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# NUMERICAL SIMULATION OF FLUID FLOW BEHAVIOUR ON SCALE UP OF OSCILLATORY BAFFLED COLUMN

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## Abstract

The fluid dynamics of oscillatory flow in a baffled column of 145 mm diameter was investigated numerically in this work. This numerical simulation was carried out by a 2D laminar unsteady solver using CFD package Fluent® 6.3. From the simulation, data on surface velocity were collected and velocity ratio was calculated to determine the intensity of mixing which were the main operating parameters in oscillatory flow in a baffled column. The suitable operating parameters of oscillatory baffled column of 145 mm diameter were also determined in this work. It was found that the oscillation amplitude was more dominant for obtaining desirable mixing results compare to oscillation frequency.

Keywords: Oscillatory baffled column, Velocity ratio, CFD modeling,
Flow pattern, Oscillation amplitude, Oscillation frequency.

## 1. Introduction

With the recent advancement of computational fluid dynamics (CFD), fluid flow behaviour in oscillatory baffled column can be easily understood. Previous computational fluid dynamics (CFD) modelling of oscillatory baffled column was done on a 50 mm diameter oscillatory baffled column [1] followed by scale up of baffled column [2]. This paper reports numerical simulation of fluid flow in larger scale of oscillatory baffled column and compares the data with previously reported results. The results are potentially useful and relevance in order to design and operate a larger scale oscillatory baffled column which is a novel mixing technology.

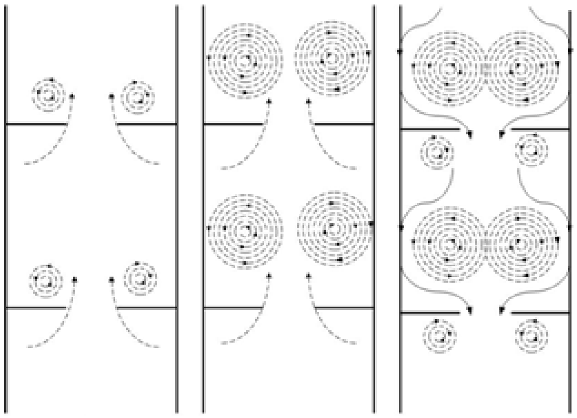
## Nomenclatures

| | |
|---|---|
| $D$ | Column diameter, m |
| $d$ | Orifice diameter, m |
| $f$ | Oscillation frequency, Hz |
| $L$ | Cell length, m |
| $\mathrm{Re}_o$ | Oscillatory Reynolds number |
| St | Strouhal number |
| $U_o$ | Initial velocity, m/s |
| $V$ | Fluid velocity component, m/s |
| $x_o$ | Oscillation amplitude, m |

*Greek Symbols*

| | |
|---|---|
| $\delta$ | Baffled thickness (m) |
| $\mu$ | Fluid viscosity (kg/ms) |
| $\rho$ | Fluid density (kg/m$^3$) |

Oscillatory baffled column is a cylinder with evenly spaced orifice baffles in which a liquid or multiphase fluid are oscillated axially by means of diaphragm, bellows or piston at one or both ends of the column [1]. For batch operations, the column is usually operated vertically, where the fluid oscillation is achieved by means of piston or bellows at the base of the column or by moving a set of baffles up and down the column at the top of the column [1]. The mechanism of mixing in oscillatory baffled column is illustrated in Fig. 1 [3].



(a)
Piston
upstroke

(b)
End of piston
upstroke

(c)
Piston
downstroke

**Fig. 1. Mechanism of Mixing in Oscillatory Baffled Column.**

The essential feature is that sharp edges (provided by the baffles) are presented transverse to an oscillating, fully reversing flow. Flow of fluid across a transverse baffles as shown in Fig. 1(a) forms clockwise and counter clockwise vortices downstream of the baffles. The vortices are pushed away from the baffles by the fluid flow and reaching their furthest position at the peak of the upward velocity, Fig. 1(b). On flow reversal, the vortices encourage the flow to flow between them and the inner wall. This in turn forces the vortices into the main flow area and new vortices are from on the new downstream of the baffles as shown in Fig. 1(c). The described flow behaviour provides a mechanism for forming eddies and moving the fluid in the wall area to the main body of the fluid. The repeating cycles of vortex formation and of similar magnitude to the axial velocities gives uniform mixing in each inter-baffle zone and cumulatively along the length of the column [4-6].

The fluid mechanics of oscillatory baffle column is governed by two dimensionless parameters which are oscillatory Reynolds number ($\mathrm{Re}_o$) and Strouhal numbers (St), defined as

$$\mathrm{Re}_o = \frac{2\pi f x_o \rho D}{\mu} \tag{1}$$

$$St = \frac{D}{4\pi x_o} \tag{2}$$

where $D$ is the column diameter (m), $\rho$ the fluid density (kg/m$^3$), $\mu$ the fluid viscosity (kg/ms), $x_o$ the oscillation amplitude (m) and $f$ the oscillation frequency (Hz). Fluid Oscillatory Reynolds number ($\mathrm{Re}_o$) is a modification of Reynolds number to describe the nature of oscillating fluid behaviour. For $\mathrm{Re}_o < 250$, low mixing intensity was observed which also known as 'soft' mixing regime. For $\mathrm{Re}_o > 250$, the flow becomes progressively turbulent like and a fully turbulent nature can be achieved with $\mathrm{Re}_o > 2000$ [7]. In short, the oscillatory Reynolds numbers is used to define the mixing intensity in oscillatory baffled column. On the other hand, Strouhal number represents the ratio of column diameter to stroke length, measuring the effective eddy propagation [8]. In this case, Strouhal number is used to describe the oscillating flow mechanism with vortex shredding [9]. For $St > 0.1$, a collective oscillating movement of the 'plug' fluid can be found where the increment in St reduces relative length of fluid transportation. These dimensionless parameters can be used as primary reference in order to achieve the chaotic mixing in oscillatory baffled column.

## 2. Numerical Simulation Setup

The scale up of oscillatory baffled column involves increasing the column diameter. The aspect ratio of related parameter such as percent baffle opening and baffle spacing is maintained in the scaled up column. In previous works, scale up factors of 2 and 4 that corresponds to 100 mm and 200 mm are used in the simulation with a base column diameter of 50 mm [2]. In this work, oscillatory baffled column with diameter of 145 mm with a scale up factors of 2.9 is used and the oscillating amplitude required is predicted to be 5.7 mm to achieve efficient mixing. To further investigate suitable operating condition for the scaled up oscillatory baffled column, oscillation amplitude of 10 mm is used as a basis to determine the suitable oscillation frequency. Table 1 summarizes the operating conditions used in previous and this work in the simulations. Before the simulations were conducted, the respective St and $\mathrm{Re}_o$ were calculated for all oscillation frequencies and oscillation amplitudes to ensure the turbulent nature and the vortex formations were sufficient to produce efficient mixing in oscillatory baffled column. From Table 1, it can be found that the minimum requirement of $\mathrm{Re}_o$ [7] and St [9] in the operation of oscillatory baffled column was fulfilled. These numerical simulations were conducted in 2-D unsteady laminar simulations of oscillatory baffled column to understand the model behaviour and obtained sufficient amount of information before proceeding to 3-D numerical simulation.

**Table 1. Working Conditions in the Scale-up Simulations.**

| Diameter (mm) | 50 [2] | 100 [2] | 145 | 145 | 200 [2] |
|---|---|---|---|---|---|
| $x_o$ (mm) | 4.0 | 5.0 | 10.0 | 5.7 | 6.4 |
| St | 0.995 | 1.592 | 1.154 | 2.024 | 2.487 |
| $f$ (Hz) | 1 | 1 | 0.51 | 1 | 1 |
| $x_o f$ (mm/s) | 4 | 5 | 5 | 5.7 | 6.4 |
| $U_o$ (=$2\pi x_o f$) (mm/s) | 25.1 | 31.4 | 32.0 | 35.8 | 40.2 |
| $Re_o$ | 1257 | 3142 | 4624 | 5168 | 8043 |

## 2.1. Boundary conditions

In previous studies, [5, 10, 11] both oscillatory and periodic conditions were used. In the former, spatially periodic condition are used [1, 2]. In this paper, a user defined function (UDF) code is written to model the oscillatory and periodic conditions. The idea was to simulate the piston movement which can be defined as oscillation velocity as shown in Eq. (3)

$$u = 2\pi f x \tag{3}$$

where

$$x = x_o \sin(2\pi f t) \tag{4}$$

By substituting Eq. (4) into Eq. (3), a sinusoidal velocity time function describing piston movement can be defined as in Eq. (5)

$$u = 2\pi f x_o \sin(2\pi f t) \tag{5}$$

This UDF code was subjected to the axial velocity components at the inlet and outlet of oscillatory baffled column to ensure the fluid flow as well as the grids at inlet and outlet were configured to be identical for each time steps. Numerical simulations were carried out to solve the governing equations using pressure based solver with unsteady time condition. Within the discretization schemes, the pressure was a body force weighted scheme, the momentum is a second-order upwind scheme, and the SIMPLE algorithm was employed in the pressure-velocity coupling scheme. Although SIMPLEC algorithm can provides a faster converged solution, however it might also lead to instability due increasing pressure-correction due to under-relaxation at 1.0. To avoid this, SIMPLE algorithm was chosen by compensating the convergence time required.

## 2.2. Model configuration and grid generation

In the 2-D numerical simulations of the oscillatory baffled column, a single plane of a channel flow containing two orifice baffles was used and is shown in Fig. 2. The column model was 145 mm in width and 652.5 mm in length with baffle spacing of 217.5 mm and the orifice diameter of 75 mm. This model was designed in such a configuration in order to compare with previous work [2]. The working fluid was water at room temperature (density 998.2 kg/m$^3$, viscosity 0.001003 kg/ms). A uniform grid with 11,810 cells was used in the simulation, and generated by Gambit 2.3.16. The grid was tested through mesh refinement using fast Fourier transform analysis prior to simulation in order to eliminate grid dependence on the model.

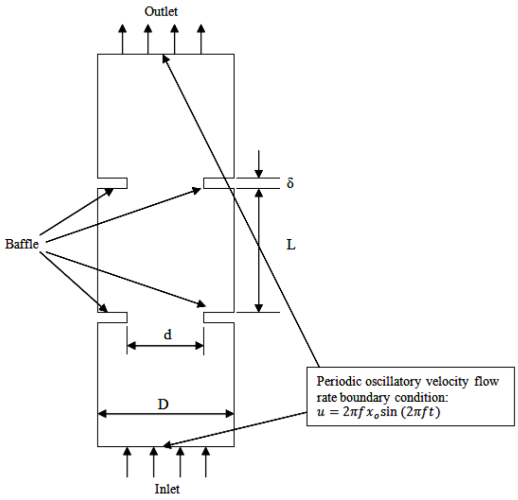


**Fig. 2. Basic Configuration of Oscillatory Baffled Column and Periodic Boundary Conditions, *L*/D=1.5, *D*=145 mm, *d*=75 mm, *δ*=3 mm.**

## 3. Numerical Results

In this work, each oscillation cycle was divided into three upward strokes phases and three downward strokes phases as shown in Fig. 3 to further elaborate the fluid flow in oscillatory baffled column. Figures 4 to 6 show comparisons of velocity contour of flow characteristics within oscillatory baffled column at various times with respect to different oscillation cycle at different operating parameters. These results were taken from large number of simulation runs. Colour bands differences in Figs. 4 to 6 show different velocity magnitudes in the oscillatory baffled column. At the beginning of oscillatory baffled column operation, the 1st cycle of Fig. 4 clearly shows the formation of vortices in both.

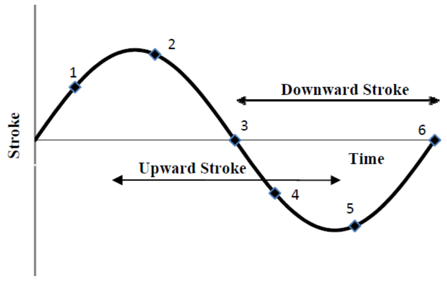


**Fig. 3. Phase Position in a Complete Oscillation Cycle.**

Combination of frequencies and amplitudes ($f$ = 1.0 Hz with $x_o$ = 5.7 mm and $f$ = 0.5 Hz with $x_o$ = 5 mm) during the end of upstroke and downstroke. This vortices formation is the main mixing mechanism in oscillatory baffled column as described in Fig. 1. At the 5th cycle of Fig. 4, the flow in oscillatory baffled column were progressively becomes complex. It was found that fluid dispersion at $f$ = 1.0 Hz and $x_o$ = 5.7 mm was much better compared to the combination of $f$ = 0.5 Hz with $x_o$ = 5 mm.

From Fig. 5 (10th cycle), it is observed that the vortices formed especially at the centre compartment were now interacting with each others. Continuous vortices formation and interaction are the main phenomena in creating the chaotic flow of oscillatory baffled column. At the 10th cycle, it was also observed that for a combination of $f$ = 1.0 Hz and $x_o$ = 5.7 mm the fluid mixing was outstanding compared to the other combination of frequency and amplitude. This can be further emphasizes by the flow pattern during the 20th cycle where the vortices already approached the outlet of oscillatory baffled column in a shorter time. The only similarity found in both configurations is the complex mixing at the centre compartment of oscillatory baffled column.

At the 30th cycle (Fig. 6), vortices formed were getting greater and bigger compared to the 20th cycle which also indicate more efficient mixing. However, the vortices formation at $f$ = 0.5 Hz with $x_o$ = 5 mm were not satisfactory compared to at $f$ = 1.0 Hz and $x_o$ = 5.7 mm. The observations indicated that efficient mixing can be achieved in oscillatory baffled column by carefully selecting the combination of oscillation frequency and amplitude. At the 40th cycle (Fig. 6), it is observed that the flow is fully developed and becomes chaotic. The interaction of vortices formed are now occupied the whole oscillatory baffled column and this is the key mechanism that enhance the mixing and mass transfer in oscillatory baffled flow.

From the numerical simulation results, surface velocities which were taken from three different points on the same plane were divided equally throughout the time taken as surface average velocity. The surface average velocity was around 0.07 m/s for oscillatory baffled column with diameter of 145 mm and consistent with previous works [2]. By increasing the column diameter, surface average velocity should decrease under a constant oscillatory Reynolds number. The effect of increasing column diameter on average velocity can be compensated by increasing the oscillation amplitude [2]. In this study, a column with a diameter of 145 mm needed oscillation amplitude of 5.7 mm (Table 1) which was about 14% increment in oscillation amplitude. To further explore the suitable operating condition, oscillation frequency of 0.51 Hz was found suitable for oscillation amplitude of 10 mm giving a surface averaged velocity of 0.05 m/s. To further ensure the importance role of surface averaged velocity, oscillation frequency of 0.51 Hz was tested with oscillation amplitude of 5 mm giving surface average velocity of 0.016 m/s. The results deviated too much from the previous works [2] indicates an unsuccessful scale-up operating parameters. Hence this suggests that maintaining surface averaged velocity is one of the major factors to scaling-up oscillatory baffled column.

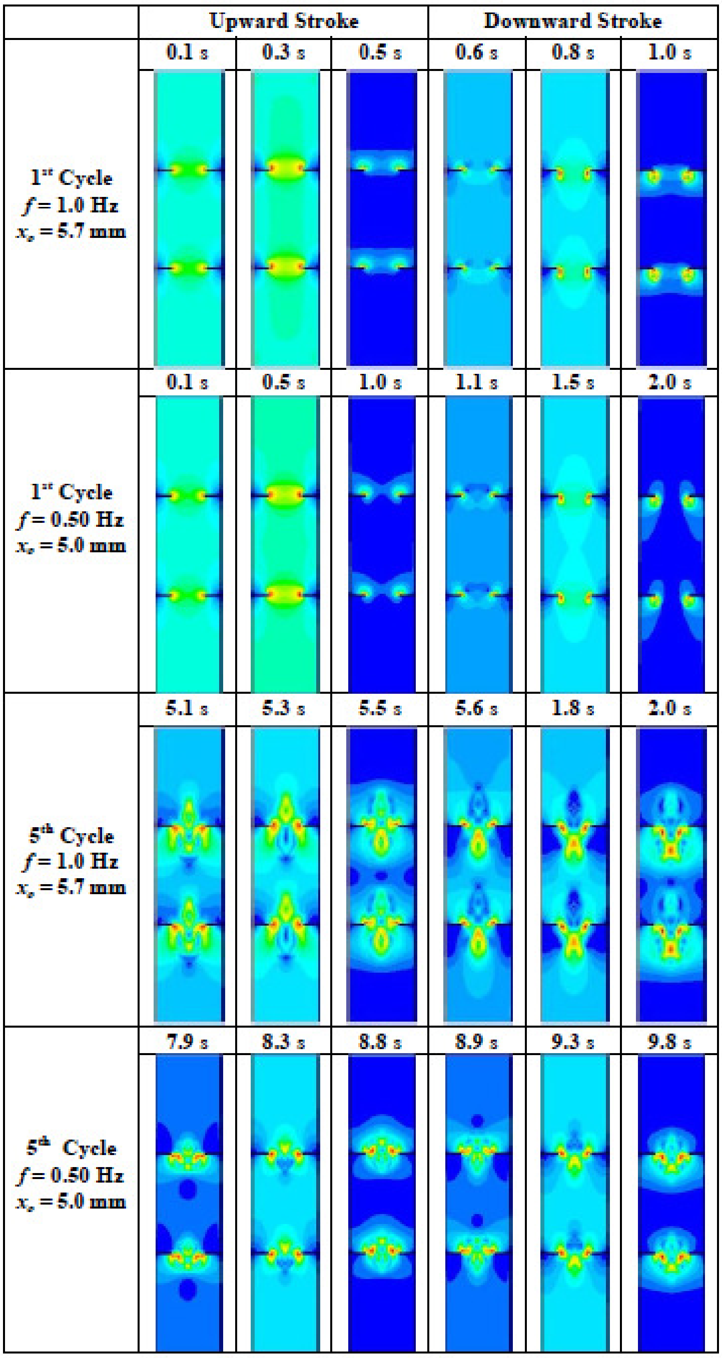


**Fig. 4. Comparison of Velocity Contour Map of Oscillation Baffled Column for 1st and 5th Cycle at Oscillation Frequency of 1 Hz and 0.5 Hz with Oscillation Amplitude of 5.7 mm and 5.0 mm.**

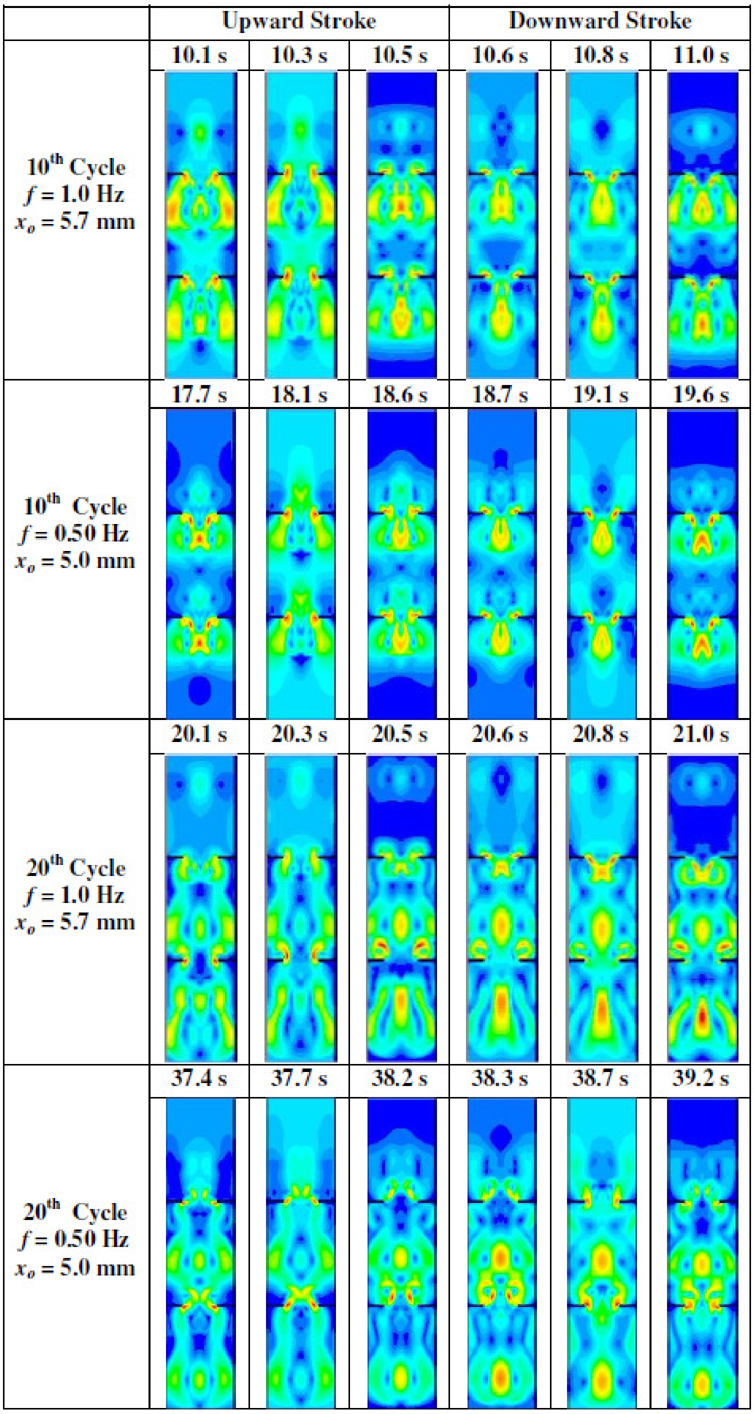


**Fig. 5. Comparison of Velocity Contour Map of Oscillation Baffled Column for 10th and 20th Cycle at Oscillation Frequency of 1 Hz and 0.5 Hz with Oscillation Amplitude of 5.7 mm and 5.0 mm.**

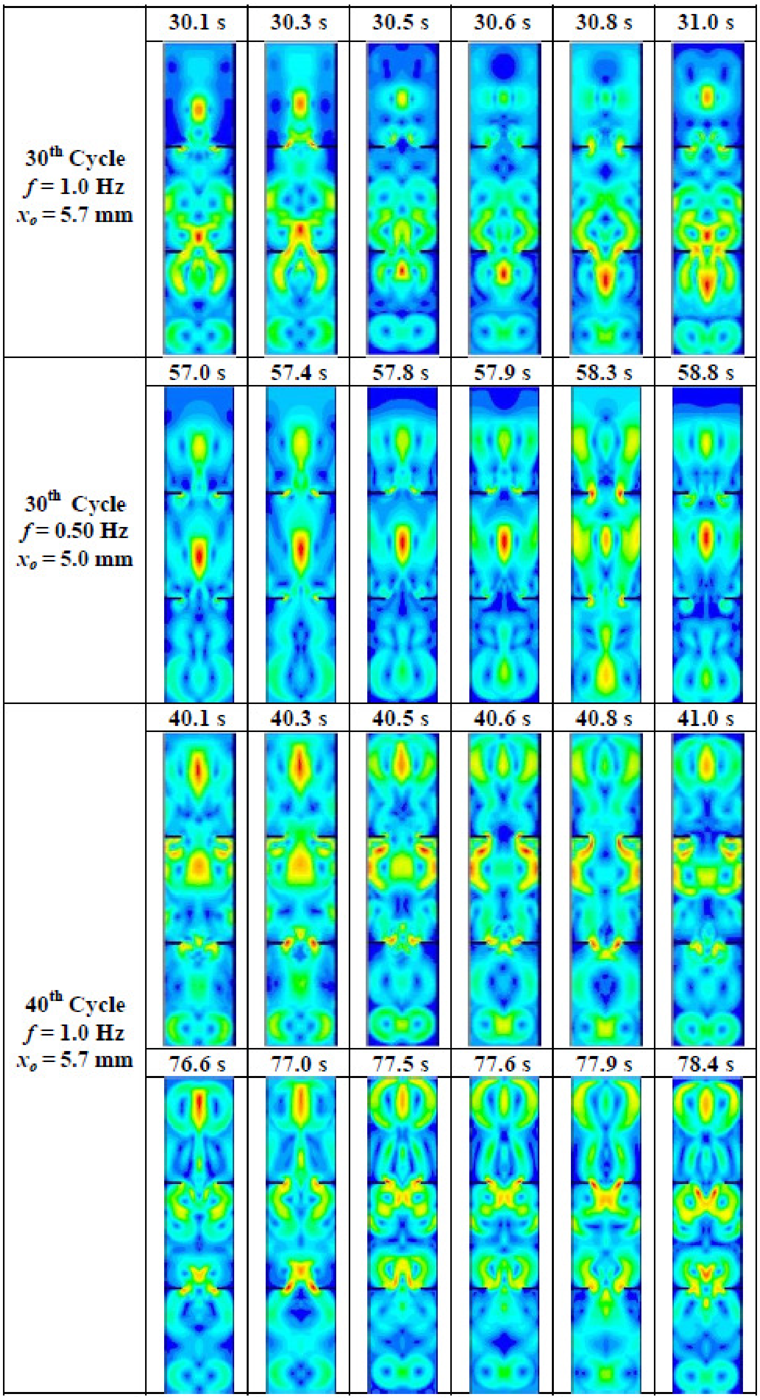


**Fig. 6. Comparison of Velocity Contour Map of Oscillation Baffled Column for 30th and 40th Cycle at Oscillation Frequency of 1 Hz and 0.5 Hz with Oscillation Amplitude of 5.7 mm and 5.0 mm.**

Another key factor for scaling up in oscillatory baffled column was the efficiency of mixing in oscillatory baffled column. This can be calculated through the axial and radial velocities collected from the simulation. The characteristic of mixing in oscillatory baffled column can be defined as:

$$\text{Ratio of velocity} = \frac{\text{Surface averaged axial velocity}}{\text{Surface averaged radial velocity}} \tag{6}$$

It was recommended that the averaged ratio should be kept between 2.0-2.5 for oscillatory baffled column scale-up [2]. It is interesting to note that at oscillation amplitude around 5.7 mm, the velocity ratio was 2.0 as shown is Fig. 7 whereas others oscillation amplitude giving a higher axial dispersion indicates a poor mixing. This suggests that to scale-up oscillatory baffled column with constant frequency, it can be done only with certain oscillation amplitude, e.g. oscillation amplitude of 5.7 mm with oscillation frequency of 1.0 Hz. Varying the oscillation amplitude at constant oscillation amplitude at 10 mm gave satisfactory results of velocity ratio which is 2.2-2.3 at 0.50 Hz and 0.51 Hz. However, at oscillation frequency of 0.51 Hz and oscillation amplitude of 5 mm, velocity ratio of 0.761 was obtained. In this case, radial dispersion was higher than axial dispersion which implies a poor mixing. It was noted that velocity ratio should not be more than 3.5 [2] because high axial dispersion resulted in insufficient mixing.

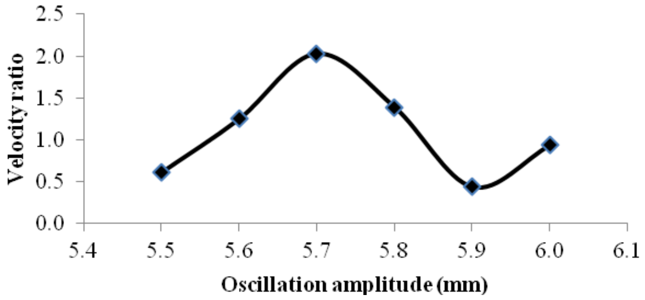


**Fig. 7. Comparison of Velocity Ratio with Different Oscillation Amplitude in Oscillatory Baffled Column (*f*=1.0 Hz).**

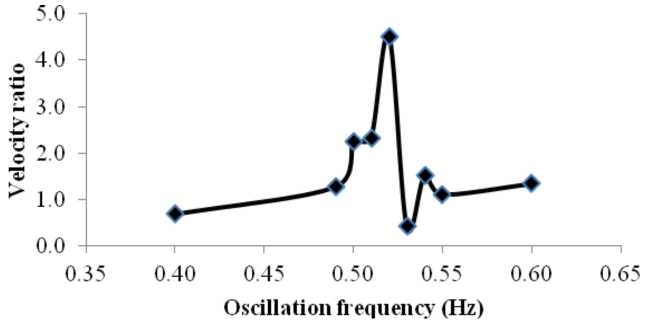


**Fig. 8. Comparison of Velocity Ratio with Different Oscillation Frequency in Oscillatory Baffled Column ($x_o$=10 mm).**

The results suggest that main consideration in the scaling up of oscillatory baffled column were to maintain the surface average velocity and velocity ratio. It was also found that it was easier to control the fluid mechanics behaviour in oscillatory baffled column through oscillation amplitude which results in less fluctuation in the velocity ratio as shown in Figs. 7 and 8. The CFD simulation of different scales of oscillatory baffled column can be used to predict mixing characteristic and determine the operating condition of oscillatory baffled column in a larger scale.

## 4. Conclusions

The fluid dynamics and scale-up characteristic of oscillatory baffled column was successfully investigated numerically in this work. The surface average velocity and velocity ratio were found to be important parameters in the scaling up oscillatory baffled column. It was also found that it was easier to control the fluid mechanics behaviour in oscillatory baffled column through oscillation amplitude which results in less fluctuation in the velocity ratio.

## Acknowledgement

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