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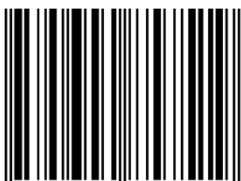
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CONTROL OF POLYETHYLENE'S RADIATION CROSS-LINKING BY GAMMA IRRADIATION IN ACETYLENE ATMOSPHERE

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Abstract. To produce cross-linked polyethylene using the radiation method, a lengthy procedure for irradiating the polyethylene is required. Reducing the time spent on irradiation will increase the yield of finished products per unit time and increase production efficiency. It has been experimentally confirmed that irradiation of polyethylene in the presence of hydrocarbon gases (for example, in the presence of acetylene) makes it possible to achieve the required degree of intermolecular cross-linking in less time. The article presents a modified algorithm for the production of cross-linked polyethylene, and identifies parameters whose changes can influence the speed of the production process. The problem of managing the production process is formulated in order to minimize the time spent on the production of cross-linked polyethylene. A description of mathematical models is given that make it possible to develop a control system for the production process of polyethylene modification using radiation exposure.

Keywords: cross-linked polyethylene, radiation technology, gas diffusion, production management.

1. Introduction

The development of modern production is difficult to imagine without organic polymer materials, in particular polyethylene. Radiation cross-linked polyethylene is one of the most popular materials. It has a number of unique physical characteristics, such as wear resistance, inertness, heat resistance and, of course, the shape memory effect. These qualities are especially in demand in the electrical industry, in particular in the production of electrical couplings and cables with special properties. Also, pressure pipes for cold and hot water supply, heat-shrinkable tubes and anti-corrosion tapes, prostheses, catheters, and

implants are made from cross-linked polyethylene (PEX). The use of radiation technology for the production of polyethylene, in contrast to chemical technology, allows us to obtain a chemically pure material, which reduces the toxicity of the product. In addition, this technology significantly increases the service life of products (up to 30 years).

2. Literature Review

The production of the noted polyethylene is associated with the process of gamma irradiation of the material, which causes certain radiation-chemical reactions. First of all, it is necessary to distinguish between the reactions of the formation of cross-links between polyethylene macromolecules and the reactions of breaking molecular chains with the formation of radicals and subsequent oxidation (formation of peroxide groups, $-O-O-$ bonds) [1, 2]. The noted processes occur in parallel. The dominance of cross-linking reactions leads to structuring (cross-linking) of the polymer, the formation of a new material – cross-linked polyethylene, and the predominance of oxidation reactions leads to destruction of the material [1-4].

One of the quantitative characteristics of the quality of PEX is the degree of crosslinking - the proportion of the insoluble fraction formed in the polymer during radiation-chemical reactions [3, 4].

Cobalt 60 (^{60}Co) is used as a source of radiation exposure in the PEX manufacturing process. An alternative technology involves irradiation with accelerated electrons. In this version, radiation exposure is carried out in an open atmosphere, which promotes active oxidation of the resulting radicals. Polyethylene tubes treated with gamma irradiation have a higher shrinkage coefficient and a higher elasticity index. In addition, they have a low shrinkage temperature and higher wear resistance and inertness. It is important to note the significant penetrating ability of gamma rays compared to accelerated electrons. This allows thick-walled products to be modified without compromising quality.

However, radiation sources are quite expensive production elements. Cobalt 60 (^{60}Co) is produced from Cobalt 59 (^{59}Co) in a nuclear reactor by bombarding nuclei with thermal neutrons. The power of the sources decreases over time in accordance with the half-life (5.27 years for ^{60}Co). In this regard, there is a production need to speed up the process of manufacturing PEX, which allows increasing the yield of finished products per unit of time.

According to previously conducted experimental studies, the process of cross-linking polyethylene can be significantly accelerated by

irradiating the material in the presence of hydrocarbons, in particular acetylene C_2H_2 [5-7]. Acetylene molecules are relatively small in size and, during the process of diffusion, penetrate deeply into polyethylene. Here they serve as material for the formation of additional cross-links between macromolecules. The rate of formation of intermolecular bonds, other things being equal, is probably proportional to the concentration of mobile radicals.

3. Data and Methodology

As part of this work, it is proposed to modify the production process for manufacturing PEX by adding additional steps that will speed up the process of obtaining the finished product. In addition, it is necessary to develop a technological process model that will provide recommendations on the processing time of raw materials in order to obtain finished products of the required quality.

Currently, when manufacturing PEX in production, a sequence of actions is performed, which is shown in Fig. 1 [8, 9]. The irradiation procedure for polyethylene is the longest step in the production process. Depending on the power of the radiation sources, this operation can take from seven days to a month. It is proposed to change the production process of PEX, supplementing the sequence of steps with several stages that can significantly reduce the duration of the polyethylene irradiation procedure to obtain products of the required quality (that have reached the required degree of gel fraction).

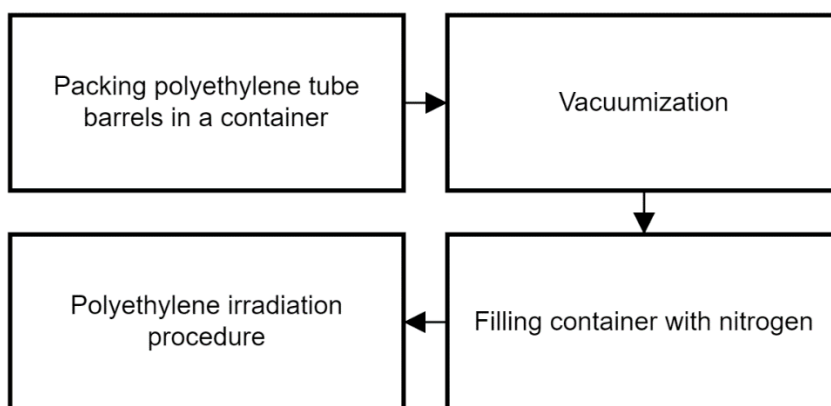


Fig. 1 Scheme of the current production process

Firstly, it is proposed to carry out the procedure of repeated vacuumization of the starting material (polyethylene). It would be able

to achieve the required concentration of oxygen dissolved in polyethylene in less time. Reducing the oxygen concentration in polyethylene, in turn, will reduce the intensity of oxidation reactions, which will slow down the process of destruction of the material and increase its service life.

Secondly, it is proposed to keep the source material in the acetylene presence for some time before the radiation exposure procedure. This will allow the polyethylene to absorb a certain volume of gas. Acetylene molecules, due to their size and mobility, will act as additional material in the formation of new intermolecular bonds. In this way, acetylene molecules are chemically incorporated into the structure of polyethylene. Next, the containers are filled with inert nitrogen in order to reduce the acetylene concentration in the volume to a certain value. The sequence of actions for the proposed modified production process is presented in Fig. 2.

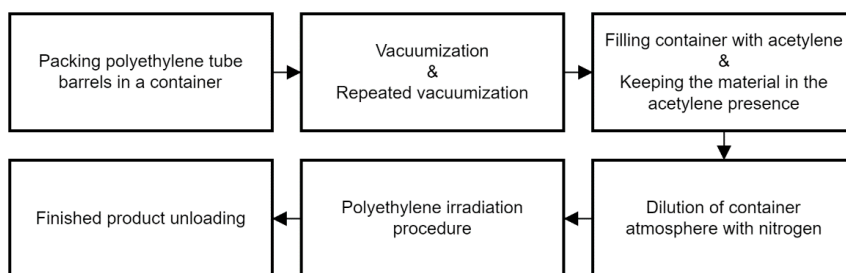


Fig. 2 Proposed production process diagram

Since the physical and mechanical characteristics and volume of the starting material might be different for each production batch, it makes sense to consider the modified production process as a control object. Let us introduce the following notation:

- \mathbf{X} – vector of uncontrolled, observable, input parameters;
- \mathbf{Z} – vector of control parameters;
- y^* – model response.

The vector of input parameters is formed by a set of characteristics of the material, containers, the state of gamma radiation sources and the atmosphere inside the container:

$$\mathbf{X} = \{D_{O_2}, D_{C_2H_2}, k_{O_2}, k_{C_2H_2}, h, L, \xi, V_s, \dot{D}_0\}$$

Here $D_{O_2}, D_{C_2H_2}$ are the diffusion coefficients of oxygen and acetylene in polyethylene, $k_{O_2}, k_{C_2H_2}$ are the solubility constants of the corresponding gases, h, L are the linear dimensions of a polyethylene tube, ξ is a degree of crystallinity of polyethylene, V_s is the volume of the container

free from the polyethylene tube, \dot{D}_0 is the dose rate at the moment the irradiation process begins.

The vector of control parameters is formed from the varied parameters of the control object:

$$\mathbf{z} = \{C_{C_2H_2}^{(0)}, C_{C_2H_2}^*\}$$

Here $C_{C_2H_2}^{(0)}$ is concentration of acetylene in the container during gas absorption by the tube, $C_{C_2H_2}^*$ is acetylene concentration in the container at the start of the irradiation procedure.

The response of the model y^* is the predicted degree of cross-linking of polyethylene (share of gel fraction). The criterion for completing the production process is to achieve a certain required degree of polyethylene cross-linking (share of gel fraction):

$$0 \leq y^*(\mathbf{x}, \mathbf{z}, t(\mathbf{x}, \mathbf{z})) - \bar{y} < \varepsilon$$

Where \bar{y} is the required degree of crosslinking of the finished product, ε is a small value.

To determine the degree of crosslinking of the finished product, it is necessary to keep the PEX in a solvent for a long time. Therefore, it is not possible to obtain any information about product quality in real time. Thus, at this stage, only software control of the PEX manufacturing process is considered (Fig. 3).

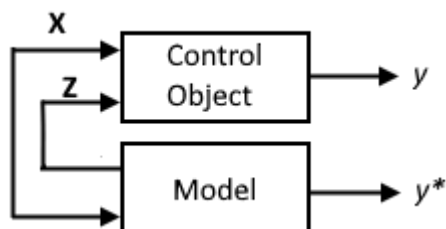


Fig. 3 Scheme of the manufacturing process software control

We assume that t is time required for the production process to achieve the required degree of crosslinking \bar{y} , then process control consists of solving the following optimization problem:

$$\hat{\mathbf{Z}} = \left\{ \hat{C}_{C_2H_2}^{(0)}, \hat{C}_{C_2H_2}^* \right\}, \hat{C}_{C_2H_2}^{(0)} \in \left[0, C_{C_2H_2}^{(\max)} \right], \hat{C}_{C_2H_2}^* \in \left[0, C_{C_2H_2}^{(\max)} \right]$$

$$t = t(\mathbf{X}, \hat{\mathbf{Z}}) \rightarrow \min$$

$$J: \sim^2 \rightarrow \sim$$

$$0 \leq y^*(\mathbf{X}, \hat{\mathbf{Z}}, t(\mathbf{X}, \hat{\mathbf{Z}})) - \bar{y} < \varepsilon$$

Where $C_{C_2H_2}^{(\max)}$ is a certain maximum permissible concentration of acetylene.

The total time of the production process consists of the sum of the time spent on performing the stages of evacuation, exposure of polyethylene in acetylene and irradiation of the material:

$$t(\mathbf{X}, \mathbf{Z}) = t_1(\mathbf{X}) + t_2(\mathbf{X}, \mathbf{Z}) + t_3(\mathbf{X}, \mathbf{Z})$$

Where t_1 is the time of the vacuum stage, t_2 is the required exposure time of polyethylene in acetylene, t_3 is the required irradiation time of the material to achieve the target degree of cross-linking \bar{y} .

To describe evolution of the oxygen concentration in polyethylene at the vacuum stage, a mathematical model of gas diffusion in polyethylene is used [9]:

$$\frac{\partial C_{O_2}(x, t)}{\partial t} = D_{O_2} \nabla \cdot (\nabla C_{O_2}(x, t)), \quad x \in \Omega$$

$$C_{O_2}(x, t) = k_{O_2} P_{O_2}(t), \quad x \in \partial\Omega$$

$$C_{O_2}(x, 0) = C_{O_2}^{(0)}, \quad x \in \Omega$$

$$P_{O_2}(t) = f(C_{O_2}(x, t), h, L, \xi, V_s), \quad P_{O_2}(0) = 0, \quad x \in \Omega_s$$

where $C_{O_2}(x, t)$ is the distribution function of oxygen concentration in a closed system, t is time, x is the coordinate of an arbitrary point from Ω , P_{O_2} is the partial pressure of oxygen in the container, Ω_s is the area of the container free of polyethylene. We believe that during this process the properties of the material do not change, therefore, the diffusion coefficient D_{O_2} remains unchanged.

The progress of this stage does not depend on the control parameters of the original problem. Its goal is to achieve the lowest possible concentration of dissolved oxygen. The vacuum process is modeled in two stages.

On the first - up to a certain point in time t_1^* , at which a given closed system reaches equilibrium. The next iteration of the simulation is then performed, taking into account the repeated removal of air from the container by resetting the boundary conditions.

This iteration is also simulated until the system reaches equilibrium (time point t_1^{**}). Therefore, the duration of the vacuum stage is the sum of the iteration durations:

$$t_1(\mathbf{X}) = t_1^*(\mathbf{X}) + t_1^{**}(\mathbf{X})$$

At the stage of filling the container with acetylene, the evolution of the acetylene concentration in the material is also described by a mathematical model of gas diffusion in polyethylene [9]:

$$\begin{aligned} \frac{\partial C_{C_2H_2}(x, t)}{\partial t} &= D_{C_2H_2} \nabla \cdot (\nabla C_{C_2H_2}(x, t)), \quad x \in \Omega \\ C_{C_2H_2}(x, t) &= k_{C_2H_2} P_{C_2H_2}(t), \quad x \in \partial\Omega \\ C_{C_2H_2}(x, 0) &= 0, \quad x \in \Omega \\ P_{C_2H_2}(t) &= f(C_{C_2H_2}(x, t), h, L, \xi, V_s), \quad x \in \Omega_s \\ P_{C_2H_2}(0) &= f(\hat{C}_{C_2H_2}^{(0)}, h, L, \xi, V_s), \quad x \in \Omega_s \end{aligned}$$

Where $C_{C_2H_2}$ is the distribution function of acetylene concentration in a closed system, and $P_{C_2H_2}$ is the partial pressure of acetylene in the container. It is assumed that the coefficient $D_{C_2H_2}$ does not change during the gas absorption process.

The duration of exposure of polyethylene in the acetylene presence is determined by modeling the diffusion process until the system reaches an equilibrium state.

To describe the behavior of the material at the irradiation stage, it is necessary to model not only the process of acetylene diffusion, but also the process of formation and destruction of cross-links between polyethylene macromolecules. To describe the diffusion process, one can also use a mathematical model of gas diffusion in polyethylene [9], which needs to be supplemented because:

1. some part of acetylene participates in radiochemical reactions;
2. the formation of cross-links limits the freedom of movement of gas molecules, which leads to a decrease in the diffusion coefficient and an increase in the solubility constant [10-13].

$$\frac{\partial C_{C_2H_2}(x,t)}{\partial t} = D_{C_2H_2}(t) \nabla \cdot (\nabla C_{C_2H_2}(x,t)) - k_r C_{C_2H_2}(x,t), \quad x \in \Omega$$

$$C_{C_2H_2}(x,t) = k_{C_2H_2}(t) P_{C_2H_2}(t), \quad x \in \partial\Omega$$

$$C_{C_2H_2}(x,0) = \hat{C}_{C_2H_2}(x), \quad x \in \Omega$$

$$P_{C_2H_2}(t) = f(C_{C_2H_2}(x,t), h, L, \xi, V_s), \quad x \in \Omega_s$$

$$P_{C_2H_2}(0) = f(\hat{C}_{C_2H_2}^*, h, L, \xi, V_s), \quad x \in \Omega_s$$

Where k_r characterizes the intensity of radiation-chemical reactions involving absorbed acetylene, $\hat{C}_{C_2H_2}(x)$ is the distribution function of the concentration of acetylene in polyethylene, obtained during modeling of the previous stage of the production process. The diffusion coefficient and solubility constant depend on the current degree of cross-linking of the material:

$$D_{C_2H_2}(t) = D_{C_2H_2}^* (1 - \xi(y^*(\mathbf{X}, \mathbf{Z}, t)))$$

$$k_{C_2H_2}(t) = k_{C_2H_2} (y^*(\mathbf{X}, \mathbf{Z}, t))$$

Where $D_{C_2H_2}^*$ is the diffusion coefficient of acetylene in the amorphous part of polyethylene, $y^*(\mathbf{X}, \mathbf{Z}, t)$ is a model that describes the change in the degree of cross-linking of the material, $\xi(y^*(\mathbf{X}, \mathbf{Z}, t))$ is a function that describes the change in the proportion of the crystalline phase of polyethylene depending on the current degree of cross-linking.

4. Conclusion

As part of this work:

1. based on experimental data, a technology for accelerating the existing cross-linked polyethylene production process has been proposed;
2. a modified algorithm for the production of PEX using the radiation manufacturing method is proposed;
3. based on the modified algorithm, the problem of managing the production process of PEX manufacturing is formulated;
4. mathematical models are presented that make it possible to describe the behavior of the material at the stages of evacuation and saturation of polyethylene with acetylene;
5. The description and requirements for the mathematical model describing the behavior of the material at the irradiation stage are given.

Further research will be aimed at developing and verifying a mathematical model that describes the behavior of the material during irradiation, as well as the implementation of a production process control system.

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