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Melt index prediction by neural networks based on independent component analysis and multi-scale analysis

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Abstract

Reliable estimation of melt index (MI) is crucial for the production of polypropylene. Propylene polymerization process is highly nonlinear and characterized by multi-scale nature with lots of variables and information that are highly correlated and derived at different sample rates from different sensors. A novel soft-sensor architecture based on radial basis function networks (RBF) combining independent component analysis (ICA) as well as multi-scale analysis (MSA) is proposed to infer the MI of polypropylene from other process variables. In the proposed model, ICA is carried out to select the most independent process features and to eliminate the correlations of the input variables, MSA is introduced to acquire approximate and detailed scale information of the process and make the model more robust to mismatches, and RBF networks are used to characterize the nonlinearity in every scale. The approach is evaluated and the results are compared with simplified approaches built with the same data set. The research results confirm the validity of the proposed model.

Keywords: Propylene polymerization; Radial basis function network; Independent component analysis; Multi-scale analysis

1. Introduction

Production of polypropylene is a multi-billion business, which moves around 15 billion US$ per year, with average annual consumption growth rate at 5%. Melt index (MI), the most important parameter in determining the product's grade and quality control of polypropylene produced in practical industrial processes, is usually evaluated off-line with an analytical procedure that takes almost 1 h to complete in the laboratory, leaving the process without any real-time quality indicator during this period. An alternative is to develop on-line estimators based on available process information to supervise the process and avoid any mismatch of product quality during product grade transitions. Normally an on-line analyzer can be constructed with the mechanism of polymerization. However, it is often challenged by the engineering activity and the relatively high complexity of the kinetic behavior and operation of the polymer plants as shown in Fig. 1 [11,12,19].

In a situation when a considerable amount of data about the studied process is available, as it is in the case with propylene polymerization, it is possible to exploit the available data using machine learning methods such as artificial neural networks (ANN) [6,14,18]. ANN has found wide application in the fields of process identification and process control due to its superb ability in representing arbitrary nonlinear relationships [2,5]. Propylene polymerization is a well-know highly nonlinear process which is obvious in the mechanism analysis of the reactions and plants [13]. So ANN is a reasonable choice for the currently studied problem. Unfortunately, neural networks often suffer from poor ability of generalization as the predictive accuracy depends on the data presented to it during training.

In the propylene polymerization plants, the number of the measured variables is large, which implies the generation of large datasets containing a large amount of features and the variables may be highly correlated, which would

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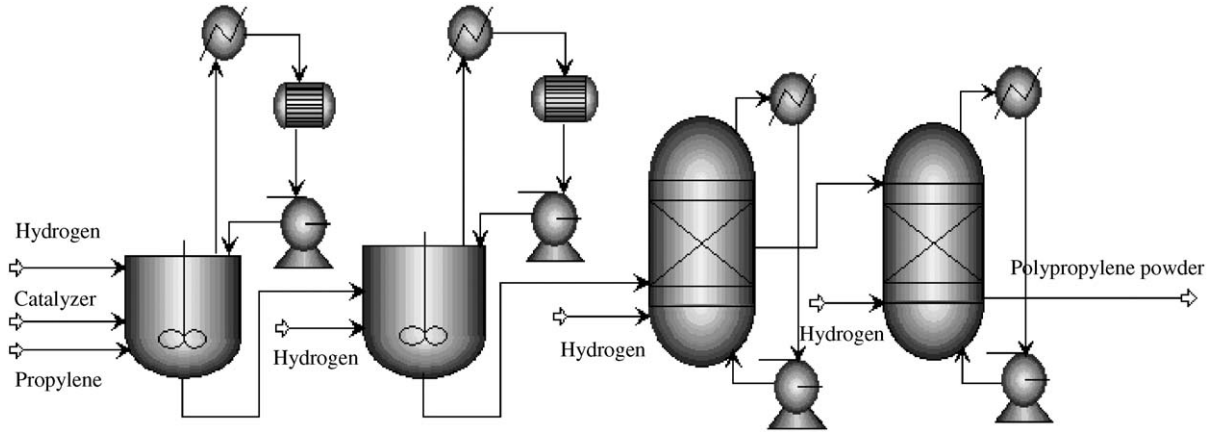

Fig. 1. General diagram of propylene polymerization.

ruin the performance of the model. Independent component analysis (ICA) is a very general-purpose projection technique in which observed random data are linearly transformed into components that are maximally independent from each other [7]. This is a widely used method to perform blind-source separation and feature extraction, developed in recent years and with a wide range of applications [20,22]. The present study adopts ICA to perform the selection of relevant features and information. In addition, a reduction in the dimension of the input space is derived, which will simplify the neural architecture and reduce the time needed for training.

Propylene polymerization is characterized by multi-scale nature with respect not only to space but also to time, showing dissipative structures induced by inherent nonlinear and non-equilibrium interactions and stabilized by exchanging energy, matter and information with their surroundings. The process ranges form molecular scales through reactor scales to factory scales, and the process data are derived at different sample rates from different sensors [9,10]. On the other hand, a signal or a function may be better understood if expressed as a decomposition over a basis. Multi-scale analysis (MSA) uses wavelets and corresponding scaling functions as basis functions to decompose a set of data into components described by wavelet coefficients. Signal decompositions with MSA have near-optimal properties in quite a wide range of non-homogeneous function spaces. MSA is thereby employed to acquire much more information from the process data, which will reduce the uncertainty and complexity of the studied problem [1].

As the above-mentioned methods have accordant property to the studied process, it is expected that the modeling of the process with the combination of the three methods would provide promising predictive accuracy of the melt index of polypropylene. The purpose of this study is to develop a virtual soft sensor to infer MI of polypropylene from other more easily measured process variables using neural network architecture combining ICA and MSA. Up to now, little literature about the integration of ICA, MSA and neural networks is reported. All aspects concerning the design are described, highlighting the basic architectures and algorithms. The performance of soft sensor has been illustrated and evaluated with an actual propylene polymerization. The results obtained are then discussed and concluding remarks about the design are finally presented.

2. Soft-sensor modeling

2.1. Neural networks

The neural network is a universal approximator that learns from the past to predict the future values. ANN is a broad term covering a large variety of network architectures, the most common of which is the feed-forward network. The Radical basis function (RBF) network is a typical feed-forward network, whose global approximation and convergence make it the primary choice for process product quality prediction [17,21]. RBF neural networks allow the parametrization of any function $f(x)$ as a linear combination of non linear basis functions,

$$f(x) = p + \sum q_j G(||x - x_j||), \tag{1}$$

where j is the function index, the norm $|\cdot|$ is the Euclidean distance, x_j are the centers of the proposed basis functions, p and q are adjustable parameters and G is a radial kernel function. In the current model a Gaussian activation function is used,

$$G(r_j) = \exp(-r_j^2/2\sigma_j), \tag{2}$$

where r_j is the Euclidean distance to the center and σ_j is the dispersion of the Gaussian. For each activation function (11) the center position x_j and its width σ_j must be determined to define a receptive field around the node. In this work the center position is obtained by the orthogonal least square (OLS) algorithm [3] and the width is determined by experience.

2.2. ICA

ICA is a very general-purpose statistical technique in which observed random data are linearly transformed into components that are maximally independent from each other, and simultaneously have "interesting" distributions.

Assume that n process variables indicated by x_j, $j = 1, \ldots, n$ represent a combination or mixture of n independent, nonGaussian and unknown sources s_i, $i = 1, \ldots, n$,

$$x_j = a_{j1}s_1 + a_{j2}s_2 + \cdots + a_{jn}s_n, \quad \text{for all } j. \tag{3}$$

Using this vector–matrix notation, the above mixing model is written as $\mathbf{X} = \mathbf{AS}$. One may now attempt to estimate the sources $\mathbf{S}$ with the mixing matrix $\mathbf{A}$. All we observe is $\mathbf{X}$, and both $\mathbf{A}$ and $\mathbf{S}$ must be estimated using it. After estimating the matrix $\mathbf{A}$, its inverse $\mathbf{W}$ can be computed, and the independent components are obtained simply by $\mathbf{S} = \mathbf{WX}$.

Entropy is the basic concept of information theory. The more independent, i.e., unpredictable and unstructured a variable is, the larger its entropy, and the ICA algorithms calculate the independent components based on this criterion. Negentropy J, often used as a slightly modified version of the definition of differential entropy H, is defined as follows:

$$J(s) = H(s_{\text{gauss}}) - H(s), \tag{4}$$

where s is a random vector and s_{gauss} is a Gaussian random variable of the same covariance matrix as s. The problem in using negentropy is, however, that it is computationally very difficult. A generally used approximation of negentropy is developed:

$$J(s) \approx \sum k[E\{(G(s)\} - E\{(G(v)\}]^2, \tag{5}$$

where k is some positive constant, v is a Gaussian variable of zero mean and unit variance (i.e. standardized) and E is the expectation. The variable s is assumed to be of zero mean and unit variance, and the functions G is some non quadratic function. The following choices of G have proved very useful:

$$G_1(u) = \frac{1}{a_1}\log\cosh a_1 u, \quad G_2(u) = -\exp(-u^2/2), \tag{6}$$

the derivatives of the functions in Eq. (6) are:

$$g_1(u) = \tanh(a_1 u), \quad g_2(u) = u\exp(-u^2/2), \tag{7}$$

where $1 \leqslant a_1 \leqslant 2$ is some suitable constant.

In this work the de-mixing matrix $\mathbf{W}$ will be calculated by FastICA algorithm [8] based on a fixed-point iteration scheme:

(1) Choose an initial (e.g. random) weight vector w_i, if $i \geqslant 2$, $w_i = w_i - W_{i-1}W_{i-1}^{\mathrm{T}}w_i$, where $W_{i-1} = [w_1\ w_2\ \ldots\ w_{i-1}]$, $i = 1, \ldots, m$. Usually $m \leqslant n$ instead of $m = n$.
(2) Let $w_i^+ = E\{xg(w_i^{\mathrm{T}}x)\} - E\{g'(w_i^{\mathrm{T}}x)\}w_i$.
(3) Let $w_i = w_i^+/||w_i^+||$.
(4) If not converged, go back to 2, else do the iteration until $i = m$.

The independent components then can be obtained by $\mathbf{S} = \mathbf{WX}$.

Here m means the number of independent components that is desired while n means the number of observed signals. Convergence means that the old and new values of w point in the same direction, i.e. their dot-product is (almost) equal to 1. It is not necessary that the vector converges to a single point, since w and $-w$ define the same direction.

2.3. MSA

Signal decompositions with MSA have near-optimal properties in quite a wide range of non homogeneous function spaces. The main idea behind wavelets is that, in representing a function belonging to a general space, space–time and frequency resolution analyses are pursued. The increased localization power yields advantages of more spatial adaptability. The approximate and detailed scale information conduces to better description of original signals and contributes to the modeling of the propylene polymerization process with the above described multi-scale nature.

The wavelet MSA is based on the scaling function $\phi(x)$ and the corresponding mother wavelet $\psi(x)$ [4]. The scaling function and the mother wavelet are localized both in time and frequency domain, which allows for explicit capture of the local dynamics of signals. By dilation and translation of the scaling function and the mother wavelet the following functions are derived:

$$\phi_{j,k}(x) = 2^{j/2}\phi(2^j x - k) \quad \text{and} \quad \psi_{j,k}(x) = 2^{j/2}\psi(2^j x - k), \tag{8}$$

with the subscript j denoting the scale or corresponding resolution of the functions and the subscript k localizing the functions in time. On each scale j, the functions $\phi_{j,k}(x)$, $k\varepsilon Z$ and $\psi_{j,k}(x)$, $k\varepsilon Z$ form an orthonormal basis in the spaces of the square integrable functions $L_2(R)$. An arbitrary signal $f(x)\varepsilon L^2(R)$ can be written as

$$f(x) = \sum_k a_{J,k}\phi_{J,k}(x) + \sum_{j \leqslant J}\sum_k d_{j,k}\psi_{j,k}(x), \tag{9}$$

where the first term represents the approximation on the scale J and the second term the details on the scale J and all finer scales. Together the wavelet coefficients $a_{j,k}$ of the approximation and the wavelet coefficients $d_{j,k}$ of the details form the discrete wavelet transform of the original signal $f(x)$.

In the wavelet MSA the wavelet coefficients $a_{j,k}$ of the approximation and the wavelet coefficients $d_{j,k}$ of the details on adjacent scales are related by the decomposition

$$a_{j,k} = \sum_{n\in Z} h^*_{n-2k}a_{j-1,n}, \quad d_{j,k} = \sum_{n\in Z} g^*_{n-2k}a_{j-1,n}, \tag{10}$$

as well as by the reconstruction

$$a_{j-1,k} = \sum_{n\in Z}(h_{k-2n}a_{j,n} + g_{k-2n}d_{j,n}), \tag{11}$$

where * denotes complex conjugates. Pyramidal schemes of decomposition and reconstruction are graphically presented in Fig. 2.

Coefficients h_n and g_n used in the decomposition and the reconstruction formulae are given as

$$h_n = \int_{-\infty}^{+\infty} \phi(x)\phi_{-1,n}(x)\,\mathrm{d}x \quad \text{and} \quad g_n = (-1)^n h^*_{1-n}. \tag{12}$$

The information in every scale will be used as input to the sub-RBF networks.

In the wavelet-based representations of signals, the goal of obtaining more information and reducing the uncertainty of the system is achieved.

2.4. Structure

Assume a data set $S = \{(X, Y)_k; k = 1, 2, \ldots, N\}$, where N is the number of the sample data, and $X = (x_1, x_2, \ldots, x_n)$, $Y = (y_1, y_2, \ldots, y_m)$, where n and m represent the dimension of input and output variables. The structure of the model can be expressed as follows:

As shown in Fig. 3, the ICA procedure is employed as a signal preprocessing step in the architecture. The decorrelation of the input space is realized by ICA, which would not only decrease the feature dimensions and the complexity of model, but also enhance the model practicability and forecast accuracy [23]. MSA is carried out here to decompose the independent components by wavelet theory to scale information, where a represents the approximate information and d represents the detailed information. Multi-scale presentation of the information is considered robust to mismatches and usually exhibits good performance [15]. The RBF network is the basis of the proposed model which characterizes the nonlinear relationship between the measured variables and the melt index of the product. The number of the sub-RBF networks is $J+1$ as the decomposition scale is set to J. For each subnetwork the number of inputs nodes is equal to the desired number of independent components and the number of hidden nodes is determined by the above-mentioned OLS algorithm. The wavelet reconstruction is carried out finally to get the prediction of the target output.

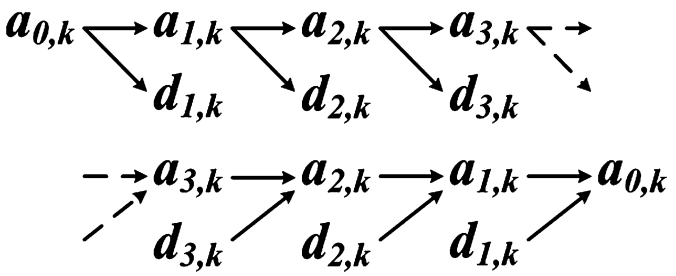

Fig. 2. Pyramidal schemes of decomposition and reconstruction.

3. Results

A pool of process information, formed by process variables formed by 9 process variables ($t, p, l, a, f_1, f_2, f_3, f_4, f_5$), has been chosen to develop the soft sensor, where t is the process temperature, p the pressure, l the level of liquid, a the percentage of hydrogen in vapor phase, f_1–f_3 are flow rates of 3 streams of propylene, f_4 is the flow rate of catalyzer and f_5 the flow rate of aid catalyzer, respectively. The data used for training and testing the virtual sensor have been acquired from the historical logs recorded in a real propylene polymerization plant. Data are filtered to discard abnormal situations and to improve the quality of the predictive system. The input and output variables are normalized with respect to their maximum operation values. Data from the records of the process variables and MI are separated into training, test and generalization sets. All the data sets are constructed from the time series of recorded plant data, 57 of which are used as the training

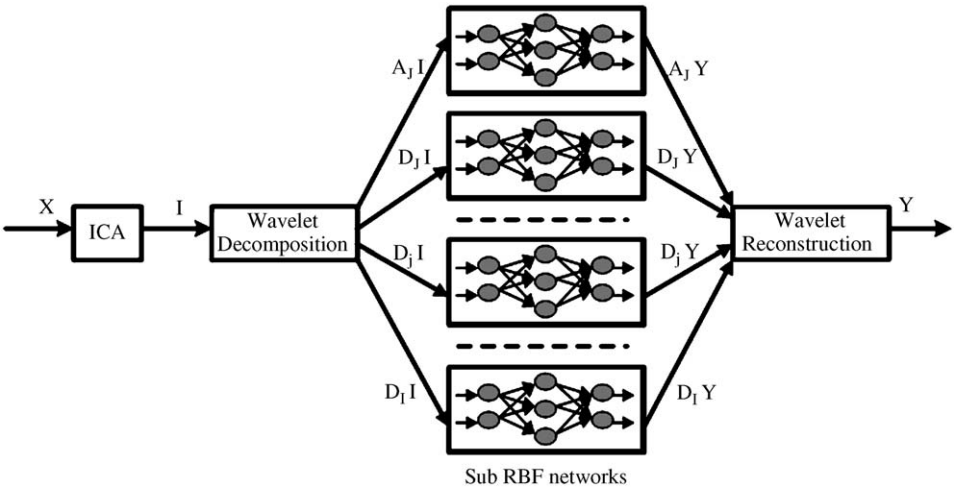

Fig. 3. General scheme of the proposed architecture.

set, 19 are used as the test set, and the remaining data points are used as generalization set. It is noted that the test set is obtained from the same batch as the training set, while the generalization set is derived from another batch.

The training accuracy and the agreement level of the proposed model are quite acceptable as shown in Fig. 4. In this case study MSA is carried out by employing Daubechies3 wavelet and the decomposition scale is set to 5. The corresponding number of sub-RBF networks is 6.

Models without ICA (MS-RBF) and MSA (ICA-RBF) have been developed simultaneously to compare with the performance of the architecture currently under consideration (ICA-MS-RBF). The results obtained for all models considered are summarized in the following section.

3.1. Models built with independent components and original variables (ICA-MS-RBF and MS-RBF)

The ICA of input variables has the advantages of (i) dealing with a lower-dimensional problem, (ii) cutting back any noise that could contaminate the measurements of the discarded variables, and (iii) avoiding variables that could provide conflicting information with respect to more relevant variables in relation to the MI.

Table 1 summarizes the test performance of models developed with independent components and original input process variables after training with the sequential sets of data given above. The difference between the output of the models and the desired output (analytic MI from laboratory) is referred to as the error and can be measured in different ways. In this study, the following measures are used for model evaluation: MAE, MRE, MXAE, MXRE, RMSE and TIC. The MAE values are mean absolute errors while MRE values represent mean relative errors. The MXAE and MXRE values indicate maximum absolute and relative errors. RMSE value is root of mean square error and TIC values are calculated as

$$\mathrm{TIC} = \frac{\sqrt{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}}{\sqrt{\sum_{i=1}^{N} y_i^2} + \sqrt{\sum_{i=1}^{N} \hat{y}_i^2}}, \quad i = 1, \ldots, N, \tag{13}$$

where y_i, $\hat{y}_i$ denote the measured value and predicted result, respectively.

The training results of the model are pretty well, and the test results are a little worse in comparison. The reason lies in the fact that the studied process is characterized by high complexity (described in introduction section) and uncertainty. There exists lots of uncertainty such as the inherent analysis errors, measurement errors and operation errors for a practical industrial process of propylene polymerization. These lead to the model/plant mismatch. Thereby it is usually considered that the relative prediction errors $\leqslant 10\%$ is quite well for a practical industrial propylene polymerization process.

The data listed in Table 1 indicates that the ICA-MS-RBF model functions better than the MS-RBF model on the overall, with mean absolute error for the former being 0.0848 and the latter 0.1092, respectively. An increase of approximately 20% in prediction accuracy is obtained when the ICA technique is applied. The RMSE listed also in Table 1 for both models have confirmed the prediction accuracy of the proposed method. TIC of ICA-MS-RBF is quite acceptable compared to that of MS-RBF, which indicates a good level of agreement between the proposed model and the studied process [16]. A visual impression of the agreement between the measured MI and the model output can be obtained from Fig. 5. It can be seen that the agreement level of ICA-MS-RBF is quite good.

To illustrate the universality of the proposed model, a detailed comparison of the generalization set is presented in Table 2. It is noted that the performance is consistent with the above test results, with a slight increase in predictive precision. The mean relative error of ICA-MS-RBF is 2.98%, compared to 6.05% of MS-RBF, whose accuracy increases by 50% approximately. The maximal relative errors have a similar result with 4.59% compared to

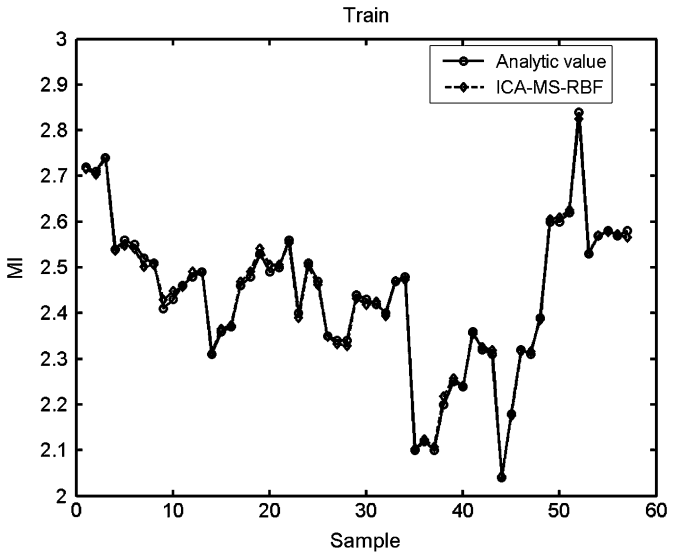

Fig. 4. Training results of the proposed ICA-MS-RBF model.

Table 1
Performance evaluation of models built with IC and original variables during test process

Performance	MAE	MRE (%)	MXAE	MXRE (%)	RMSE	TIC
ICA-MS-RBF	0.0848	3.50	0.1779	8.22	0.1034	0.0211
MS-RBF	0.1092	4.54	0.3134	14.65	0.1334	0.0272

9.37%, showing an increase of approximately 50% in prediction accuracy.

3.2. Models with and without MSA (ICA-MS-RBF and ICA-RBF)

Table 3 summarizes the results predicted by models developed with MSA and without MSA. The MSA of information has the advantages of (I) obtaining much more information and (II) reducing the uncertainty of the system. The average performance indicate that ICA-MS-RBF yields better results than ICA-RBF with mean relative error of the former being 3.50%, and the latter 5.27%. An error decreasing of approximately 30% is obtained by applying MSA. The maximal errors listed in Table 3 are of the same order of magnitude as the mean errors. The better performance of ICA-MS-RBF is clearer in the time sequence of the measured MI as shown in Fig. 6, where the model yields consistently good predictions.

Similarly, a detailed comparison of the generalization set is carried out. Table 4 shows accordant results with the generalization set. ICA-MS-RBF yields predictions with mean relative error of 2.98%, which is much better than the corresponding 3.69% obtained from ICA-RBF. Similar behaviors are observed in the term of MXAE, MXRE, RMSE and TIC.

4. Conclusions

This paper has presented a method for using neural network to design and build soft-sensor architecture based on ICA and MSA to infer MI of polypropylene from other process variables.

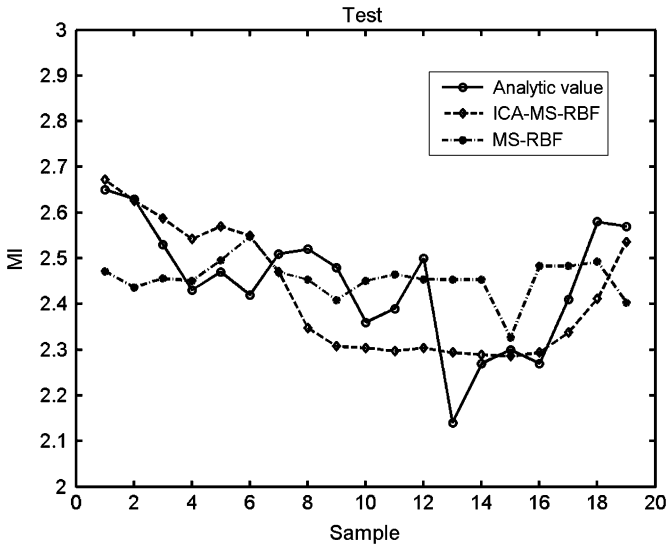

Fig. 5. Comparison of measured MI with predictions obtained using ICA-MS-RBF and MS-RBF.

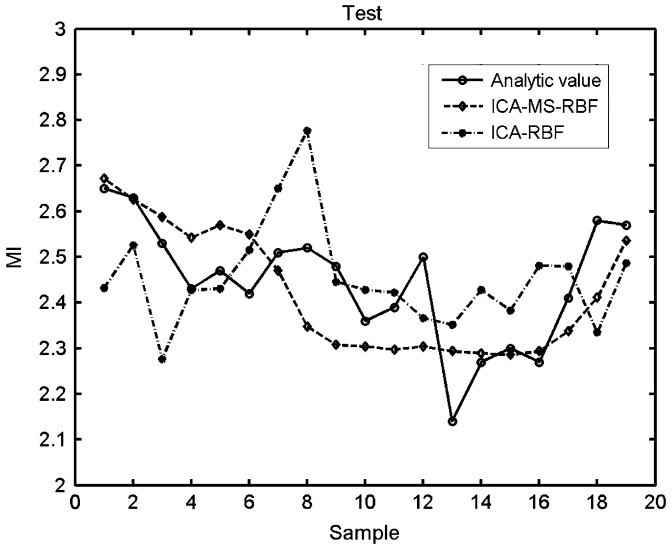

Fig. 6. Comparison of measured MI with predictions obtained using ICA-MS-RBF and ICA-RBF.

Table 2
Performance evaluation of models built with IC and original variables during generalization process

Performance	MAE	MRE (%)	MXAE	MXRE (%)	RMSE	TIC
ICA-MS-RBF	0.0757	2.98	0.1138	4.59	0.0799	0.0156
MS-RBF	0.1550	6.05	0.2379	9.37	0.1710	0.0346

Table 3
Performance evaluation of models built with MSA and without MSA during test process

Performance	MAE	MRE (%)	MXAE	MXRE (%)	RMSE	TIC
ICA-MS-RBF	0.0848	3.50	0.1779	8.22	0.1034	0.0211
ICA-RBF	0.1285	5.27	0.2566	10.18	0.1517	0.0309

Table 4
Performance evaluation of models built with MSA and without MSA during generalization process

Performance	MAE	MRE (%)	MXAE	MXRE (%)	RMSE	TIC
ICA-MS-RBF	0.0757	2.98	0.1138	4.59	0.0799	0.0156
ICA-RBF	0.0945	3.69	0.1444	5.57	0.1014	0.0202

ICA has been introduced and proven effective to estimate the relevance of certain features needed as input to the model. MSA is carried out to acquire more information and reduce the uncertainty of the studied problem. In order to demonstrate the validation of the proposed method, models without ICA and MSA procedure have been developed simultaneously.

The ICA-MS-RBF model predict MI with mean relative errors of approximately 3% when appropriately trained, compared with the mean errors of approximately 4% and 5% obtained from the corresponding MS-RBF and ICA-RBF models, respectively. The results obtained indicate that the proposed method provides prediction reliability and accuracy, which is capable of learning the relationships between process variables and the target MI of the polypropylene and supposed to have promising potential for practical use.

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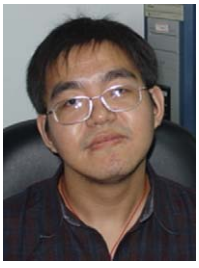

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