An effective parameter optimization technique for vibration flow field characterization of PP melts via LS-SVM combined with SALS in an electromagnetism dynamic extruder

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Abstract. A method for predicting the optimal vibration field parameters by least square support vector machine (LS-SVM) is presented in this paper. One convenient and commonly used technique for characterizing the vibration flow field of polymer melts films is small angle light scattering (SALS) in a visualized slit die of the electromagnetism dynamic extruder. The optimal value of vibration vibration frequency, vibration amplitude, and the maximum light intensity projection area can be obtained by using LS-SVM for prediction. For illustrating this method and show its validity, the flowing material is used with polypropylene (PP) and fifteen samples are tested at the rotation speed of screw at 36rpm. This paper first describes the apparatus of SALS to perform the experiments, then gives the theoretical basis of this new method, and detail the experimental results for parameter prediction of vibration flow field. It is demonstrated that it is possible to use the method of SALS and obtain detailed information on optimal parameter of vibration flow field of PP melts by LS-SVM.

1. Introduction

Very recently, the intelligent characterization methods for flow field of polymer melts are intensely researched. The intelligent methods can react on inner stimuli like changes in maximum light intensity projection area according to change of the vibration frequency and amplitude.

Because of carrying structural information of polymer melts, the approach of small angle light scattering (SALS) has been applied to characterize vibration field of polymer melts. During the study, the experimental device is used to analyze the pattern of small angle light scattering in the extrusion process [1-3]. Such an approach [4-6] provides a means of characterization of the flow field of polymer melts, allowing calculation of light intensity in relation to the molecular orientation of polymer. The experiment uses He-Ne laser as light source. The scattering profiles thorough the visual slit die of the electromagnetism dynamic extruder are recorded by a charge coupled device (CCD) industrial high-resolution monochrome camera, equipped with lens and positioned on the optical rails. The SALS image processing software captures and analyzes the obtained images containing information about intensities at various scattering and azimuthal angles [7].

Support vector machine (SVM) [8] proposed by Vapnik [9-10] is a valuable tool to solve pattern recognition and classification problem [11-13]. By introducing an alternative loss function, SVM can be used to regression problems. Due to its advantages and remarkable generalization performance over other methods, SVM has attracted attention and gained extensive application [9]. SVM shows excellent performances because it can lead to global models that are often unique by embodying the structural risk of minimization principle [9], which has been shown to be superior to the traditional empirical risk minimization principle. In addition, due to their specific formulation, sparse solutions can be found, and both linear and nonlinear regression can be performed. However, it is very difficult to find the final SVM
model in calculation, because it needs to solve a set of nonlinear equations (quadratic programming problem). As a simplification, Suykens and Vandewalle [14] proposed a modified version of SVM called least-squares SVM (LS-SVM) [15-21], which resulted in a set of linear equations instead of a quadratic programming problem, which can extend the applications of the SVM [22].

The least square (LS) version of the SVM is described in Suykens and Vandewalle [14]. LS-SVM is extensively used in complex system studies for modeling, regression or parameter prediction [22]. However, there is no applications [23-27] to the parameter optimization for vibration field for polymer melts.

A new method is put forward in this study, based on LS-SVM for predicting optimal the vibration field parameters. Using this method, the scattering angle must remain in an angular range that is easily obtained [28]. To illustrate this method and show its validity, scattered light is applied to characterize the vibration flow field of polypropylene (PP) melts in a visual slit die of the electromagnetism dynamic extruder. The paper first gives the theoretical basis of SALS and LS-SVM method, then describes the process to perform the experiments and details the experimental results.

2. Material and experimental process

2.1. Material
In this study polypropylene is used to characterize flow field of polymer melts in a visual slit die. PP melts is transparent and melts at high temperatures.

2.2. Experimental process
The experimental setup used for small angle light scattering experiments consisted of a He-Ne laser source, a beam expander, an optical lens, a visual slit die, an electromagnetism dynamic extruder, a CCD camera, and a personal computer as its major hardware components and a series of photosensitive detectors. Polymer melts in the visualized slit die pass through the expanded parallel beam. The optical lens focuses the nonscattered light and detectors are positioned in the focal plane at various angular positions [29]. Small angle light scattering was used to characterize the vibration flow field. Two parameters (vibration amplitude, vibration frequency) are input in LS-SVM to predict the maximum light intensity projection area of SALS. The experimental process diagram is shown in Fig.1.

![Figure 1. The experimental process diagram](image-url)
3. Small angle light scattering method
Scattering intensities are recorded at 19 different angles $\delta$, resulting in angular-dependent scattering curves [30]. The scattering vector $v$ indicated of these scattering curves as below.

$$v = (4\pi n / \lambda) \sin(\delta / 2)$$  \hspace{1cm} (1)

where $n$ is the refractive index of the solvent and $\lambda$ is the wavelength of the laser light source [31].

The small angle data was evaluated using an indirect Fourier transform [32-34] followed by deconvolution [33-35]. The overall shape and size of the scattering particles is determined by the pair distance distribution function (PDDF), $p(d)$.

The electron density contrast, $\Delta \rho(d)$, is related to the PDDF by the following equation

$$p(d) = d^2 \Delta \rho^2(d)$$  \hspace{1cm} (2)

where $\Delta \rho^2(d)$ indicates the convolution square of $\Delta \rho(d)$ averaged for all directions in space [33-34]. This averaging for the case of a spherical particle will not result in the loss of information [36].

The SALS apparatus consisting of a He-Ne laser, and a set of optics to collimate the beam. SALS measurements were carried out using a light scattering apparatus, which is illustrated in Fig. 2. The laser beam is focused through a polarizer, hitting the sample in the visualized slit die of the electromagnetism dynamic extruder, and then through the analyzer. The laser light first passes the polarizer, which removes one orthogonal component of the light [34]. The scattered light is collected and recorded using a CCD camera. The beam is then shone through a polarizer which acts as a neutral density filter and cuts out a part of the light, preventing any damage to the CCD camera. In the experiment, it is assumed that the total intensity is proportional to orientation of molecular chain.

![Figure 2. A typical set-up for SALS](image)

4. Least square support vector machine (LS-SVM)
In 1995, Vladimir Vapnik at AT&T Bell Laboratories developed the theory of SVM which is applicable to both classification and regression. The SVMs based on the principle of structural risk minimization is a new supervised learning approach [10].

It is considered that a given training set $D = \{(x_i, y_i)\}_{i=1,2,\cdots,n}, x \in R^n$ with class labels $y \in \{-1, +1\}$ and linear classifier

$$f(x) = \text{sign}[\omega^* \cdot x + b^*]$$  \hspace{1cm} (3)

When the data of the two classes are separable one can say

$$\begin{align*}
\{ \omega^* \cdot x_i + b - 1 \geq 0, & \quad \text{if} \quad y_i = +1 \\
\omega^* \cdot x_i + b - 1 \leq 0, & \quad \text{if} \quad y_i = -1 
\end{align*}$$  \hspace{1cm} (4)

The two sets of inequalities are combined into one single set as below.

$$y_i(\omega \cdot x_i + b) - 1 \geq 0, i = 1, \cdots, n$$  \hspace{1cm} (5)

The theory of SVM is to start formulating the problem as a constrained optimization problem, next formulate the Lagrangian and then take the conditions for optimality, finally solve the problem in the dual space of Lagrange multipliers. With resulting classifier
\[ f(x) = \text{sgn}\left[ \sum_{i=1}^{N} \alpha_i y_i \langle x_i, x \rangle + b \right] \quad (6) \]

Cortes and Vapnik extended linear SVM classifier to non-separable case [10]. It is done by taking additional slack variable in the problem formulation. One modifies the set of inequalities into

\[ y_i (\omega \cdot x_i) + b - 1 + \xi_i \geq 0, \quad i = 1, \cdots, n \quad (7) \]

Considering the equality type constraints instead of inequalities as in the classic SVM approach, Suykens and Vandewalle proposed the least square version of the SVM classifier [14]. The reformulation procedure above greatly simplifies a problem such that the LS-SVM solution follows directly from solving a set of linear equations rather than from a convex quadratic program.

According to the optimization function, the Lagrangian function can be defined as below.

\[ L(\omega, b, e, \alpha) = J(\omega, e) - \sum_{k=1}^{N} \alpha_k \left\{ \omega^T \varphi(x_i) + b + e_k - y_i \right\} \quad (8) \]

where support vector \( \alpha_i \in \mathbb{R} \). After optimization the above equation, we can get

\[
\begin{align*}
\frac{\partial L}{\partial \omega} = 0 & \Rightarrow \omega = \sum_{k=1}^{N} \alpha_k \varphi(x_i) \\
\frac{\partial L}{\partial b} = 0 & \Rightarrow \sum_{k=1}^{N} \alpha_k = 0 \\
\frac{\partial L}{\partial e_k} = 0 & \Rightarrow \alpha_k = \gamma e_k \\
\frac{\partial L}{\partial \alpha_k} = 0 & \Rightarrow \omega^T \varphi(x_i) + b + e_k - y_i = 0
\end{align*}
\]

where \( k = 1, \cdots, N \).

For nonlinear classification, the LS-SVM classifier in the dual space can be expressed as below,

\[ y(x) = \text{sgn}\left[ \sum_{i=1}^{N} \alpha_i y_i K(x_i, x) + b \right] \quad (10) \]

where \( \alpha_i \) are positive real constants and \( b \) is a real constant, in general, \( K(x, x_i) = \langle \varphi(x), \varphi(x_i) \rangle \) is inner product, and \( \varphi(x) \) is the nonlinear map from original space to the high-dimensional space. For function estimation, the LS-SVM model can be describe as follows.

\[ y(x) = \sum_{i=1}^{N} \alpha_i K(x, x_i) + b \quad (11) \]

When radius bias function (RBF) kernels are used, two tuning parameters \((\gamma, \sigma)\) are added. Where \( \gamma \) is regularization constant and \( \sigma \) is width of RBF kernel [37].

5. Results and discussion
To further demonstration the effectiveness of the existing LS-SVM algorithm and make it be more feasible to be used in polymer characterization application, this paper introduces LS-SVM algorithm combined with small angle light scattering method to characterize the vibration flow field of PP polymer melts in an electromagnetism dynamic extruder.

The LS-SVM is trained with two inputs and one outputs, where the output denotes the maximum light intensity projection area. To check correctness and efficiency of the algorithm, tested 15 samples are tested with rotation speed at 36 rpm. The experimental data of frequency, amplitude and maximum light intensity projection area used in this study is shown in Fig.3.
Parameter of amplitude ranges from 0.08 to 0.36 mm. Parameter of frequency ranges from 5 to 20 Hz. Fig. 4 shows the 3D plots of the generalization performance of the optimally trained support vector regression. LS-SVM predicts that the optimal value of amplitude, frequency are 0.204 mm and 9.65 Hz, respectively. And the maximum light intensity projection area is predicted to be 22577 pixels. Simulation examples show the good performance of the proposed LS-SVM for parameter optimization for vibration flow field of PP melts.
6. Conclusion
The experiments described in this work demonstrate a rapid, economic screening method for characterizing polymer melts of vibration field in an electromagnetism dynamic extruder. Using SALS combined with LS-SVM, it is possible to optimize parameters for vibration conditions of polymer melts of quickly and effectively. Optimum conditions of vibration field of polymer melts can be discovered this way. Such screening techniques may be used for many applications of different kinds of polymer melts. The results reported in this study are obtained with polypropylene with rotation speed at 36 rpm. The proposed techniques can be used to monitor the processing of material under a variety of conditions. SALS can be used, as described, to monitor the polymer melts structure as a function of molecular orientation. Such applications will depend highly on the prediction ability of LS-SVM for materials of vibration flow field, which may also be probed using scattering methods coupled with such technology.

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