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On-line Neural Network Estimator of Polymerization Plant

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Abstract

A major difficulty affecting the control of product quality in industrial polymerization is the lack of suitable on-line measurements of polymer properties such as melt flow rate (MFR), polymer density and molecular weight distribution. Therefore traditional polymerization control has been carried out by sampling, off-line characterization of polymer quality in a laboratory and manual recording results. This approach is very time consuming and then causes lots off specification products. A practical on-line inferential scheme for estimating the melt flow rate and the polymer density proposed in this paper is a neural network approach based on input-output information of an industrial polyethylene plant. Available on-line temperature, pressure, flow rate, gas composition and other variables measurements of the process have been used to develop the network models; the neural networks have been trained based on actual operating data with backpropagation and Levenberg-Marquart techniques. Simulation results show that the developed neural network process models with two hidden layers can successfully predict both the melt flow rate and the density. Then the models can be applied to predict these quality variables on-line. Information regarding the on-line estimation of the quality variables can be useful in the formulation of advanced model based control techniques to achieve good control of product specifications as desired.

Keywords Neural networks, Polymerization, Polyethylene, Estimation

1. Introduction

Due to a growing demand for consistent and high quality polymer, there is strong need to control polymer properties as specified with optimal cost. Generally, the polymer's quality is defined in term of properties such as melt flow rate, molecular weight distribution and density. The melt flow rate of a polymer is vital to designing and controlling its processing; the flow of a plastic material is used as an indication of whether its final properties will be consistent with those required by an application. For the polymer density, it is empirically correlated to weight percent co-monomer incorporated in the polymer. Many polymer end-use properties are also dependent upon molecular weight distribution (MWD) because MWD is largely responsible for rheological properties. However, these quality variables are rarely available at frequent interval with substantial delays between sampling and analysis. Especially, off-line analyzing of melt flow rate is time consuming around 1 to 4 hours in a laboratory. Such a delay can result in product quality inconsistency and process control difficulty. One of solutions for improving on-line measurement is using a dynamic model based upon the mathematics-physics-chemistry of the process to predict the effect of changes in the reactor condition including the polymer properties. The use of mechanistic approach leads to less accurate prediction or large discrepancy because of process-model mismatch [1,2,3]. An alternative technique which can reduce the problematic of process-model mismatch is the use of an empirical technique to predict the polymer properties.

Here, the quality of polymer: melt flow rate (MFR) and density, have been predicted on-line by neural network models based on actual plant data.

2. Polyethylene process

The polyethylene process has a simplified schematic illustrated in Figure1. Ethylene, co-monomer and hydrogen are fed along with the prepared catalyst and hexane to the first reactor of a polymerization section. The product from the first reactor is then fed to the second reactor. Polymerization occurs in the reactors forming the polyethylene slurry. The slurry containing hexane proceeds to the separation and drying section. Polyethylene cake with some hexane and hexane are obtained from separation using a centrifuge. The polyethylene cake then leaves the vessel and proceeds to a rotary dryer. The obtained dried polymer flows to the purge column. Hot nitrogen flows through the purge column to remove most of the remaining hexane. Some of the hexane in the nitrogen is removed and then sent to the hexane recovery column. As the polyethylene passes through the separation and drying section, it is completely separated from solvent and takes a form of a powder. The polyethylene in powder form is fed to the pelletizing section to mix and stabilize the powder by a homogenizer. After that, the obtained powder is fed into a pelletizer to make polyethylene pellet. For the hexane recovery section, the hexane which contains low molecular weight polymers is separated by a distillation column and the purified hexane is returned to the reactor as recycle.

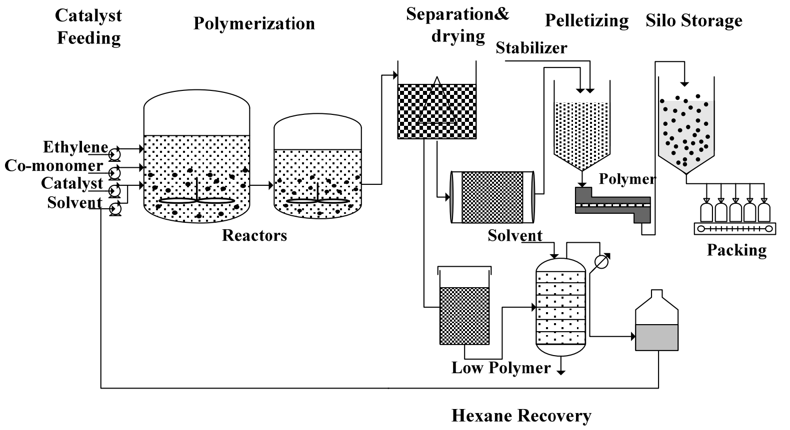

Figure 1 Simplified Schematic of polyethylene Plant

As the key properties: melt flow rate (MFR) and density are either rarely available or at best available rather infrequently, neural network models have been developed to provide the estimates of those on-line based on available information such as temperature, flow rate and concentration.

3. Neural network models for estimation of the polymer quality variables

Neural networks (NNs) have been applied to nonlinear process modeling and control recently [4,5,6,7]. They have the ability of learning the behavior of the process and the relationships between variables, without having a model of the phenomenological underlying laws. In this work, multi-layered feed forward neural networks are used as on-line estimators to estimate the polymer quality variables. The feed forward neural networks are trained by Levenberg-Marquardt technique; they are fed with the actual available input-output polymerization plant data obtained by both recoding on DCS (Distributed Control System) and analyzing samples in a laboratory on the actual plant. After training, the trained neural networks are validated by validation data sets. If the validation test is not satisfactory, the neural network requires more training by re-initializing the weights and biases.

Here, four network models have been developed with respect to key process variables shown in Table 1. The Neural Network with two hidden layers structure has been chosen due to the complexity of the process. To achieve proper neural network training, a sufficient number of data points must be used depending on the complexity of the process. In this work, about 1,600 samples are used for network training, and 200 samples for validation for modelling of four networks. The optimum structures of NNs are selected by the Sum of Squared Error (SSE) minimization method. The optimal configurations of the NNs that give the best estimates of the key properties on training and validating the networks are shown in Table 2. The obtained neural network models are then used as on-line estimator in the actual polyethylene plant.

Table 1 List of major process variables of model inputs and outputs

Model No.	Model inputs and outputs
Model #1	**Inputs:** H_2 to C_2 ratio **,** % H_2 **,** C_3/C_2,C_4/C_2 molar ratio (gas phase)**,** temperature**,** pressure **,** ethylene feed rate **,** past data **Output:** MFR in the Reactor 1
Model #2	**Inputs:** H_2 to C_2 ratio **,** % H_2 **,** C_3/C_2,C_4/C_2 molar ratio (gas phase)**,** temperature**,** pressure **,** ethylene feed rate **,** past data **Output:** MFR in the Reactor 2
Model#3	**Inputs:** H_2 to C_2 ratio of the Reactor 1 and Reactor 2, %H_2 of the Reactor 1 and Reactor 2, C_3/C_2,C_4/C_2 molar ratio (gas phase), temperature, pressure, ethylene feed rate, temperature of powder , temperature of resin in pelletizer, past data **Output:** MFR of pellet
Model#4	**Inputs:** H_2 to C_2 ratio of the Reactor 1 and Reactor 2, % H_2 of the Reactor 1 and Reactor 2, C_3/C_2,C_4/C_2 molar ratio (gas phase), temperature,, pressure, ethylene feed rate, slurry concentration, temperature of powder, temperature of resin in pelletizer, past data **Output:** polymer density

Table 2 The configuration of the neural networks for estimation of the polymer quality variables

Estimated polymer quality variables	Obtained NN configuration
MFR in the first polymerization reactor	**Model#1 =** 1-3-5-11 NN
MFR in the second polymerization reactor	**Model#2 =** 1-3-7-11 NN
MFR of polyethylene pellet	**Model#3** = 1-3-7-27 NN
Polyethylene density	**Model#4** = 1-9-11-25 NN

4. Results and discussion

The optimal network models with two hidden layers are chosen and in the on-line inferential system to provide the estimates of the MFR and the density of the properties in the actual plant with the frequency of one minute sampling interval. Figure 2 shows the estimates of the MFR in the Reactor 1 by 11-5-3-1 NN models. It can be seen that the error between actual and output values in the first 1,000 data points are rather high due to the lack of past values of output data. Additionally, if operating condition or process variables lies outside the training range, the models usually provides bad estimates; neural network models are rarely applicable to carry out extrapolations. After the first 1,000 data points, the networks can predict the MFR precisely.

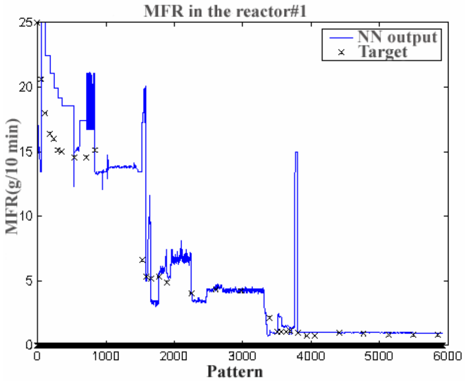

Figure 2 On-line estimation of MFR in the Reactor 1 by 11-5-3-1 NN, SSE=7.5617

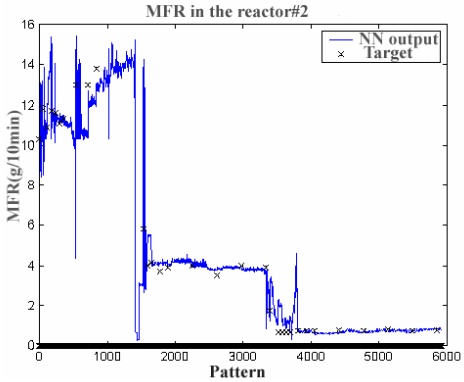

Figure **3** On-line estimation of MFR in the Reactor 2 by 11-7-3-1 NN, SSE=1.4463

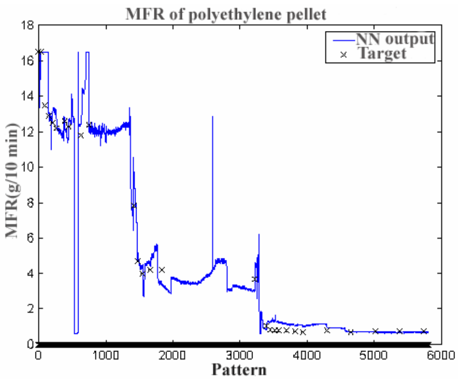

Figure 4 On-line estimation of MFR of polymer pellet by 27-7-3-1 NN, SSE =0.58188

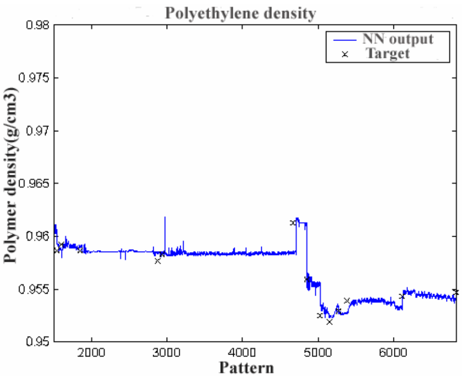

Figure 5 On-line estimation of polyethylene density by 25-11-9-1 NN, SSE =54.1295

The estimates of the MFR in the second reactor are almost identical to the actual data for the whole region (Figure 3). This shows that the 11-7-3-1 model can be confidently used for estimation purposes. Figure 4 illustrates that with the feedback calculated outputs, the model can still provide good estimates of the MFR of polyethylene pellet even though the estimates of the MFR in the Reactor 1 and 2 are not good; the deviations between the NN outputs and the plant values are fairly high. For the estimation of polyethylene density shown in Figure 5, it gives excellent estimates of the density with respect to the actual input data. This result, therefore, demonstrates that the neural network is applicable to estimate the trajectory of polyethylene density.

For all cases, the influence of the learning sets is also considered because learning sets with redundant data during training usually lead to poor performance. This is because the networks will tend to overfit the given data and the output and then provide estimates which highly depend on the given data. However, there is still no formula to define the number of data points required to train neural networks. In addition, the number can be varied depending on the complexity of the problem and the quality of the data.

5. Conclusions

Polymer properties: the Melt Flow Rate (MFR) and the density can be used to classify their physical and chemical properties. Therefore, they are needed to be controlled at a defined set point. However, they are rarely available or measured with sufficient frequency in the control point of view. To overcome the lack of on-line measurement of this information without process-model mismatch, neural network models based on actual input-output information of the process are used to provide the estimates of the MFR and the polymer density in industrial polymerization process. It was observed that the neural network models provide good estimates of both the MFR and the polyethylene density; the polymer properties obtained by networks have profiles almost identical to those gathered from the actual process. It should be noted that appropriate numbers of learning data and data range for training are required to achieve good models for the property inferential system.

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