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Soft computing applications in dynamic model identification of polymer extrusion process

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Abstract

This paper proposes the applications of soft computing to deal with the constraints in conventional modelling techniques of the dynamic extrusion process. The proposed technique increases the efficiency in utilising the available information during the model identification. The resultant model can be classified as a 'grey-box model' or has been termed as a 'semi-physical model' in the context. The extrusion process contains a number of parameters that are sensitive to the operating environment. Fuzzy rule-based system (FRBS) is introduced into the analytical model of extrusion by means of sub-models to approximate those operational-sensitive parameters. In drawing an optimal structure for each sub-model, a hybrid algorithm of genetic algorithm with fuzzy system (GA-fuzzy) has been implemented. The sub-models obtained show advantages such as linguistic interpretability, simpler rule-base and less membership functions (MFs). The developed model is adaptive with its learning ability through the steepest decent error back-propagation algorithm. This ability might help to minimise the deviation of the model prediction when the operational-sensitive parameters adapt to the changing operating environment in the real situation. The model is first evaluated through simulations on the consistency of model prediction with the theoretical analysis. Then, the usefulness of adaptive sub-models during the operation is further explored in existence of prediction error.

Keywords: Dynamic modelling; Soft computing; GA-fuzzy algorithm; Steepest decent error back-propagation; Semi-physical modelling; Distributed parameter system; Adaptive; Polymer extrusion

1. Introduction

Extrusion is a critical operation in the thermoplastic processing industry since all commercial polymers are compounded [1]. During the process of extrusion, the quality of the product fluctuates within a certain range due to the variation in the properties of materials, or the operating environment including the system disturbances. This may introduce defects to the end product. A number of control methodologies have been proposed to regulate the product quality [2–5]. A simple methodology can be a single-input–single-output (SISO) feedback control linking the output at the die to the input parameter such as the screw speed. However, this technique is not efficient as the product quality is greatly affected by the flow history inside the extruder. Further complication includes the strong interactions between process parameters. For example, changes in the screw speed can lead to changes not only in the melt temperature, but in the flow rate as well.

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Consequently, a feasible control methodology shall consider the process as a multivariable and distributed parameter system.

The design of an appropriate controller requires a dynamic model of the extrusion. The model identification is restricted by the lack of access of some process parameters. For instance, the true temperature of the melt is expensive, if possible, to be gauged directly due to the operational constraints. In common with many other chemical processes, the polymer processing contains a few parameters that are improper to be expressed in deterministic manners. These parameters are referred to as the 'operational-sensitive parameters'. An example could be the polymer viscosity during the process. The viscosity of the melt varies due to the inconsistency of the input material properties.

The aforementioned modelling problems limit the application of either empirical or analytical technique to model the dynamic extrusion process. If the combination of both modelling techniques is possible, the flexibility will improve the utilisation of the available information rather than having the need to conduct a series of dedicated experiments for the model identification. It is speculated that the semi-physical or semi-mechanistic modelling technique can be a potential solution [6]. The technique shall integrate different sources of knowledge and technology during the model development.

In this paper, the fuzzy rule-based system (FRBS) is applied as the sub-models to approximate the operational-sensitive parameters. The optimal structures of the sub-models are produced by executing the genetic algorithm with fuzzy system (GA-fuzzy). The sub-models thus obtained are integrated with the analytical model, forming a semi-physical model. The semi-physical model is adaptive to the varying operating environment through its learning ability while preserving the natures of multivariable and distributed parameter process. In the following sections, a brief description of the extrusion process is given, to be followed by soft computing applications in developing a semi-physical model. The model evaluation is performed from two bases. Firstly, the predictions on the melt temperature and the pressure are compared to the theoretical analysis. Then, the usefulness of adaptive sub-models in approximating the operational-sensitive parameters is further investigated.

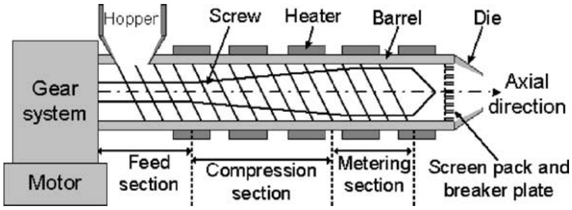

Fig. 1. Single screw extruder.

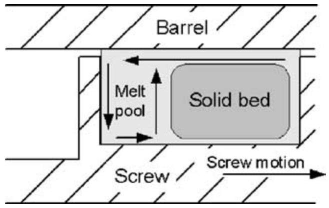

Fig. 2. Melting of solid bed.

2. The process description

The schematic diagram of a single screw extruder is illustrated in Fig. 1. The extruder consists of a barrel, which is heated by a series of wall-mounted heaters and a rotating screw; the latter is linked to a gear system and a motor. Polymer particles are fed in through the hopper, by gravity, into the helical screw channel. The screw has a varying channel depth along the axial direction. The melt flowing through the die is formed into an end product. Fig. 2 illustrates the content of a typical helical cross section of the screw channel in the compression section. It consists of a solid bed and a melt pool. The size of the solid bed diminishes as the solid bed travels in the axial direction along the screw and eventually ends when it reaches the metering section. The variation of the width of the solid bed along the screw channel in helical direction is called the solid bed profile (SBP) while the variation of the melt temperature along the helical screw channel is called the melt temperature profile.

3. The development of semi-physical dynamic extrusion model

An analytical dynamic model of the extrusion process is available [7]. However, its application in the controller design is limited since it is not adaptive to the varying operating conditions. The variation could be due to the instability of the power supply affecting the screw speed and the barrel temperature, the changes of ambient conditions such as humidity, temperature, etc. In addition, the properties of the polymer to be processed may vary from batch to batch, depending on the regrind level, drying condition, etc. A number of process parameters are sensitive to the variation, particularly the polymer viscosity during the extrusion. The viscosity of melt is approximated by means of a power law model in the analytical model. The coefficients of the power law model are predetermined based on the experiments conducted on a rheometer. The application of the power law model to describe the viscosity of melt has several shortcomings. Its validity is limited to the intermediate shear rate range and its coefficients are not adaptive accordingly to the variation in the operating conditions. In the present study, a semi-physical model is developed by extending the analytical model so that the FRBS is applied as sub-models to approximate the operational-sensitive parameters.

Fig. 3 provides an overview of development of the semi-physical model for the extrusion process [8]. The analytical model provides simulated data only for the initialisations of the FRBS sub-models. The optimal sub-models thus obtained are incorporated into the analytical model forming the semi-physical model. The model is then simulated and the predictions are compared to the experimental measurements on the melt temperature and the melt pressure. In existence of prediction error, a model adaptation algorithm will commence to minimise the error by tuning the parameters of the FRBS sub-models.

3.1. The analytical model

The semi-physical dynamic model in the case study is an extension of the analytical model of the work in [7]. The following assumptions are made for the analytical model:

- States of the process dynamic can be described by the transient responses of the solid bed profile (SBP), represented as $X(z, t)$ and the melt temperature profile (MTP), represented as $T(z, t)$ where z and t are the helical down channel distance and time instant, respectively. Dynamic condition prevails only when the melting starts, i.e. in the melting and melt conveying mechanisms;
- Local melting rate, heat transfer rate through barrel wall, viscous dissipation rate and pressure profile (PP) can be calculated using steady-state equations accordingly to local instantaneous conditions.

On the basis of the above assumptions, the analytical dynamic model is formulated. Two main equations in which the dynamic SBP governed by the differential mass balance on the solid bed is expressed in Eq. (1) whereas the dynamic MTP governed by the differential energy balance on the melt pool is written as Eq. (2).

$$\frac{\partial X}{\partial t} + v_{\mathrm{sz}}\frac{\partial X}{\partial z} = \frac{\phi X^{1/2}}{\rho_{\mathrm{s}} H} + \frac{A v_{\mathrm{sz}}}{H} X \tag{1}$$

$$\frac{\partial T}{\partial t} + v_{\mathrm{mz}}\frac{\partial T}{\partial z} = \frac{\phi X^{1/2}(T_{\mathrm{f}} - T)}{\rho_{\mathrm{m}} H(W - X)} + \frac{q_{\mathrm{tr}} + q_{\mathrm{vc}}}{C_{\mathrm{m}}\rho_{\mathrm{m}} H(W - X)} \tag{2}$$

where X is the solid bed width and T is the melt temperature; v_{sz} and v_{mz} are the down channel velocities

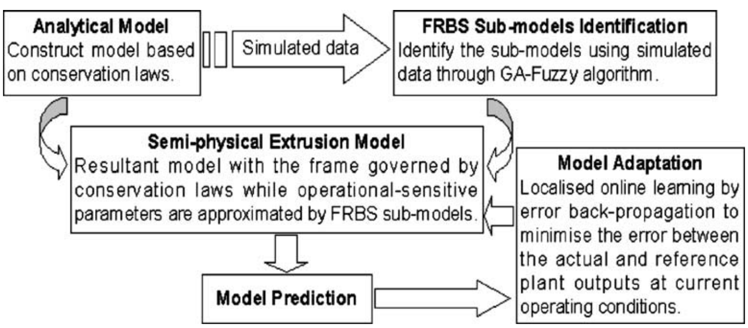

Fig. 3. Overview of development of semi-physical model.

of solid and melt, respectively; ρ_s and ρ_m are the densities of solid and melt; A is the slope of compression section; H is the channel height; T_f is the film temperature; ϕ is the melting coefficient; C_m is the heat capacity of melt; W is the channel width; q_{tr} is the heat transfer rate through barrel wall and q_{vc} is the viscous dissipation rate.The process parameters that are sensitive to the operating conditions are ϕ and q_{vc}. Similar concern is applied for q_{tr} due to the uncertainty in the heat transfer duration. These parameters have been expressed in the analytical model as the following functions [9]:

$$\phi = f_{\phi}(\omega, T_b, G, \alpha) \tag{3}$$

$$q_{tr} = f_{q_{tr}}(\omega, T_b, X, T, \alpha) \tag{4}$$

$$q_{vc} = f_{q_{vc}}(\omega, T, X, G, \alpha) \tag{5}$$

where ω is the screw speed, T_b is the barrel temperature, G is the total mass flow rate, α is a set of parameters specifying the physical properties of polymer and the geometry of the extruder including the viscosity of melt η. The value of η is expressed by the power law model with reference to the local melt temperature and a set of coefficients θ. The equation can be simplified as

$$\eta = f_{\eta}(T, \theta) \tag{6}$$

where θ is the coefficient set predetermined by the offline experiments on a rheometer.

The deterministic equations (Eqs. (3)–(6)) used in the analytical model to approximate those varying operational-sensitive parameters are considered inappropriate, since they are not adaptive when the actual parameters are varying. The FRBS is introduced as an alternative to describe the behaviours of those parameters.

3.2. The FRBS sub-models identification

Eqs. (7)–(10) express the fuzzy functions of the operational-sensitive parameters. A hybrid GA-fuzzy algorithm is adopted to identify the optimal structures for the FRBS sub-models. Data from the simulation of the analytical model is used as the training data during the identification process.

$$\phi = f_{fz}(\omega, T_b) \tag{7}$$

$$q_{tr} = f_{fz}(\omega, T_b, X) \tag{8}$$

$$q_{vc} = f_{fz}(\omega, T_b, T, H) \tag{9}$$

$$\eta = f_{fz}(\omega, X, T) \tag{10}$$

where f_{fz} is the fuzzy function.

3.2.1. The GA-fuzzy algorithm

The GA-fuzzy algorithm employed to identify the structures of sub-models is similar to the Pittsburgh approach [10]. In the algorithm, each chromosome in the population represents a complete knowledge base (KB), which consists of data base (DB) and rule base (RB). The potential solution for a sub-model of n input, m output and k rules is coded into a chromosome with a fixed binary number of l bits. Each parameter of the input and the output has its own set of membership functions (MFs). The identification process begins with a sub-model of maximum MFs, i.e. $q_i = k$, $i = 1, \ldots, n + m$. As the FRBS sub-models are of zero-order Sugeno type with symmetric Gaussian MFs (two MF parameters), the total length of a chromosome is $L = l(2 \times (m + n) \times k)$. The algorithm is programmed with a flexible coding length to deal with the deducting number of rules and MFs during the structure optimisation. Apart from the chromosome representation, the genetic operators are important to enrich the possible solutions for the optimal structure. The commonly used operators include *selection*, *crossover* and *mutation*.

3.2.2. The optimisation process

Fig. 4 shows the flow diagram for the optimisation of the structure of a FRBS sub-model. The structure is

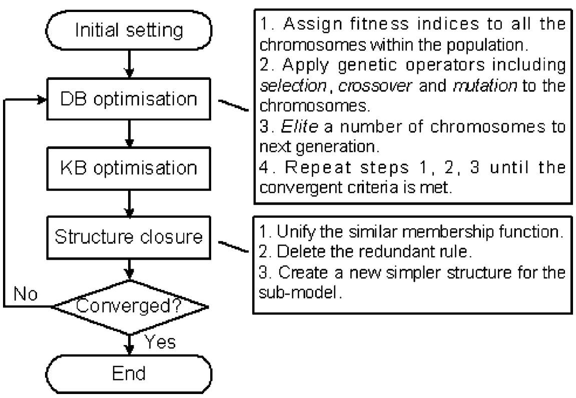

Fig. 4. GA-fuzzy algorithm for optimisation of sub-model structure.

defined as a set of rules that constituting the sub-model and the way of each MF of the input and output parameters associated in the rules. The initial setting defines the criteria of the optimisation. For example, the maximum number of rules desired, type of genetic operators, definition of convergences, etc. It is possible to translate the expert knowledge to the construction of a FRBS sub-model in the initial setting.

During the data base (DB) optimisation, fitness indices are assigned to all chromosomes within the population. The definition of the best fitness depends on several conditions as proposed by [11]. In the present study, the fitness index is determined by the inverse of mean square error between the predicted and the desired results. A few chromosomes with high fitness are kept for the next generation and the genetic operators are applied to the current population. The optimisation process is repeated until the convergent criterion is met. When this happens, the population with the selected chromosomes proceeds to the knowledge base (KB) optimisation.

The KB optimisation procedure is similar to that of the data base (DB) optimisation except that three extra fitness indices, namely the entropy of a FRBS ($F_{\mathrm{I}}^{\mathrm{E}}$), the membership function (MF) similarity ($F_{\mathrm{I}}^{\mathrm{S}}$), and the rule activation ($F_{\mathrm{I}}^{\mathrm{Z}}$), are included with assigned weights and are evaluated in a single convergent criterion. Introducing $F_{\mathrm{I}}^{\mathrm{E}}$ into the criterion encourages an adequate overlapping of MFs of the sub-models, while $F_{\mathrm{I}}^{\mathrm{S}}$ and $F_{\mathrm{I}}^{\mathrm{Z}}$ search for similar MFs and the redundant rules of the sub-models.

Upon convergence of the KB optimisation, only the best chromosome is selected for the structure closure step. A new simpler structure is obtained by unifying similar MFs and deleting the redundant rules. Then, a new generation of the chromosomes having this new structure is created and the entire GA-fuzzy optimisation process is then repeated. While the convergences of DB and KB optimisations maybe decided by a predefined number of generations or an error tolerance, the optimisation of the structure of a sub-model is deemed to have converged only if the closure step cannot be further executed.

Table 1 tabulates the settings of GA parameters for the structure identifications and the final structures obtained for the FRBS sub-models. The size of the population is set accordingly to the number of inputs in each sub-model. Larger population enhances the probability of variation, which is especially important for a lengthy chromosome. The parameters of MF are encoded into six bits binary code, in which a range of 64 discretised values is produced. The resolution should be sufficient as the parameters represent only the width and the location of the membership function (MF) within a bounded operating range. The strategy for applying the genetic operators is *tournament selection*, *multiple-points crossover* with the crossover rate of 1 and *randomised mutation* with a trigger weight of 0.1. *Elitism* is applied as a special policy to each generation. The properties of elite chromosomes are exceptional and excluded from the treatment of the genetic operators. Five chromosomes of the highest fitness within the current generation are elite to the next generation. The elitism policy might help to ensure the fitness of chromosomes in the next generation will be at least maintained as, if not higher than, the current

Table 1
Settings of GA parameter and resultant FRBS sub-models structure

Properties	Sub-model			
	ϕ	q_{vc}	q_{tr}	η
Number of inputs	2	4	3	3
Size of population	40	60	50	50
Bit number	6	6	6	6
Crossover rate	1	1	1	1
Mutation rate	0.1	0.1	0.1	0.1
Elite chromosomes	5	5	5	5
Initial number of rules	27	36	30	30
Initial number of MFs	27^3	36^5	30^4	30^4
Final number of rules	5	3	5	2
Final number of MFs	$5 \times 5 \times 5$	$2 \times 3 \times 2 \times 3 \times 3$	$5 \times 5 \times 5 \times 5$	$2 \times 2 \times 1 \times 2$

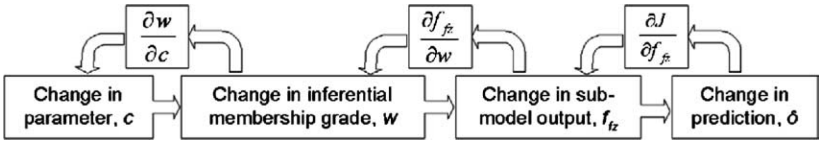

Fig. 5. Causal relationship of MF parameters to model prediction.

generation. To an extent, if all the chromosomes of the current generation are elite to the next generation, the fitness of the chromosomes in the next generation will never be improved.

It is clear that the sub-models contain fewer MFs and rules. For instance, the q_{tr} sub-model is initialised with 30 fuzzy rules and 30 MFs per parameter. After the structure optimisation, the sub-model contains only five rules and five MFs per parameter. The advantages of the simpler structure include easier model interpretation, less computational demanding and higher efficiency during the model adaptation.

3.3. The model adaptation

The sub-models with the optimised structures are incorporated into the semi-physical model for further adaptation. The commencement of the adaptation process is dependent on the errors of the model predictions when compared with the actual melt temperature and the pressure. The model adaptation is complicated since the sub-models approximate only the operational-sensitive parameters but not directly the melt temperature and the pressure. These approximations will then be part of the semi-physical model in generating the predicted melt temperature and pressure as depicted in Fig. 6. Therefore, the model adaptation is executed by back-propagating the prediction errors to the corresponding sub-model through level by level. The concept of error back-propagation from the prediction to each parameter of the MF is depicted in Fig. 5. In the forward sequence (left to right), a small change in the MF parameter c will affect the inferential membership grade w of an input. The influence is further reflected on the approximation of the FRBS sub-model f_{fz}, which will in turn affect the prediction of the semi-physical model, $\hat{o}$. It can be seen that the prediction error can be minimised if the effects of change at individual level are known, which are the gradient vectors of the causal relationship. The derivative information is passed from the output level, and going backward level by level, to the first level as shown in the backward sequence (right to left) of Fig. 5.

The total derivative information in the backward sequence can be effectively represented by a chain rule, which is generalised as Eq. (11). MF parameters are then updated by the steepest descent algorithm. The tuning of the MF parameters is accomplished by minimising the sum of squared errors between the desired, o and predicted, $\hat{o}$ results as written in Eq. (12).

$$\frac{\partial J}{\partial c_{qi}^{p}} = \frac{\partial J}{\partial f_{fz}^{p}} \sum \frac{\partial f_{fz}^{p}}{\partial w_{k}^{p}} \frac{\partial w_{k}^{p}}{\partial c_{qi}^{p}} \tag{11}$$

$$J = \sum (o - \hat{o})^2 \tag{12}$$

where J and p are the square error index and the sub-model index, respectively.

3.4. The model simulation

Fig. 6 illustrates the computation path of the semi-physical dynamic model. The program is initially provided with the following input data:

- Geometry parameters such as channel depth;
- Material properties such as density of solid polymer;
- Settings of screw speed $\omega(t)$ and barrel temperature $T_b(t)$ as a function of time;
- Initial profiles at time t_0 for the solid bed, $X(z, t_0)$ and the melt temperature $T(z, t_0)$;
- Location where the melting process commences;
- Initial estimation of the output flow rate, $G(t_0)$.

The output flow rate G is initialised with the flow rate taken from the previous steady-state condition. When the operating condition changes with time, the program is iterated until a new steady-state condition is reached. The estimation on the output flow rate improves during the iteration. The relationship between

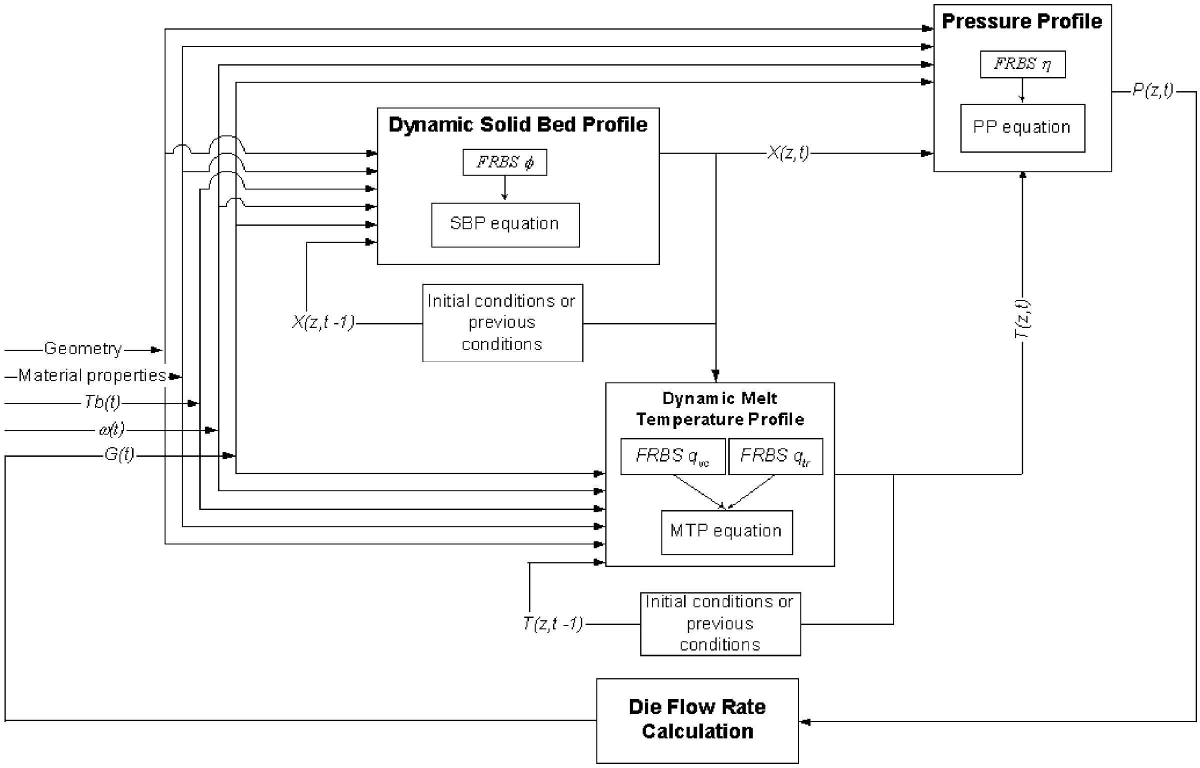

Fig. 6. Diagram of model computation.

flow rate and pressure-drop at the die ΔP_{die} is shown in Eq. (13).

$$G = K_{\text{die}}\rho_{\text{m}}\frac{\Delta P_{\text{die}}}{\eta_{\text{die}}} \tag{13}$$

where K_{die} and ρ_{m} are the die constant and the density of melt, respectively, while η_{die} is the apparent viscosity of the melt at the die.

4. The model evaluation

Evaluation of the developed model is performed by first checking the consistency of the model prediction with the theoretical analysis. The model is simulated when step changes in the screw speed and the barrel temperature are applied separately. Figs. 7 and 8 show the responses of the temperature and the pressure at the die when the screw speed is changed. The screw initially rotates at a speed of 60 revolutions/min (rpm) and the extrusion process is assumed to be operating under a steady-state condition. The dashed lines represent the steady-state responses of the process; the dotted lines denote the responses of the system to a positive step change from 60 to 70 rpm, whereas the solid lines are the responses to a negative step change from 60 to 50 rpm. In Fig. 7, the model predicts a slow temperature increment when a positive change of screw speed is applied. The increase in the temperature of melt is chiefly attributed to the heat generated from the viscous dissipation, which increases with the screw speed and vice versa. The viscous dissipation occurs when the polymer melt is sheared by the relative motion of the rotating screw and the stationary barrel. Fig. 8 depicts an immediate change in the melt pressure at the die; an overshoot is observed before the pressure decaying to a new steady-state value.

The model is also evaluated for an ideal case of altering the melt temperature at the die by manipulating the barrel temperature; assuming that step changes in the barrel temperature can be achieved in practice. The barrel temperature settings are indicated in the

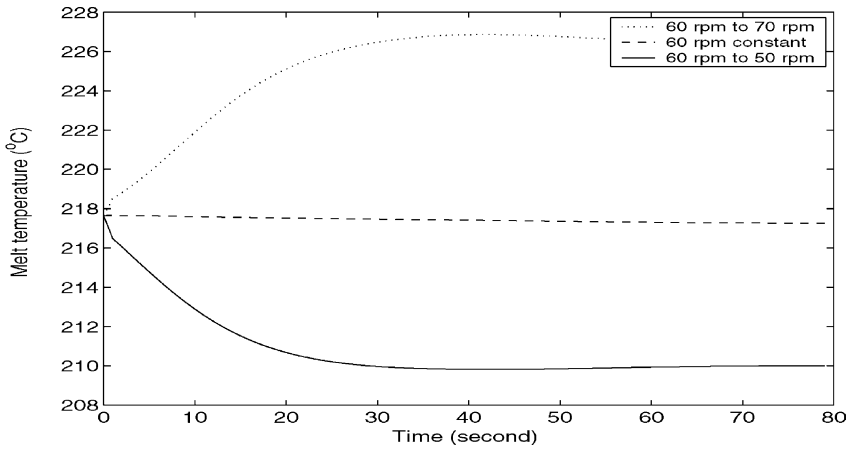

Fig. 7. Transient responses of melt temperature for step changes in screw speed.

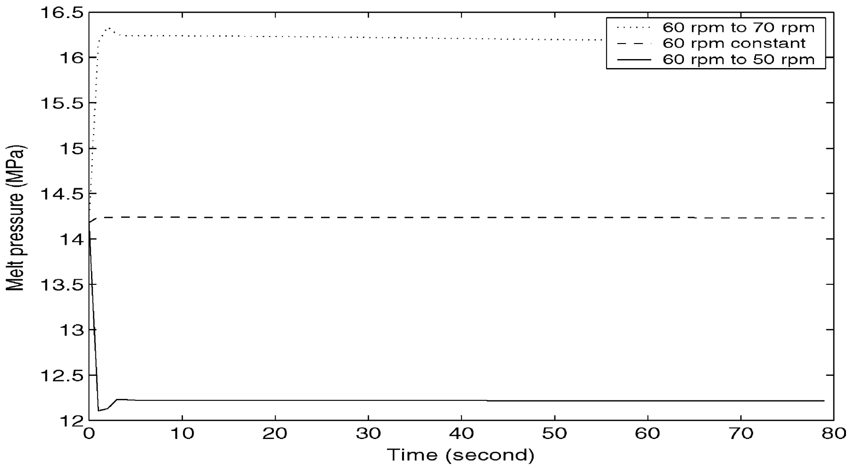

Fig. 8. Transient responses of melt pressure for step changes in screw speed.

legend of Fig. 9. The model predicts an increase in the melt temperature when the barrel temperature is set to a higher value. The higher barrel temperature results in more heat energy being transferred from the barrel wall to melt the solid polymer. Consequently, the melting mechanism commences earlier and the solid is completely melted sooner than the case where lower barrel temperature is applied. The melt temperature shows an inverse response at the early stage when a step change of 180–190 °C is applied to the barrel temperature. Logically, the inverse response should not appear when the barrel temperature is increased. This error is mainly due to the simplifying assumptions of the semi-physical model. It is obvious especially when the step change of the barrel temperature is small.

The evaluations presented earlier are with the assumption that the model truly describes the behaviour of the extrusion. The assumption might invalid as the actual operating conditions are subjected to the disturbances. Fig. 10 shows the results of evaluating the effectiveness of model adaptive capability when the properties of input material vary during the operation. The evaluation is performed to an extent that different input material is being processed. The star–dotted points represent the published experimen-

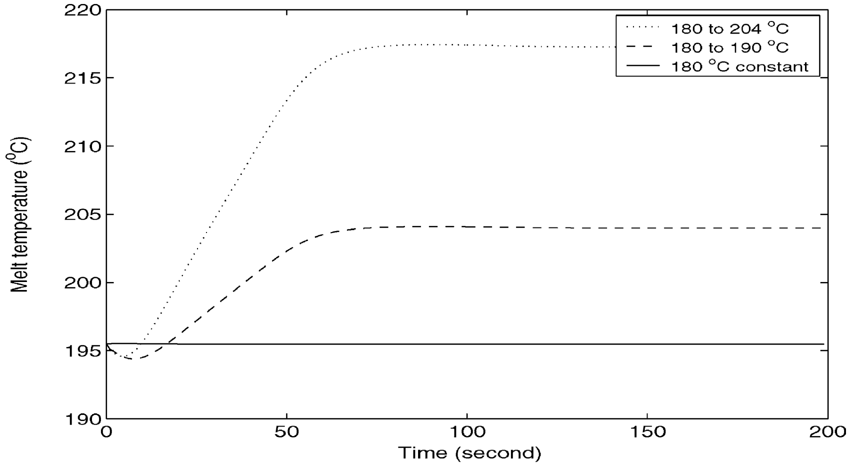

Fig. 9. Transient responses of melt temperature in changing barrel temperature.

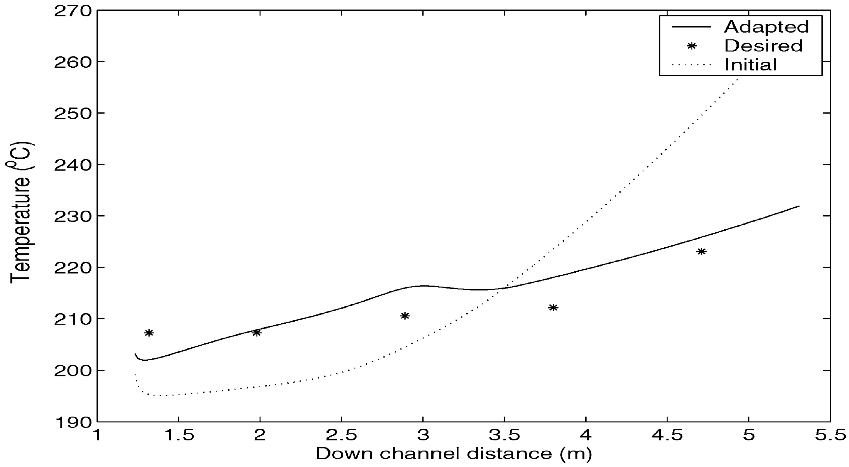

Fig. 10. Effectiveness of model adaptive capability for different processing material.

tal measurements of the melt temperatures at five locations distributed along the barrel, when the new material (high density polyethylene) is being processed. The dotted line shows the initial prediction of the semi-physical model. The prediction error is obvious as the approximations of the sub-models are based on the information of old material (low density polyethylene) before the adaptation. The smooth line shows a reasonable good prediction after the adaptation. The sub-models have been tuned automatically to approximate the operational-sensitive parameters in the new operating environment.

The model is further evaluated when it is employed as the predictive model in the control scheme namely as the fuzzy supervisory indirect learning predictive controller (FsiLPC) [12]. Fig. 11 indicates that without the adaptation, both of the plant outputs at die diverge if the prediction error exists. When the model adaptation commences, specifically when the approximations of the sub-models have been tuned automatically according to the varying operating conditions, the melt temperature and the pressure are regulated within tolerances as shown in Fig. 12a and b, respectively.

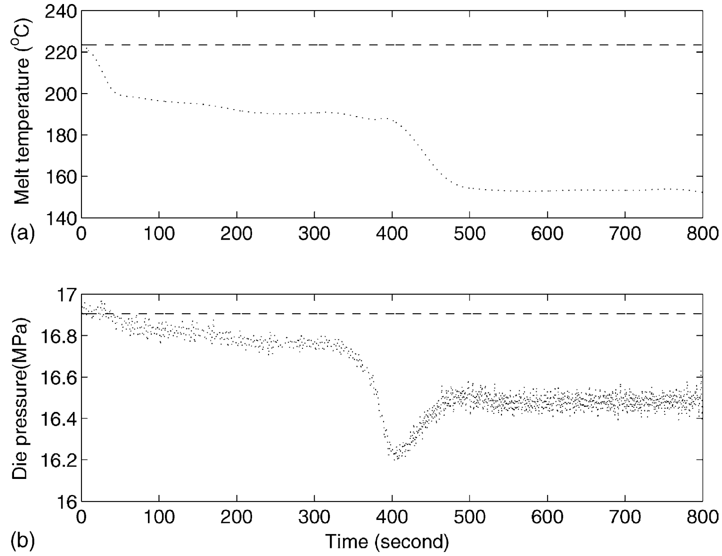

Fig. 11. Extrusion control with prediction error without model adaptation: (a) melt temperature at die and (b) melt pressure at die.

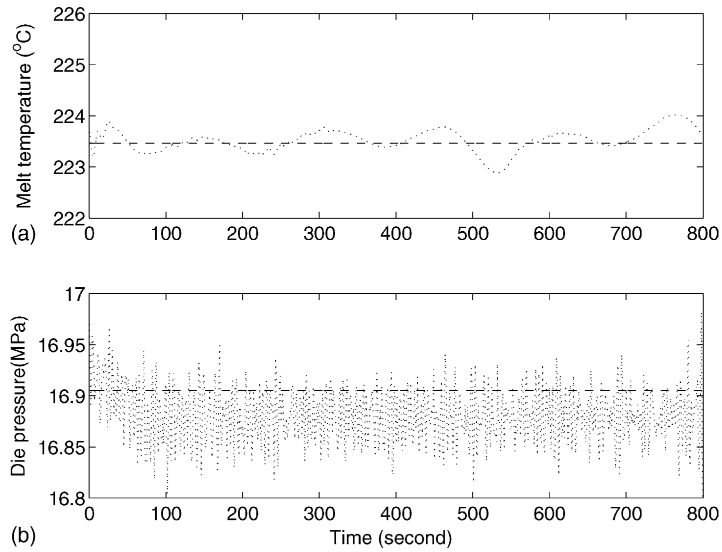

Fig. 12. Extrusion control with prediction error with model adaptation: (a) melt temperature at die and (b) melt pressure at die.

5. Conclusions

The paper highlighted some of the problems associated with the polymer extrusion modelling for real-time control applications. A semi-physical dynamic model has been developed to estimate the melt temperature and the pressure at the die. These parameters are regarded as the quality indicators of the extrusion operation. Fuzzy rule-based sub-models were applied as a means to capture the non-linearity characteristics of the operational-sensitive parameters. The optimal structures for the sub-models were established by a GA-fuzzy algorithm. The gradient-based error back-propagation algorithm was implemented only to stimulate the parameters convergence by 'climbing the remaining hill' and to equip the sub-models with an adaptive capability. The optimised structure with smaller number of membership functions and rules would help to increase the interpretability while avoiding the problem of over-parameters. Besides, the speed of simulation would also improve as the sub-models contain fewer parameters.

The model was first evaluated in the basis of consistency with the theoretical analysis. The model predictions in general adhered to the theory when step changes in the manipulating parameters such as the screw speed were simulated. Further evaluations were performed to check the usefulness of sub-models adaptations. The results showed that the sub-models, which represent the operational-sensitive parameters had effectively adapted to the changing environment.

Future work is planned to fully evaluate the conditions for employing the semi-physical model in the design of fuzzy supervisory indirect learning predictive controller in the extrusion process. The advantage of the methodology lies on its multivariable supervisory ability; the effects on the output parameters are considered before a control action such as altering the screw speed is implemented. With this ability, an optimum control function can be ascertained.

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