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# Experimental Verification for Numerical Flow Analysis in Mixing Vessel

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## ABSTRACT

Visualization of a streak line pattern in a mixing vessel is quite useful for understanding the mixing mechanism and designing an optimal mixing vessel. However, conventional experimental methods for visualizing streak lines require a lot of time to construct impellers and prepare solutions. Although various commercial fluid analysis software has been developed, there are still no examples of its use for calculating streak lines in mixing vessels. A simulation method was developed to quickly evaluate the streak line pattern in a laminar mixing vessel by numerical analysis with commercial code. A commercial CFD code can calculate streak line patterns in a laminar mixing vessel. It was found that a lattice method was more suitable than a particle method for the simulation of the streak line.

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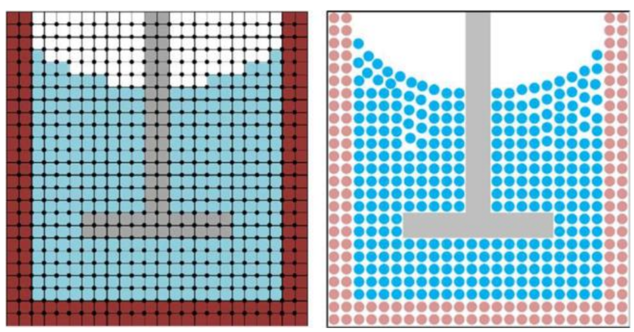
# 1. Introduction

Visualizing the streak line and clarifying the mixing mechanism enables the setting of optimal conditions for the mixing process, leading to cost reductions and improved production efficiency [1–4]. However, the conventional experimental method of visualizing a streak line requires a large amount of time for impeller construction and solution conditioning. Numerical analysis effectively visualizes the streak line without conducting experiments to solve this problem. However, the flow pattern in a mixing vessel is unsteady, and the number of tracer particles increases as time passes to draw the streak line, making the calculation heavy and increasing the calculation time [5, 6]. To solve this problem, our proposed method was developed to calculate the streak line as a two-dimensional unsteady velocity field from a three-dimensional velocity field [7]. However, this method is not yet common. Various commercially available fluid analysis software has been developed and is becoming more accurate [8], but there are still no examples of its use in calculating streak lines in mixing vessels.

Although the lattice method that brown keys indicate solid walls and no-slip conditions. Light blue keys indicate fluid., as shown in Figure **1a**, is the most common method for numerical analysis in mixing vessels, the particle method, as shown in Figure **1b**, is also effective for the calculation of flows with free surfaces and unsteady flows [9]. Compared to the lattice method, this method calculates the motion of fluid particles in a Lagrangian manner, eliminating the need to calculate an advection term and simplifying the computation [10]. Therefore, we attempted to develop a simulation method that can rapidly calculate the streak line in the laminar region and evaluate the mixing performance by numerical analysis using the particle method. Ultimately, we aim to shorten the process design period and improve the design accuracy by using the simulation. Currently, many cases exist where experiments are conducted on a laboratory scale to evaluate mixing performance, performance is re-evaluated on a pilot scale, and the actual plant design is attempted [11]. By applying simulation to this process, it will be possible to evaluate the plant's performance simultaneously from the design stage, which will not only shorten the design period but also reduce the number of experiments by improving design accuracy.

Therefore, the purpose of this study is to verify the accuracy of the numerical results by comparing the streak line visualized by experiments and those are visualized by numerical analysis.



(a) Lattice method (b) Particle method

**Figure 1:** Simulation methods.

**Table 1: Parameters and algorithms in the particle method.**

| **Method of discretization** | |
|---|---|
| Viscosity | Implicit |
| Pressure | Implicit |
| Diffusion | Laplacian |
| **Resolution** | |
| Influence radius | 3.1 |
| Particle size [mm] | 2.0 |
| Time step [s] | $1.0 \times 10^{-4}$ |

# 2. Numerical Analysis

Flow patterns were calculated using commercially available fluid analysis software, Ansys Fluent 2021 R2 (lattice method) using the finite volume method and Particleworks 7.0 (particle method) using the MPS method. These software programs are generally used in mixing analysis [12, 13]. However, using this method, the number of tracer particles increases with time, which increases the computation time and makes the computation heavy. Therefore, we used a method in which another fluid with the same physical properties is discharged from the impeller tip, and the streak line is expressed by its concentration. The governing equation is as follows.

Equation of continuity:

$$\nabla \cdot u = 0 \tag{1}$$

Equation of momentum:

$$\rho \left(\frac{\partial u}{\partial t} + u \cdot \nabla u\right) = -\nabla p + \mu \nabla^2 u + \rho g \tag{2}$$

Species transport equation:

$$\rho \left(\frac{\partial Y_i}{\partial t} + \nabla u Y_i\right) = -\nabla \cdot J_i \tag{3}$$

$$J_i = -\rho D_{i,m} \nabla Y_i \tag{4}$$

$J_i$ is the diffusive flux of species i caused by the concentration gradient. $D_{i,m}$ is the mass diffusion coefficient of the chemical species in the mixture, and $D_{i,m} = 1.4 \times 10^{-10}$ m$^2$/s.

## 2.1. Particle Method

Figure **2** shows the method of drawing a streak line using the particle method. First, the flow pattern is calculated until a steady state is achieved. Then, virtual parameters that imitate the uranine concentration are assigned to the calculation points located at the impeller tip. Since there is no need to solve for the advection term in the particle method, the value of the virtual parameter Y is simplifies the following diffusion equation.

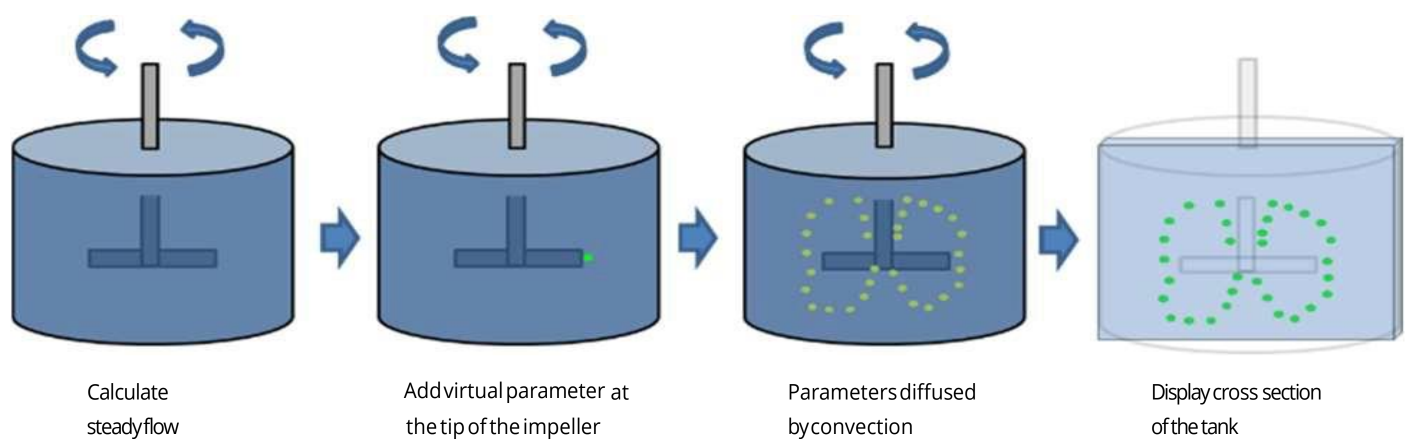



**Figure 2:** Drawing method of Streak Line by the particle method.

$$\frac{\partial C}{\partial t} = D \Delta Y \tag{5}$$

**Table 2: Computing environment in the particle method.**

| | |
|---|---|
| OS | Windows 10 pro |
| CPU | Intel(R)Xeon(R) Gold 6128 CPU @3.40GHz 3.39GHz (2 processors) |
| Computer memory | 256GB |
| Cluster PC cores | none |
| Cluster PC memory | none |
| GPU | NVIDIA(R) Quadro(R) GP100 |
| Software | Particleworks v7.0 |

This equation is calculated by solving the following diffusion equation using a Laplacian model. The Laplacian model was implemented using the Software Development Kit (SDK), an extension of Particleworks. The streak line was plotted by displaying only the calculation points with parameters above a certain value in a longitudinal section of the tank passing through the mixing shaft. Table **1** shows the algorithm and parameters used in the calculations. In this calculation, the rotation speed of the impeller was set empirically to 300~600 rpm for ease of observation of the streak line. The viscosity on this simulation was adjusted to various viscosities (0.34~1.05 Pas) to match the Reynolds number with the experiment. The density ρ was set to 1000 kg/m$^3$. All walls in the simulation are treated as a nonslip conditions. Following the general setup of particle methods, the pressure of the particles on the free surface is set to 0 Pa [14].

Particleworks uses a semi-implicit algorithm as the method of an algorithm for the calculation of incompressible flow. Therefore, the viscosity and pressure gradient terms are calculated separately. This time, the implicit algorithm was used for the viscosity term calculation and the implicit algorithm for the pressure gradient calculation. The number of particles is about 450,000 for the Max-blend impeller and 350,000 for the other systems. The particle size was changed from 1.0 mm to 4.0 mm, and the time step was changed from 5.0 × 10$^{-5}$ s to 1.0 × 10$^{-4}$ s, and it was confirmed that there was no significant change in the obtained streak line. In particular, for the paddle impeller (Re=80), of the three calculations with different particle sizes (4mm,3mm,2mm), the torque average value in the case study was 1.89× 10$^{-2}$ Nm, the maximum value was 2.04 × 10$^{-2}$ Nm, and the minimum value was 1.68× 10$^{-2}$ Nm. These results suggest that changing the particle size does not have a fatal effect on the flow field. We confirmed that the "particle number density," used to judge the accuracy of convergence calculations, is less than 80 in all calculations. The above calculation conditions were adopted as the conditions under which the streak line pattern can be captured in one to two days of calculation time. A Dell Precision 7920 tower was used as the calculation workstation. Table **2** shows the computing environment. The calculations were performed using a GPU.

## 2.2. Lattice Method

In the lattice method, a liquid with the same physical properties as the bulk liquid is injected from the impeller tip. As in the particle method, the streak line was plotted by displaying the concentration of the liquid above a certain value in a longitudinal section of the vessel passing through the agitator axis. In this calculation, the rotation speed of the impeller was set empirically to 300 rpm for ease of observation of the streak line. The viscosity on this simulation was adjusted to various viscosities (0.18~0.85 Pas) to match the Reynolds number with the experiment. The density ρ was set to 1000 kg/m$^3$. A pressure boundary (0 Pa) was set above the liquid surface, and diffusion between fluids was calculated by solving the transport equation for the chemical species. Table **3** shows the algorithm and parameters used in the calculations. A tetra mesh was used as the mesh geometry, with a minimum mesh size of 2 mm, and the sliding mesh method was used for the unsteady calculations. The mesh geometry for a paddle impeller is shown as an example in Figure **3**. The number of meshes is about 800,000 for the paddle impeller. As with the particle method, analysis was performed by changing the mesh size and time step, and it was confirmed that there was no significant change in the streak line shape. In particular, for the paddle impeller (Re=80), of the three calculations with different minimum mesh sizes (4mm,3mm,2mm), the torque average value in the case study was 1.20× 10$^{-2}$ Nm, the maximum value was 1.21× 10$^{-2}$ Nm, and the minimum value was 1.18× 10$^{-2}$ Nm. These results suggest that changing the mesh size does not have a fatal effect on the flow field. The maximum number of iterations per timestep is 40. We ensure that the relative error of all variables involved in the convergence calculation is less than 2.62× 10$^{-5}$ during the calculation in all cases. A Dell Precision 7920 tower was used as the calculation workstation. A cluster computer was used for parallel computation. The execution environment is shown in Table **4**.

**Table 3: Parameters and algorithms in the lattice method.**

| Calculation method | |
|---|---|
| Solver | Segregated-Steady |
| Model | Laminar |
| Coupling method | Coupled |
| **Method of discretization** | |
| Gradient | Least Squares Cell-Based |
| Pressure | Pressure Staggering Option |
| Momentum | Second Oder Upwind |
| Species | Second Oder Upwind |
| **Resolution** | |
| Minimum mesh size[mm] | 2.0 |
| Time step[s] | $1{,}0 \times 10^{-3}$ |

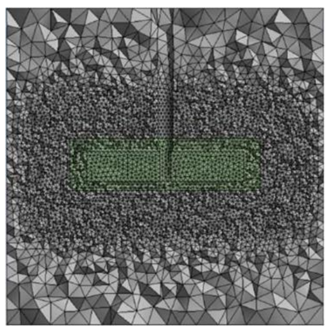


**Figure 3:** Shape of meshes of Paddle impeller.

**Table 4: Computing environment in the lattice method.**

| | |
|---|---|
| OS | Windows 10 pro |
| CPU | Intel(R)Xeon(R) Gold 6138 CPU @2.00GHz |
| Computer memory | 256GB |
| Cluster PC cores | 132core |
| Cluster PC memory | 377GB |
| GPU | none |
| Software | Fluent 2021 R2 |

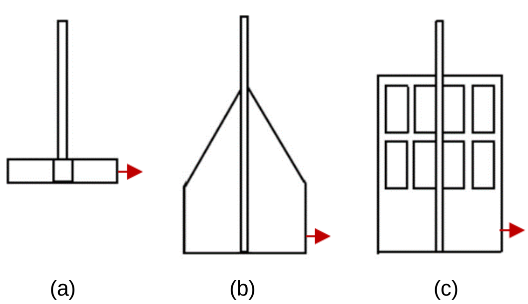



**Figure 4:** Used Impeller. (a) Paddle impeller; (b) HB-type Impeller; (c) MAXBLEND Impeller.

# 3. Experimental

## 3.1. Experimental Apparatus

Figure **4** shows the mixing impellers used for experimental verification. In this study, a two-bladed paddle impeller (impeller diameter d = 74 mm, blade width b = 14 mm), a home base (HB) impeller (impeller diameter d = 111 mm, blade width b = 141 mm, blade thickness 6 mm) [15], and a Maxblend (MB) impeller (impeller diameter d = 96 mm, blade width b = 146 mm) were used. An acrylic resin flat-bottomed cylindrical vessel with a diameter of D = 150 mm was used as the mixing vessel, and the ratio of liquid height H to vessel diameter H / D was 1.0 for the paddle and HB impellers and 1.3 for MB impellers (liquid high to better performance for MB impellers [16]). The streak lines were visualized in the laminar to transition region (Re = 50~225), where the streak lines can be clearly visualized. Reynolds number was calculated from Eq. (6).

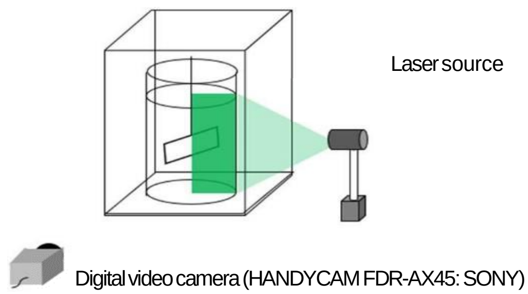



**Figure 5:** Schematic diagram of experimental apparatus.

$$Re = \frac{d^2 n \rho}{\mu} \tag{6}$$

The aqueous syrup solution was adjusted to various viscosities (0.012~0.036 Pas) to adjust the Re number. The density ρ was 1200~1400 kg/m$^3$. The rotation speed of the impeller was set empirically to 24~27 rpm for ease of observation of the streak line. The arrows in the figure indicate the position of tracer generation.

## 3.2. Experimental Method

A hollow shaft and impeller were used to visualize the streak line, and the colored liquid was discharged from the impeller tip. A fluorescent aqueous solution of uranine syrup (viscosity was the same as that of the bulk fluid) was used as the coloring liquid to enable observation of a two-dimensional cross-section of the streak line. The streak line was visualized in a vertical cross-section by irradiating a laser slit light (LCD PROJECTOR: EPSON) onto a mixing shaft placed in the center of the vessel shown in Figure **5**. Basically, the streak line pattern is the same regardless of where the tracer is discharged in the tank, but the method in which the tracer is discharged from the impeller tip is the easiest to visualize the streak line pattern beautifully. In the calculations, the tracer discharge position was set at the impeller tip shown in Figure **4** for both the lattice and particle methods.

# 4. Results and Discussion

## 4.1. Comparison Streak Line of the Non-Baffle Mixing Vessel

To verify the validity of the calculation results, the streak line pattern of a two-bladed paddle impeller is shown in Figure **6** after two to six rotations. In the numerical analysis, Re=80 was assumed, but in the experiment, the measured physical properties were not exactly Re=80, but Re=77.

The streak line patterns were qualitatively consistent using lattice and particle methods.

## 4.2. Comparison Streak Line of the Baffled Mixing Vessel

Figure **7** shows a horizontal cross-sectional view of a mixing vessel with a baffle. Two baffle plates were placed on the wall, and the position at which the streak line pattern observed was at 45˚.

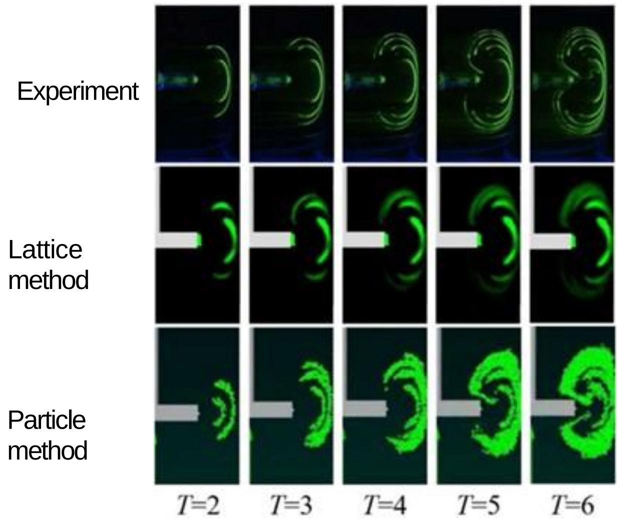



**Figure 6:** Streak line pattern in an unbaffled vessel with paddle impeller.

The streak line pattern in this cross-section is shown in Figure **8**. The numerical analysis showed Re=150, but the experimental results did not show Re=150 exactly, but Re=154.

Comparing Figure **6** and Figure **8**, the baffle affected the streak line pattern. The streak line pattern calculated by the lattice method agreed qualitatively well, with the experimental results, the particle method failed to reproduce the symmetrical streak line pattern.

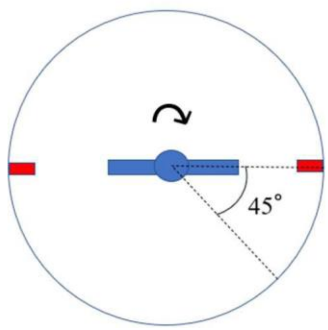



**Figure 7:** Horizontal view of the baffled vessel.

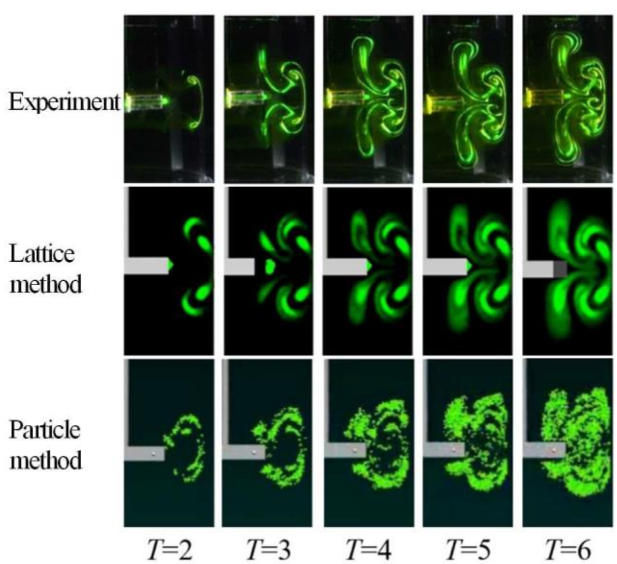



**Figure 8:** Streak line pattern in a baffled vessel (45˚).

To investigate why the particle method could not reproduce the symmetrical streak line patterns at the top and bottom of the paddle impeller, simulations were performed under various calculation conditions. The simulation was able to reproduce the dents in the upper half of the streak line, which is characteristic of the streak line when a baffle is inserted, but the accuracy of the lower half was low. We tried changing the bottom boundary conditions but could not identify the cause of the problem. The upper and lower halves were asymmetrical from the velocity vector stage, which is an issue to be re-examined in the future.

### 4.3. Comparison Streak Line of HB Impeller

Figure **9** shows the streak line of the HB impeller, which is not vertically symmetrical because the streak line pattern is vertically symmetrical when the paddle impeller is placed in the center of the tank in laminar flow. Re = 50 was used in both the experimental and numerical analyses. Both methods reproduced the streak line pattern from the vessel bottom to the liquid-free surface along the vessel wall. In addition, the flow characteristic of the HB impeller after 10 rotations was reproduced in good agreement with the experimental results.

### 4.4. Comparison Streak Line of Max-blend Impeller

Figure **10** shows the streak line pattern of the MB impeller at Re=100. Both calculation methods reproduced the streak line running up the vessel wall toward the liquid-free surface after stagnating at the bottom of the tank, in good qualitative agreement with the experimental results.

The particle method was able to calculate the streak line pattern of large two-bladed impellers such as the HB and MB impellers but was unable to reproduce the streak line pattern of a paddle impeller in a baffled mixing vessel.

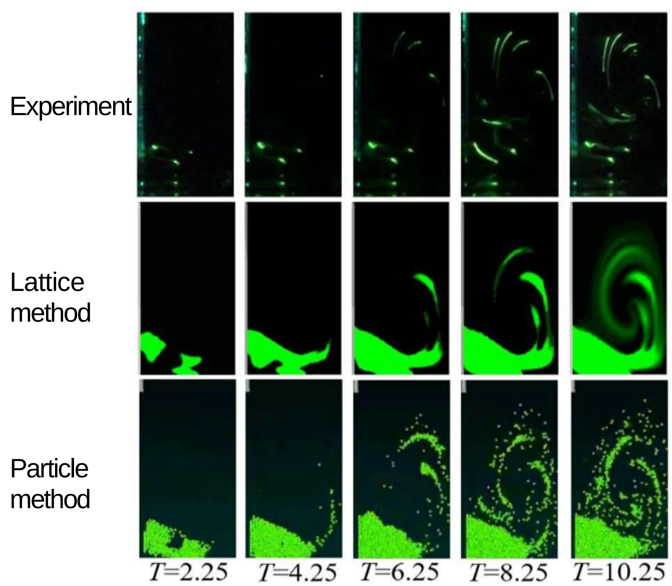



**Figure 9:** Streak line pattern of HB-type impeller.

## 5. Conclusion

Aiming to shorten the process design period and improve the design system using simulation, we developed a numerical analysis method to draw streak lines in a laminar region. A comparison of calculation and experimental results showed that commercially available software is sufficient to reproduce the streak line of large two-bladed impellers such as the HB and MB impellers. However, when we tried to reproduce the streak line pattern of a paddle impeller in a baffled mixing vessel, the lattice method was more advantageous than the particle method for vertically symmetric flows.

In the future, if we can reproduce the streak line pattern in a broader range of conditions, we expect to establish this method as the practical numerical analysis method that can be used in the actual plant design.

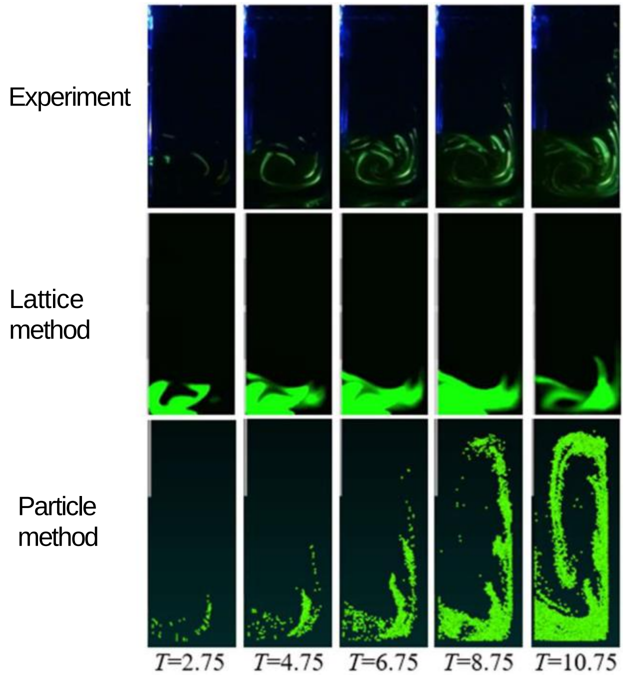



**Figure 10:** Streak line pattern of MAXBREND impeller.

## Nomenclature

| | | |
|---|---|---|
| $b$ | = height of impeller blade | [m] |
| $D$ | = vessel diameter | [m] |
| $d$ | = impeller diameter | [m] |
| $g$ | = gravitational acceleration | [$m \cdot s^{-2}$] |
| $H$ | = liquid depth | [m] |
| $n$ | = rotational number | [$s^{-1}$] |
| $p$ | = static pressure | [Pa] |
| $Re$ | = impeller Reynolds number (= $d^2 n\rho/\mu$) | [−] |
| $T$ | = impeller period | [−] |
| $u$ | = velocity | [$m \cdot s^{-1}$] |
| $\rho$ | = liquid density | [$kg \cdot m^{-3}$] |
| $\mu$ | = liquid viscosity | [$Pa \cdot s$] |

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