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Soft Sensing of Melt Temperature in Polymer Extrusion

Chamil Abeykoon

Abstract—Precise monitoring techniques are invaluable to any process for diagnosing its operational health, safety concerns and also for achieving good process control. In polymer extrusion, it is quite difficult to visually observe the melt inside barrel during the process operation and hence the level of control of the process operational quality is highly dependent upon the process monitoring techniques. Currently, a number of physical sensing devices are widely available in industry for monitoring of parameters such as melt temperature, melt pressure, screw speed and so forth. However, there are some limitations to use physical sensors in process measurements due to several constraints such as their access requirements, disruptive effects on the melt flow, fragility, complexity, etc. Thus, the application of soft sensing techniques should be highly useful for improved process monitoring and hence for advanced process control. In this work, a general discussion is made on the soft sensors and soft sensing applications in polymer extrusion. Then, a soft sensor concept is proposed for the die melt temperature profile prediction in polymer extrusion. The simulation results showed that the proposed technique can predict the temperature profile across the melt flow in real-time with good accuracy. Eventually, the importance of developing of such soft sensing techniques is discussed while providing some of the possible directions for future research.

Index Terms—Polymer extrusion, Process monitoring, Infrared sensor, Soft sensor, Melt temperature profile, Modelling.

I. INTRODUCTION

Polymer extrusion is a fundamental technique of processing of polymeric materials and is involved in the production of various commodities in the diverse industrial sectors. Since materials are processed inside a closed barrel, process monitoring techniques are highly important in determining the process health and also for ensuring the process safety. Basically, the melt pressure and temperature (i.e., point or bulk measurements) monitoring techniques are well-established in industrial applications and these are used as the major measures of determining the process functional quality and the quality of the melt output. Obviously, the melt pressure is a good indication on process functional quality and the variations of melt pressure would result in fluctuations in melt temperature and process output rate. However, the commonly used melt temperature sensors are flush mounted to the barrel wall and also they are highly affected by the barrel wall set temperature. Moreover, they are not capable of measuring a melt temperature profile or detecting rapid variations in melt temperature [1], [2]. Melt temperature profile measurements are highly difficult in industry as it disturbs the smooth motion of the melt flow and also due to the factors such as access requirements, complexity, fragility

of the sensors, etc. Currently, no technique is available for making melt temperature profile measurements in industry. Furthermore, the melt viscosity (which is another important process parameter of indicating the melt quality) is also not possible to directly measure by using a physical sensor. The in-line rheometers, a common method of making viscosity measurements, are also not industrially attractive due to their possible disruptions on the steadiness and rate of the melt flow. Therefore, soft sensors and soft sensing should be highly invaluable for a process like polymer extrusion as it has a number of parameters which are difficult to directly monitor by a physical sensor. More details on the process operation and mechanisms of polymer extrusion can be found in the literature [2], [3].

A. Soft sensor

A soft sensor, a virtual sensor or an inferential estimator is a technique of estimating some particular parameter/s (e.g., quality measures, functional variables) in various applications when a hardware sensor is unavailable or unsuitable. Moreover, soft sensors are used in real-time process monitoring and control; fault detection; process diagnostics; etc. Currently, soft sensors are widely used in chemical processes such as reactors, distillation columns, cement kilns, food processing, paper and pulp industry, etc, to estimate the product quality parameters [4]. In the majority of these previous soft sensing applications, the non-linear behaviours of the industrial processes have been modelled with the techniques such as artificial neural network (ANN); fuzzy systems; partial least squares (PLS); support vector machine (SVM) and support vector regression (SVR) and some of these are discussed in the next section. Currently, soft sensors are becoming widely popular in various industrial applications due to their advantages such as:

- It can be highly useful in the applications where physical sensors may not be applicable or unsuitable.
- It offers real-time estimations while handling time delays.
- It is a low cost alternative for expensive online analysers.
- It can be easily implemented on the existing hardware platform and no additional investment may be required.

However, a few barriers/complexities are also attributed to the design/application of the soft sensors:

- It requires a considerable process expert knowledge, effort and time to design.
- Its performance depends on the quality of the training/validation data (may have problems due to outliers, noise and missing data).
- It may be specific only for a given machine, material or processing conditions.

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Obviously, the expert knowledge is playing a key role in the design and application of a soft sensor. The designer should have a sound knowledge in the areas such as process monitoring; data collection/processing; modelling and model training/validation; soft sensor design/adaptation/maintenance; etc. In the long run, the drifts of the process may be a major problem on the performance of the soft sensor and hence it should be compensated either by adapting or re-developing the model/s [5]. Therefore, designing and maintaining of a soft sensor is an extensive task and more details relating to this area can be found in the literature [4], [6], [7].

B. Inferential process monitoring in polymer extrusion

Although some of the key process parameters such as melt viscosity and temperature profile across the die melt flow are difficult to measure/monitor using physical sensors only a few previous work has been reported so far on inferential prediction of such parameters in polymer extrusion.

A previous work by the author [8], [9] made an attempt to predict the process thermal stability inferentially. Correlations between the screw load torque, melt pressure and melt temperature fluctuations were examined by analyzing experimentally measured signals. However, no strong correlations between these signals could be observed. It was found that the screw load torque signal is not sensitive enough to identify unstable melting issues as it is dominated by the solids conveying torque. However, melt pressure fluctuations had slight correlations with melt temperature fluctuations particularly at low screw speeds. Nevertheless, none of these signals showed sufficiently good performance for them to be used as a powerful tool of monitoring the process thermal stability inferentially. To the author's knowledge, there is no other reported work in the literature on inferential thermal monitoring in polymer extrusion.

Wang et al. [10] used a soft sensing approach for making online measurements of the degree of orientation of polymer materials incorporating ultrasonic velocity measurements and infrared spectroscopy. The relationship between the ultrasonic velocity and the degree of orientation were established based on a SVM approach. The authors mentioned that the soft sensing system was able to make accurate measurements with a relative error of around 5%.

Chitrakleha and Shah [11] proposed a steady-state melt flow index soft sensor for an industrial scale polymer extrusion process by using a SVR approach. The authors claimed that the SVR-based soft sensor was valid over a wide range of melt indices and outperformed the existing nonlinear least-square-based soft sensor in terms of lower prediction errors. Furthermore, they mentioned that the proposed technique is having a few tuning parameters (compared to neural network approaches) and good generalization capabilities over other nonlinear black-box modelling techniques.

Gonzaga et al. [12] developed a soft sensor for viscosity prediction of a polyethylene terephthalate (PET) production process. The soft sensor which was based on a feed-forward artificial neural network performed its predictions with a relative error of approximately 0.3%. Then, the sensor was

integrated with an industrial process control system through a supervisory system and the authors mentioned that the controller gave good performance by allowing an effective and feasible operation of the PET production plant.

Sharmin et al. [13] designed a PLS based soft sensor to predict the melt flow index of polymeric materials. In the development of the PLS model, 48 process variables and the corresponding time delays were considered. The sensor was implemented on an industrial reactor and the authors claimed that the successful results were achieved. Moreover, they have discussed about the difficulties associated with the data-driven modelling of industrial data.

McAfee et al. [14] proposed a soft sensor which consists of two models to estimate the melt viscosity. The first model predicts the viscosity based on the processing conditions while the second model predicts the pressure based on the estimated viscosity. The estimated pressure is compared with the actual die pressure and the error signal is used to compensate for errors in the viscosity prediction model. A grey box modelling technique was used to develop dynamic models and the sensor gave predictions within 2% error.

Shi and Liu [15] proposed a melt index (MI) prediction soft sensor for a polypropylene (PP) polymerization process. The model included in the soft sensor was developed by a weighted least squares support vector machines (weighted LS-SVM) approach and it predicts the MI based on nine input process variables. Moreover, this model predicted the MI with a mean relative error (MRE) of approximately 3.27% and outperformed the accuracy of the sensors based on LS-SVM and SVM approaches. In other work by Li and Liu [16], a MI soft sensor was proposed for the same polymerization process based on a radial basis function (RBF) neural network incorporating an adaptive ant colony optimization algorithm. As was mentioned by the authors, this sensor was able to predict the MI with an MRE of 0.44% which was superior in performance to their previous work.

Ogawa et al. [17] proposed a MI sensor for an industrial high density polyethylene process using a few on-line measurements. In general, two models were used in the inferential MI measurement system: (i) an MI model which presents the relationship between the process variables and the MI (ii) a cumulative model that describes the relationship between the MI of the total polymer in the reactor. The soft sensor was combined with a model predictive controller which was aiming at the process quality control. The authors claimed that the controller with the MI soft sensor performed well with less quality deviation but they are still undertaking trials prior to its application in industrial processes.

Few other work [5], [18]–[21] also attempted to inferentially predict some process parameters in polymer extrusion.

II. A SOFT SENSOR FOR DIE MELT TEMPERATURE PROFILE PREDICTION IN POLYMER EXTRUSION

A. Background

Melt thermal homogeneity/stability is a key requirement in polymer processing and hence the melt temperature is a commonly measured parameter in polymer processes.

Currently, a number of point/bulk measurement techniques are well-established in the industrial applications while a few thermal profile measurement techniques have been attempted in research. More details on these existing thermal measurement techniques in polymer processing were previously discussed by the author [3], [22], [23]. As was revealed by the previous work [3], [8], [22]–[25], temperatures at the different radial locations of the extruder output melt flow are significantly different and also these variations are dependent upon processing conditions, material being processed and the machine geometry. Obviously, point/bulk thermal measurement techniques are not capable of detecting these thermal variations across the melt flow although these are widely used in the current industrial applications. Hence, the melt temperature profile measurement is highly suitable for determining the actual thermal homogeneity/stability across the extruder output melt flow. Some of the measurement techniques in research (e.g., a thermocouple mesh [26], [27], a fluorescence technique [28]) are capable of measuring a temperature profile across the melt flow but these techniques are not yet suitable for use in a production environment due to constraints such as their complexity, limited durability, access requirements, disruptiveness on the melt flow and output, etc. Hence, it is clear that the physical sensors are not suitable for making die melt temperature profile measurements in practice and also a soft sensing technique is not yet available for this purpose. Thus, a novel approach for developing a temperature profile prediction (across the extruder die melt flow) soft sensor is presented in this study.

B. Concept

From the previous thermal monitoring studies [3], [22], [23], it has been realized that a thermocouple mesh technique [26], [27] is good in providing detailed and accurate information on the thermal homogeneity of the extruder output melt flow. Therefore, it was felt that it is better if it is possible to inferentially predict the melt temperatures at different melt flow radial locations to obtain similar types of measurements to the thermocouple mesh. In fact, thermocouple mesh technique can be used to collect experimental data and then the data can be used to develop a dynamic model to predict the melt temperature profiles across the melt flow during the process operation (i.e., in real-time). Although such a model can predict the melt temperature profile, it is still good to have some reference or correction for the predicted melt temperatures at the different radial locations to ensure the prediction accuracy. From the experimental results achieved by evaluating the commonly used melt temperature sensors in polymer processing [3], [23], it was found that an Infrared (IR) temperature sensor follows the process thermal dynamics in a similar way to the thermocouple mesh better than the other temperature sensors which were used in the evaluation. Specifically, it is not required to add any modification to the existing extruders to use an IR temperature sensor as it can be attached to a standard sensor port which is designed to attach typical temperature/pressure sensors. Moreover, the non-invasive melt temperature measurements with a fast

response time can be made by using IR sensors near to the screw tip or in the die during the process operation and hence it is industrially compatible. Therefore, an IR temperature sensor should be good to obtain a temperature feedback to correct the possible errors of the soft sensor's temperature predictions at the different melt flow radial positions.

C. Process investigation

Prior to designing a soft sensor, it is essential to understand the basic process mechanisms and functional principles while identifying the key process variables. To obtain the required background knowledge, a large number of experiments were performed on industrial scale extruders using industrially common polymeric materials and processing conditions, and a detailed review of the literature was also carried out.

D. Selection of the key process variables, model structure and modelling technique

It was planned to use two dynamic models within the novel temperature profile prediction soft sensor. One model is to predict the melt temperature at the different radial positions of the melt flow (i.e., the T_P model) and the other is to predict the melt temperature given by an IR temperature sensor (i.e., the T_{IR} or feedback model). From the details gathered, it was realized that the melt temperature of a given point across the melt flow which is j mm away from the melt flow centre ($T_{m,j}$) can be modelled as a function of screw speed (ω_{sc}), barrel set temperatures (T_b , subscript b represents a number of barrel set temperature zones: T_1, T_2, \dots, T_n) and die radial position ($R_{p,j}$):

$$T_{m,j} = f(\omega_{sc}, R_{p,j}, T_b) \quad (1)$$

Previous studies have shown that the die melt temperature profile is dependent upon a number of processing, material and machine parameters [8], [22], [24], [25], [29]. However, the three variables given in Eq. (1) were identified as the major influential variables to the die melt temperature profile for a given machine and a material, and hence these were selected to use as inputs to the T_P model. At this stage, the soft sensor is proposed for a given machine and a material (as this is the first approach of its kind) and then in future, it can be generalized for other machines and materials as well.

Based on the experimental observations, the melt temperature measured by an IR temperature sensor (T_{IR}) can be represented as a function of ω_{sc} , $T_{m,act}$ and T_b :

$$T_{IR} = f(\omega_{sc}, T_{m,act}, T_b) \quad (2)$$

The $T_{m,act}$ is the mean value of the predicted melt temperatures at the different radial positions by the T_P model. Then, the difference between the predicted and measured IR temperature measurements ($T_{IR,Error}$) is given by:

$$T_{IR,Error} = T_{IR} - \hat{T}_{IR} \quad (3)$$

where \hat{T}_{IR} is the predicted melt temperature relating to the IR temperature sensor.

The selection of an appropriate modelling technique is the next step after choosing the key process variables and the structures of the models. A few important factors should be considered for making this choice as the developed models:

- should be simple and compact (i.e., less computational complexity).
- should be compatible for using in real-time applications.
- should take the corresponding process delays into account.
- should predict the corresponding variable/s with an acceptable accuracy over the full process operating window.

After considering a number of possible techniques, a two-stage algorithm which can be used to develop simple and compact linear/nonlinear polynomial models with a linear-in-the-parameters (LITP) structure was chosen to develop the models. The functions given in Eqs. (1) and (2) can be modelled as a general nonlinear discrete-time dynamic multi-input-single-output (MISO) system as given by Eq (4):

$$y(t) = f(y(t-1), y(t-2), \dots, y(t-n_1), \dots, y(t-n_a), u_i(t-n_{ik}), u_i(t-n_{ik}-1), \dots, u_i(t-n_{ik}-n_1), \dots, u_i(t-n_{ik}-n_{ib})) \quad (4)$$

where $y(t)$ is the system output at time t , $u_i(t)$, $i = 1, \dots, m$ are the system inputs at time t (m is the total number of inputs to the system), n_a is the number of poles, n_{ib} is the number of zeros plus 1 and n_{ik} is the corresponding delays (i.e., the number of input samples that occur before each input affects the output) of each input. More details on the modelling technique is not provided as the author has used the same technique for modelling of the melt pressure [30], melt temperature [24], [25], [31], and power consumption [32] in polymer extrusion where good results were achieved.

III. EQUIPMENT, PROCEDURE & MATERIALS

All measurements were carried out on a medium scale industrial extruder. Melt temperature profiles at the 38 mm diameter die were measured using a thermocouple mesh with seven junctions which were placed across the die melt flow (distances from the die centreline to each mesh wire/junction: 0 mm, ± 3.0 mm, ± 4.5 mm, ± 8.8 mm, ± 11.0 mm, ± 14.7 mm, ± 16.5 mm, and ± 19.0 mm). The die wall set temperature was used as the melt temperatures at the ± 19 mm radial positions. As it was previously confirmed [29], the die melt temperature measurements are symmetrical across the centerline of the thermocouple mesh when averaged over sufficient time. Thus, the melt temperatures measured at these seven points across the die melt flow were mirrored over the die centreline to obtain the complete die melt temperature profile. The structure of the experimental set-up is shown in Figure 1. A data acquisition (DAQ) programme developed in LabVIEW was used to communicate between the experimental instruments and a PC. Screw speed and all temperature signals were acquired at 10 Hz sampling speed.

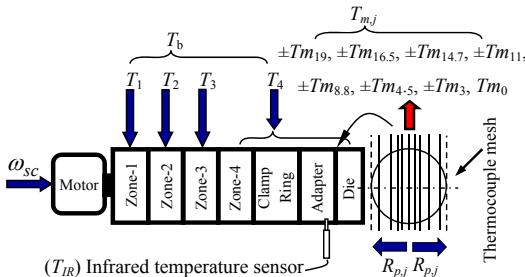


Fig. 1. A schematic of the experimental set-up

More details on the experimental set-up and procedure were discussed by the author previously [22], [24].

A. Materials and experimental conditions

Experimental trials were carried out on a virgin high density polyethylene (HDPE), (ExxonMobil HYA 800), (density: 0.961 g/cm³, melt flow index (MFI): 0.7 g/10min @ (190 °C, 2.16 kg)). The extruder barrel temperature settings were fixed as described in Table I under three different set conditions denoted as A (high temperature), B (medium temperature) and C (low temperature).

TABLE I
EXTRUDER BARREL TEMPERATURE SETTINGS

Temperature settings	Set temperatures (°C)					
	Barrel zones				Clamp ring	Adapter
A	110	130	180	230	230	230
B	105	125	175	215	215	215
C	100	120	170	200	200	200

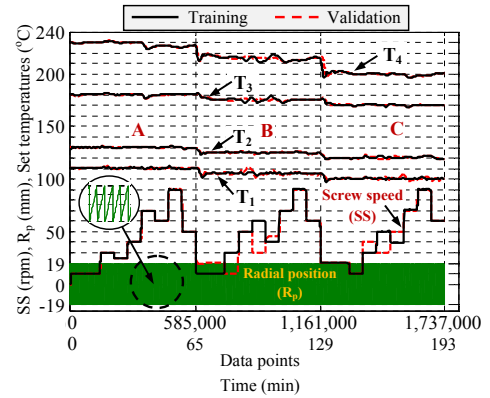


Fig. 2. The process settings matrices of training and validations tests

The experiments were started with the temperature setting A and data was recorded with the screw stationary for 1 minute. Then, the screw speed was increased up to 90 rpm with random steps of between ± 5 -40 rpm and in different barrel set temperatures with the extruder running for about 193 minutes continuously as shown in Figure 2. The extruder was allowed to stabilise for 15 minutes after each set temperature change while the extruder was hold for about 7 minutes at each other different condition. All of these settings were selected in order to generate realistic processing conditions whilst covering the full operating range of the extruder (i.e., 0-100 rpm). Separate tests were carried out to obtain the data for model training and validation.

B. Model training and validation

After studying a number of models, a 2nd order model with six terms (i.e., with a 0.25% of normalized prediction error (NPE) on the validation data) and a 2nd order model with fifteen terms (i.e., with a 1.22% of NPE on the validation data) were selected as the T_P and T_{IR} models, and these are given in Eqs. (6) and (5), respectively.

$$\begin{aligned} \hat{T}_{IR}(t) = & 0.9507 \times \hat{T}_{IR}(t-1) + 0.0003 \times T_1(t-150) \times T_2(t-120) \\ & + 0.00276 \times \hat{T}_{m,act} - 0.0001 \times T_1(t-150) \times T_4(t-60) \\ & + 9.9513 \times 10^{-05} \times T_3(t-90) \times T_4(t-60) \\ & - 8.8588 \times 10^{-06} \times \omega_{sc}(t-10)^2 \end{aligned} \quad (5)$$

$$\begin{aligned}
\hat{T}_{m,j}(t) = & 0.8207 \times \hat{T}_{m,j}(t-1) - 0.0012 \times \hat{T}_{m,j}(t-1) \times T_2(t-120) \\
& - 0.0223 \times R_{p,j}(t)^2 - 0.0008 \times \hat{T}_{m,j}(t-1) \times \omega_{sc}(t-10) \\
& + 0.0006 \times \omega_{sc}(t-10)^2 + 0.0081 \times R_{p,j}(t) \times T_4(t-60) \\
& + 0.0638 \times T_3(t-90) - 0.0037 \times \omega_{sc}(t-10) \times T_3(t-90) \\
& + 0.3096 \times T_4(t-60) - 0.0113 \times \hat{T}_{m,j}(t-1) \times R_{p,j}(t) \\
& + 0.0033 \times \omega_{sc}(t-10) \times T_2(t-120) \\
& + 0.0134 \times R_{p,j}(t) \times T_2(t-120) \\
& + 0.0008 \times \omega_{sc}(t-10) \times R_{p,j}(t) \\
& + 0.0043 \times \omega_{sc}(t-10) \times T_1(t-150) \\
& + T_{IR,Error} \pm bias
\end{aligned} \tag{6}$$

In fact, the models with suitable size (i.e., from the model order and number of terms) can be selected based on the requirements of the soft sensor design.

C. Soft sensor design

The soft sensor design was performed by combining the dynamic process models and the feedback mechanism. The structure of the newly proposed melt temperature profile prediction soft sensor concept is shown in Figure 3. This

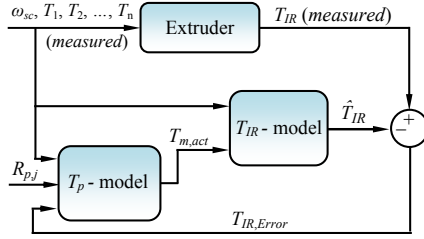


Fig. 3. The structure of the die melt temperature profile soft sensor

predicts the melt temperatures of the user defined radial locations across the melt flow when the required inputs are feed into the T_P model. The $T_{m,act}$ can be obtained by taking the average value of the T_P model's predictions and this value can be feed into the T_{IR} model together with other relevant parameters. Consequently, the T_{IR} model will predict the temperature given by the IR temperature sensor and this can be compared with the actual value measured to generate the $T_{IR,Error}$. If an error is available, it will be feed into the T_P model together with a bias specific to the each radial position for compensating the error. These steps will be repeated throughout the process operation and hence the temperature profile across the melt flow can be predicted in real-time. The number of radial positions required to generate the melt temperature profile and the sensor's output updating frequency can be defined as suitable.

IV. RESULTS AND DISCUSSION

The proposed soft sensor was implemented in Matlab-Simulink to check its performance and both the measured (i.e., temperatures measured under the barrel set temperature conditions A and B given in Table I) and predicted temperature signals at 0 mm, 3.0 mm, 8.8 mm and 16.5 mm radial positions are shown in Figure 4. All figures have plotted in the same scale and the time intervals shown along the X-axis are relevant to the times of the applied screw speed step changes. A step change of the barrel set temperatures was applied at the time of 65 minutes. Overall, the soft sensor predicts the melt temperatures at the different melt

flow radial locations with good accuracy and some of the slight deviations can be seen only over a few processing conditions. To further confirm the performance/reliability of the proposed soft sensor, its responses over the disturbances were checked by adding different size of negative and positive step changes (i.e., 10, 20 and 30 units) to each individual process variable from their set value while others remained unchanged and also by applying similar types of disturbances to the feedback model. The results confirmed that the soft sensor can settle back to the normal operating conditions just after removing the applied disturbances on its input variables and the feedback model which showed good disturbance rejection ability. In fact, these experiments were carried

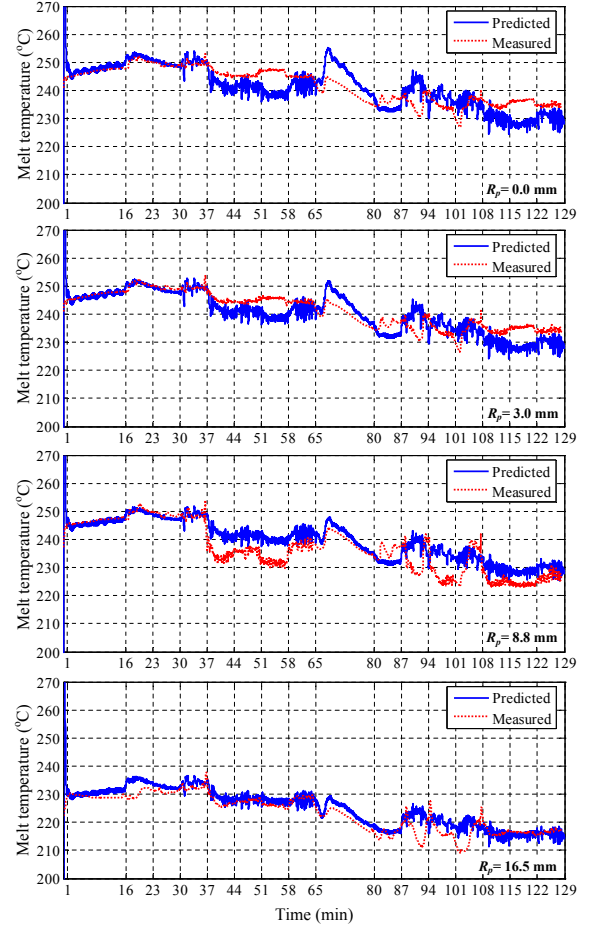


Fig. 4. Measured and predicted melt temperatures at the 0.0 mm, 3.0 mm, 8.8 mm and 16.5 mm melt flow radial positions

out by applying frequent screw speed step changes and a large step change of the barrel set temperature (see Figure 2). However, there will be no such frequent screw speed changes in industry as the processes are usually operated at a constant temperature and speed for a long period of time. Obviously, the soft sensor may have much better performance under such constant process operating conditions. Moreover, as the newly proposed melt temperature profile prediction soft sensor showed good performance in predicting a melt temperature profile across the die melt flow, it should be used to develop a control strategy to manipulate process settings to achieve the desired average melt temperature

across the extruder output melt flow while minimising the melt temperature variance. Some of the initial results relating to the development of a process controller incorporating this soft sensor have been presented by the author recently [33].

V. CONCLUSIONS AND FUTURE WORK

A. Conclusions

It was realized that the soft sensing approaches are highly useful for the processes like polymer extrusion due to the limitations of using physical sensors for making some of the important process parameters such as die melt temperature profile, melt viscosity, etc. In this study, a novel soft sensor concept was proposed to predict the temperature profile across the die melt flow in polymer extrusion. Mainly, the newly proposed soft sensor employs two dynamic process models and a feedback mechanism incorporating a physical IR temperature sensor. The soft sensor can predict the melt temperature values of a number of radial positions across the melt flow (and hence the melt temperature profile) in real-time based on five process variables. The simulation results of the proposed soft sensor confirmed that it can predict the melt temperatures at different die radial positions with good accuracy. Moreover, the process variables required for the operation of the soft sensor can be readily measured in any practical environment to a good accuracy by using commercially available physical sensors. Therefore, this will be a promising strategy for making real-time melt temperature profile measurements in polymer extrusion which is highly difficult to perform by using a physical sensor.

B. Future Work

In future, the proposed soft sensor will be implemented in a software platform and then on an industrial scale extruder for evaluating its performance. Moreover, the possible approaches for narrowing its current limitations will be explored. Also, an attempt will be made to investigate soft sensing approaches for predicting other important parameters which are difficult to measure physically.

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