Application of support vector regression for optimization of vibration flow field of high-density polyethylene melts characterized by small angle light scattering

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Abstract. In this paper, the vibration flow field parameters of polymer melts in a visual slit die are optimized by using intelligent algorithm. Experimental small angle light scattering (SALS) patterns are shown to characterize the processing process. In order to capture the scattered light, a polarizer and an analyzer are placed before and after the polymer melts. The results reported in this study are obtained using high-density polyethylene (HDPE) with rotation speed at 28 rpm. In addition, support vector regression (SVR) analytical method is introduced for optimization the parameters of vibration flow field. This work establishes the SVR for predicting the optimal parameters of vibration flow field.

1. Introduction
Small angle light scattering (SALS) [1-5] is a quantitative tool for studying vibration flow field of polymer melts in a visual slit die. Through the utilization of small angle light scattering, important chemical processes can be integrated onto a computer aided system.

Small angle light scattering, carrying structural information of polymer melts, is widely used in vibration fields where take decisive roles in affect the flow field of polymer melts. During the process of study, experimental device performs real-time image analysis of the evolving light-scattering pattern during extrusion. The scattering light generated by the He-Ne laser was recorded by a CCD camera and analyzed in-line. Intensities at various scattering and azimuthal angles are plotted at each time [6]. The light intensity in relation to the molecular orientation of polymer can characterize the flow field of HDPE melts.

Support vector regression (SVR) [7-11], motivated by statistical learning theory, have recently received considerable attention in the field of pattern recognition and regression [12-14]. Their foundation has been developed by Vapnik and has obtained popularity [7-8]. The main feature of SVR is that they use the structural risk minimization rather than the empirical risk minimization. Unlike the well-known multilayer perceptron (MLP) and radial-basis function (RBF) networks, training an SVM is equivalent to solving a linearly constrained convex quadratic programming problem. Since the MLP and RBF networks rely on the minimization of a nonlinear error function which may be nonconvex, the localminima problem in training can be avoided by using the SVM approach [15].

A new method based on SVR is proposed for predicting optimal the vibration field parameters. By this method, the scattering angle must remain in an angular range that is easily obtained [16]. To illustrate this method and show its validity, scattered light is used to characterize the vibration flow field of high-density polyethylene (HDPE) melts in a visual slit die. The paper first gives the theoretical basis of SALS and SVR method, then describes the process to perform the experiments and details the experimental results.
2. Material and experimental setup

2.1. Material
The results reported in this study are obtained with high-density polyethylene. It is transparent, which is necessary to perform visualization experiments. As it is commercial polymers that melt at high temperatures, they enabled the study to be performed under quasi-industrial conditions.

2.2. Experimental setup
The experimental setup (Fig.1) 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 extruder, a CCD camera, and a personal computer as its major hardware components and a series of photosensitive detectors. HDPE melts in the visual 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 [17].

![Experimental setup diagram](image)

**Figure 1.** The experimental setup.

3. Small angle light scattering method
SALS measures the time-averaged intensity of scattered light, \( \langle I_s(q,t) \rangle \), where \( q \) is called the scattering vector [18-19]. The magnitude of the scattering vector is given by

\[
q = \frac{4\pi n}{\lambda} \sin \left( \frac{\theta}{2} \right)
\]

(1)

where \( \lambda \) is the wavelength of the incident light, \( n \) is the refractive index of the scattering medium, and \( \theta \) is the scattering angle. Light scattering by particles in polymer melts is characterized by a scattering function, \( S(q) \), that depends on the size and structure of the particles. (See supporting information for more details.) One important measure of the particle size is the radius of gyration \( R_g \). When \( qR_g \leq 1 \), the scattering function can be expressed as

\[
S(q) = 1 - \left( \frac{qR_g}{3} \right)^2
\]

(2)

If the particles have a self-similar (i.e., fractal) internal structure, the scattering function in the limit that \( qR_g \geq 1 \) takes the form
where $d_f$ is called the fractal dimension of the structure [20-21].

Fluctuations of the scattering intensity come from fluctuations of the concentration due to the Brownian motion of the scatterers [22-23].

The SALS apparatus consisted of a He-Ne laser, and a set of optics to collimate the beam. SALS measurements are carried out using a light scattering apparatus. The laser beam is focused through a polarizer, hitting the sample in the visualized slit die, and then through the analyzer. The laser light first passes the polarizer, which removes one orthogonal component of the light [24]. 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 our experiment, we assume that the total intensity is proportional to orientation of molecular chain. In order to simply visualize the extent of rotation speed of the extruder screw, a constant speed is prepared.

4. **Support vector regression** [28 – 29]

Consider the problem of approximating a set of data

$$\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$$  

with a regression function of the form as below

$$g(X) = \sum_{i=1}^{N} \alpha_i \Phi_i(X) + b$$  

where $\{(\Phi_i(X))_{i=1}^{N}\}$ are called feature functions defined in a high dimensional space, $b$ and $\{\alpha_i\}$ are parameters of the model to be estimated. An SVR is to find the unknown parameters by minimizing the following regularized risk function

$$R_{emp}(\alpha) = \frac{1}{N} \sum_{i=1}^{N} L(g(X_i) - y_i) + c \|\alpha\|^2$$  

where $L(g(X_i) - y_i)$ is called a loss function which indicates how the difference between and should be penalized. Here the following Huber loss function is used below

$$L(g(X) - y) = \begin{cases} \frac{1}{2} (g(X, \alpha) - y)^2 & \text{if } |g(X, \alpha) - y| < \varepsilon \\ \varepsilon |g(X, \alpha) - y| - \frac{\varepsilon^2}{2} & \text{otherwise} \end{cases}$$  

where $\varepsilon > 0$ is a scale constant. Let a kernel function $K(x, y)$ satisfying $K(x, x_i) = \Phi(x_i)^T \Phi(x_i)$. Then the regression function defined in equation (5) can be written as

$$g(X) = \sum_{i=1}^{N} (\zeta_i - \alpha_i) K(X, X_i) + b$$  

where $\zeta_i$ and $\alpha_i$ are optimal solutions to the following quadratic optimization problem

$$\max - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} (\alpha_j - \zeta_j)(\alpha_j - \zeta_j) K(X, X_j) + \sum_{i=1}^{N} (\alpha_i - \zeta_i)y_i - \frac{\varepsilon}{2c} \sum_{i=1}^{N} [\alpha_i]^2 + (\zeta_i)^2$$\ s.t. \begin{align*}
\sum_{i=1}^{N} (\zeta_i - \alpha_i) = 0 \\
0 \leq \zeta_i, \alpha_i \leq c, i = 1, \cdots, n.
\end{align*}$$  

By the complementary property that $\zeta_i \alpha_i = 0$, it can be seen that $(\alpha_i)^2 + (\zeta_i)^2 = (\alpha_i = \zeta_i)^2$. Then the above optimization problem can be equivalently expressed as
\[
m \in \min \left\{ \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} (\alpha_i - \zeta_j)(\alpha_j - \zeta_j)K(X_i, X_j) - \sum_{i=1}^{N} (\alpha_i - \alpha_j)y_i - \frac{\epsilon}{2c} \sum_{i=1}^{N} [(\alpha_i)^2 + (\zeta_j)^2] \right\}
\]
\[\text{s.t.} \quad \sum_{i=1}^{N} (\zeta_i - \alpha_i) = 0 \]
\[\quad 0 \leq \zeta_i, \alpha_i \leq c, i = 1, \ldots, n. \quad (10)\]

Let \( \alpha_i = \alpha_i - \zeta_i \). Then \(-c \leq \alpha_i \leq c\) and (10) can be simply written as

\[
m \in \min \left\{ \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j K(X_i, X_j) - \sum_{i=1}^{N} \alpha_i y_i + \frac{\epsilon}{2c} \sum_{i=1}^{N} (\alpha_i)^2 \right\}
\]
\[\text{s.t.} \quad \sum_{i=1}^{N} \alpha_i = 0 \]
\[\quad -c \leq \alpha_i \leq c, i = 1, \ldots, n. \quad (11)\]

Therefore, the learning problem in SVR is equivalent to the quadratic programming problem in equation (11) with bounded variables.

Remark 1: All training data are “support vectors” because of using the Huber loss function in SVR. When the epsilon insensitive function is used in SVR like in [30], it may lead to a sparse solution with \(2N\) variables: half of its variables are zero. As a result, both using the Huber loss function and using the epsilon-insensitive function all lead a solution with \(N\)-nonzero elements. On the other side, the problem (11) has only variables instead of \(2N\) variables like in [15, 30].

5. Results and discussion

These experiments provide demonstrations of how SALS on a device can be used as a rapid screening tool to optimize processing conditions for HDPE melts. To study the effect of parameters of vibration field, the algorithm of SVR is used and kept at a rotation rate of screw at a constant 28rpm.

Fig.2 (a) shows light scattering image of HDPE at 24 rpm screw rotate speed without vibration. Fig.2 (b), (c), (d), (e) and (f) show light scattering image of HDPE at the same rotate speed with vibration amplitude 0.04, 0.08, 0.12, 0.16 and 0.20 mm, respectively (vibration frequency 10 Hz). These figures are meant for illustrative purposes of the research and it is attempt to quantify the optimum conditions for vibration field of HDPE melts using this approach.

**Figure 2.** The largest light intensity projection area images of HDPE at 24 rpm screw rotate speed. (a) without vibration, (b), (c), (d), (e) and (f) with vibration amplitude 0.04, 0.08, 0.12, 0.16 and 0.20 mm, respectively (vibration frequency 10 Hz).
It can be seen that the largest light intensity projection area with vibration is larger than image with out vibration. It is also illustrated that the orientation of molecular chain increases because light intensity is proportional to orientation of molecular chain.

The SVR is trained with two inputs and one output, where the output denotes the maximum light intensity projection area. To check correctness and efficiency of the algorithm, 15 samples are tested with rotation speed at 28 rpm. The experimental data of frequency, amplitude and maximum light intensity projection area used in this study is shown in Fig.3.

**Figure 3.** Experimental data of amplitude, frequency, and maximum light intensity projection area.

**Figure 4.** The 3D plots of the generalization performance of the optimally trained regularization SVR.
Parameter of amplitude ranges from 0.08 to 0.20 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. SVR predicts that the optimal value of frequency, amplitude are 11.72 Hz and 0.1503 mm, respectively. And the maximum light intensity projection area is predicted to be 13783 pixels.

6. Conclusion
In this study, support vector regression method has been utilized to predict the vibration field parameters of small angle light scattering. This work aims at developing an accurate measurement of characterization flow field of high-density polyethylene melts by small angle light scattering. A laser light passes through polymer melts in the visual slit die. In the experiment, the results are obtained using HDPE with rotation speed at 28 rpm. A polarizer and an analyzer are placed before and after the HDPE melts for capturing the scattered light. SVR inputs consist of vibration amplitude and frequency, which are used as input parameters to predict the maximum light intensity projection area. SVR predicts that the optimal value of frequency, amplitude is 11.72 Hz and 0.1503 mm, respectively. And the maximum light intensity projection area is predicted to be 13783 pixels. These experiments provide demonstrations of how SVR can be used as a prediction tool to optimize vibration flow field conditions for a visual slit die of HDPE melts.

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