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ANN-based soft-sensor for real-time process monitoring and control of an industrial polymerization process

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A B S T R A C T

This paper presents the development and the industrial implementation of a virtual sensor (soft-sensor) in the polyethylene terephthalate (PET) production process. This soft-sensor, based on a feed-forward artificial neural network (ANN), was primarily used to provide on-line estimates of the PET viscosity, which is necessary for process control purposes. The ANN-based soft-sensor (ANN-SS) was also used for providing redundant measurements of the viscosity that could be compared to the results obtained from the process viscometer. It was shown that the proposed ANN-SS was able to adequately infer the polymer viscosity, in such a way so as this soft-sensor could be used in the real-time process control strategy. The proposed control system has successfully been applied in servo and regulatory problems, thus allowing an effective and feasible operation of the industrial plant.

1. Introduction

Polyethylene terephthalate (PET) is a thermoplastic polymer resin of the polyester family that is used in synthetic fibers, beverage, food and other liquid containers, thermoforming applications, and engineering resins often in combination with glass fiber. It is one of the most important raw materials used in man-made fibers. Polymerization is carried out through a polycondensation reaction of the monomers with ethylene glycol as the byproduct. The majority of the world's PET production is for synthetic fibers (60%) with bottle production accounting for around 30% of global demand. In discussing textile applications, PET is generally referred to as simply "polyester" while "PET" is used most often to refer to packaging applications.

Large-scale industrial PET line sizes reached the 800–1000 T/d rate in mid-2003, at M&G's PET resin plant located in Mexico. Additional world scale process units in this capacity range are in operation with on stream dates since 2005. The current trend is toward 1000 T/d single melt phase units coupled with two individual 500 T/d SSP (solid state polymerization) lines. While the driving forces toward maximum capacity plants are very strong, it is critical that with scale-up the plants must run reliably and continuously near its design capacity and without waste or off-specification product. With the modern, high-capacity SSP units, the financial consequences of producing un-saleable product are enormous. The key process factors that can influence the cost of production are: (i) ineffective equipment utilization; (ii) unscheduled down-time and upsets; (iii) transitions during product grade changes, as well as start-up and shutdowns; (iv) variations in product quality (McGehee, Johnson, & Bertelli, 2004).

Regarding only the product quality factor, one of the most important specifications that must be maintained is the intrinsic viscosity (IV). The viscosity is the main controlled variable of the PET polymerization process (Gonzaga, 2003). Intrinsic or relative solution viscosities and melt flow index are widely used in the specification of many polymer resins used in the fiber industry. The solution viscosity provides a measure of the molecular weight of a polymer, but the precision of these measurements can be relatively poor (De Laney & Oliver, 2002). Although the viscometers relating to this work usually provide reliable on-line viscosity measurements, special care must be taken to ensure their perfect operation, e.g., adequate temperature control, and regulation of the pump velocity during process operation. Despite all efforts to avoid such problems, capillary obstruction and subsequent pump malfunction often occurs. In these occasions, viscometers provide incorrect values of the PET viscosity and this problem is only detected by

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laboratory analysis, with a considerable time delay. This delay causes problems such as production of out-of-specification polymer, and interventions in the viscometers to proceed accurate capillary cleaning, pump exchanges, gauging the pressure transmitters, etc. (Gonzaga, 2003).

To overcome the technical difficulties associated with real-time measurement of the PET viscosity, the authors proposed the development and on-line application of an artificial neural network (ANN)-based soft-sensor (ANN-SS) to provide reliable estimations of this property. The estimated viscosity was then used in the control strategy of this industrial polymerization process.

The remainder of this paper proceeds as follows: Section 2 introduces the industrial polymerization process, describes the main equipments, as well as the digital distributed control system. Soft-sensors are presented in Section 3 , while the results concerning the development of the proposed ANN-based soft-sensor, its performance, and the resulting control system are discussed in Section 4. Finally, the concluding remarks are addressed in Section 5.

2. The polymerization process

The case study is the M&G PET resin plant located in Poços de Caldas, State of Minas Gerais, Brazil. This plant is composed of four production lines with total capacity of 180.000 ton a year. Although the whole production process of the PET resin is carried out in two stages: liquid and solid state polymerization; only the liquid polymerization stage is presented in this paper. The process flow diagram of the plant investigated in this work is shown in Fig. 1.

In this process, polyethylene terephthalate resin is produced from a paste composed of purified terephthalic acid (PTA), ethylene glycol (EG), and purified isophtalic acid (PIA). The chemical reactions that occur in liquid polymerization stage are esterification and polymerization. The final product of this stage is the PET resin in amorphous state, which should still pass through the SSP for attainment of the necessary characteristics required in the production of packings. During liquid polymerization stage, water, EG and solids are generated as by-products.

Since this process involves a significant amount of equipments and process variables, a distributed control system (DCS) was designed to allow the automatic supervision and control of the main process variables. In this full-automated plant, the supervisory system was built by using a net structure interconnecting programmable logical controllers (PLC), which actuate directly on process equipments, with human-machine user interfaces (HMI). The use of this structure makes possible the development of several control loops and their integration to the proposed soft-sensor. The main process variables of the liquid polymerization stage, highlighted in Fig. 1, are shown in Table A.1 in Appendix A.

2.1. Process description and plant equipments

In order to obtain PET resin, it is necessary that two chemical reactions happen: esterification and polymerization. The esterification is the chemical reaction that occurs between (mono) EG and PTA, yielding the monomer bishidroxyethyl terephthalate (BHET). Since the PET produced to packing manufacturing is a copolymer, PIA is used as copolymerization agent in small amounts, which also reacts with EG producing the monomer bishidroxyethyl isophtalate (BHEI).

In the *paste mixing tank* (RM), PTA is mixed with EG and PIA in carefully metered amounts, automatically controlled by a PLC through the distributed control system of the plant. The resulting paste is fed to the first reactor, the *primary esterification reactor* (PE). The reactions of production of the monomers BHET and BHEI occur inside PE and in the *secondary esterification reactor* (SE) under specific and controlled conditions of residence time, temperature and pressure. In the esterification process, PE is responsible for nearly 80% yield of the polymerization reaction. Monomers produced inside PE are transferred to the SE by differential pressure, where the reaction is completed and esterification rate grows up from 80 to 98%. Polymerization occurs after esterification is concluded, and this reaction also occurs under specific conditions of temperature, pressure and residence time. The *low polymerizer* (LP) is typically composed of a simple CSTR where chemical reactions occur between the monomers to form polymer with molecular weight of the order of 2500 g/mol and EG as the main byproduct. The polymer intrinsic viscosity (IV) in the LP is approximately about 0.2. *High polymerizer* (HP) is the final stage of the polymerization process and, at this point, it is important the accurate control of the molecular weight of the polymer. While in the LP molecular weight of the order of 2500 g/mol is obtained, in the HP the polymerization reaction continues until the molecular weight reaches a final value about 15,000–20,000 g/mol. The polymer intrinsic viscosity in the HP is about 0.6–0.64, depending on the type of the resin produced (Gonzaga, 2003).

Intrinsic viscosity (IV) is a relative measure of the resin molecular weight (or the polymer chains length), and also is a common descriptor of the PET flow-ability (De Laney & Oliver, 2002). At the M&G industrial plant, the viscosity is directly measured in the process output line by using a capillary viscometer. The *Viscometer* is installed in the polymer transfer line from the liquid to the solid state polymerization unit (see Fig. 1), close to the extrusion head. The signal from the on-line viscometer, representing the PET IV, is sent to the master viscosity controller (V-1) that, in a cascade control configuration, sets the pressure to be provided by the slave controller (P-3) in the high polymerizer. Fig. 2 shows the block diagram of the viscosity control loop.

Although these viscometers can provide quite good on-line measurements, it is necessary to carefully control some operational aspects related to this sensor during the PET production process, such as the viscometer block temperature, and the polymer pumping velocity. Despite all efforts to avoid operational problems, regular maintenance of the viscometers are necessary due mainly to capillary obstruction, pump exchange, calibration of the pressure transmitter, and correction of the conversion scales. During these malfunction periods, on-line viscometers provide incorrect measurement of the PET viscosity and this problem is only detected, with a considerable time delay, by laboratory analysis. This problem was the main driving force behind the development of the ANN-SS presented in this work.

2.2. The PET distributed control system

As described in the Section 2.1, the PET production process involves a number of equipments and process variables. In order to adequately deal with such a significant amount of process data, a DCS is used to supervise the entire plant events as well as to run algorithms that automatically control the main process variables.

This distributed control system is formed by a net of PLC and another net of HMI, the latter located in a net server, where the database is stored. The integration of these two nets (PLC and HMI) forms the industrial local net, or the Local Area Network (LAN), thus constituting the *PET Distributed Control System*. Fig. 3 illustrates the industrial LAN of the polymerization process.

A *Supervisory System* is a modularly organized structure composed of specialized programs that reside permanently in the computer's main memory and controls the processing of user's programs. In this plant, the communication interface between process engineers and PLCs is carried out through a supervisory system

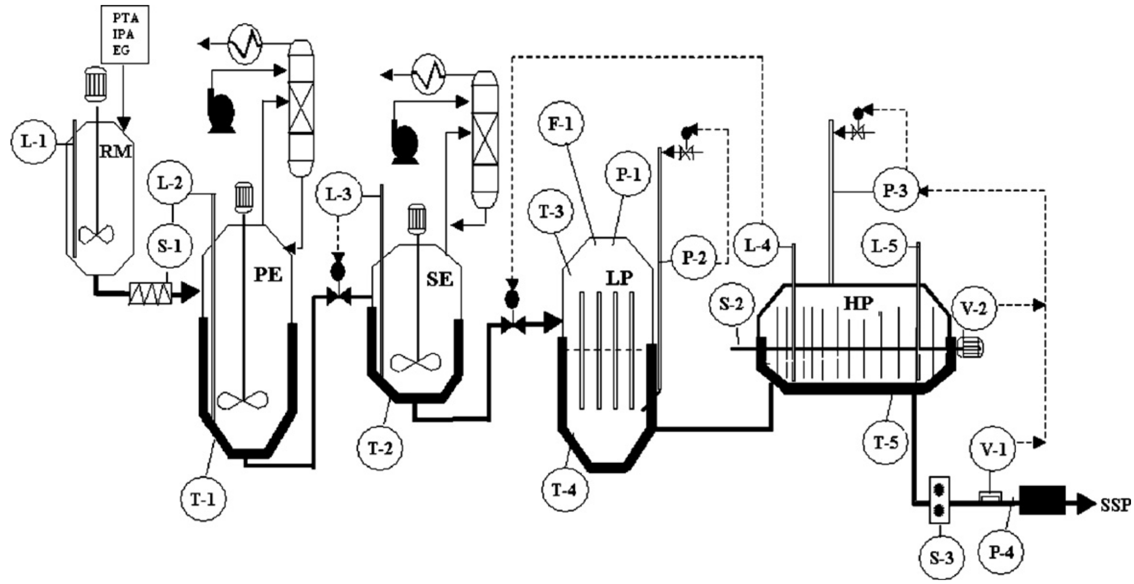

Fig. 1. General flow diagram of the PET polymerization process.

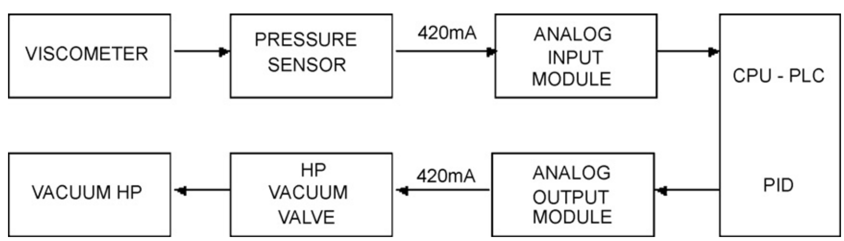

Fig. 2. Viscosity control loop.

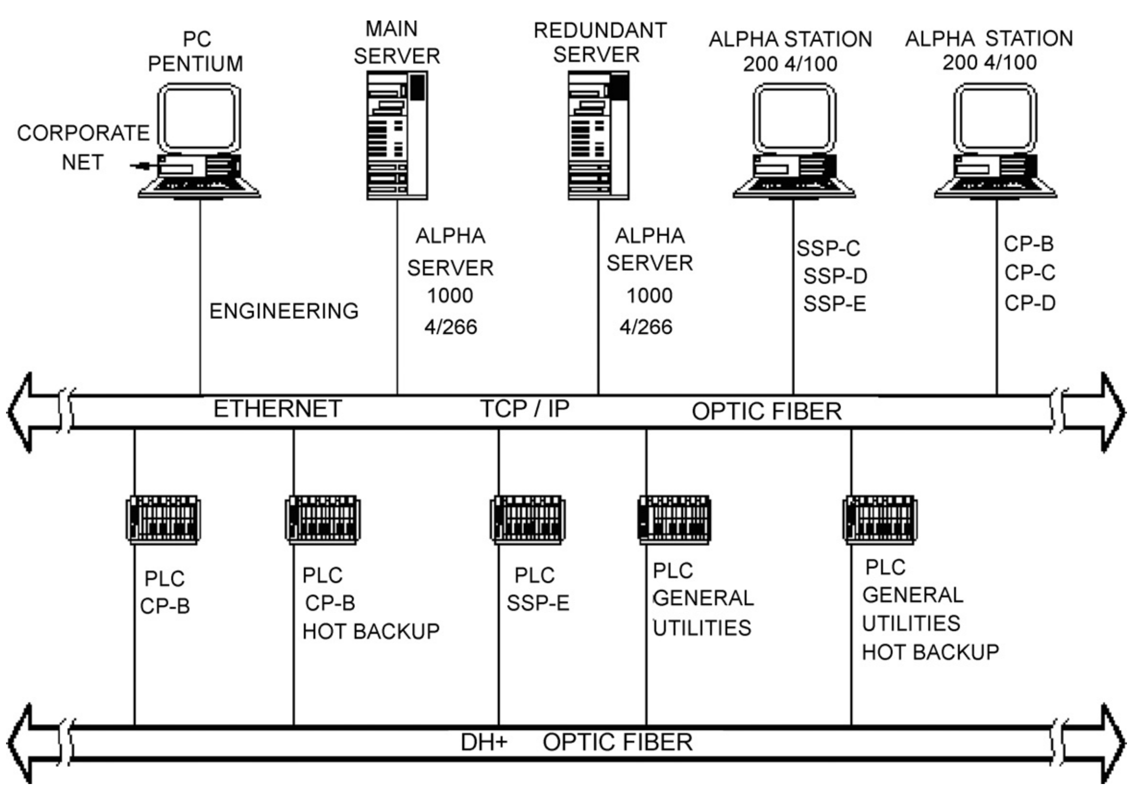

Fig. 3. Communication net topology of the industrial polymerization plant.

(SETCIM) developed by AspenTech. This *Real-Time Database System* is used for database management in such a way that the process data are updated in real-time in the resident memory in a dynamic and standard storage protocol.

3. Soft-sensors

Soft-sensor or virtual sensor is a common name for a software where several measurements are processed together. The interaction of the signals can be used for calculating or to estimate new quantities that cannot be measured. A virtual sensor is a conceptual device whose output or inferred variable can be modeled in terms of other parameters that are relevant to the same process (Rallo, Ferre-Giné, Arenas, & Giralt, 2002). Software sensors can also be understood as an association of a sensor (a hardware), which allow on-line measurements of some process variables, with an estimation algorithm (a software) in order to provide on-line estimates of immeasurable variables, model parameters or to overcome measurement delays. In fact, many authors proposed the soft-sensor approach to overcome the problem of on-line estimation of process variables (e.g. (Tham, Morris, & Montague, 1989; Martin, 1997; Févotte, McKenna, Othman, & Santos, 1998; Ohshima, & Tanigaki, 2000; Abonyi, Nemeth, Vincze, & Arva, 2003; Sharmin, Sundararaj, Shah, Griend, & Sun, 2006; Lin, Recke, Knudsen, & Jørgensen, 2007).

Several estimation techniques have been proposed in the literature. Among these techniques, four have been recognized to have strong potential in on-line estimation tasks (Assis, & Maciel Filho, 2000): (i) estimation through elemental balances; (ii) adaptive observers; (iii) stochastic techniques (e.g. Kalman filter); (iv) artificial neural networks.

According to Rallo et al. (2002), artificial neural networks have been shown to be an adequate choice because they can receive real-time readings of several process variables as well as feedback signals of downstream on-line analyzers for the target property. Once trained, this virtual sensor uses real time measurements of the selected process variables to infer the value of the product target property. The output can be redirected as information to the plant operator or to the control system to maintain optimal plant operation for a given product quality. In addition, ANN can improve performance with time, i.e., they are capable of learning real cause-effect relations between sensors stimulus and its response when historical databases of the whole process are used for training.

Since last decade, a considerable number of papers refer to the development and application of ANN as soft-sensor in polymerization process. (Lightbody, O'Reilly, Irwin, Kelly, & McCormick, 1997) investigated the performance of B-spline and MLP neural networks to predict the viscosity of an industrial polymerization reactor and hence remove the measurement time-delay introduced by the viscometer. (Wagner, Montague, & Tham, 1997) used ANN as soft-sensor in an industrial reactive plasticating extruder to enable prediction of extrudate viscosity. Zhang et al. (1997, 1998) developed a robust estimation technique to infer the polymer properties using multiple neural network representations as software sensor for a batch polymerization reactor. This technique was further improved by Zhang (1999). Rallo et al. (2002) proposed the use of a neural virtual sensor for the inferential prediction of the melt index and the quality of six different low-density polyethylene grades produced in a tubular reactor. Abonyi et al. (2003) presented a soft-computing based approach to predict the polyethylene melt index and density based on measured process variables of an industrial plant. Shi, Liu, and Sun, (2006) proposed a novel soft-sensor architecture based on radial basis function networks combining independent component analysis and multi-scale analysis to infer the melt index of polypropylene from process variables.

4. Results and discussions

In this study, an artificial neural network was used to build a soft-sensor to predict the polymer viscosity by using easily measured process variables. The study was conducted using operational data collected from the industrial polymerization process described in Section 2.

4.1. Soft-sensor development

To accomplish this work, authors used a feed-forward artificial neural network in the development of a soft-sensor aiming to provide on-line estimates of the polymer viscosity. This ANN, which uses easily measured process variables in the input layer, was trained with the historical operational dataset of the plant. The proposed ANN-SS was able to accurately infer the PET viscosity in such a way so as these estimates could be used on-line in the process control strategy. The ANN-SS was also used for providing redundant measurements of the PET viscosity that could be compared to the results obtained from the process viscometer and from laboratory analysis.

4.1.1. Selection of the input variables

In the process of building a neural inferential measurement system, a reduction in the dimension of the input space would simplify the input layer of the neural architecture and reduce the time needed for training (Rallo et al., 2002). Additionally, due to their generic structures, neural models usually require the estimation of a large number of parameters. Generally, the number of parameters and data needed to provide a desired degree of accuracy increases exponentially with the dimension of the input space of the mapping to be approximated (Meleiro, Campello, Maciel Filho, & Amaral, 2006). To avoid this problem, the so called "Curse of Dimensionality" (Kosko, 1997; Haykin, 1999), a great effort must be done in order to reduce the dimension of the input space. In this work, a preliminary set of input variables for the neural model was selected considering a priori knowledge about the process. These input variables were further analyzed considering their degree of correlation with the polymer viscosity by using sensitivity analysis. Based on these considerations, eight variables were selected for the input layer of the neural model (see Fig. 1): PE temperature (T-1); SE temperature (T-2); LP second stage temperature (T-4); HP temperature (T-5); LP first stage pressure (P-1); LP second stage pressure (P-2); HP pressure (P-3); Additive flow rate into LP (F-1). The patterns used in the output layer of the ANN (the target variable) during the training stage were the actual viscosity obtained from the plant viscometer (V-1) data records.

4.1.2. Selection of the historical data

In the present study, a representative dataset containing 6500 input/output patterns, corresponding to approximately 2 months of process operation, was used for ANN training. Considering the ANN-SS development, special care was taken for selecting all significant information from the complete set of available patterns contained in the data records. The effects of outliers (Sharmin et al., 2006; Lin et al., 2007) were reduced by filtering the training data using the three standard deviation confidence interval (3σ rule) as specification criterion. The key idea was to include as learning examples those data that contain most of the important information about the PET polymerization process. These patterns, which are those that best represent the different process operating conditions, were included in the training set to supply the neural model with suitable examples. A different sequence of process data, consisting of 2250 patterns, was further used to evaluate the performance of the ANN-SS.

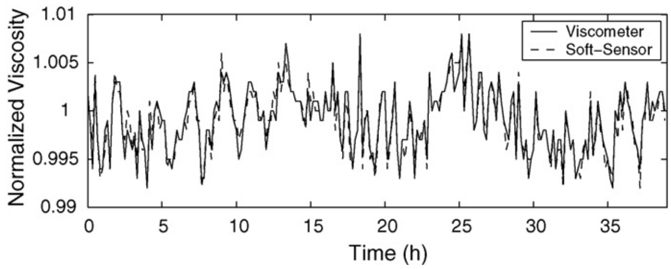

Fig. 4. Performance of the ANN-SS using the validation dataset.

4.1.3. *Neural network structure selection*

One-hidden-layer feed-forward neural network using hyperbolic tangent as activation functions was selected as the neural paradigm. ANNs were configured for training using the Levenberg–Marquardt optimization algorithm together with the cross validation based early stopping mechanism to prevent over-fitting (Haykin, 1999). Several feed-forward ANNs were investigated considering different number of hidden neurons, ranging from 3 to 25. Each network was trained at least three times using different sets, randomly generated, of initial weights. The number of neurons in the hidden layer was chosen considering the performance of the network giving the least error on the test data. The neural model selected in this work was an one-hidden-layer feed-forward neural network with eight neurons in the input layer (see Section 4.1.1), nine hyperbolic tangent hidden neurons, and one linear neuron in the output layer, representing the estimated PET viscosity. The predictions provided by the selected neural model, exhibited in Section 4.1.4, showed a quite good agreement with the validation process data.

4.1.4. *Soft-sensor performance*

The datasets used for training and testing the proposed soft-sensor were acquired from the historical logs recorded at the M&G PET polymerization plant, and the reliability of the ANN-SS predictions is illustrated by comparing their estimates with actual process data from the validation set. Fig. 4 shows the estimates of the PET viscosity provided by the ANN-SS using the test data collected from the industrial polymerization process. This figure illustrates the good performance of the virtual sensor when their predictions are compared with actual data, obtained from the process viscometer, in the course of approximately 40 h of process operation. Viscosity values were normalized for the sake of trade secret.

It should be highlighted that the maximum absolute prediction error observed in this time interval of process operation was equal to 4 poise. This value corresponds to a relative error of approximately 0.3%. According to the histogram of the estimation errors shown in Fig. 5, most of prediction errors belong to the 0–1 poise interval.

4.2. *On-line soft-sensor implementation*

Soft-sensor implementation aimed to allow its use directly in the PET supervisory control system. Once trained, this soft-sensor was able to use real time measurements of the selected process variables to infer the viscosity of the PET leaving the high polymerizer. The ANN-SS output was then sent to the control system that used this information to maintain the optimal plant operation for a pre-specified value of viscosity. Fig. 6 illustrates the soft-sensor-based control system proposed in this work.

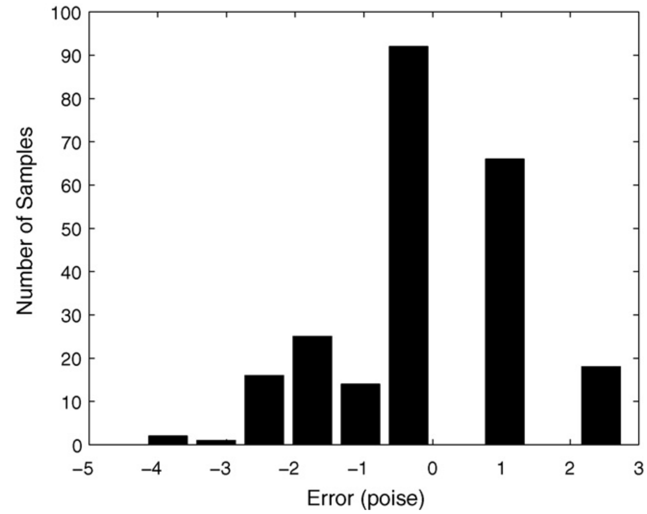

Fig. 5. Histogram of the estimation errors using validation dataset.

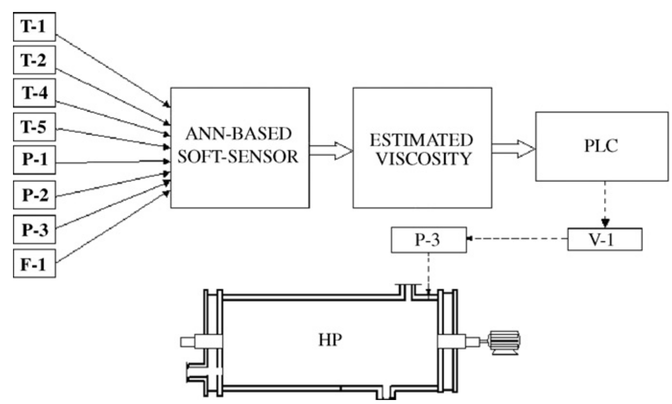

Fig. 6. Structure of the ANN-SS and its integration with the viscosity control system.

4.2.1. *Integration of soft-sensor and SETCIM*

One of the main features offered by SETCIM is the possibility of complex application development (external tasks) using scientific programming languages, such as FORTRAN and C, and associate them to the process database. The use of this kind of programming structure makes possible, if necessary, the development and use of several soft-sensors. Fig. 7 shows an application example of the SETCIM in the PET polymerization process.

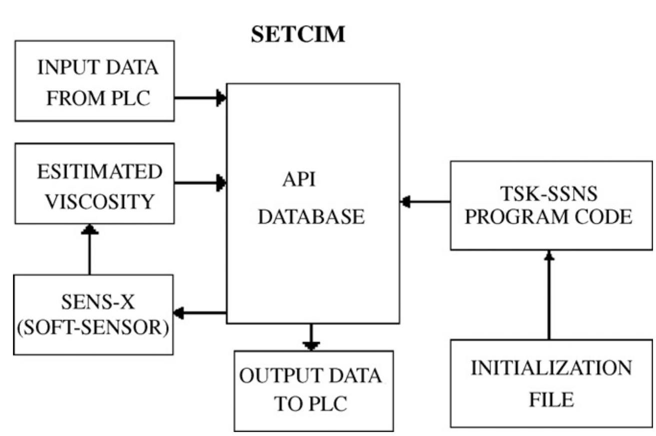

Fig. 7. Schematic representation of SETCIM data management.

As described in Section 2.2, SETCIM is used for database management in such a way that the process data is updated in real-time in the resident memory. In order to integrate ANN-SS into SETCIM environment, an external task (TSK-SSNS) was created to link online process data and the soft-sensor code through the Application Programming Interface (API). Input process data are processed inside the soft-sensor module (SENS-X) and the inferred viscosity is sent to the PLC used in the viscosity control system, as illustrated in Fig. 6.

4.2.2. Soft-sensor in the process control strategy

The main motivation behind the development of the soft-sensor for on-line use in the viscosity control strategy was to supply an alternative way to deal with the operational problems occurring with the viscometers (see Sections 1 and 2.1) at the M&G polymerization plant. The initial approach proposed by the process engineers to overcome this problem was to use the electric current demand (V-2) from the motor attached to the rotating shaft of the high polymerizer (see Fig. 1) as an indicator of the degree of polymerization, since the required amperage increases as the polymerization reaction proceeds. However, this strategy was not successful. Considering the necessity to provide a more robust and reliable control of the PET viscosity, the ANN-SS described in this work was used to replace the viscometer measurements. Since the soft-sensor shown to be able to supply accurate inferences of viscosity, it was used in the main control loop, while the viscometer was kept operating in parallel, for the sake of security. To guarantee the quality of the soft-sensor predictions, a safety plant operation procedure was implemented to detect eventual operating fails in both sensors, the viscometer and the ANN-SS: when the absolute error between the measured and estimated viscosity is greater than 50 poise, a polymer sample is analyzed in the laboratory to check which value is the more accurate. This safety procedure shown to be helpful to identify if the ANN-SS should be re-trained, by updating the database, or if the viscometer should be sent to the maintenance department. Another procedure was further implemented to avoid possible incorrect evaluation that may occur when the error analysis is based upon a single sample. This strategy considers mean errors taken from longer time intervals. Figures below show different scenarios for testing the industrial process control systems.

Fig. 8 shows the performances of the two proposed control strategies, i.e., the soft-sensor and the stirrer amperage based controllers. This figure is useful to examine the decreased product variability resulting from the use of the ANN-SS based control strategy in the course of approximately 24 h of industrial plant operation. Fig. 9 shows the corresponding absolute values of the closed-loop errors when using both control strategies.

Since ANN-SS based control provided the best performance, this strategy was adopted at the M&G polymerization plant. Fig. 10 shows the closed-loop responses of the process control system in a typical regulatory problem, i.e., when the controller must be able to reject disturbances acting on the process, and the controlled variable should be kept in a prespecified setpoint.

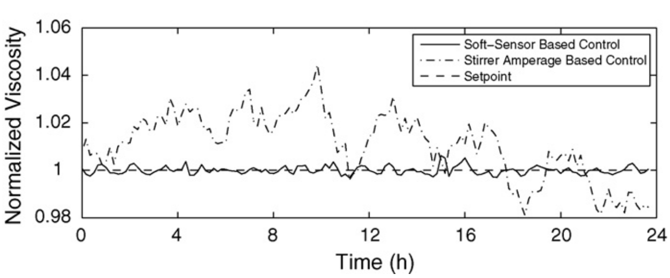

Fig. 8. Closed-loop performances of the two proposed control strategies.

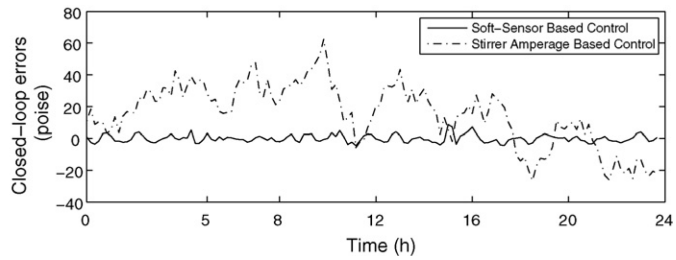

Fig. 9. Closed-loop errors (absolute values) in the regulatory problem.

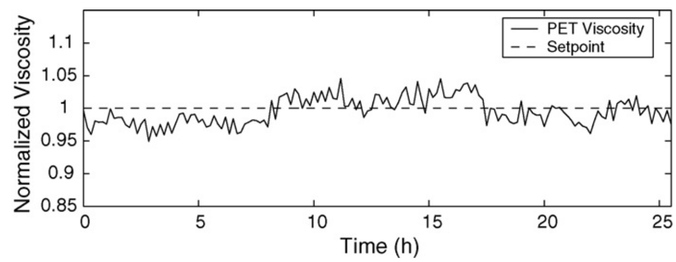

Fig. 10. ANN-SS based control in regulatory operation mode.

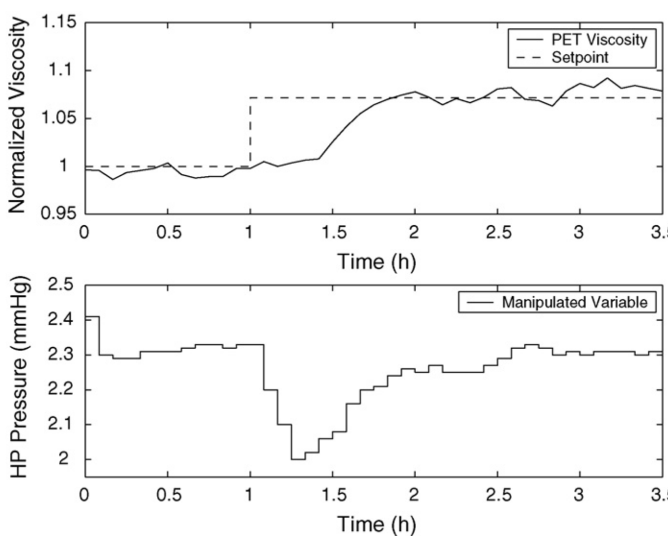

Fig. 11. ANN-SS based control in servo operation mode: reference and process output (above), and manipulated variable (below).

Fig. 11 presents the closed-loop performance of the control system when the process was required to track an imposed setpoint change, i.e., the servo control problem.

5. Concluding remarks

In the present work, an alternative way to deal with operational problems occurring with process viscometers in an industrial polymerization plant was proposed. A feed-forward ANN has been used in the development of a soft-sensor to predict the polyethylene terephthalate viscosity in the polymerization process. Off-line and real-time results have shown that the proposed ANN-SS can accurately infer the PET viscosity by using easily measured process variables. ANN-SS was integrated in the industrial process control system through a supervisory system developed by the M&G's

process engineers. Based on the ANN-SS predictions, the proposed control strategy shown good performances in both servo and regulatory problems, thus allowing an effective and feasible operation of the industrial polymerization plant.

Appendix A

See Table A.1.

Table A.1
Main process variables of the liquid polymerization stage

RM	Paste mixing tank
PE	Primary esterification reactor
SE	Secondary esterification reactor
LP	Low polymerizer
HP	High polymerizer
F-1 (kg/h)	Additive flow indication and control
L-1 (%)	RM tank level indication and control
L-2 (%)	PE level indication and control
L-3 (%)	SE level indication and control
L-4 (%)	HP input level indication and control
L-5 (%)	HP level indication
P-1 (mmHg)	Vacuum in the first stage of the LP
P-2 (mmHg)	Vacuum indication and control (LP second stage)
P-3 (mmHg)	Vacuum indication and control (HP)
P-4 (bar)	Pressure indicator of the extrusion process
S-1 (rpm)	Feed pump speed indication and control (PE)
S-2 (rpm)	Stirrer speed indication and control (HP)
S-3 (rpm)	Polymer pump speed indication and control (HP)
T-1 (°C)	Temperature indication and control (PE)
T-2 (°C)	Temperature indication and control (SE)
T-3 (°C)	Temperature indication and control (LP first stage)
T-4 (°C)	Temperature indication and control (LP second stage)
T-5 (°C)	Temperature indication and control (HP)
V-1 (poise)	Viscosity indication and control (HP)
V-2 (amperage)	Stirrer amperage indication and control (HP)

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