Development and Application of Mathematic Models to Control Quality of Thermal Shrinkage Polymer Materials in Innovative Production

A. M. Araztaganova
Saint-Petersburg State Institute of Technology
St. Petersburg, Russia
alinaami@mail.ru

T. B. Chistyakova
Saint-Petersburg State Institute of Technology
St. Petersburg, Russia
chistb@mail.ru

***Abstract*— Exploitation of innovative equipment, technologies and materials (including nanotechologies) as well as production of polymer materials with wide range of consumptive qualities allow considering modern polymer productions as innovative. To control these productions advanced digital technologies are applied. The technologies include big data processing, prediction of the properties of production and control of the processes using mathematical models. A software solution, based on the library of mathematic models, is developed. The models can be set for variety of production equipment, different types of materials and thermal shrinkage properties of polymers. Databases of the solution contain information about configurations of production lines, properties of materials, production technological regulations and coefficients of mathematical models. A visualization unit of the solution displays trends of variation of thermal shrinkage properties, calculated using mathematical models, and of control values, initiated them. Predicted values, based on current values of the regulations, and trends of difference from the required values are also represented. The software solution includes the unit for exploration the dependency of thermal shrinkage properties on control values. The solution and mathematical models were tested on data from innovative productions in Russia and Germany. The testing on wide range of quality requirements proved their accuracy and adequacy. The software solution and the models can be applied to control and reconfiguration of the modern polymer productions so digital technologies are integrated in control of innovative productions.**

Keywords*— *innovative production; simulation; control; mathematic models; software solution

I. Object of the Exploration

Innovative productions of thermal shrinkage (TS) polymer materials are the object of exploration and simulation. Production volume of the TS polymers is hundreds thousands tons a year. The key characteristics of these productions are:

- the production is continuous;
- different configurations of equipment are used: calander and extrusion lines, including 20 – 200 rolls;
- source materials (including nanomaterials) with different properties are used;
- wide range of quality requirements in condition of their simultaneous combination (color, thickness, TS properties, etc);
- frequent reconfigurations to the new quality requirements [1].

TS properties of polymer films are described by the following indicators: values of length and width shrinkage (as measure of size variation) and strength of the shrinkage – speed of size variation.

Therefore, application of software and mathematical models (MM) supporting control flexible multiproduct productions with wide range of quality requirements is required [2–3].

So, development of MM, allowing to control PS polymer films obtaining processes, using variety of equipment configurations, different types of materials with wide ranges of quality requirements.

II. Formalized Description of the Object of Exploration and Control. Task Statement for Quality Control of Polymer Films

Obtaining process of the TS polymer materials as exploration and control object can be represented as following (Fig. 1).

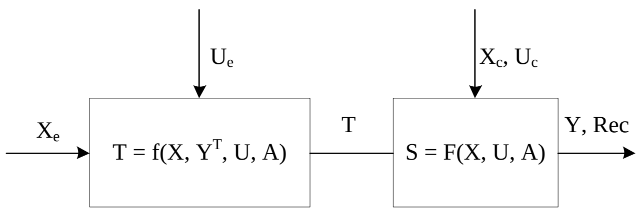

Fig. 1. Formalized description of the polymer materials obtaining process as exploration and control object

Input parameters of the exploration object X_e are configuration of the laboratory line and properties of the material and heat-transferor. Control values U are consumption rate, a temperature of the heat-transferor and quality requirements. Output parameters are reference temperature curves. The curves provide obtaining polymer materials with required TS properties Y^T. The curves are input parameters for control object. Input values for control object X_e are configuration of production line, material parameters and quality requirements. Control parameters include rotation speeds and temperatures of the rolls of the line. Output parameters – TS values and control recommendations.

Obtaining processes control task includes optimal control task and control in abnormal situations.

Optimal control task can be stated as following. For the specified configuration of production line K, material type M and required TS properties Y^T, using MM $Y_j = F_j(X, U, A_j)$, $j = 1, \ldots, N_m$, values of control actions $U = \{V_i^{opt}, T\}$, $i = 1, \ldots, N_d$ to must be found. The control values are limited by regime regulations: $V_i^{min} \le V_i^{opt} \le V_i^{max}$, $T_{ht}^{min} \le T_{ht}^{opt} \le T_{ht}^{max}$, $G_{ht}^{min} \le G_{ht}^{opt} \le G_{ht}^{max}$ and provide obtaining materials with required TS properties. N_m – number of MMs in the library, $A_j = \{A_j^{str}, A_j^{sol}\}$ – parameters of a model; A_j^{str} – coefficients of the equations of a model; A_j^{sol} – parameters of the solution of the model; V_i^{opt} – optimal value of the rotation speed of the i-th drive of the line; V_i^{min} – minimal value of the rotation speed of the i-th drive of the line; V_i^{max} – maximum value of the rotation speed of the i-th drive of the line; T_{ht}^{opt} – optimal temperature of the heat transferor; T_{ht}^{min} – minimal temperature of the heat transferor; T_{ht}^{max} – maximal temperature of the heat transferor; G_{ht}^{opt} – optimal flow rate of the heat transferor; G_{ht}^{min} – minimal flow rate of the heat transferor; G_{ht}^{max} – maximal flow rate of the heat transferor; N_d – number of drives of the calander line; $Y^T = \{S_\Sigma, P_\Sigma\}$ – required values of TS properties; S_Σ – shrinkage value; P_Σ – strength of the shrinkage [4].

Control task in abnormal situation is stated as following. For specified configuration of production line K, material type M and variation from required values Y^T, abnormal situation must be determined and recommendations Rec for its neutralization must be proposed.

III. Development of Mathematic Models for Calculation of Thermal Shrinkage Properties of Polymer Materials

The library of mathematic models was developed. The library provides calculation of TS properties for the polymer materials, obtained on production line with specified configuration K of material M [4]. The structure of the model and values of the coefficients can be selected so the MMs can be applied to calculate TS properties of films, produced on different configurations of equipment and of variety of materials.

IV. Description of the Library of Mathematic Models

To control modern production of polymer films a MM, providing calculation of TS, considering configuration of production line, parameters of material and quality requirements. To solve this problem different approaches to simulation of physical (rheological) parameters and to simulation of physical properties of polymer compositions during their processing were reviewed [5].

The library includes a model for calculation of geometric parameters of production line. The parameters include lengths of material on different production stages, material covering angles on the rolls and etc.

There is also a model for obtaining reference temperature curves. The curves are used for obtaining polymer films with specified TS properties. The lines are formed as a result of processing experimental data about dependencies of TS properties on temperature profile of a line. The experiments are performed on laboratory equipment. He curves are saved in a database for future use.

The library includes empirical and functional models for calculation of the TS properties of materials. Functional, or deterministic, models consider different characteristics of the material: viscous, elastic, and visco-elastic.

Based on result datasets from quality control of produced polymer materials an empirical model a production line is developed. Using this model, value of length shrinkage is calculated as $S_l = a_0 + a_1 \cdot H + (\Sigma_j(a_{2j} \cdot T_j) + (\Sigma_j(a_{3j} \cdot V_j))$, value of width shrinkage is calculated as: $S_w = a_4 + a_5 \cdot H + (\Sigma_j(a_{6j} \cdot T_j) + (\Sigma_j(a_{7j} \cdot V_j))$. The development and calculation of the coefficients are not difficult, but the model has narrow range of validity. Testing showed, that the model can be applied for calculation of TS properties of materials, produced on the line with 27 rolls, the model was designed on, and no more than 10% of length shrinkage.

Empiric models are simple in calculations and best for describing experimental data [1]. However, they can be applied to configuration line and material, they were designed for.

The models of elastic bodies can be applied for simulation of polymer materials properties with strong elastic properties and little or without viscous properties. Usually, these models are invariant to the configuration of the production line, but sensitive to the type, and, consequently, to the characteristics of the material. If the source materials changes, it may be necessary to recalculate the values of the model coefficients. A wide range of materials with elastic properties and the simplicity of the calculations cause application of these models [6]. Since the models consider all control actions applied in real productions, they are most suitable for control of TS properties of polymer materials. The models can be conveniently used for control the TS properties of films produced on lines of different configurations. The model allows calculation of the length shrinkage and force of shrinkage using input and control actions between rolls of the production line. The value and force of shrinkage in the end of production line is calculated as the sum of values, obtained on all gaps between rolls.

Shrinkage value is function of input and control values. Between each pair of rolls value of obtained shrinkage is calculated as root of the equation

$$a_2 \cdot S_{l_i}^6 + a_0 \cdot S_{l_i}^4 + \\ + \left(a_1 - a_2 - \frac{2^{n+1} \cdot V_{i-1}}{L_i^{air} \cdot (n-1)} \cdot \left(1 - \frac{V_{i-1}}{V_i}\right)^{1-n} \cdot \mu \right) \cdot S_{l_i}^3 - \\ - a_0 \cdot S_{l_i}^2 + a_2 = 0$$

where a_0, a_1, a_2 – coefficients of mathematic model; n – polymer flow index; $\mu = \mu_0 \cdot e^{-b(Tr - Ti)}$ – viscosity of the polymer, Pa·sec; μ_0 – viscosity coefficient, Pa·sec^n; b – temperature coefficient, 1/°C; T_r – representative temperature of the polymer, °C [6].

The model is used to control TS properties of PVC films, with length shrinkage less than 10% produced on the line, including less than 30 rolls.

The most descriptive are MMs, considering both elastic and viscous properties and influence of deformation intensity of deformations saved in the material [6]. Usually, these models can be applied for any material, processed on the line, if all the required parameters of the material are calculated. But calculations for the models can be difficult, because start values and the roots of equations of more than 3rd grade with high accuracy must be found. Also, required parameters of the material can be found only by difficult viscosimetric experiments.

The relaxation specter and three-linked model belong to this class of models.

Using model based on relaxation specter, shrinkage value is calculated as $S_\Sigma = (\alpha - 1) \cdot 100\%$, where α – relative size variation, defined as root of the equation $\alpha^3 - \alpha \cdot \sigma_N / G_0 = 0$ in case of biaxial stretching $\alpha = \sqrt{\left(\frac{\sigma_N + \sqrt{\sigma_N^2 + 4 \cdot G_0^2}}{2 \cdot G_0}\right)}$ in case of single-dimensional stretching, where σ_N is a strain of the not relaxed film, G_0 – coefficient of elasticity of the polymer. σ_N – sum of the strains, obtained on each gap between rolls, the strain between the i^{th} and the $i+1^{th}$ roll is $\sigma_i = 4\mu \cdot \left\{\frac{2}{t_i} \cdot \left(1 - \frac{V_{i+1}}{V_i}\right)\right\}^n \cdot \frac{1}{t_i} \cdot \left(1 - \frac{V_{i+1}}{V_i}\right)$, where t_i – time interval of the movement of material between the i^{th} and the $i+1^{th}$ roll, sec, if $V_i / V_{i+1} < 1$, and 0 otherwise [6]).

Testing of the model showed the variation of calculated values from measured ones was less than 15% for PVC materials and different configurations of lines (20–50 rolls).

Using three-linked model shrinkage is calculated as $S_\Sigma = \frac{\varepsilon_2}{1 + \varepsilon}$, where ε_2 – high elastic component of deformation, calculated as a root of the equation:

$$\varepsilon_2 + \frac{\mu \cdot \varepsilon_2}{G_0} - 3^{(n+1)/2} \cdot \frac{\mu \cdot \varepsilon_2}{G_0} \cdot \left|\varepsilon - \varepsilon_2\right| = 0,$$

$$\varepsilon = \hat{e} \cdot \frac{V_{i+1}}{V_i} \cdot t, \quad \hat{e} = \frac{|V_i - V_{i+1}|}{t_i}$$

where ε – normal strain; $\hat{e}$ –speed of logarithmic strain.

The model was tested on PVC films, with length shrinkage less than 10% produced on the line, including 27 rolls.

Both the relaxation specter and three-linked model require difficult experiments to determine material properties [6].

The developed library of MMs provides setting it for different types of materials and configurations of equipment.

V. Functional structure of the software solution

To control the shrinkage value, the operator and administrator interfaces and program modules for simulation of the control object, have been developed [7].

The following databases have been developed for the software package: database of production lines and their configurations, database of materials and their properties, database of technological regulations, database of mathematical models and their parameters, database of reference curves and database of abnormal situations, their reasons recommendations for their neutralization.

A user authorized in the solution as an administrator can edit data and knowledge bases of the complex. The database contains information about production lines, their structure and characteristics of the components of their drives and rolls, materials and their properties, mathematical models and their parameters, recommendations for quality management of shrinkable polymer films in contingency situations.

Users with the role of operators, can set the control actions for obtaining polymeric materials with specified shrinkage properties, as well as obtaining control recommendations.

For the selected configuration of the production line, its geometric parameters are calculated. Based on the given values of the input parameters and quality requirements, a reference temperature curve used for control the TS properties is constructed or loaded from the database.

The operator sets the values of the control parameters. For the selected production line, the type of material and the specified control actions using the selected mathematical model, the shrinkage properties are calculated. Based on the calculated values, plots of the dependence of the values of the TS properties on the control actions are constructed, as well as the trends of the dependence of the shrinkage characteristics on the control actions. If the difference between the calculated and required values is more than permissible, the abnormal situation is recognized, using the knowledgebase. The reasons are analyzed and recommendation for its neutralization is given.

The software complex is integrated into the system of intellectual analysis of big data. The system allows to analyze big production data, to determine the dependence of output parameters on control actions, to build trends in the dependence of quality indicators on the influence of control actions exerting on them.

VI. Testing of library of mathematic models and the software solution

The software solution was tested to control TS properties of PVC films, produced on production lines of polymer plants in Russia and Germany. The testing showed the adequacy of the models and recommendations for quality control of polymer films [4–5].

VII. Conclusion

The developed MMs and the software solution provide control of TS properties of polymer films, produced on different configurations of production lines on modern innovative productions with wide range of quality requirements and source materials and for reconfiguration of production for new quality requirements [8].

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