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# Dynamic Gray-Box Modeling for On-Line Monitoring of Polymer Extrusion Viscosity

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**Melt viscosity is a key indicator of product quality in polymer extrusion processes. However, real time monitoring and control of viscosity is difficult to achieve. In this article, a novel "soft sensor" approach based on dynamic gray-box modeling is proposed. The soft sensor involves a nonlinear finite impulse response model with adaptable linear parameters for real-time prediction of the melt viscosity based on the process inputs; the model output is then used as an input of a model with a simple-fixed structure to predict the barrel pressure which can be measured online. Finally, the predicted pressure is compared to the measured value and the corresponding error is used as a feedback signal to correct the viscosity estimate. This novel feedback structure enables the online adaptability of the viscosity model in response to modeling errors and disturbances, hence producing a reliable viscosity estimate. The experimental results on different material/die/extruder confirm the effectiveness of the proposed "soft sensor" method based on dynamic gray-box modeling for real-time monitoring and control of polymer extrusion processes. POLYM. ENG. SCI., 52:1332-1341, 2012. © 2012 Society of Plastics Engineers**

## INTRODUCTION

Extrusion is a widespread practical method in polymer processing, but controlling the quality of an extrudate material and hence the final product, presents various problems. The feed materials can be highly variable and unpredictable in nature, and the selection of appropriate operating conditions for each material to obtain a desired

extrudate quality is a complex task. This results in large amounts of energy and material being wasted during long set-up times, by using nonoptimum operating conditions. Real-time monitoring of the quality of the extrudate material during the extrusion process is therefore desirable to achieve reduced set-up times and improved operation of the extrusion system. In comparison with melt temperature and pressure, melt viscosity is largely recognized as one of the most relevant indicators of melt quality as it is directly related to the esthetic/dimensional properties of the melt and the molecular orientation relating to the functional properties of a polymeric extrudate [1, 2]. However, on-line viscosity measurement to a required standard has proved difficult to achieve due to the highly nonlinear and significant time delay behaviors of the process.

Currently there are a few types of melt viscosity measurement, including (1) off-line laboratory capillary rheometer (LCR), which is most accurate but involves significant time delay; (2) on-line side-stream rheometer, in which melt is taken as a side stream from the flow line by a gear pump for sampling, and results in time delay of several minutes. Besides, the side stream may not always represent the property of the bulk flow [3]; (3) in-line rheometer, which is more relevant to the process control than the above two methods since it is directly mounted in the main process flow and has advantage of real time monitoring. However, the cross section of the in-line rheometer is usually small, which results in a limitation to use in mass production [1]; (4) torsional viscometer, which gives reliable real time measurements but is expensive, particularly for producers with several extrusion lines to instrument.

For the above reasons, an alternative approach to obtain the viscosity, in the name of "soft computing," "inferential modeling," or "soft sensor" has been proposed and recently attracted significant academic and industrial interests. This method involves the estimation

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of the melt viscosity based on the system inputs, such as temperature and screw speed. Because of the inherent nonlinearities of the extrusion process, linear modeling techniques are limited in their effectiveness. Currently, the majority of nonlinear modeling methods are based on neural networks which have demonstrated their ability in producing adequate nonlinear dynamic inferential models for viscosity [4, 5]. The drawbacks of those methods are that too many parameters need to be tuned with a limited data set available; moreover, the black box modeling methods lack physical insight into the applied process. Therefore, the development of combining mechanistic and parametric models has been investigated recently. A rheological model based on first principles of power-law equation was proposed by Chen et al. [1]. However, the parameters were obtained by off-line experiments and it is not possible to adapt the model to varying operational conditions and hence limits its application in real time control. For a better solution, a gray-box model combined with a hybrid method of genetic algorithm with fuzzy system has been implemented, and the model parameter is adaptive to the changing working conditions based on simulation data [6]. It was also demonstrated that the genetic programming algorithm not only outperforms the neural network method, but also has a simple transparent model structure [5].

In spite of the effectiveness of the gray-box modeling technique assisted with genetic algorithms (GA), which combines both fundamental first principles and experimental data-driven approach, the existing methods are inherently open-loop, and therefore suffer from all the problems associated with open-loop systems, i.e., they are intolerant to any changes in the extrudate material or processing conditions. To tackle this problem, a soft sensor with a feedback structure was proposed in previous work [2, 7]. The soft sensor structure is based on that of a state observer [8] where an open-loop estimator (viscosity model) is combined with a feedback correction mechanism performed by a pressure model. The novel feedback structure enables the online adaptability of the viscosity model in response to modeling errors and disturbances, hence producing a reliable viscosity estimate. Both pressure and viscosity models were developed using gray-box modeling with GA [2, 7]. Potential to relate model parameters on different grades of the same polymer (low density polyethylene) has been demonstrated. However, extension of the technique to materials exhibiting significantly different properties and to processing in more complex industrial extruders would result in more complex models and loss of physical meanings. In this study, greater use of first-principle models is employed with the aim of identifying a simple model structure which, in combination with a mechanism to correct for oversimplifications in the model, can capture the viscosity dependence of a wide range of polymeric materials and different machines and dies. More precisely, the dynamic models in the proposed soft sensor structure are further investi-

gated and improved in this article: (1) the barrel pressure, which can be applied to any extrusion process but also is less dependent on the die design, is examined instead of the die pressure; (2) a NFIR (nonlinear finite impulse response) model for the pressure and the viscosity model was identified respectively by the GA-based dynamic gray-box modeling method instead of the NARX (nonlinear autoregressive with exogenous input) model, which has the advantage of inherent stability, without the need for feedback but exhibiting good performance; (3) both pressure model and viscosity model are simplified to a fixed structure with adaptable linear parameters which can be easily and quickly adapted to different polymers, extrusion machines and dies without extensive remodeling, resulting in good practical applicability in industry.

It is worth noting that, from the control point view, it is known that both the barrel temperature and screw speed have significant effect on the quality of the final product and the energy efficiency of the process [7]. Thus, both barrel temperature and screw speed have been used as input variables in this study. It is noted that similar work has been reported recently in [9, 10] which developed dynamic gray-box models relating melt pressure and melt temperature to screw speed (or feed rate) along with random binary sequence (or stair) type excitation for twin screw extrusion. Different from [9, 10], in this study, four input variables including three barrel temperatures and screw speed, have been excited simultaneously with a pre-designed pseudorandom signal (PRS) and hence a wide range of operating conditions has been covered for a single screw extruder. Both pressure model and viscosity model have been developed based on dynamic gray-box models acting as a soft sensor for viscosity monitoring.

The article is organized as follows: The general description of the extrusion process and the concept of soft sensor are briefly explained next, followed by the first principles and the methodology of the GA-based dynamic gray-box modeling method. Then the experiment for data generation with different materials, dies and extruders is described in detail. Then the pressure model and the viscosity model identified by the dynamic gray-box modeling method are presented, followed by the integrated soft sensor test and implementation. Conclusions are given at the end of the article.

## SOFT SENSOR FOR EXTRUSION PROCESS

### *Single Screw Extrusion Process*

Single screw extrusion is one of the core operations in polymer processing and therefore is the focus of this study. A conventional single screw extruder is divided into three main functional zones: a feed zone, a melting zone and a metering zone. Each of the three zones must perform a specific function to achieve a successful deliv-

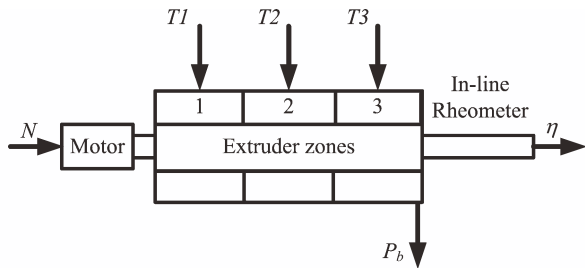


FIG. 1. The diagram of a single screw extruder with input (screw speed  $N$ , and barrel temperature  $T_1, T_2, T_3$ ) and output variables (barrel pressure  $P_b$ , and viscosity  $\eta$ ).

ery of the polymer melt to the die at a desired constant melt temperature, pressure and viscosity [11].

Figure 1 depicts the diagram of a typical single screw extruder with process input and output variables. The input variables, including the screw speed,  $N$ , and the barrel temperature  $T_1, T_2, T_3$ , can be used as manipulated variables to control the extrusion process. The output variables, such as the melt viscosity,  $\eta$ , and the barrel pressure,  $P_b$ , can be used as control variables to design a closed loop control scheme. The ultimate goal of any control scheme in a polymer extrusion process is to control the final product quality. Melt viscosity is largely recognized as one of the most relevant indicators of melt quality. However, on-line viscosity measurement to a required standard has proved difficult to achieve. Thus, controlling the melt viscosity requires good understanding of the process and prediction of it from available process variables.

### Soft Sensor

The principle of the soft sensor is based on a feedback observer mechanism, which was introduced in the previous work in [7, 12] as shown in Fig. 2. A viscosity model was identified based on the process inputs, such as barrel temperatures and screw speed, to infer the melted viscosity. The estimated melt viscosity, together with the screw speed, is then used as input variables for the pressure model to predict the barrel pressure. Finally, the predicted barrel pressure is compared with the actual measured value, and the generated error used as a feedback signal to correct the estimated viscosity. This novel feedback structure enables the online adaptability of the viscosity model in response to modeling errors and disturbances, hence producing reliable viscosity estimate. In Fig. 2,  $T_i$  is the barrel temperature in zone ( $i = 1, 2, \dots, n$ );  $e$  is the error signal of the predicted barrel pressure,  $\tilde{P}_b$ , and the measured barrel pressure,  $P_b$ . The accuracy of the feedback soft sensor depends largely on the accuracy of the pressure model as it corrects deviations in the viscosity model. The accuracy of the viscosity model is more relevant to achieving precise control of the process. To carry out the proposed method it is necessary that viscosity data for the polymer must be determined in advance to initially

identify the viscosity model using a capillary rheometer or equivalent equipment, such as in-line rheometer. The data evaluated by the proposed method is compared with that obtained by the in-line rheometer.

## MODELING TECHNIQUE

### First Principles

The extrusion process is characterized by strong interactions between mass, energy, and momentum transfer, coupled with physiochemical transformations which determine the properties of the final product [9]. To obtain robust models for the barrel pressure and the melt viscosity, it is essential to understand the underlying behavior of process variables using first principles knowledge.

**Pressure Model.** The physical relationship of the back pressure with the throughput rate and the melt viscosity is recalled by the Poiseuille equation [13]:

$$P_b = \alpha Q \eta \quad (1)$$

where  $\alpha$  is a parameter related to die resistance, and  $Q$  is volumetric throughput. Note that this equation holds for laminar flow in a capillary or slit die—in general laminar flow will not be fully achieved in a practical situation, also more complex dies will not follow this relationship. However it does give an approximation. As  $Q$  was proportional to screw speed for the plant and material used in this article, under these conditions the barrel pressure is

$$P_b = \alpha \beta N \eta \quad (2)$$

where  $\beta$  is a parameter related to the material and the machine.

**Viscosity Model.** The viscosity of a polymer melt can generally be considered as a function of shear rate, temperature, and pressure. In extrusion, polymer melts are in a predominantly shear flow regime where the viscosity follows a power-law relationship with shear rate

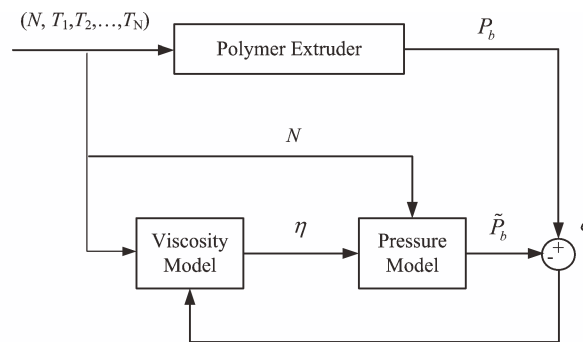


FIG. 2. Soft sensor with a feedback structure.

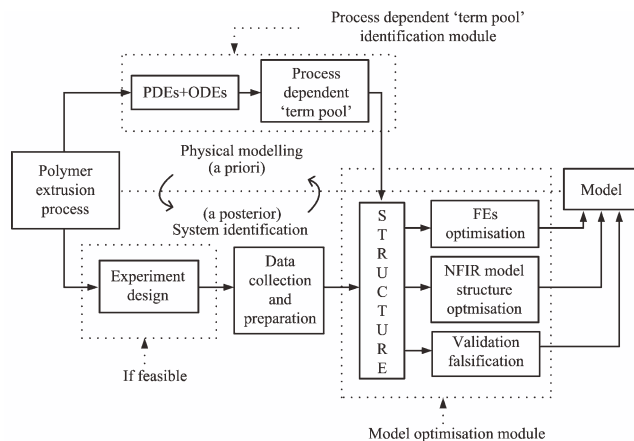


FIG. 3. Dynamic gray-box modeling framework for a polymer extrusion process.

$$\eta = m\dot{\gamma}^{\bar{n}-1} \quad (3)$$

where  $\eta$  is the shear viscosity,  $\dot{\gamma}$  is the shear rate, and  $m$  and  $\bar{n}$  are material-specific parameters (consistency index and power-law index). The relationship between viscosity and temperature is less explicitly defined; increasing temperature tends to decrease viscosity, but the nature of this behavior varies with the polymer type and state. A number of physical and empirical relationships have been proposed in the literature to describe behavior at various conditions. For a material in the power law region, an Arrhenius-type representation of the consistency index as a function of temperature is commonly applied

$$m = m_0 e^{-b(T-T_0)} \quad (4)$$

where  $m_0$  is the consistency index at a reference temperature,  $T_0$ .  $b$  is a constant in the range of [0.01, 0.1] [14].

### GA-Based Dynamic Gray-Box Modeling

In this subsection the GA-based dynamic gray-box modeling method [15] which was used both for the pressure and the viscosity modeling in the soft sensor structure is reviewed. It involves a genetic algorithm approach to identify the model structure and unknown parameters which best fitted the measured process output, based on a priori knowledge of process fundamental mechanism and empirical data. A priori “term pool” including candidate model terms is defined to capture the fundamental relationship between the system input and the output variables. More details on the methodology of the dynamic gray-box modeling and the GA approach are presented below [15–17].

**Methodology.** Within the context of nonlinear model using linear-in-parameter polynomial structure, fuzzy method, neural networks etc, the underlying principle is to use simple linear or nonlinear functions as the basis to approximate a complex process. Every process has its

own particular characteristics and may exhibit particular behavior. It is possible to select the approximation basis, such as the nonlinear terms in a linear-in-parameter generalized polynomial model structure or the activation function in the neural networks, according to a priori knowledge of the process. However, how much success a model can achieve largely depends on the form of the chosen approximation basis or functions.

These basic approximation functions acquired from the fundamental a priori knowledge of the studied process was referred to as fundamental elements (FEs) [16] and they formed the candidate model terms or the process “term pool.” Once the FEs are collected, a process model which reflects the dynamics of the process may be appropriately determined combining these FEs. At this model construction stage experimental data is required. Therefore, the applied dynamic gray-box modeling technique involves a search for the FEs from the “term pool” of the process, and then constructing the process model using appropriate combinations of these FEs.

Most system modeling methods would assume that the model structure is known or partially known, and that the main modeling task is to identify unknown parameters and unmodeled dynamics. Such methods may be suitable for simple systems, however, for complex polymer extruder processes, it is impossible to build a simplified model as the process fundamental knowledge only partially known. In the applied dynamic gray-box modeling method proposed by Li et al. [15], physical modeling and system identification form two interacting paths, as shown in Fig. 3. The essential part of this method aims to produce a simple NFIR model structure for the polymer extrusion process with only the “term pool” being proposed from a priori knowledge of process fundamental mechanism.

As shown in Fig. 3, for complex polymer extrusion processes where it is impractical to obtain a simple model structure, the main task in the physical modeling path (the upper part in Fig. 3) is to establish the fundamental “term pool.” Such a “term pool” is formed with appropriate static nonlinear functions that are uniquely identified from a priori process knowledge. The main task for the model optimization module in the lower part of Fig. 3 is to optimize the NFIR model structure and the associated parameters. The genetic algorithms for example were used for this purpose. The identification function in the lower part of Fig. 3 is for data collection and preprocessing, which is used later in the optimization module to obtain the optimal model.

These fundamental functions in the “term pool” can be power, exponential etc, which depend on the studied process, or the mathematical equations describing the fundamental laws governing the process behavior. A NFIR model can then be identified to represent the original process through appropriate composition and recombination.

**Optimization of NFIR Model by the Dynamic Gray-Box Modeling With GA.** As mentioned in the previous subsection, to obtain a NFIR model reflecting the special

nonlinear characteristics of the process, one of the solutions is essentially to extract process-dependent fundamental static functions, which are then incorporated into the NFIR structure as the fundamental elements, resulting the mathematical formulation of the identified NFIR model given by

$$y(t) = \sum_{i=0}^p \theta_i \phi_i(t) \quad (5)$$

where

$$\begin{cases} \phi_0(t) = 1 \\ \phi_i(t) = \phi_i(f_{u_1}(u_1(t - d_{u_1}), \bar{\theta}_{d_{u_1}}), \dots, f_{u_m}(u_m(t - d_{u_m}), \bar{\theta}_{d_{u_m}})) \\ i = 1, 2, \dots, p \end{cases} \quad (6)$$

and  $y$  and  $u_j$  ( $j = 1, 2, \dots, m$ ) are the process outputs and the inputs,  $\theta_i$  and  $\bar{\theta}_{d_{u_j}}$  is the linear and nonlinear parameter respectively,  $f_{u_j}$  and  $\phi_i(t)$  denote the fundamental elements and the candidate model terms respectively, and  $d_{u_j}$  is the time delay for the process inputs  $u_j$  with its range identified based on the physical knowledge of the process.

Given a performance index, optimization of the nonlinear NFIR model formulated in Eq. 5 is a mixed integer nonlinear hard problem including the following possible issues: (1) selection of model inputs (2) selection and optimization FES (3) optimization of the NFIR model structure (4) NFIR model training. Conventional optimization methods often fail to search and find the optimal solution for a mixed integer hard problem as stated above. As a stochastic optimization tool, the genetic algorithm was used for the above problem, and more details can be found in [16, 17].

Based on the above analysis, a GA-based dynamic gray-box modeling software has been developed [16, 17] and formed a platform for the dynamic modeling of the soft sensor proposed in this article.

## EXPERIMENTAL

### Materials

The six polymers including low density polyethylene (LDPE), high density polyethylene (HDPE) and polypropylene (PP) used in this study and some of their properties, such as the melt flow index (MFI-g/10 min) and melt density ( $\text{g/cm}^3$ ), are listed in Table 1. The MFI values for LDPE1 (LD159AC), HDPE1 (HHM TR114), and PP (Capilene M45F) are measured according to the ASTM D1238 procedure, and for the rest (LDPE2 and LDPE3: Dow352E and Lupolen 2426H, HDPE2: Sabic B6246LS) the ISO 1133 procedure was used. Both procedures were based on a weight of 2.16 kg, and a tem-

TABLE 1. Polymer resins and melt index.

Polymer	Trade name	Source	MFI	Density
LDPE1	LD159AC	ExxonMobil Chemical	1.2	0.923
LDPE2	Dow352E	Dow Chemical Company	2.0	0.925
LDPE3	Lupolen 2426H	LyondellBasell Industries	1.9	0.925
HDPE1	HHM TR114	Marlex Polyethylene	0.18	0.946
HDPE2	Sabic B6246LS	Saudi Basic Industries	0.5	0.962
PP	Capilene M45F	Carmel Olefins Ltd.	8.0	0.950

perature of 230°C for PP and 190°C for the rest. The selected polymers for testing are general purpose polyethylene/polypropylene. To check if the identified model structure is still valid to material blends that are commonly used in industrial plant, the experiment on HDPE blends (50% HDPE1 with 50% HDPE2) was also carried out.

### In-Line Rheometer Slit-Die and Capillary-Die

To carry out the proposed “soft sensor” approach, it is necessary that viscosity data for the polymer is obtained in advance using a laboratory capillary rheometer or in-line rheometer. A schematic of the designed in-line rheometer slit-die (slit channel height,  $H = 2$  mm, width,  $W = 39.25$  mm) and the capillary-die (bore radius  $R = 4.7$  mm) used for measuring viscosity is shown in Fig. 4 in which the pertinent dimensions and spacing of the pressure transducers are shown. Three pressure transducers are equidistant along the length of the die to identify the pressure drop. More details of the in-line-rheometer design can be found in the previous work [18]. For a capillary die, the melt viscosity calculation is based on the relation between the pressure drop  $\Delta P$

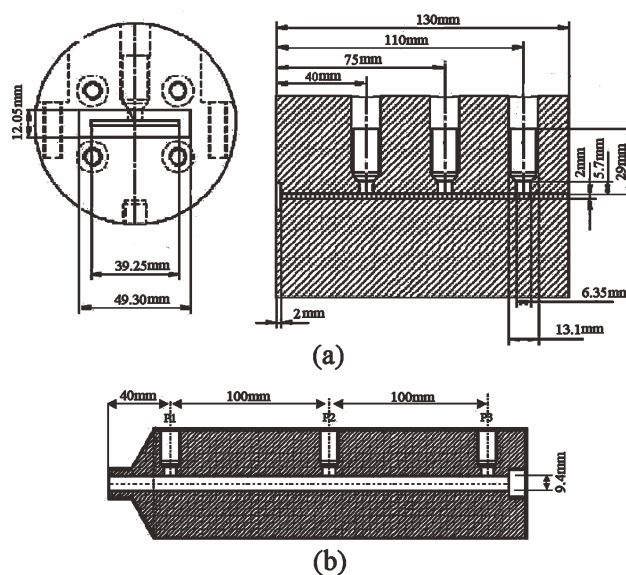


FIG. 4. (A) Slit die, (B) capillary die.



FIG. 5. Photograph of the laboratory Killion KTS-100 single screw extruder with in-line-rheometer die.

across the in-line capillary die and the flow rate  $Q$  as follows [19]:

$$\eta = \frac{\Delta P \pi R^4}{2LQ} \frac{\bar{n}}{3\bar{n} + 1} \quad (7)$$

For the slit die, the viscosity is formed as [19]

$$\eta = \frac{\Delta P W H^3}{12LQ} \frac{3\bar{n}}{2\bar{n} + 1} \quad (8)$$

where  $L$  is the length between the adjacent pressure transducers. To enable real-time calculation of viscosity, the throughput was modeled offline. The polyethylene examined in this study showed a simple linear relationship between mass throughput and screw speed when the operating temperatures are fixed.

### Single Screw Extruder

The research was performed on two single screw extruders, one is 25.4 mm, Killion KTS-100 and the other is 38 mm, Killion KN-150. Both extruders used in this study have three heating zones (feed zone, melting zone, and metering zone) controlled by the Eurotherm 808 PID controller. An in-line rheometer die for viscosity measurement is connected at the barrel exit by the clamp ring and the adaptor. The feed section is water-cooled to prevent an early rise in polymer temperature. The in-line rheometer, the clamp ring and the associated adaptor were kept at constant temperature. Typical sensing elements such as thermocouples and pressure transducers are located on the barrel and the die to provide continuous data on the state of the polymer. Figure 5 shows a photograph of the 25.4 mm extruder instrumented with a capillary in-line-rheometer die.

A LabVIEW software programme was developed to communicate between the experimental instruments and a

computer. All signals were acquired at a 10-Hz sampling rate using a 16-bit DAQ card through a SC-2345 connector box, but averaged over every 10 samples to reduce the sampling frequency to 1 Hz.

### Input Excitation

As mentioned in the previous section, both the barrel temperature and screw speed have significant effect on the quality of the final product and the energy efficiency of the process [7]. Thus, both barrel temperature and screw speed have been used as input variables in this study. For obtaining some information-rich data sets of process inputs, the screw speed,  $N$ , and the temperature settings at the three heating zones,  $T_1$ ,  $T_2$ ,  $T_3$ , were excited using a PRS (pseudorandom signal) applied in a “random walk” algorithm, respectively. It is the signal excited by a Gaussian sequence and the period of input change was also defined by a Gaussian sequence where the mean and standard deviation ( $\sigma$ ) were defined based on the measured pressure and viscosity response time to step changes in the inputs. Thus a wide operating range, including both the low frequency and high frequency spectra, was covered in the sequences while consecutive input changes were within practical operating limits [2]. The defined input sequence parameters are given in Table 2. Figure 6 shows an example of the filtered screw speed and the three-zone barrel temperature signals excited by the designed PRS.

Six different tests, as illustrated in Table 3, were performed under the designed PRS excitation, using six polymers, two dies and two extruders. Dynamic gray-box modeling based on GA was applied for both pressure and viscosity model structure identification, using data of Test A. Both model structures were further investigated and generalized from modeling of different material, die, and extruder using data of Tests B–F. More details of model identification are presented next.

TABLE 2. Excitation sequence parameters.

	Amplitude		Period (s)		Limit	
	Mean	$\sigma$	Mean	$\sigma$	Upper	Lower
<b>LDPE</b>						
$N$	65	5.0	30	3.0	105	30
$T_1$	155	3.5	120	5.0	175	135
$T_2$	160	3.5	120	5.0	180	140
$T_3$	160	3.5	120	5.0	180	140
<b>HDPE</b>						
$N$	60	5.0	60	3.0	105	30
$T_1$	190	3.0	150	5.0	195	185
$T_2$	200	3.0	150	5.0	205	195
$T_3$	210	3.0	150	5.0	215	205
<b>PP</b>						
$N$	80	5.0	30	3.0	105	45
$T_1$	195	4.0	120	5.0	205	185
$T_2$	200	3.5	120	5.0	210	180
$T_3$	210	3.5	120	5.0	215	185

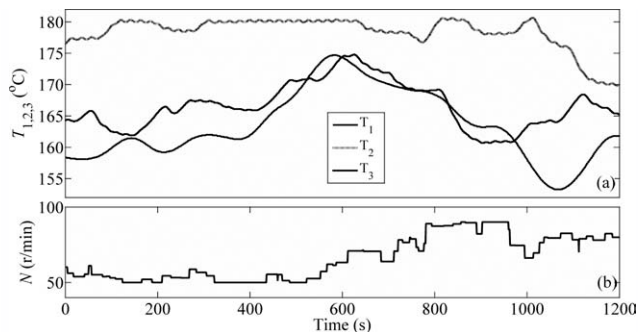


FIG. 6. Filtered screw speed and three-zone barrel temperature signals excited by designed PRS.

## RESULTS AND DISCUSSIONS

The dynamic gray-box modeling method presented in the modeling technique section was used for pressure and viscosity model in the previous work [7, 12]. Here, both models have been further improved and generalized to a broader material range with different die and extruder. The improvements include (1) the barrel pressure, which is widely measured in industrial processes and less dependent on the die design, is examined instead of the pressure inside the die; (2) The NFIR model was used instead of previous NARX model, which has a few advantages, for example, the NFIR model is inherently stable, and requires no feedback of the model output; (3) The motor power and other terms in the form of  $N^{k_i} \eta^{k_j}$  ( $k_i, k_j$  is a constant) were considered in the previous work and resulted in a random model structure. The NFIR model presented in this study has less terms in the predefined “term pool” based on the first principles which results in a simplified model structure; (4) The NFIR model has a linear-in-the-parameter structure, where the linear parameters are fairly easy to update by the least square method [20] on-line for different materials. Moreover, with the requirement of identifying only the linear parameters for different die and extruder, this NFIR structure performs well without employing the expensive GA-based dynamic gray-box modeling method.

### Dynamic Gray-Box Model for Barrel Pressure

The priori “term pool” for the dynamic gray-box modeling method is paramount to the success of the identified

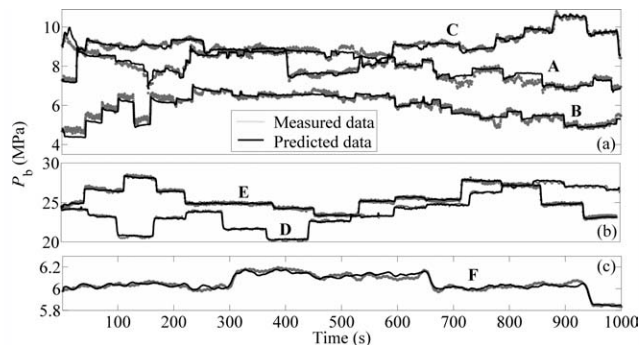


FIG. 7. Barrel pressure model performance on data of Test A-F.

model. Based on the above physical relationship between the barrel pressure and the screw speed and the melt viscosity in Eq. 2, the “term pool” for the pressure model is defined by the products of screw speed and viscosity:  $N(t - d_N)\eta(t - d_\eta)$ , where,  $d_N, d_\eta$  represents the time delay. Using the dynamic gray-box modeling method, the pressure model is generated with a time series of system inputs based on Test A data

$$\tilde{P}_b(t) = \theta_1 + \theta_2 N(t-1)\eta(t-1) \quad (9)$$

where  $\theta_1 = 1.45$  and  $\theta_2 = 1 \times 10^{-3}$ . The error residual of the above model based on data of Test A has zero mean and variance 0.03, which can be approximated by a normal distribution. Its performance on the unseen validation measured barrel pressure data of Test A is shown in Fig. 7, with the root mean square (RMS) percentage error, 2.3%. The RMS percentage error (RMSPE) here is used for evaluation purpose and is defined as

$$\text{RMSPE} = \frac{\sqrt{\sum_{i=1}^S (y_i - \tilde{y}_i)^2 / S}}{\bar{y}} \times 100\% \quad (10)$$

where  $S$  is the number of samples,  $y_i, \tilde{y}_i$  and  $\bar{y}$  is the measured value, the predicted value, and the mean value, respectively.

The effect of changes in material, die or machine on the pressure model is further investigated to adapt this model to different material or machine without extensive remodeling. Other five tests (B-F), as shown in Table 3, on five

TABLE 3. Experimental material/die/extruder.

	Material					Die		Extruder		
	LDPE1	LDPE2	LDPE3	HDPE1	HDPE blends	PP	Capillary	Slit	25.4 mm	38 mm
A	✓						✓		✓	
B		✓					✓		✓	
C			✓					✓	✓	
D				✓				✓		✓
E					✓			✓		✓
F						✓	✓		✓	



TABLE 4. Linear in parameters and the RMS percentage errors (RMSPE) of the pressure and the viscosity model on different tests using different methods.

	Proposed dynamic gray-box NFIR		Black-box polynomial NFIR	
	$\theta$	RMSPE	$\theta$	RMSPE
<b>Pressure model</b>				
A	$[1.45, 1 \times 10^{-3}]$	2.45%	—	—
B	$[0.47, 1 \times 10^{-3}]$	3.41%	—	—
C	$[-0.66, 2 \times 10^{-3}]$	1.80%	—	—
D	$[-0.97, 4 \times 10^{-3}]$	0.65%	—	—
E	$[-3.69, 3 \times 10^{-3}]$	0.64%	—	—
F	$[-0.09, 1 \times 10^{-3}]$	0.03%	—	—
<b>Viscosity model</b>				
A	$10^3 [3.05, -0.12]$	0.96%	$[232.85, 16.25, -0.03, -0.05]$	1.30%
B	$10^3 [1.87, -0.07]$	1.28%	$[802.86, -8.31, 0.01, -0.0007]$	54.87%
C	$10^3 [2.78, -0.12]$	2.05%	$[1.19 \times 10^3, -6.4, 0.30, -0.88]$	3.63%
D	$10^3 [8.18, -0.39]$	1.31%	$[3.54 \times 10^3, -31.4, -3.5, -1.2]$	8.01%
E	$10^3 [6.57, -0.30]$	1.62%	$[3.36 \times 10^3, -16.2, -9.2, -1.8]$	42.88%
F	$10^3 [3.01, -0.11]$	0.05%	$[1.28 \times 10^3, -12.6, 0.02, -0.01]$	55.59%

polymers, two dies, and two extruders were carried out for this purpose. The linear parameters and the root mean square percentage errors of the pressure model on different tests using the proposed NFIR, are presented in Table 4.

When the model was applied on different materials but with the same die and extruder, there is an offset of 0.98 and the RMS percentage error is 3.4%. When the model was applied on different die and extruder in Test C–F, the RMS percentage error is less than 2%. The model performance on these tests is illustrated in Fig. 7. Based on the above analysis, it can be seen that the predicted pressure value of Test B–F matches the measured value very well. Thus the above NFIR structure based on the dynamic gray-box modeling reflects the fundamental physical relationship between viscosity and extruder pressure, and only the linear parameter  $\theta = (\theta_1, \theta_2)$  needs to be updated when the material, machine or die changes.

### Viscosity Model

In this subsection, the prediction model is generated to estimate the melt viscosity based on the process inputs. To reduce model complexity and to improve the performance, the dynamic gray-box modeling approach is also applied here for identification of a dynamic model which is a function of the properties of the material and the physical processes inside the extruder. To determine the “term pool” for viscosity model, a complex term approximating to an Arrhenius-type relationship may be appropriate. But as this involves a difficult problem of tuning several parameters, the “term pool” with power law terms,  $N^{k_1} T_3^{k_2}$  ( $k_1, k_2$  is a constant) [2] is selected. For a continuous nonlinear function a general power law element could potentially fit the relationship accurately if enough terms are included. However, it should be noted that a viscosity

model with more terms does not necessarily have better generalization ability. Using data of Test A, a NFIR viscosity model is identified

$$\tilde{\eta}(t) = \bar{\theta}_1 + \bar{\theta}_2 \mathbf{N}(t-1)^{0.22} \mathbf{T}_3(t-38)^{0.36} \quad (11)$$

The model performance of Eq. 11 on the unseen data of Test A is shown in Fig. 8, with the RMS percentage error 0.96%. It can be seen that the identified model (Eq. 11) by dynamic gray-box modeling method is able to describe the dynamic behavior of the LDPE1 material and hence tracks the viscosity change on the same material. Similar to the pressure model, the viscosity model with a fixed structure (Eq. 11) was applied on the data of Test B–F, to check the model performance on different material, die and machine, and the results are shown in Table 4 and Fig. 8. If the melt viscosity estimate  $\eta$  is used as an input to the pressure model, and then it might give an inaccurate predicted pressure value due to changes in feed material properties. For a better solution, the error  $e$  generated by the predicted and the measured pressure value

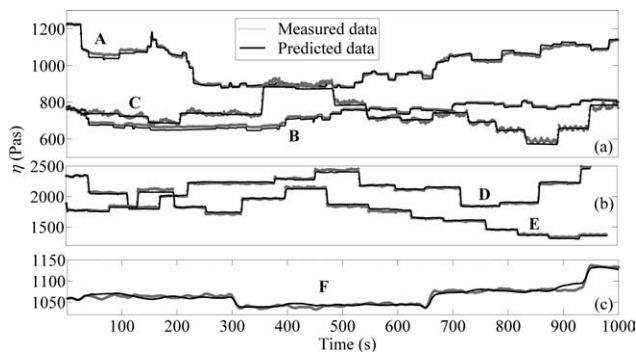


FIG. 8. Viscosity model performance on unseen data of Test A–F.

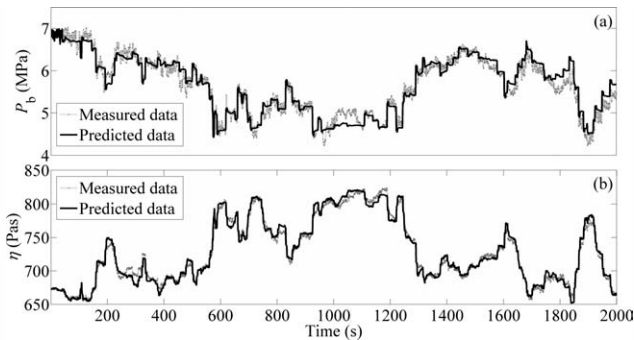


FIG. 9. Soft sensor performance on LDPE2 unseen data.

is used as a feedback signal to correct the melt viscosity estimate  $\tilde{\eta}$  of Eq. 11.

$$\hat{\eta}(t) = \tilde{\eta}(t) + k_p \mathbf{e}(t) + k_I \sum_{k=1}^{\infty} \mathbf{e}(t-k) \quad (12)$$

where the last two terms in Eq. 12 are in the forms of PI (proportional gain and integration) of the error signal,  $\mathbf{e}$ . To minimize the error signal between the predicted and measure barrel pressure value, the parameters in Eq. 12 can be identified.

The effectiveness of the soft sensor based on the pressure model and the viscosity model developed above is then tested on the unseen data of LDPE2 in the following section.

### Soft Sensor Testing

Applying the pressure model in Eq. 9 and the viscosity model in Eqs. 11–12 on the unseen LDPE2 data, the soft sensor performance on the barrel pressure and the viscosity is shown in Fig. 9.

The difference between the measured viscosity and the prediction value in terms of RMS percentage error is 0.46%. A satisfactory match between the estimated and the measured value validated the developed soft sensors for real time monitoring of the polymer extrusion process. Therefore, it has been verified that using the error between the predicted and the measured barrel pressure as a feedback to correct the viscosity estimate made the real time monitoring of viscosity feasible and reliable.

To better understand the advantage of the dynamic gray-box NFIR model proposed in this article over a general black-box polynomial NFIR model which does not incorporate first principle knowledge [21], the performance of the viscosity models based on the above two different approaches is illustrated in Table 4, with the identified black-box polynomial NFIR model

$$\tilde{\eta}(t) = \bar{\theta}_1 + \bar{\theta}_2 \mathbf{N}(t-1) + \bar{\theta}_3 \mathbf{N}(t-1) \mathbf{T}_3(t-5) + \bar{\theta}_4 \mathbf{N}(t-1) \mathbf{T}_3(t-8) \quad (13)$$

The polynomial NFIR model performance is good on the unseen LDPE1 data, with RMSE 1.3%; however, this model has poor generalization to data from different

materials of LDPE2 as well as PP even using the same machine and die, with RMSE 54.87 and 55.59%, respectively. Further, poor generalization performance is also observed on data from a different machine using HDPE blends, with RMSE 42.88%. This is due to the fact that the black-box modeling methods do not use physical knowledge. In comparison, the proposed NFIR model combines the first principles with the data-driven identification method, and hence the model terms reflect the physical relationship between the input and output variables, leading better model prediction performance.

### Soft Sensor Implementation

Implementation of the proposed “soft sensor” approach on any material/die/machine configuration involves off-line modeling and online monitoring. In model development, a data set describing the dynamic process behavior is first recorded to acquire the linear parameters of both pressure and viscosity models. In the on-line monitoring procedure, a feedback correction mechanism in the form of the PI of the error signal is employed and used to correct the predicted melt viscosity. The construction of the off-line models and the on-line implementation procedures can be summarized by the following steps.

For the off-line modeling, it involves: (i) Record dynamic data including the screw speed,  $\mathbf{N}$ , the barrel pressure,  $\mathbf{P}_b$ , the barrel temperature,  $\mathbf{T}_3$ , and the melt viscosity,  $\eta$  (measured by the in-line-rheometer in this study). (ii) Identify the parameters  $\theta_1$  and  $\theta_2$  of the pressure model in Eq. 9, based on the recorded screw speed,  $\mathbf{N}$ , the barrel pressure,  $\mathbf{P}_b$ , and the melt viscosity,  $\eta$ . (iii) Identify the parameters  $\bar{\theta}_1$  and  $\bar{\theta}_2$  of the viscosity model in Eq. 11 based on the recorded screw speed,  $\mathbf{N}$ , the barrel temperature,  $\mathbf{T}_3$ , and the melt viscosity,  $\eta$ .

For on-line monitoring, it involves: (i) Record normal operating data including the screw speed,  $\mathbf{N}$ , the barrel pressure,  $\mathbf{P}_b$ , the barrel temperature,  $\mathbf{T}_3$ . (ii) Compute the melt viscosity  $\tilde{\eta}$  based on Eq. 11 and the identified parameters  $\bar{\theta}_1$  and  $\bar{\theta}_2$ . (iii) Compute the barrel pressure  $\hat{\mathbf{P}}_b$  based on Eq. 9, the identified  $\theta_1$  and  $\theta_2$ , and the predicted melt viscosity  $\tilde{\eta}$ . (iv) Compute the error signal  $\mathbf{e}$  between the measured barrel pressure,  $\mathbf{P}_b$ , and the predicted barrel pressure,  $\hat{\mathbf{P}}_b$ . (v) On-line identification of  $k_p$  and  $k_I$  in Eq. 12 to minimize the predicted and the measured pressure values. (vi) Recompute the corrected melt viscosity  $\hat{\eta}$  based on Eq. 12.

## CONCLUSIONS

This article presents the latest progress and a comprehensive coverage of the soft sensor approach developed in the group, which has shown to be able to accurately estimate the viscosity using industrially available measurements, including barrel pressure, barrel temperatures, and screw speed, and is robust to process disturbances and adaptive to operation variations such as the change of materials. The proposed soft sensor structure is simple to

implement and has shown to be capable of tracking of polymer viscosity in extrusion based on the experimental data with RMS percentage error less than 1%. The success of the structure is due to (1) the identification of a pressure model with a simplified fixed structure (NFIR) which captures the fundamental physical relationship between the viscosity, screw speed and extruder barrel pressure by a dynamic gray-box modeling technique; (2) a NFIR model identified for the estimation of the melt viscosity based on the process inputs such as screw speed and temperature; (3) the viscosity model with adaptable linear parameters to different material; (4) using the error between the predicted and the measured barrel pressure as a feedback to correct the viscosity estimate which has made the real time monitoring of viscosity feasible and reliable. The developed soft sensor can greatly help to reduce the need for measuring devices and to develop robust on-line system identification and real time control of feed material changes in future work. It should also be noted that the soft-sensor framework presented in this article and in our previous research works is generic and can be extended to online prediction of many process variables which can not be directly measured online or are too expensive to measure in real-time.

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