm computes density in output area with the model for each pass of the first area for set temperature value and finds amount of emitted heat. Gradually increasing temperature, the algorithm brings the process to an acceptable level of emitted heat and computes density on the output of the first stage. Then, in the same way, maximum possible temperature is obtained in all other areas.

If density on the last area output exceeds the set value (initial values are set in a way, that density on output does not exceed the set value), then fiber pass rate is increased by outer loop and again each area is brought to a maximum acceptable temperature. This way, increasing the temperature in areas and fiber pass rates,

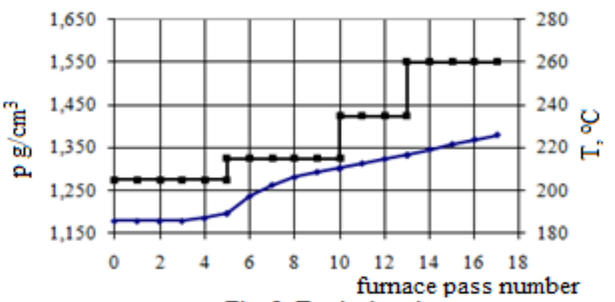

Fig. 2. Typical regime.

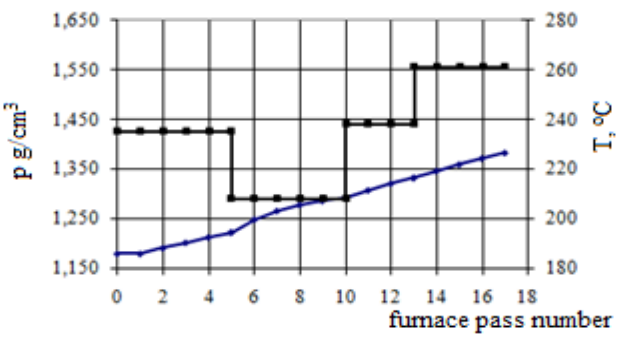

Fig. 3. Regime with temperature activation.

algorithm selects by mathematical model the most effective fiber treatment regime with set parameters.

4. Results of PAN-fiber thermal treatment optimization.

Fig. 2 shows treatment temperature and density charts by areas with typical temperature regime. Fig. 3 shows treatment temperature and acrylic fiber density variation charts, found with the algorithm. For considered acrylic fiber, temperature in the first area may be increased up to 236 degrees without exceeding allowed exoeffect heat flow. At the same time, unlike with typical regime, when density starts to grow on last passes of the first area, it happens on first passes of the first area, when regime, selected with the algorithm, is applied. At the same time, thermostabilisation process duration becomes 1.5 times shorter.

Summary:

1. Optimal thermostabilisation temperature regime, corresponding to the regime with thermal activation [3,4], is obtained with mathematical modeling.
2. Obtained temperature regime provides maximum possible treatment temperature, which contributes to process starting in maximum possible number of points by precursor volume, i.e. to achieving of maximum possible process uniformity without exceeding allowed exoeffect heat flow.
3. Treatment with maximum possible temperature also corresponds to maximum performance of a production line.

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