Research Article

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Chaotic characteristics and mixing performance of pseudoplastic fluids in a stirred tank

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Abstract: The key for improving the mixing efficiency of pseudoplastic fluids is to enhance the chaotic degree in the flow field. The xanthan gum solution was used to study the chaotic characteristics and mixing performance in a stirred tank with the impeller of perturbed six-bent-bladed turbine. Based on the velocity time series collected by the experiment of particle image velocimetry (PIV), the distributions of the largest Lyapunov exponent (LLE) and Kolmogorov entropy (K entropy) of the system were obtained through the programming calculation using the software MATLAB (R2016a) for characterizing the chaotic degree. The mixing performance of the fluid was numerically investigated using the Computational Fluid Dynamics package, and the velocity distributions were compared with the results obtained by the experiment of PIV. The relevance between the chaotic degree and the mixing performance was clarified. Results showed that the numerical results of velocity distributions agreed well with the experimental data which validated the Computational Fluid Dynamics model established. When the speed reached 600 rpm, the LLE and K entropy climbed the maximal values at the same time, which meant the greatest degree of chaos, and the mixing energy per unit volume was minimal at that moment, which was corresponding to the highest mixing efficiency. As the speed increased further, the LLE and K entropy decreased instead, which meant the chaos reduction, and the corresponding mixing energy per unit volume increased with the low mixing efficiency.

Keywords: pseudoplastic fluid, chaotic characteristics, mixing efficiency, largest Lyapunov exponent, Kolmogorov entropy

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>b</td>
<td>impeller blade width (m)</td>
</tr>
<tr>
<td>C</td>
<td>off-bottom clearance (m)</td>
</tr>
<tr>
<td>D</td>
<td>impeller diameter (m)</td>
</tr>
<tr>
<td>d</td>
<td>shaft diameter (mm)</td>
</tr>
<tr>
<td>H</td>
<td>fluid height (m)</td>
</tr>
<tr>
<td>K</td>
<td>consistency index (Pa s^n)</td>
</tr>
<tr>
<td>K entertopy</td>
<td>Kolmogorov entropy</td>
</tr>
<tr>
<td>LLE</td>
<td>largest Lyapunov exponent</td>
</tr>
<tr>
<td>M</td>
<td>torque (N m)</td>
</tr>
<tr>
<td>m</td>
<td>embedding dimension</td>
</tr>
<tr>
<td>N</td>
<td>impeller speed (rpm)</td>
</tr>
<tr>
<td>n</td>
<td>rheological index</td>
</tr>
<tr>
<td>PIV</td>
<td>particle image velocimetry</td>
</tr>
<tr>
<td>P</td>
<td>average period</td>
</tr>
<tr>
<td>P_v</td>
<td>mixing power per unit volume (W m^-3)</td>
</tr>
<tr>
<td>R</td>
<td>radial distance (m)</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>T</td>
<td>inner diameter (m)</td>
</tr>
<tr>
<td>V</td>
<td>volume (m^3)</td>
</tr>
<tr>
<td>W_v</td>
<td>mixing energy per unit volume (J)</td>
</tr>
<tr>
<td>w</td>
<td>flat baffles width (m)</td>
</tr>
<tr>
<td>w_t</td>
<td>mass concentration (%)</td>
</tr>
<tr>
<td>z</td>
<td>axial height (m)</td>
</tr>
<tr>
<td>6PBT</td>
<td>perturbed six-bent-bladed turbine</td>
</tr>
<tr>
<td>y</td>
<td>shear rate (s^-1)</td>
</tr>
<tr>
<td>η</td>
<td>apparent viscosity (kg m^-1 s^-1)</td>
</tr>
<tr>
<td>θ</td>
<td>impeller backswept angle (°)</td>
</tr>
<tr>
<td>τ</td>
<td>time delay</td>
</tr>
</tbody>
</table>

1 Introduction

Pseudoplastic fluids play an important role in many industrial mixing operations, such as petrochemical, polymer engineering, and biopharmaceutical engineering [1,2]. For such pseudoplastic fluids with the shear-thinning properties, usually there are viscosity changes in different regions...
of the stirred tank, which will lead to an unique flow field characteristics [3–5], resulting in lower heat or mass transfer efficiency. Therefore, it is important to improve the mixing efficiency in the mixing of pseudoplastic fluids [6–8]. The mixing efficiency is closely related to the structure of the flow field. It has been found that the main way of improving mixing efficiency is to induce the chaotic flow and enhance chaotic degree in a stirred vessel [9–13]. According to the chaos theory, the characteristic parameters of the strange attractor, acting as the chaotic signal in the system, are usually used to reveal and characterize the degree of chaos. It mainly includes two key parameters: the largest Lyapunov exponent (LLE) and Kolmogorov entropy (K entropy) [14–16]. For instance, Liu et al. [17,18] analyzed the chaotic mixing characteristics in a water stirred tank with the rigid-flexible combination impeller. They found that the LLE and K entropy of the flow field produced by the combination impeller were obviously higher than those by the rigid impeller, which resulted in the higher mixing efficiency. Li [19] studied the chaotic characteristics of the power load time series by calculating the distribution of the LLE and K entropy in the system. Kashif et al. [20,21] studied the chaotic systems with hidden attractor and self-excited attractor. The numerical schemes of chaotic models were presented using the Adams–Bashforth–Moulton method. The main purpose of the agitation is to improve the mixing efficiency, and mixing time is a key index to evaluate the mixing performance. So the measurement of the mixing time is crucial for evaluating the mixing efficiency [22,23]. From the literature review, it has been found that most studies mainly focused on the chaotic characteristics and mixing performance of the flow field in Newtonian fluids [24,25]. There are relatively few studies on the chaotic mixing performances of the pseudoplastic fluid with the complex rheological properties, especially the correlation between the degree of chaos and the mixing efficiency [26,27].

The impeller of perturbed six-bent-bladed turbine (6PBT) can generate the asymmetric flow field structure and induce the chaotic flow in stirred tank, which is especially suitable for improving the mixing efficiency of the pseudoplastic fluids [28,29]. In this work, the xanthan gum solution is used to study the chaotic characteristics and mixing performance in stirred tank with the 6PBT impeller. Based on the velocity time series measured by particle image velocimetry (PIV) experiment, the distributions of LLE and K entropy of the flow field at different speeds are calculated by programming using the software MATLAB (R2016a). The mixing time is numerically calculated to obtain the mixing rate and mixing efficiency at different speeds. As a result, the relevance between the chaotic degree of flow field and the mixing performance is clarified. The research results provide a theoretical basis for improving the mixing efficiency of the pseudoplastic fluid.

2 Experimental setup and procedure

The experimental setup is shown in Figure 1. The mixing vessel was a flat-bottomed cylindrical tank with an inner diameter (7) of 210 mm fitted with four equally spaced flat baffles. The 6PBT impeller with a blade thickness of 2 mm and backswept angle \( \theta = 30^\circ \) was mounted on a centrally positioned shaft of diameter \( d = 16 \) mm. P1, P2, and P3 were three speed detecting points, their distances from the axis were all 70 mm, and the off-bottom clearance was 150, 100, and 40 mm, respectively. P0 was the initial tracer point, its location was 70 and 50 mm from the axis and the top, respectively. Further details of the geometrical characteristics of the stirred tank are shown in Figure 2.

The PIV system (Dantec Dynamics A/S company, Denmark) was used to measure the velocity profiles within the stirred tank by determining trajectory of the tracer particles (from which the laser is reflected) with two CCD cameras. The accuracy of the measurement depends on the following behavior of the tracer particles, i.e., the particle density should be closer to the fluid density and the particle diameter should be as small as possible in the case of ensuring imaging [30]. So the polystyrene microspheres of diameter equal to 1–5 \( \mu m \) and density 998 kg \( m^{-3} \) (approximating to the test fluid density) were selected as tracer particles in PIV measurement owing to its good imaging visibility and the behavior of not losing particle pairs between two exposure times. The CCD camera exposure time was set to 1.8 ms through calculation according to the biggest linear velocity of the blade tip. The sampling frequency was all set on 10 Hz at different collection conditions. The laser sheet thickness was adjusted to 1 mm. The experiment was carried out with the deionized water at a speed of 60 rpm (the Reynolds number \( Re = \rho ND^2/\mu = 10,972 \)), corresponding to the turbulent flow. The structure and size of the stirred apparatus used in the experiment are exactly the same as that of the calculation model. The velocity distributions obtained by PIV experiment were compared with the computational results to verify the simulated model.


3 Calculation method

3.1 Mesh formation of stirred tank

Gambit (Fluent Inc.) was used to discretize the computational domain with a tetrahedral mesh. The increased mesh density was used in order to have a very refined mesh near the impeller. Grid independence was confirmed by demonstrating that additional grid cells did not change the calculated velocity magnitude and power number by more than 3% [31], so 1,004,727 cells were employed in this study, as shown in Figure 3.

3.2 Numerical model

In this work, the Xanthan gum solution in water at 0.5% mass concentration was employed, and the rheological parameters were measured under a temperature of 30℃ with DV3T rheometer, as shown in Table 1.

The continuity equation is expressed as follows:

$$\frac{\partial p}{\partial t} + \frac{\partial (p\mu_i)}{\partial x_i} = \rho \frac{\partial u_i}{\partial x_i} = 0,$$  \hspace{1cm} (1)

The momentum equation is expressed as follows:

$$\frac{\partial (p\mu_i)}{\partial t} + \frac{\partial (p\mu_i u_j)}{\partial x_j} + \frac{\partial p}{\partial x_i} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).$$  \hspace{1cm} (2)

The viscosity of xanthan gum solution can be described by power law model in turbulent flow. Its apparent viscosity $\eta$ is defined as follows:

$$\eta = K(y)^{n-1}.$$  \hspace{1cm} (3)

The average shear rate can be related to the rotation speed of the impeller according to the Metzner–Otto’s correlation [32,33] as follows:

$$\gamma = K_N.$$  \hspace{1cm} (4)

The shear rate constant can be defined as follows [34]:

$$K_i = B \left( \frac{3n + 1}{4n} \right)^{\frac{1}{n(n-1)}}.$$  \hspace{1cm} (5)

$$B = 9.5 + \frac{9 \times \left( \frac{r}{2} \right)^2}{\left( \frac{r}{2} \right)^2 - 1}.$$  \hspace{1cm} (6)

Figure 1: Schematic of the stirred experimental apparatus: (a) PIV measurement, (b) System apparatus: 1. stirred equipment, 2. Encoder, 3. laser transmitter, 4. Synchronizer, 5. Computer, and 6. CCD camera, and (c) stirred equipment.
Then, the apparent viscosity $\eta$ is described as follows:

$$\eta = K \left( \frac{3n + 1}{4n} \right)^n B^{n-1} N^{n-1}. \quad (7)$$

The apparent Reynolds number is defined as follows:

$$\text{Re} = \frac{\rho N D^2}{\eta}. \quad (8)$$

The model of Detached eddy simulation (DES) is employed to calculate the turbulent flow field for accurately capturing the flow characteristics [35–37]. The method of dynamic mesh was adapted in the velocity field calculation, which is well suitable for dealing with unsteady flow problems [38]. The solutions were considered converged when the normalized residuals for each transport equation were below $1 \times 10^{-5}$. Computations were carried out using Dell workstation with 3.2 GHz processor and 32 GB RAM and convergence was achieved after 96 h. When the flow behavior index $n$ and consistency coefficient $K$ are set to 1.0 and 0.001 Pa·s$^n$, respectively, in power law model, this means that the flow of Newtonian fluid (deionized water) can be calculated using the power law model [31] in order to compare the computed data with PIV experimental results.
4 Validation of calculation method

A comparison of the velocity data distribution from the PIV experiment at different heights of the longitudinal section with the computed velocities using the model of DES at $N = 60$ rpm is shown in Figure 4. It can be seen that the computed data agreed well with the measured results and the DES calculations accurately picked up the features of the flow field, which validated the model of DES.

5 Results and discussion

5.1 Velocity time series

The xanthan gum solution in water at 0.5% mass fraction was used to carry out the numerical calculation of the flow field. The radial velocities of the three monitoring points were collected over 200 s record, respectively. Owing to limited space, the time series of radial velocity at P1 point...
are shown only in Figure 5. It can be found that the fluctuation range of the velocity increases with the rotational speed, which shows the enhanced turbulent characteristics.

### 5.2 Chaotic characteristics

The chaos theory points out that the characteristic parameters of strange attractor in the system, as the chaotic signal, can be used to distinguish chaos and characterize the degree of chaos. The LLE and K entropy are two key parameters for determining the chaotic degree of the mixing system. If the values of LLE and K entropy of the system are all positive numbers, it indicates that the system is in a definitely chaotic motion. The bigger the values of LLE and K entropy, the higher the chaotic degree of the system.

The embedding dimension \( m \) and time delay \( \tau \) may be solved by the programming calculation using the software MATLAB (R2016a) based on the velocity time series of the detecting point. The calculation process is as follows:

The velocity time series should be divided into \( t \) different sub-sequences, each sub-sequence \( S(m, r, t) \) may be described as follows:

\[
S(m, r, t) = \frac{1}{t} \sum_{i=1}^{t} [C(m, r, t) - C_{m}^{\text{max}}(1, r, t)],
\]

\[
\Delta S(m, t) = \max \{S(m, r, t)\} - \min \{S(m, r, t)\},
\]

where \( r \) is the range radius of the time series, \( t \) is the time interval, and \( C \) is the relevant integral function of time series for reconstructing the phase space.

According to the study by Brock et al. [39], the following three sequences can be solved out by the programming calculation using the software MATLAB.

\[
\bar{S}(t) = \frac{1}{16} \sum_{m=2}^{5} \sum_{j=1}^{4} S(m, r, t),
\]

\[
\Delta \bar{S}(t) = \frac{1}{4} \sum_{m=2}^{5} \Delta S(m, t),
\]

\[
S_{\text{cor}}(t) = \Delta \bar{S}(t) + |\bar{S}(t)|,
\]

where \( S_{\text{cor}} \) is the statistical variable used to calculate the time window \( \tau_{w} \) by the C–C method.

Taking \( N = 300 \text{ rpm} \) as an example, the variations in \( \Delta \bar{S} \) and \( S_{\text{cor}} \) with \( t \) are shown in Figure 6. The C–C method is usually used to determine the width of the embedding window and the best time delay, and finally obtain the

**Figure 5:** The velocity time series at different speeds. (a) \( N = 300 \text{ rpm} \), (b) \( N = 500 \text{ rpm} \), (c) \( N = 600 \text{ rpm} \), and (d) \( N = 800 \text{ rpm} \).
embedding dimension through the embedding window width. According to the C–C method, the corresponding \( t \) value at the position of the first minimum value in the curve graph is the time delay, i.e., \( \tau = 17 \), and the corresponding \( t \) value at the position of the minimum value in the \( S_{\text{cor}} \) curve graph is the time window, i.e., \( \tau_w = 91 \). So the embedding dimension \( m \) can be obtained according to \( \tau_w = (m - 1)\tau \), i.e., \( m = 6 \).

The maximum likelihood algorithm not only solves time delay \( \tau \) and embedding dimension \( m \), but also needs the average period \( P \) [35]. The velocity time series are conducted at different speeds through the fast FFT transform for acquisition of the average period \( P \). The embedding dimension \( m \), time delay, and average period \( P \) of the velocity time series at different speeds are shown in Table 2.

These data are reconstructed in the phase space according to the time series. At last, LLE and K entropy of the system can be solved out using the C–C method and maximum likelihood algorithm, respectively, as shown in Figure 7.

**Table 2**: Embedding dimension \( m \), time delay \( \tau \), and average period \( P \) of velocity time series at different speeds

<table>
<thead>
<tr>
<th>Speed ( N ) (rpm)</th>
<th>Time delay ( \tau )</th>
<th>Time window ( \tau_w )</th>
<th>Embedding dimension ( m )</th>
<th>Average period ( P )</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>17</td>
<td>91</td>
<td>6</td>
<td>61</td>
</tr>
<tr>
<td>400</td>
<td>15</td>
<td>110</td>
<td>8</td>
<td>68</td>
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<tr>
<td>500</td>
<td>19</td>
<td>150</td>
<td>9</td>
<td>87</td>
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<tr>
<td>600</td>
<td>21</td>
<td>120</td>
<td>7</td>
<td>67</td>
</tr>
<tr>
<td>700</td>
<td>15</td>
<td>85</td>
<td>7</td>
<td>89</td>
</tr>
<tr>
<td>800</td>
<td>16</td>
<td>140</td>
<td>10</td>
<td>92</td>
</tr>
</tbody>
</table>

It can be seen that both the LLE and K entropy increase with the speed at the beginning. When the speed reaches 600 rpm, the LLE and K entropy of the system are at the maximum values simultaneously, corresponding to 0.61 and 0.94, respectively, which indicates that the chaotic degree of the flow field reaches the highest level. However, as the speed further increases, the LLE and K entropy decreases instead, which leads to the reduction in the chaotic degree. This is because the highly regular and repetitive coherent structures (such as cylindrical reflux, etc.) appear in the flow field.

**Figure 6**: The variations in \( \Delta S \) and \( S_{\text{cor}} \) curve with \( t \) by C–C method.

**Figure 7**: The distribution of LLE and K entropy of flow field at different speeds.
5.3 Mixing performance

5.3.1 Mixing time

The numerical simulations of the mixing procession are conducted through detecting the tracer concentration (taking water as a tracer in this work). The mixing time can be obtained based on the 95% principle [40]. Taking $N = 600$ rpm as an example, the tracer concentration response curve at three monitoring points are shown in Figure 8.

![Concentration response curve at different detecting points.](image)

It can be seen that the concentration response curve of tracer fluctuates greatly at the beginning. It rises sharply, then descents rapidly, and finally it tends to be a straight line which means the completion of the mixing process. The value at P3 point is adopted as the final mixing time $t_{95} = 1.48$ s.

5.3.2 Mixing efficiency

The mixing efficiency is usually characterized by mixing energy per unit volume. The smaller the mixing energy per unit volume, the higher the mixing efficiency, its expression is as follows:

$$W_V = \frac{P_v}{V} = \frac{2\pi NM}{V}. \quad (14)$$

The expression of the stirring power per unit volume is as follows:

$$P_v = \frac{W_V}{t_{95}}. \quad (15)$$

The torque values ($M$) of stirring shaft and impeller can be obtained by numerical simulation. The computational fluid dynamics results of power consumption and mixing energy per unit volume at different speeds are shown in Table 3.

<table>
<thead>
<tr>
<th>$N$ (rpm)</th>
<th>Mixing time (s)</th>
<th>$M$ (N m)</th>
<th>$P_v$ (W m$^{-3}$)</th>
<th>$W_V$ (J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>4.89</td>
<td>0.0042</td>
<td>18.14</td>
<td>88.71</td>
</tr>
<tr>
<td>400</td>
<td>3.17</td>
<td>0.0046</td>
<td>26.52</td>
<td>84.07</td>
</tr>
<tr>
<td>500</td>
<td>1.99</td>
<td>0.0051</td>
<td>36.72</td>
<td>73.07</td>
</tr>
<tr>
<td>600</td>
<td>1.48</td>
<td>0.0056</td>
<td>48.37</td>
<td>71.59</td>
</tr>
<tr>
<td>700</td>
<td>1.32</td>
<td>0.0068</td>
<td>68.53</td>
<td>90.46</td>
</tr>
<tr>
<td>800</td>
<td>1.18</td>
<td>0.0079</td>
<td>90.99</td>
<td>107.37</td>
</tr>
</tbody>
</table>

It can be observed that the variation trend of mixing energy per unit volume is consistent with that of LLE and K entropy at different speeds. At the speed of $N = 600$ rpm, the mixing energy per unit volume is the smallest ($W_V = 71.59$ J), at the time, corresponding to the maximum value of LLE and K entropy, which means the highest mixing efficiency and the greatest degree of chaos. At other speeds, the mixing efficiency will decline with the decrease in the chaotic degree. Therefore, the mixing efficiency is determined by the chaotic degree of the flow field, and the chaotic characteristics of the flow field are directly correlated with the mixing performance of the fluid.

6 Conclusion

In this work, the chaotic characteristics and mixing performance of pseudoplastic fluid in a stirred tank with 6PBT
impeller are studied. The relevance between the chaotic degree and the mixing efficiency is analyzed. The conclusions are as follows:

1) Both the LLE and K entropy increase with the increase in the speed at the beginning. When the speed increases to 600 rpm, the LLE and K entropy of the system are at the maximal value, corresponding to 0.61 and 0.94, respectively, which indicates the greatest degree of chaos at this time. As the speed increases further, both the LLE and K entropy tend to decline instead with the decreasing degree of chaos.

2) The mixing rate is proportional to the speed, but the mixing efficiency has a maximal value at $N = 600$ rpm. As the speed increases further, the mixing efficiency will decrease instead.

3) The variation in mixing efficiency is consistent with that of LLE and K entropy at different speeds. The highest mixing efficiency corresponds to the greatest degree of chaos. When the chaotic degree decreases, the mixing efficiency also declines correspondingly. Therefore, the chaotic degree of the flow field determines the mixing efficiency and there is a direct relevance between them.

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References


