MODELLING OF LOCAL CRYSTALLINITY IN POLYMER EXTRUSION PROCESS

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ABSTRACT

The dynamic model between crystallinity and process input is obtained corresponding to a particular position which is located in polymer film during extrusion process. To attain this local model, the process is perturbed by the process input around the operating conditions. Data of change of crystallinity and of process inputs at that position are collected and applied to determine the model by process indentification technique. The simulation result shows that the proposed methodology can obtain the discrete transfer function between crystallinity and process input which can represent the dynamics of the non-linear model (regarded as real process) quite well around the given operating conditions.

1. INTRODUCTION

It is found that different dynamics of crystallinity yield different morphology during the extrusion process [1]. This can shape the different properties of finished polymers [2]. The steady crystallinity control [3] is presented where the boundary conditions that correspond to a given desired crystallinity distribution are optimally determined. If there are no disturbances acting on the system, then application of these boundary conditions under the open loop control keeps the crystallinity at their desired levels. However, in real life applications, a variety of random disturbances can change the transients of crystallinity, one needs to know the transfer functions between the process inputs and the resulting crystallinity. The proposed process identification technique can be obtained in order to approximate the unknown dynamics. With experimental data driven model, the obtained model can then provides a knowledge of transient behaviour for design a feedback control system to control crystallinity on-line.

2. PROCESS IDENTIFICATION ALGORITHM

The process identification techniques are based on the observed system data and result in data driven black box models[4]. The approach is briefly explained as the follows. Process input/output data is first generated. These data will be obtained by exciting the process by a Pseudo Random Binary Sequence (PRBS)[5]. The PRBS can be generated by using shift registers. It is a periodic signal that shifts between two levels around the operating point. Generally, the process input/output data are divided to two portions: the first half of the data is used to determine the model structure and the model parameters and the second half is used in order to validate the obtained model structure and the parameters. A linear dynamic model is fitted to process input/output data. The primary assumption made here is that the process has linear behaviour around the operating condition where the data is collected. The Box-Jenkins model [6] is used and can be expressed as:

$$\alpha(k) = \frac{H(z)}{G(z)} u(k\text{-}nk)+\varepsilon(k) \qquad (1)$$

with the denominator polynomial

$$G(z) = 1 + g_1 z^{-1} + ...+g_{ng} z^{-ng} \qquad (2)$$

and the numberator polynomial of the transfer function as

$$H(z) = 1 + h_1 z^{-1} + ...+h_{nh} z^{-nh} \qquad (3)$$

where u, α, and ε are the input process, the process output and the noise of the process respectively. ng, nh and nk are the number of parameters in G and H polynomials and of delay respectively. z^{-1} is the delay operator. Assume that equation (1) represents the true structure of the process, a process model can be found in the form as

$$\alpha_m(k) = \frac{\tilde{H}\ (z)}{\tilde{G}(z)} u(k\text{-}n\tilde{k}) \qquad (4)$$

with

$$\tilde{G}(z) = 1 + \tilde{g}_1 z^{-1} + ...+\tilde{g}_{n\tilde{g}}\ z^{-n\tilde{g}} \qquad (5)$$

$$\tilde{H}(z) = 1 + \tilde{h}_1 z^{-1} + ...+\tilde{h}_{n\tilde{h}}\ z^{-n\tilde{h}} \qquad (6)$$

An estimate of the process output error is given by :

$$e = \alpha - \alpha_m \qquad (7)$$

where α and α_m are the process output vector and the model output vector respectively. The loss function is defined as:

$$V = e^T e \qquad (8)$$

This loss function will be minimized by adjusting the parameter $\tilde{g}_{n\tilde{g}}$, $\tilde{h}_{n\tilde{h}}$, $n\tilde{g}$, $n\tilde{h}$, and $n\tilde{k}$) and a Gauss-Newton minimization procedure is carried out to minimize (8).

In the next section, the process output is referred to the crystallinity at a particular position while the process input can be one of the boundary conditions.

3. CRYSTALLIZATION DURING CASTING FILM POLYMER PROCESS

In this section, the mathematical model of crystallization is established to used as the real process. Figure 1 illustrates the casting film extrusion process.

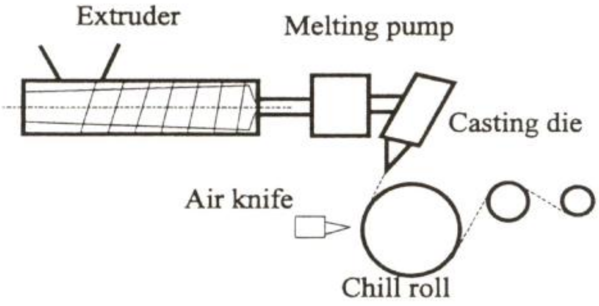

Figure 1 Sketch of film extrusion process

The semi-crystalline polymer is melted in the extruder and extruded though the casting die. It is cooled over the chill roll. The air knife is sometimes added to make a good contact between the polymer film and the chill roll. It is found that crystallization takes place on the chill roll[7]. Mathematical model of casting film polymer process is described by kinetic theory and principle of energy conservation [8, 9, 10]. Here, a stress induced crystallization [11] can be ignored. The crystallinity distribution inside the casting film polymer over the chill roll for non-isothermal crystallization can determined by the follows. The energy equation is written as:

$$\rho\ (C_p\frac{\partial T}{\partial t} - H_\infty\frac{\partial \alpha}{\partial t}) + \rho v_x (\mathrm{C}_\mathrm{p}\frac{\partial T}{\partial x} - \mathrm{H}_\infty\frac{\partial \alpha}{\partial x}) = k\ \frac{\partial^2 T}{\partial z^2} \qquad (9)$$

where T is the temperature, $\alpha \in [0,1]$ is crystallinity, t is the time, x and z are the coordinates correspond to the flow direction and film thickness respectively, ρ is the density, C_p is the constant pressure specific heat, H_∞ is the actual specific enthalpy of crystallization and k is the thermal conductivity and v_x is the velocity of polymer film.

The temperature of surface which is cooled by chill rool T_{sc} is determined by the following equation[1]:

$$T_{sc} = \frac{b_r T_r + b_p T_p}{b_r + b_p} \tag{10}$$

wher b_r and b_p are the thermal effusivities of metallic roll surface and of the polymer respectively, T_p is the mean temperature of the polymer at abscissa x. and T_r is the temperature of the chill roll.

The other side is cooled by air and air knife convection:

$$-k \frac{\partial T}{\partial Z} = h(T_{sa} - T_{a,ak}) \tag{11}$$

where T_{sa} and $T_{a,ak}$ are respectively the temperature of surface of the film and of the air or air knife.

The local convection heat transfer coefficient between air and polymer is calculated by [12]:

$$\mathrm{h} = 0.402 \frac{k_a}{x} \sqrt{\mathrm{Re}} \frac{\mathrm{Pr}^{1/3}}{\left(1+\left(\frac{0.0336}{\mathrm{Pr}}\right)^{2/3}\right)^{1/4}} +0.45 \tag{12}$$

where k_a is the conductivity of air, Pr is the Prandtl Number and Re is the Reynolds Number. x is the distance between the first point of contact polymer-roll and the abascissa x. Between the air knife and polymer film, the convection heat transfer coefficient of a single nozzle is determined from the Nusselt Number Nu [13]:

$$Nu = \frac{3.06}{x_e / W_e + H / W_e + 2.78} \mathrm{Re}^s \, \mathrm{Pr}^{0.42} \tag{13}$$

$$s = 0.695 - \left[\left(\frac{x_e}{2W_e}\right) + \left(\frac{H}{2W_e}\right)^{1.33} + 3.06\right]^{-1} \tag{14}$$

where W_e is the width of the slot nozzle, H is the height of the slot-nozzle exit and x_e is distance from the center of the single slot. The non-isothermal crystallization kinetics can be expressed as [14]:

$$\frac{d\alpha}{dt} = nK\ (T)\ (1-\alpha)\ [-\ln(1-\alpha)]^{(n-1)/n} \tag{15}$$

$$K(T) = \ln 2^{1/2} \left(\frac{1}{t_{\frac{1}{2}}}\right) \exp\left(-\frac{U^* / R}{(T - T_\infty)}\right) \exp\left(-\frac{K_g}{T \Delta T f}\right) \tag{16}$$

$$\Delta T = T_m^0 - T \tag{17}$$

$$f = \frac{2T}{(T + T_m^0)} \tag{18}$$

$$T = T_g - 30 \tag{19}$$

where n is the Avrami index, T_m^0 is the equilibrium melting temperature, $t_{\frac{1}{2}}$ is the isothermal crystallization half time, U* is the activation energy, R is the universal gas constant, K_g is the nucleation exponent and T_g is the glass transition temperature. The induction time can be determined by:

$$\bar{t} = \int_0^{t_i} \frac{1}{b\ (T_m^0 - T\ )^{-\gamma}}\, d\tau = 1 \tag{20}$$

where $\bar{t}$ is the dimensionless induction time index, γ and b are the constant values. As soon as this time index reaches one, the corresponding length of delay time t_i is the non-isothermal induction time.

The integration of equation (20) starts when the temperature of polymer below the equilibrium melting temperature.

4. RESULTS

The non-linear model of energy equation (9)-(14) and crystallization kinetic (15)-(19)

including the non-isothermal induction time (20) is regarded as the real process. The process identification technique given in section 2 is performed at x=25 mm and z=3.56 mm. and the position is illustrated in Figure 2.

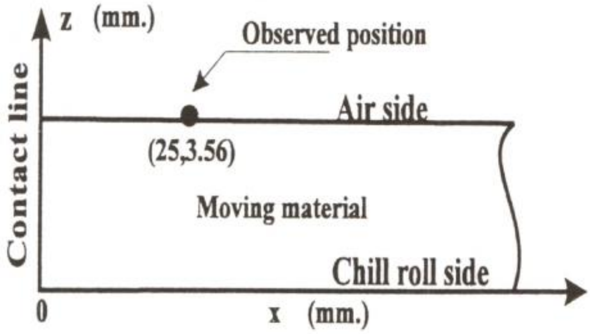

Figure 2 Model of crystallinity in a given position

The values of parameters are given in Appendix 1. The initial chill roll temperature is 350 K and the air temperature is 293 K. Fig. (3) shows the change of crystallinity and temperature.

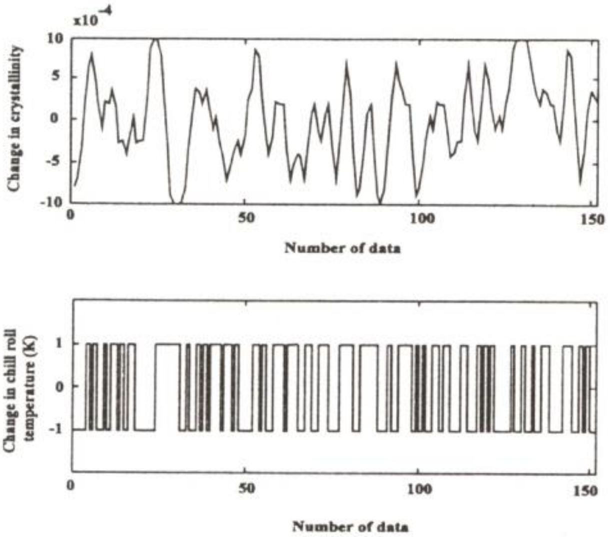

Figure 3 Changes in crystallinity following PRBS changes in chill roll temperature at position (x=25mm., z=3.56 mm.)

Now, figure 3 shows the change of crystallinity when the chill roll temperature is changed following a PRBS of magnitude 1K around the operating condition of 350. The clock period of the PRBS signal is 5 seconds. By simulation, total 150 input/output data are obtained. The first 90 data are selected for building a model. The remaining 50 data are used to validate the model. The order and parameters of model, obtained according to equation (4), are shown in Table 1. These parameters are obtained using Box and Jenkins Model.

Table 1 Model obtained by the process identification technique

$\frac{h_0+h_1z^{-1}+h_2z^{-2}+h_3z^{-3}+h_4z^{-4}+h_5z^{-5}}{1+g_1z^{-1}}$	Values
h_0	0
h_1	-4.86x10^{-6}
h_2	-8.77x10^{-5}
h_3	-2.21x10^{-4}
h_4	-2.67x10^{-4}
h_5	-2.36x10^{-4}
g_1	-1.72x10^{-1}

The numerical optimization algorithm is available is System Identification Toolbox of MATLAB. Figure 4 show how well the output of model fits the independent remaining 50 data which are not used to generate the model. The solid line presents the remaining 60 data points whereas the dotted form feeding the same 50 input data points into the model. The dynamics of output from the model are closed to the dynamics of output data. The error at beginning is due to the lack of initial input data points at initial iteration for equation (4).

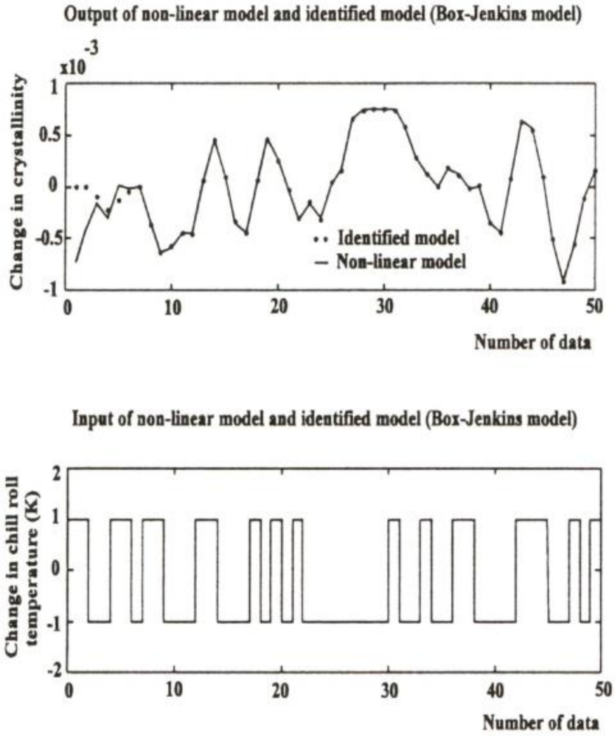

Figure 4 Comparison between the output of non-linear model and identified model around operating condition of α= 3.9x10^{-2} and T_r=350 K at position (x=25mm., z = 3.56 mm.)

5. CONCLUSION

An experimental process model can be obtained for a given position. The data does not actually come from a physical polymer sheet over the chill roll, instead the dynamics is simulated by the partial differential equations for the process. The same technique can also be extended to real process and multi point measurements. As the results demonstrate, the model is quite capable of describing the process around the chosen operating points. The application of the obtained model is illustrated by incorporating it in a feedback control design.

6. REFERENCES

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7. APPENDIX

b, γ : Constant material for induction time, b=8.0x10^{11}, γ=6.

b_p : Thermal effusivity of polymer, b_p= 609.69 (Js$^{-1/2}$ K^{-1} m^{-2}).

b_r : Thermal effusivity of chill roll, b_r = 7520 (Js$^{-1/2}$ K^{-1} m^{-2}).

C_p : Constant pressure specific heat, C_p=2140 (J kg^{-1} K^{-1}).

e : Thickness of the polymer sheet, e=3.56x10^{-3} (m).

H : Height of the slot air-knife jet to material on the chill roll, H=0.1 (m).

H_∞ : Actual specific enthalpy of crystallization, H_∞=83800 (J kg^{-1}).

K_g : Nucleation exponent, K_g=2.99x10^5 (K^2).

k : Conduction heat transfer coefficient, k=0.193 (J m^{-1} s^{-1} K^{-1}).

n : Avrami index, n=3.

T_g : Glass transition temperature, T_g=255 (K).

T_o^m : Equilibrium melting temperature, T_o^m =445 (K).

t_m : Material constant for induction time, t_m = 8.0x10^{11}.

$(1/t_{1/2})_0$: Isothermal crystallization half time, $(1/t_{1/2})_0$ = 2.07x10^6 (s^{-1}).

R : Universal gas constant, R=0.831 (J mol^{-1}K^{-1}).

U* : Activation energy, 6284 (J mol^{-1}).

u : Polymer velocity, u=0.001 (m s^{-1}).

V_e : The velocity of air jet at slot nozzle exit, V_e=40 (m s^{-1}).

W_e : The width of a slot nozzle, W_e=0.02 (m).

ρ : Density, ρ=900 (kg m^{-3}).