Journal Article

A Novel Soft Sensor for Real-Time Monitoring of the Die Melt Temperature Profile in Polymer Extrusion

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Chamil Abeykoon

***Abstract*—Polymer extrusion is the most fundamental technique for processing polymeric materials and its importance is increasing due to the rapid growth of worldwide demand for polymeric materials. However, the process thermal monitoring is experiencing several problems resulting in poor process diagnostics and control. Most of the existing process thermal monitoring methods in industry only provide point/bulk measurements which are less detailed and low in accuracy. Physical thermal profile measurements across the melt flow may not be industrially compatible due to their complexity, access requirements, invasiveness, etc. Therefore, inferential thermal profile monitoring techniques are invaluable for obtaining detailed, accurate and industrially compatible measurements and hence to achieve improved process control. In this work, a novel soft sensor strategy is proposed to predict the real-time temperature profile across the die melt flow in polymer extrusion to the first time in industry or research. It is capable of determining the melt temperature at a number of die radial positions only based on six readily measurable process parameters. A comparison between the simulation results of the novel melt temperature profile prediction soft sensor and the experimental measurements showed that the soft sensor can predict the real-time melt temperature profile of the die melt flow with a good accuracy. Therefore, this will offer a promising solution for making real-time melt temperature profile measurements non-invasively in polymer extrusion and also it should be applicable to other polymer processes only with a few modifications. Moreover, this technique should facilitate in developing an advanced process thermal control strategy.**

***Index Terms*—Polymer Extrusion, Melt Temperature Profile, Inferential Measurements, Process Monitoring, Dynamic Modelling, Soft Sensor, Process Control.**

I. Introduction

Polymers are one of the major raw materials in the current industry and most of the conventional raw materials such as glass, steel, wood are being replaced by polymeric materials due to their valuable properties such as high strength to weight ratio, high impact/chemical/corrosive resistance, ease of forming into complex shapes, etc. For example, currently there is a great concern on replacing the conventional materials such as metal and glass in the transport sector with advanced polymer composites or with other high performance polymer materials (which provide very high strength to weight ratio compared to other materials) as a solution for on-going global energy crisis. Likewise, polymeric materials are becoming increasingly popular in the areas such as construction, medical, electrical and electronic, household applications, and so forth. This rapid increase of the use of polymeric materials has caused to demand high quality and efficient processing procedures from the polymer industry.

Usually, polymer extrusion is used in the final production of many polymer products such as pipes, films, sheets, tubes, rods, etc. Also, it is an intermediate processing stage in injection moulded, blown film, thermoformed, and blow moulded products. An extruder is a machine which processes material by conveying it along a screw and forcing it through a die at a certain pressure. The screw is the key component of extrusion machines and it has been divided into three main functional/geometrical zones (i.e. solids conveying or feed, melting or compression, and metering or pumping) which are necessarily based on the primary operations of an extruder as shown in Figure 1. The feedstock material fed into the machine

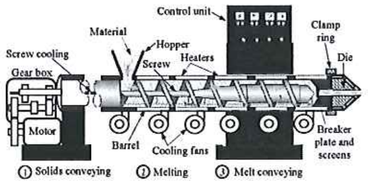

Figure 1. Basic components of a single screw extruder

through the hopper conveys along the screw while absorbing the heat provided by the barrel heaters and process mechanical work. Materials can be extruded either in the solid or molten state. However, polymers are generally extruded in the molten state by melting solid feed material in the machine. Eventually, a molten flow of material is forced into the die which forms the material into the desired shape. The main function of an extruder is to deliver a homogeneous and well-mixed polymer melt at a specified uniform temperature and pressure. In all cases, the melt output from the machine is expected to be homogenous in composition, colour and temperature. To achieve this dominant requirement, extruders are generally equipped with an efficient drive; a feed system; a screw designed to melt and convey the polymer; and devices such as temperature and pressure transducers required to monitor the system for troubleshooting and control. Moreover, some processes use devices such as mixers, gear pumps, controlled feeding devices, etc, with the purpose of improving the quality of the melt output [1].

In general, the temperature across the extruder output melt flow cross-section should be homogeneous and also it should be uniform over the time. Therefore, accurate process thermal monitoring is highly invaluable as this helps not only for diagnosing process thermal instabilities but also for accurate

Manuscript received October 28, 2013 ; revised January 13, 2014, March 8, 2014 and April 13, 2014; accepted April 17, 2014.

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process control. It is difficult to achieve the process control accurately if the problems relating to the process cannot be properly diagnosed. Despite the significant developments in polymer extrusion over the last few decades, process thermal monitoring and control still remain issues. Process operators have to face challenges in achieving the required thermal quality of the melt output with the existing knowledge and technology. Indubitably, achieving of good thermal stability is a major requirement of the extrusion process to form a high quality product [1]. Even small variations in melt temperature can cause to have poor quality products [2]. Therefore, continuous monitoring of the process thermal behaviour is an essential requirement for advanced process control to maintain the process thermal stability at a desired level. More details on the functional requirements and the mechanisms/theories of polymer extrusion can be found in the literature [1], [3].

As revealed by the previous work [4]–[7], melt thermal homogeneity in polymer extrusion is considerably affected by the process settings, and the melt flow temperature is differed depending on the radial location of the die. Therefore, the study of the entire melt temperature profile as a measure of the process thermal stability is more appropriate than a single point or bulk measurement to ensure high quality products. Typical wall mounted thermocouples (i.e. based on the thermoelectric effect) are the most commonly used melt temperature measurement method in the present industry and few processes use infrared (IR) and ultrasonic temperature measurement techniques as well. Unfortunately, all of these industrially well-established temperature sensors provide low accuracy single point or bulk measurements only and they are incapable of detecting thermal variations across the melt flow [1], [3], [8]. As these thermal variations cannot be detected accurately, these cannot be controlled and hence industrial processes experience poor melt quality leading to high defect rates, long downtimes, material and energy waste, etc. Some thermal measurement techniques (e.g. traversing thermocouple, thermocouple mesh, florescent technique) are capable of monitoring the melt temperature at a range of points within the melt flow cross-section during the process operation. A traversing thermocouple uses the same principle as conventional wall mounted thermocouples but it has the facility to move the probe into the melt manually or mechanically. A thermocouple mesh consists of a grid of thermocouple wires, and an electromotive force (emf) is developed at each grid junction which can be correlated with the local melt temperatures across the melt flow [9]. In florescent technique, polymer is doped with a temperature sensitive fluorescent dye, allowing temperature at different points to be derived from changes in the fluorescence spectrum [10]. However, these techniques are not yet suitable for use in a production environment due to the constraints such as their complexity, limited durability, access requirements, disruptive effects on the melt flow and output while they are very useful to gather valuable process information in a research setting. Currently, no industrially well-established thermal profile measurement technique is available. Under these circumstances, inferential thermal profile monitoring techniques should be promising for the present industry to obtain detailed, accurate and industrially compatible measurements and hence to achieve improved process control.

A. Soft sensor

A soft sensor or an inferential estimator is a technique of estimating some particular parameter/s (e.g. quality measures, variables) in various applications when a hardware sensor is unavailable or unsuitable. Generally, soft sensors are used in real-time process monitoring and control; fault detection; process diagnostics and so forth. In practise, these are widely used in chemical processes such as reactors, cement kilns, distillation columns, food processing, paper and pulp industry, etc, to estimate the product quality parameters [11], [12]. In the majority of previously reported soft sensing applications, 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), etc [13]–[18]. In fact, designing of a soft sensor is an extensive task and some of the major steps can be listed as below:

- Process investigation and data collection
- Data processing
- Selection of the variables and model structure
- Model training and validation
- Design and testing of the soft sensor
- Application and maintenance of the soft sensor

Currently, soft sensors are becoming widely popular in various industrial applications particularly due to their benefits such as:

- It can be highly useful in the applications where physical sensors may not be applicable or unsuitable.
- It provides 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.

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 on all the areas listed in the above. In the long run, the drifts of the process may be a problem on the performance of the soft sensor and hence it should be compensated either by adapting or re-developing the model/s [19]. More details on soft sensor design, applications and related issues can be found in the literature [11], [20].

B. Previous work on inferential monitoring of point/bulk melt temperature or melt temperature profile in polymer extrusion

Although soft sensing techniques are widely popular in various industrial processes, only a very little work has been reported on inferential process monitoring in polymer extrusion particularly in process thermal monitoring applications.

Previous work by the author [21] reported an attempt to predict process thermal stability inferentially. Correlations between screw load torque, melt pressure and melt temperature fluctuations were examined by analysing experimentally measured signals. However, no strong correlations between these signals could be observed. It was found that the screw load torque signal is dominated by the solids conveying torque and hence it was not sensitive enough to identify unstable melting issues. Pressure fluctuations had slight correlations with melt temperature fluctuations particularly at low screw speeds. However, none of these signals showed sufficiently good performance for them to be used as a powerful tool to monitor the process thermal stability inferentially. In fact, there is no other reported work in the literature on inferential thermal monitoring in polymer extrusion according to the author's knowledge. A few researchers attempted to predict some of the parameters relating to the process quality, in other industrial applications based on polymeric materials, inferentially [13], [15]–[17], [22]–[26] and also based on other advanced techniques [27]–[29]. Therefore, it is clear that no any inferential process thermal monitoring technique is currently available in polymer extrusion which can be used in the situations where making of physical thermal measurements are difficult or unsuitable.

In this work, a highly instrumented single screw extruder was used in the experiments to make a number of real-time process measurements. Here, a single screw extruder was selected as it is the most common type using in the polymer processing industry [30]. A thermocouple mesh technique [9] was used to measure the radial temperature profile across the die melt flow over different process operating conditions as this technique was recognized as the one of the best methods to measure a melt temperature profile over several other techniques [3]–[5]. Then, the data obtained was used to develop a novel soft sensor strategy to predict a die melt temperature profile in polymer extrusion which is the main contribution of this paper [31]. Therefore, this work will provide a strong platform and an initiative for future research on investigating real-time thermal information across the die melt flow in polymer extrusion which is very important for advanced process monitoring and control, but cannot be easily obtained via a physical temperature sensor. Moreover, the optimisation of the process thermal efficiency and energy usage is timely important as energy prices have been rapidly increasing over the last few decades throughout the world. Therefore, this type of novel technique would be greatly useful to the current industry as it would contribute to minimise the process energy usage via advanced thermal monitoring and control.

II. Equipment & Procedure

All measurements were carried out on a 63.5mm diameter (D) single screw extruder (Davis Standard BC-60). A barrier flighted screw with a spiral Maddock mixer and a 2.5:1 compression ratio (feed or solids conveying - 5×D, compression or melting - 13×D, metering or melt conveying - 6×D) was used to process the material. The extruder was fitted with a 38mm diameter adapter by using a clamp ring prior to a short capillary die with a 6mm bore as shown in Figure 2. The extruder barrel has four separate temperature zones and another three separate temperature zones are available at the clamp ring, adapter and die. Each of these temperature zones is equipped with a separate temperature controller which allows individual control of the set temperature.

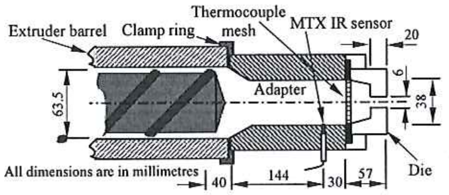

Figure 2. Extruder die, adapter and thermocouple mesh

Melt temperature profiles at the die (i.e. at the end of the 38mm diameter adapter) were measured using a thermocouple mesh which is placed in-between the adapter and the die as shown in Figure 2. As it was previously confirmed by Kelly et al. [7], the die temperature measurements are symmetrical across the centerline of the thermocouple mesh when averaged over sufficient time. Therefore, seven thermocouple junctions (i.e. with 7 positive and 1 negative thermocouple wires) were placed asymmetrically across the die melt flow along the diameter of the mesh as shown in Figure 3, and this asymmetric placement of wires gave the opportunity to increase the number of effective temperature measurements across the melt flow by mirroring them over the centreline to obtain the complete die melt temperature profile.

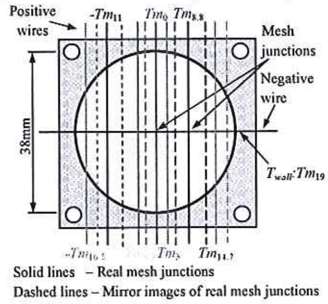

Figure 3. The thermocouple mesh arrangement

Finally, 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 die wall set temperature was used as the melt temperature at the ±19mm radial positions. Then, the final temperature profile was obtained by fifteen radial positions (distances from the die centreline to each radial position: 0mm, ±3mm, ±4.5mm, ±8.8mm, ±11mm, ±14.7mm, ±16.5mm, and ±19mm) across the melt flow as illustrated in Figure 3. In addition to the thermocouple mesh measurements, an IR temperature sensor (Dynisco MTX 922-6/24) was used to make bulk temperature measurements of the melt in the adapter close to the thermocouple mesh as shown in Figure 2.

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 10Hz using a 16-bit DAQ card (National Instruments PCI-6035E) through a TC-2095 thermocouple connector box and a low-noise SCXI-1000 connector box.

A. Materials and experimental conditions

Experimental trials were carried out on a virgin high density polyethylene (HDPE), (ExxonMobil HYA 800), (density: $0.961 g/cm^3$, melt flow index (MFI): 0.7g/10min @ (190°C, 2.16kg)). 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	Die
	1	2	3	4			
A	110	130	180	230	230	230	230
B	105	125	175	215	215	215	215
C	100	120	170	200	200	200	200

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 90rpm with random steps of between ±5-40rpm and in different barrel set temperatures with the extruder running for about 193 minutes continuously as shown in Figure 4.

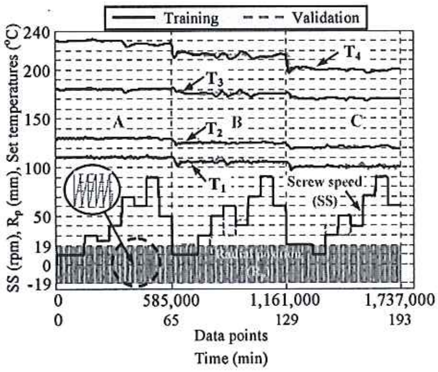

Figure 4. The process settings matrices of training and validations tests

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. 0-100rpm). This therefore allowed investigation of melting performance at low throughputs where melting is dominated by conduction from the barrel and screw, and intermediate and high throughputs where melting is primarily achieved by viscous shearing. Separate tests were carried out to obtain the data for model training and validation.

III. TYPICAL DIE MELT TEMPERATURE PROFILE

As was mentioned in section 2, melt temperature profiles across the melt flow at the end of the 38mm diameter adapter were observed and profiles over some processing conditions (i.e. the average values of the data collected for the last two minutes of each speed) are shown in Figure 5. The data collected over the last two minutes at different experimental conditions were used to create these plots as the process signals were included transients during the first few minutes, followed by the applied step changes to the process variables. These temperature profiles show the effects of process settings on the temperature profile of the extruder melt output and more details relating to this area were discussed by the author previously [3]–[5].

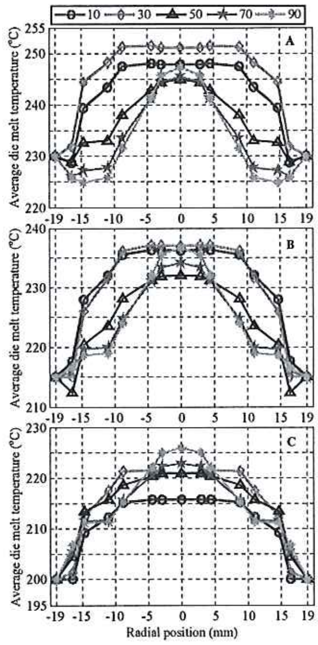

Figure 5. Average die melt temperature profiles over the last two minutes at different temperature settings (i.e. conditions A, B, and C shown in Table I) and screw speeds of 10, 30, 50, 70 and 90rpm

IV. DEVELOPMENT OF THE SOFT SENSOR TO PREDICT THE MELT TEMPERATURE PROFILE

A. Comparison of the temperature measurements of the IR sensor and thermocouple mesh

The thermocouple mesh technique is good in providing detailed and accurate information on the thermal homogeneity of the extruder output melt flow. It was felt that it is better

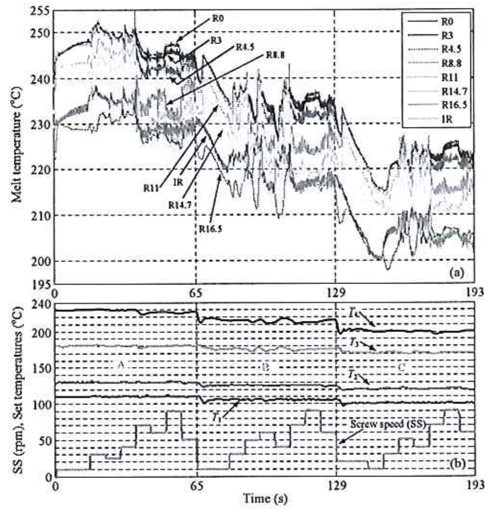

Figure 6. (a). Measured melt temperatures by the IR temperature sensor and the thermocouple mesh at different processing conditions (b). Corresponding step changes applied to the process settings during the temperature measurements (in this figure 'R' refers to the radial position and all the numbers followed by R are in millimeters)

if it is possible to inferentially predict melt temperatures at the different melt flow radial locations to obtain similar types of measurements to the thermocouple mesh. Therefore, the collected experimental data was used to develop a dynamic model which can predict a melt temperature profile across the melt flow from readily measurable process parameters during the process operation. Although this 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], [4], it was found that an IR temperature sensor had the closest relationship with the thermocouple mesh measurements among the methods evaluated. However, the experimentally measured melt temperatures in this study by using the IR temperature sensor and the thermocouple mesh were compared to confirm the suitability of using an IR temperature sensor to compensate the possible prediction errors of the melt temperature at the different radial locations of the melt flow, and these temperature signals are shown in Figure 6. As it is evident, the IR temperature sensor follows the process thermal dynamics in a similar way to the thermocouple mesh. Specifically, an IR temperature sensor is an industrially compatible thermal monitoring technique and hence it can be used on industrial extruders. Moreover, it is not required to add any modification to the existing extruders to use this method as an IR temperature sensor can be attached to a standard sensor port which has been designed to attach typical temperature and pressure sensors. Another advantage is that 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 (i.e. real-time measurements). Therefore, an IR temperature sensor was selected to obtain a temperature feedback to compensate the possible errors of the soft sensor's temperature predictions at the different melt flow radial positions.

B. *Structures of the dynamic models*

Generally, the proposed soft sensor includes two dynamic models (which are named as the MTPP model and the IRTP model) based on readily measurable process parameters and a temperature feedback based on an IR temperature sensor. Here, there are a few considerations to be made prior to selecting the structures of process models as these should be compatible with real-time applications. In general, all the parameters included in these models are required to be easily measurable during the process operation. Moreover, these models should have the capability of predicting the relevant process parameters to a good accuracy as quickly as possible.

1) Melt temperature profile prediction model (MTPP model): A detailed review of the literature [1], [32], [33] on melting in polymer extrusion (e.g. melting mechanisms, models, experimental investigations) was carried out prior to selecting the structure of the MTPP model. Moreover, a number of experiments were carried out on an industrial scale extruder to observe the real-time die melt temperature profile and some of these findings were presented in section III and in the previous publications of the author [3]–[6]. Based on the information gathered, the melt temperature ($T_{m,j}$) at a particular die radial position ($R_{p,j}$) which is $j$mm away from the melt flow centre can be represented as a function of ω_{sc}, $R_{p,j}$ and T_b:

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

where ω_{sc} is the screw speed and T_b represents the barrel set temperatures (subscript b represents different barrel zones T_1-T_4). Six inputs (ω_{sc}, $R_{p,j}$, T_1, T_2, T_3, T_4) were considered to model the melt temperature at a particular die radial position ($T_{m,j}$), $-19mm \leq j \leq 19mm$, as illustrated in Figure 7.

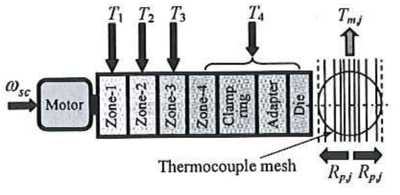

Figure 7. Extruder model with selected inputs and output

The set temperatures of the clamp ring, adapter, and die are always equal to T_4 in this study. If the set values of these zones are different from T_4, it is possible to add them as three different model inputs. Apart from these six inputs, the difference between the predicted and measured IR temperature sensor measurement ($T_{IR,Error}$) at each radial position with a suitable adjustment (i.e. a positive or a negative bias value specific to each radial position) are also taken as inputs of the MTPP model for the purpose of the compensation of the possible prediction errors. Currently, these bias values are determined off-line and the author expects to improve the modelling algorithm to select these bias values on-line under future work.

2) Infrared temperature prediction model (IRTP model): The IRTP model is used within the feedback mechanism of this soft sensor to inferentially predict the temperature which is measured from the IR temperature sensor. Based on the experimental observations, the melt temperature measured by the IR temperature sensor (T_{IR}) can be represented as a function of ω_{sc}, $T_{m,act}$ and T_b:

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

The $T_{m,act}$ is the mean value taken from the predicted melt temperatures at the different radial positions by the MTPP model as given by equation (3).

$$T_{m,act} = \frac{1}{K}\sum_{i=1}^{K}(\hat{T}_{m,j})_i \tag{3}$$

where K is the number of radial positions that have been chosen across the melt flow and $\hat{T}_{m,j}$ is the predicted melt temperature of the radial location where $j$mm away from the melt flow centre. Then, the difference between the predicted and measured IR temperature sensor measurements ($T_{IR,Error}$) is given by:

$$T_{IR,Error} = T_{IR} - \hat{T}_{IR} \tag{4}$$

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

C. Modelling technique

For this work, a modelling technique should be selected to develop simple, compact and computationally efficient models which are appropriate for real-time applications. The development of models based on the first principles were possible but these may have limitations in practical applications due to the issues such as computational complexity, difficulty of obtaining closed form solutions and so forth [34]. Alternatively, it was possible to use one of the data driven modelling approaches such as time series, transfer function, state-space, grey box, etc which could be found in the previous research and more details on these approaches were discussed previously [5], [6]. However, it was realized that an alternative modelling approach would be more appropriate as most of these previously used techniques have encountered with some problems. After considering a number of modelling techniques, a recently proposed two stage algorithm [35] which can be employed in the selection and refinement of linear/nonlinear polynomial models with a linear-in-the-parameters (LITP) model structure was selected for this study.

Here, the MTPP model should predict the melt temperature value of the each radial position assigned by the radial position input. For this study, fifteen radial positions (i.e. $K = 15$ for this study) make a complete melt temperature profile across the die melt flow. The model should estimate the melt temperature values of these fifteen positions individually by only changing the radial position input, while the screw speed and barrel set temperatures remain constant. There are twenty five different processing situations including 1,737,000 data points over 193 minutes (i.e. 193×600×15). The process settings matrices (i.e., the MTPP model input matrices) for training and validation data are shown in Figure 4. The model output contains the measured melt temperatures at the different radial positions corresponding to the relevant inputs, and the signal length is the same as the input signals length.

The process was modelled as a general nonlinear discrete-time dynamic multi-input-single-output (MISO) system which can be expressed as:

$$\begin{aligned} y(t) = & f(y(t-1), y(t-2), ...y(t-n_1), ...y(t-n_a), u_i(t-n_{ik}), \\ & u_i(t-n_{ik}-1), ...u_i(t-n_{ik}-n_1), ...u_i(t-n_{ik}-n_{ib})) \end{aligned} \quad (5)$$

where $y(t)$ is the system output at time t; $u_i(t)$, $i = 1, \cdots, m$ are the system input variables 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. number of input samples that occur before each input affects the output) of each input.

Firstly, an attempt was made to identify a linear model to correlate the output with the inputs by approximating the function *f*. However, this did not predict the temperature values accurately due to the significant nonlinearities in the process and has not been presented in this paper. Then, nonlinear polynomial models were adopted and a 2^{nd} order model was selected as the MTPP model. This model included a large number of terms which may limit its practical application. However, only a few terms were found to provide a significant contribution to the output. Sub-model selection algorithms (e.g. orthogonal least squares (OLS) [36], fast recursive algorithm (FRA) [35]) can be applied to construct a parsimonious model with satisfactory generalisation capability. Due to the lower computational complexity and improved stability over OLS, a FRA was used as a sub-model selection algorithm for this study. It solved the problem recursively and did not require matrix decomposition as was the case for OLS techniques [36]. In the first stage, the model structure selection and the estimation of the model parameters were carried out. In the second stage, a backward model refinement procedure was carried out to eliminate non-significant terms to build up a compact model. The significance of each selected model term was reviewed and compared with those remaining in the candidate term pool and all insignificant terms were replaced to obtain the improved performance without increasing the model size. Likewise, the same procedure was followed for the development of the IRTP models with different size and a 2^{nd} order model was selected to use in this study. More details on the application of the modelling technique used in this study to the polymer extrusion process was previously discussed by the author [5], [6], [37].

D. Structure and the operation of the novel die melt temperature profile prediction soft sensor

The structure of the newly proposed soft sensor for the die melt temperature profile prediction in polymer extrusion is shown in Figure 8. In operation, the soft sensor should predict

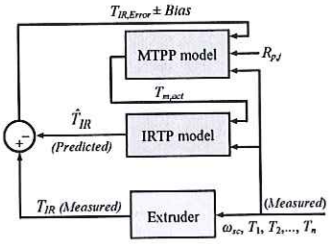

Figure 8. The structure of the proposed soft sensor to predict the melt temperature profiles across the extruder output melt flow in real-time

the melt temperatures at the different radial positions (which are defined by the user or designer) across the die melt flow by allowing to determine the melt temperature profiles in real-time. Overall, the proposed soft sensor employs two models for its operation. One model is to predict the melt temperature profile (MTPP model) across the melt flow and it takes eight inputs (ω_{sc}, $R_{p,j}$, T_1, T_2, T_3, T_4, $T_{IR,Error}$ and a $\pm$ *bias*) for its prediction as shown in Figure 8. A desired number of radial positions can be defined under the $R_{p,j}$ input as required and for this study fifteen radial positions (see Figure 3) were defined. In practice, the MTPP model would operate in place of the thermocouple mesh. The IRTP model (or feedback model) takes six inputs (ω_{sc}, $T_{m,act}$, T_1, T_2, T_3, T_4) and predicts the melt temperature given by the IR temperature sensor. Then, the measured and predicted IR temperature signals are compared to identify the possible prediction error of the die melt temperature profile. Finally, the generated error signal ($T_{IR,Error}$) is fed into the MTPP model together with a bias (which is specific to the each radial position) for compensating the prediction error at each radial position. This operation takes place throughout the process operation while updating the sensor output by user defined intervals. More importantly, the screw speed and barrel set temperatures which are used as the MTPP and IRTP models' inputs can be measured easily in any industrial polymer process during the process operation and this would be an advantage which makes it is easy to use this soft sensor in practical applications.

V. Results & Discussion

A. MTPP and IRTP models used in the soft sensor

For the selection of dynamic MTPP and IRTP models, a number of different model combinations (i.e. with different orders and number of terms) were studied. One past output term and one past input term from each model input were used to predict the current output (i.e. n_a=1 and n_b for each input is equal to 1) and these two variables can be adjusted as required. Then the maximum delays (n_k) attributed to the each model input had to be determined. Changes of the melt temperature at each radial position followed by the step changes of the screw speed and barrel set temperature were observed from the experimentally measured data. Melt temperature changed soon after any change of the screw speed. Also, the melt temperature was affected by the set temperatures of the barrel heater zones but it was taken slightly long period of time to reach to the set value once any change was made. Moreover, these changes in melt temperature depend on the size of the changes applied to the variables and also the magnitude of which the variable was before the applied change. Therefore, the selection of delays was quite complex and hence the values were selected to reflect the information collected from the measured signals and the other details which were observed during the experiments. The values which were selected for delays attributed to each input are: $d-\omega_{sc}$=10s, $d-R_{p,j}$=0s, $d-T_1$=150s, $d-T_2$=120s, $d-T_3$=90 s and $d-T_4$=60s. These delays can be adjusted as required depending on the screw geometry, material, processing conditions, etc. In fact, it is good to allow to the modelling algorithm for selecting the delays itself automatically depending on the processing conditions and this will be considered under the future work.

To test the accuracy of the developed models, the normalised prediction error (NPE) of each of them was determined by equation (6).

$$NPE \triangleq [\sum_{i=1}^{N}(\hat{y}_i(t)-y_i(t))^2/\sum_{i=1}^{N}y_i(t)^2]^{1/2}\times 100\% \qquad (6)$$

where $y_i(t)$ and $\hat{y}_i(t)$ are the measured and model estimated melt temperatures at time t respectively, and N is the number of data points.

Eventually, a 2^{nd} order model with fifteen terms (i.e. with a 1.22% NPE on the validation data) and a 2^{nd} order model with six terms (i.e. with a 0.25% NPE on the validation data) were selected as MTPP and IRTP models to use in the soft sensor and these are given in equations (7) and (8), respectively.

$$\begin{aligned}\hat{T}_{m,j}(t)=&0.8207\times\hat{T}_{m,j}(t-1) && -0.0012\times\hat{T}_{m,j}(t-1)\times T_2(t-120)\\ &+0.0081\times R_{p,j}(t)\times T_4(t-60) && +0.0134\times R_{p,j}(t)\times T_2(t-120)\\ &-0.0113\times\hat{T}_{m,j}(t-1)\times R_{p,j}(t) && -0.0008\times\hat{T}_{m,j}(t-1)\times\omega_{sc}(t-10)\\ &+0.0008\times\omega_{sc}(t-10)\times R_{p,j}(t) && +0.0043\times\omega_{sc}(t-10)\times T_1(t-150)\\ &+0.0006\times\omega_{sc}(t-10)^2 && +0.0033\times\omega_{sc}(t-10)\times T_2(t-120)\\ &+0.0638\times T_3(t-90) && -0.0037\times\omega_{sc}(t-10)\times T_3(t-90)\\ &+0.3096\times T_4(t-60) && -0.0223\times R_{p,j}(t)^2\\ &+T_{IR,Error} && \pm\, bias\end{aligned} \qquad (7)$$

$$\begin{aligned}\hat{T}_{IR}(t)=&0.9507\times\hat{T}_{IR}(t-1) + 0.0003\times T_1(t-150)\times T_2(t-120)\\ &+0.0276\times\hat{T}_{m,act} - 0.0001\times T_1(t-150)\times T_4(t-60)\\ &+9.9513\times 10^{-05}\times T_3(t-90)\times T_4(t-60)\\ &-8.8588\times 10^{-06}\times\omega_{sc}(t-10)^2\end{aligned} \qquad (8)$$

Inputs of these models can be updated in real-time to obtain the corresponding outputs.

B. Evaluation of the performance of the soft sensor

The proposed soft sensor was implemented in Matlab-Simulink to check its performance of predicting the melt temperatures at different melt flow radial locations. A comparison of the experimentally measured (i.e. temperatures measured under the barrel set temperature conditions A and B over 129 minutes (see Figure 6) at the end of the 38mm diameter adapter) and the predicted temperature signals at different radial positions is shown in Figure 9. All sub-figures are plotted on the same scale and the relevant melt flow radial position is shown at the right bottom corner of each figure. Only the temperature range of 200-270°C of the Y-axis is shown in these figures for more clarity. 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.

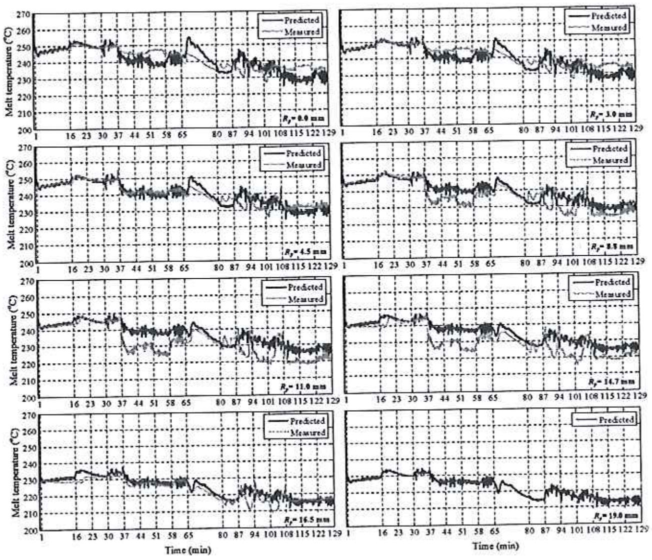

Figure 9. Measured and predicted melt temperatures at the 0.0mm, 3.0mm, 4.5mm, 8.8mm, 11.0mm, 14.7mm, 16mm and 19.0mm die radial positions (in figure 'R' refers to the radial position)

In case of accurate prediction, the predicted and measured IR temperature signals should be overlapped and hence $T_{IR,Error}$ should be equal to zero. The experimentally measured and predicted (i.e. by the soft sensor) IR temperature signals over the duration of 129 minutes are shown in Figure 10 while the corresponding IR temperature prediction error ($T_{IR,Error}$) is shown in Figure 11. As shown in Figure 10, both the experimentally measured and predicted IR temperatures are mostly overlapped and the prediction error sits around zero, i.e. in the range of -5°C to 5°C or less than ±2.25% of the full scale reading. The highest difference between the predicted and measured IR temperatures can be observed just after the applied barrel set temperature change (i.e. negative step changes to all of the barrel zone temperatures as shown in Table I) together with a 40rpm screw speed step change.

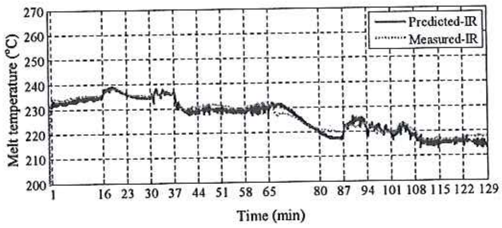

Figure 10. Measured and predicted melt temperatures signals relevant to the IR temperature sensor

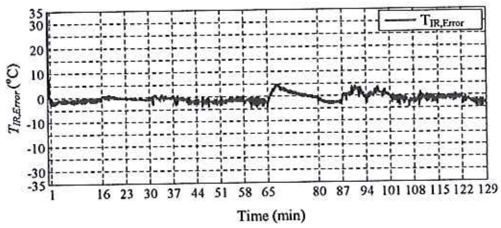

Figure 11. IR temperature prediction error (i.e. the difference between the measured and predicted IR temperatures)

Furthermore, the normalised prediction error between the experimental measurement and the soft sensor prediction at each radial position was determined based on equation (6) and the corresponding values are shown in Table II.

Table II
THE NORMALISED PREDICTION ERROR BETWEEN THE EXPERIMENTAL MEASUREMENT AND SOFT SENSOR'S PREDICTION AT EACH RADIAL POSITION

Radial position (mm)	Normalised prediction error (NPE)
0.0	1.99
3.0	1.70
4.5	1.33
8.8	2.10
11.0	2.89
14.7	2.72
16.5	1.45

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 out by applying frequent screw speed step changes and a large step change of the barrel set temperature (see Figures 4 and 6 for more details). However, there will be no such frequent screw speed changes under the industrial processing conditions 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. Here, the comparisons between the predicted and experimental measurements (as shown in Figure 9) were made only with the radial positions at which mesh junctions were placed in the experiments. However, the soft sensor can predict the melt temperature of any desired radial position across the melt flow in its normal use. Moreover, as the newly proposed 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 [38].

C. *Industrial use of the soft sensor and possible improvements*

In fact, promising results were achieved although this is the first time of introducing a soft sensor for determining a die melt temperature profile in polymer extrusion. This strategy would be very much appropriate (i.e. in its present state) for processes which use the machine to manufacture the same product, all the time by using the same screw and material. The required process models can be developed by following the same procedure as was used in this study (i.e. from the system identification experiments). Also, all the required process measurements for soft sensor's operation can be made easily by using commercially available sensors without involving modifications to the existing machine. Moreover, the good performance of the proposed technique in rejecting disturbances is also a supporting factor for its industrial use. Furthermore, there are a few possible directions for improving the soft sensors' performance and its applications in future and these are discussed in the followings.

In this study, the die melt temperature profile and the bulk melt temperature indicated by the IR temperature sensor were modelled as functions of major process variables (i.e., screw speed and barrel set temperatures) together with a machine geometrical parameter (i.e., die radial position). Although these are the variables which significantly affect the process melt temperature, proposed models may be further improved with a generalised structure (as the example shown in equation (9)) by taking all the relevant material, machine geometrical and processing parameters into account.

$$\hat{T}_{m,j} = \pm(a_1 \times \omega_{sc}^{z1} \times D^{z2}) \pm (a_2 \times k_m^{z3} \times T_{b,i}^{z4} \times R_{p,j}^{z5}) \pm(a_3 \times \omega_{sc}^{z6}), ... \pm (a_i \times C_s^{zi}), ... \pm (a_{\bar{n}} \times R_{p,j}^{z\bar{n}}) \quad (9)$$

where a_i, $i = 1, 2, \cdots, \bar{n}$, are the model coefficients of a generalised model, zi are the corresponding powers of the variables included in a generalised model, D is the diameter of the screw, $T_{b,i}$ are the barrel zone temperatures, k_m is the melt thermal conductivity, C_s is the specific heat capacity of the solid material and $\bar{n}$ is the total number of model terms of a generalised model (it should be noted that a generalised model may include several other process variables which were not included in equation (9)). Obviously, the development of these types of generalised models may allow to obtain models which are smaller in size but with good accuracy (i.e. obtaining highly accurate predictions from the models which are low in order and with less number of model terms) that can be used with any machine, material and process settings and hence will be considered in future research. Furthermore, such generalised models could represent the actual process dynamics better than the first principle models which are usually developed based on a number of simplifying assumptions.

Conversely, the performance of the IR temperature sensor may be affected by some of the material properties such as melt emissivity [39] and this is one of the possible disadvantages of the use of an IR temperature sensor within this soft sensor. However, IR temperature sensors are readily used in the present industry with a large number of materials without any problem. Nevertheless, it is possible to replace the IR temperature sensor from the proposed soft sensor if any other better technique is available which can perform the same job.

The accuracy of the process measurements is also important for the better performance of the soft sensor. That is because the models developed are based on the measured experimental data and if these measurements are poor in accuracy, resulting models would also be poor in accuracy. Moreover, the soft sensor uses a few real-time process measurements for its predictions. Therefore, the use of highly accurate equipment for process measurements is a major requirement for a model-based soft sensing or control approach. Also, all of the sensors should be calibrated properly while avoiding possible offsets of sensor readings. A careful attention should be made on the possible effects of the noise (if any) attached to the measured signals on the performance of the soft sensor. As was reported in the literature [40], [41], filtering of the signals should not be carried out for avoiding noise or large fluctuations in the measured signals to making it is easy to design the soft sensor. This may cause to filtering of the fluctuations which may really affect the process functional quality and hence the measurements made by the sensor may not be capable of indicating the real fluctuations attributed to the process. In fact, the best practice would be the achievement of the accurate measurements (i.e. measurements such as screw speed and barrel set temperatures) to the highest possible level by improving the quality of the sensors and data acquisitioning (DAQ) devices. If it is obvious that some of the information included in a measured signal is not relevant to the actual process, then these can be filtered by using a properly designed filter. Sometimes, it would be difficult for industrial processes to follow all the practices which can be followed in an experimental laboratory to make accurate process measurements. However, it would be better to check the accuracy of the physical sensors (which are engaged with the soft sensor) from time to time while observing the key process signals on a screen in real-time. Obviously, the real-time observation of process signals on a screen should allow to identify the accuracy of these measurements while determining the process functional quality.

In this stage, the soft sensor strategy is proposed only for single screw extruders. In the application of the proposed technique into the multi screw extruders, the generalised models should be developed by studying their processing behaviours. Although the same model structure can be used, additional process and machine geometrical parameters may need to be considered depending on the machine and the nature of the process. In fact, there is no fundamental issue of using the thermocouple mesh technique on multi screw extruders. However, the possibility of using of the thermocouple mesh technique may depend on the process speeds, output channel shape and size, access requirements, etc. Currently, research work is underway to test the performance of the soft sensor on an industrial extruder and also to extend this technology to other type of extruders.

VI. Conclusions

A thermocouple mesh technique was used to monitor the temperature profile across the die melt flow of an industrial polymer extrusion plant. The data obtained was used to develop a novel real-time technique to predict the temperature profile across the extruder output melt flow in polymer extrusion (i.e. a soft sensor for temperature profile prediction) for the first time in research. It predicts the melt temperatures at a number of radial positions across the die melt flow and the possible prediction errors are compensated by a temperature feedback obtained from a combined mechanism of a physical IR temperature sensor attached to the extruder and a feedback model. Basically, two computationally efficient dynamic process models are included within the newly proposed soft sensor. These models are simple in structure and can be used in real-time applications. Moreover, the predictions of these models are in good agreement with the previously reported experimental findings and hence it confirms their accuracy. Generally, only the readily measurable process parameters (i.e. screw speed, barrel zone temperatures, a temperature measurement from an IR temperature sensor) are used by the proposed soft senor for its predictions. As all of these parameters can be easily measured in any industrial/practical environment by using commercially available instruments to a reasonable accuracy, the newly proposed soft sensor can be used to make real-time measurements. In the operation of the proposed soft sensor, it compares the predicted and measured IR temperature signals (i.e. the feedback mechanism) and the difference between these two signals ($T_{IR,Error}$) is used to compensate the possible errors in melt temperature profile prediction. A simulation of the proposed soft sensor on a set of unseen data of 129 minutes of process operation showed that the predicted and measured IR temperatures were mostly overlapping while occasional prediction errors (i.e. $T_{IR,Error}$) less than $\pm 5°C$ (i.e. less than $\pm 2.25\%$ of full reading) were available. More importantly, this newly proposed soft sensor technique should help to demonstrate a potential method for determining in-process melt flow thermal homogeneity (i.e. across the melt flow cross-section) without disturbing the steadiness of the melt flow. Usually, the use of physical sensors for making temperature profile measurements across the melt flow is not industrially compatible due to several constraints. Therefore, the newly proposed soft sensor technique will be a promising industrially compatible solution to predict real-time melt temperature profile across the melt flow cross-section in polymer extrusion. Moreover, this technique allows to build-up a control strategy to obtain the required melt flow thermal homogeneity in polymer extrusion by manipulating the process settings while maintaining the desired average melt temperature across the melt flow.

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