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Application of Turbulent Model for Liquid Simulation in an Oscillatory Baffled Column

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Abstract: The Oscillatory Baffled Column (OBC) is a relatively new type of mixing device in bubble column group for chemical/biochemical reactions. It has been recognized that OBC is better in terms of mass transport rates, heat transfer, chaotic mixing and longer residence time. This paper reports the spatial and temporal behavior of oscillatory flow in baffle column. The numerical work was carried out for single phase for an unsteady three dimension using FLUENT SST k-ω, Realizable k-ε and RNG k-ε. A typical in terms of baffle spacing, baffle free area, oscillation amplitude and oscillation frequency was taken into account. A few parameters such as vertex and cycle average axial and radial velocity and turbulence kinetic energy besides the flow pattern was observed to study the ability of turbulence models. The study shows RNG k-ε is better for flow pattern, turbulent kinetic energy and mixing intensity but very sensitive to time step size. For radial velocity estimation, SST k-ε gives good predictions. Realizable k-ε gives fairly good results compared to two other models for all the parameter studies.

Keywords: CFD, flow pattern, oscillatory baffled column, turbulence model

1.0 INTRODUCTION

A substantial body of scientific papers and engineering applications now support the view that the oscillatory baffled column (OBC) is an exciting form of reactor and process technology with major commercial potential [1]. However the OBC will enter to the industry soon. Among other reasons is, research on the efficiency of this technology is still at early stages. There have been an increasing number of application's studies on OBC as widely discussed in previous research [2-6].

Oscillatory baffled column typically consists of periodically spaced annular baffles inside a long tube in which either a liquid or a multiphase mixture is oscillated axially. This induces vortices on both sides of the baffle which provide both axial and radial mixing in the tube and impart a unique form of control of mixing and transfer processes in the tube [7]. Mixing intensity of OBC can be easily controlled through manipulation of the oscillation amplitude and frequency. Besides that OBC can also be operated on both laminar and turbulent flow depending upon the process suitability.

The fluid mechanical condition in an OBC is controlled by the dimensionless parameters which are;

Reynolds number,

$$(\mathrm{Re}_n = \frac{uD}{v} = \frac{uD\rho}{\mu}),$$

Oscillatory Reynolds number,

$$(Re_o = \frac{u_o D}{v} = \frac{x_o \omega D\rho}{\mu} = \frac{2\pi f x_o \rho D}{\mu}),$$

and the Strouhal number,

$$(S_t = \frac{D}{4\pi x_o}).$$

Oscillatory Reynolds number characterizes the intensity of mixing applied to column. Strouhal number represents the ratio of column diameter to stroke length, measuring the effective eddy propagation [1]. Efficient mixing can be achieved in oscillatory flow in a baffled tube when Re_o is greater than 150 [8]. Baffle spacing on the order of 1.5 tube diameter and constriction of a ratio about 60% is optimal to achieve good mixing in oscillatory condition [9].

In this paper, computational fluid dynamics (CFD) package FLUENT was used to investigate the turbulence behavior of OBC. Three turbulence models have been used, which is SST k-ω, Realizable k-ε and RNG k-ε to study the ability of each model in characterizing the oscillatory flow in baffle column. The observed parameters are dispersions of axial and radial velocity and kinetic turbulence velocity at different positions.

2.0 NUMERICAL MODEL

Numerical modeling presented was conducted using the commercial CFD package [10]. In general, all the models were three-dimensional and considered incompressible and turbulent. The 3D domain considered is shown in Fig. 1. The channel width and length are 145 mm by 500 mm respectively with a baffle spacing of 217.5 mm and an orifice diameter of 81 mm. These scales met the Brunold *&* Roberts specifications to achieve the efficient mixing [8-9]. The working fluid is water at room temperature (density 998.2 kg/m^3, viscosity 0.001003 kg/(ms)). Hexahedral mesh were generated by Gambit 2.3. Among the baffles axial directions, five divisions were used. The operating conditions used in all simulations are shown in Table 2.

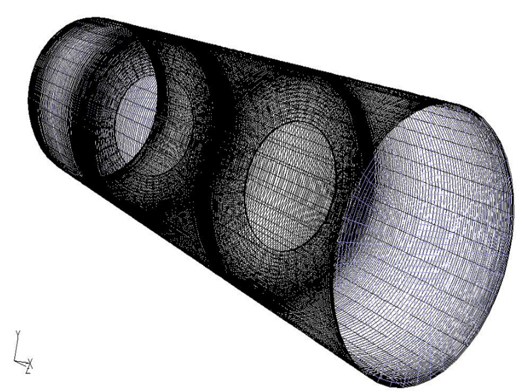

Fig. 1 3-D mesh unsteady turbulence simulation for all cases

Table 2 Operating conditions used in the all simulations

Case study	Case 1	Case 2	Case 3
Mesh size	341,300	341,300	341,300
Oscillation amplitude (mm)	10	10	10
Oscillation frequency (Hz)	1	1	1
x_of (mm/s)	10	10	10
Turbulent model	SST k-ω	Realizable k-ε	RNG k-ε
Time step size	0.01 and 0.001	0.01 and 0.001	0.01 and 0.001

Oscillatory periodic flow boundary conditions were applied using user defined function (UDF) as $u=2\pi f x_o \sin(2\pi ft)$. For the convenience of analysis, ten phases (stages) in the oscillation cycle were defined in studies, as shown in Fig. 2. Each iterative numerical integration of the model differential equations was continued until all residuals attended an average value of the final update to the solution of 10^{-6}.

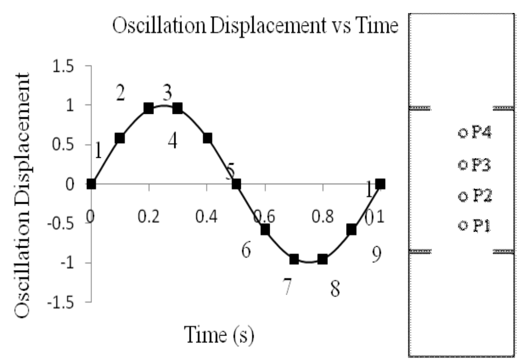

Fig. 2 (a) Periodic flow profile applied at the OBC boundaries (b) Focus point locations

3.0 RESULTS AND DISCUSSIONS

Unsteady simulations of turbulence flow have been carried out to obtain velocity vector map, average axial and radial velocity, and average turbulent kinetic energy of the oscillatory baffled column. Fig. 3 - 5 shows the results of the predicted flow patterns at various times depend on sinusoidal cycle for case 1 (Fig. 3), case 2 (Fig. 4) and case 3 (Fig. 5) by using Tecplot® respectively. To be fair, velocity scale was set to minimum velocity as 0.02 m/s and 0.3 m/s for maximum velocity. Two of ten phases were selected at higher oscillation amplitude at upstroke (phase 3) and downstroke (phase 8). Each Fig. is distinguished using time step size, which is (a) for 0.01 s and (b) 0.001 s. The highest velocity can be achieved for all three cases is 0.3 m/s and thus occurs in the baffle edges area. Mechanism of oscillatory flow is based on formation and destruction of vortices. From Fig. 3 – 5 clearly seen from the start of upstroke, vortices begin to form next to the downstream edge of the baffles. As the flow decelerates, the vortices are swept into the bulk of the baffle cell and form vortices at another side of the baffle then reach the center of the cell at the point of flow reversal. As the down stroke, these vortices unravel while new vortices are formed, on the contrary, edge of the baffle. This leads on a time-averaged basis to a uniformly mixed regime in each inter-baffle region, and the cycle repeats itself in the adverse direction of flow. This result also can be found in [12] and [13] as well. These results show that, the used of SST *k*-*ω*, Realizable *k*-*ε* and RNG *k*-*ε* model can produce similar results with LES model.

From Fig. 3 - 5, it can be observed that the effect of time step size and turbulent model on the resulting flow pattern. By reducing the time step size, the formation of vortices around baffle area and the movement of vortex in the column are clearly observable. RNG *k*-*ε* produce the sharper images than the other turbulence models.

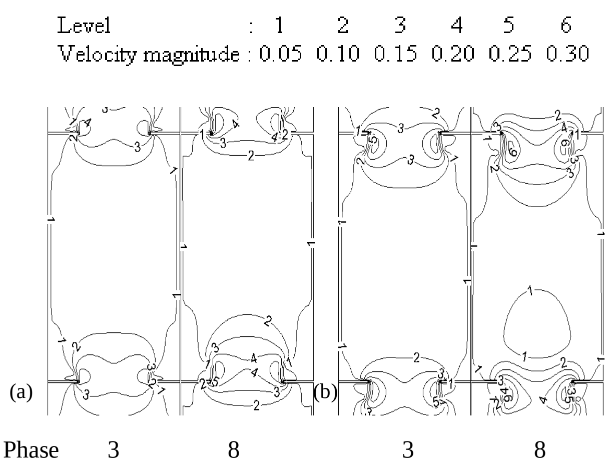

Fig. 3 Velocity vector map for SST *k*-*ω* model at different time step size (a) 0.01 (b) 0.001.

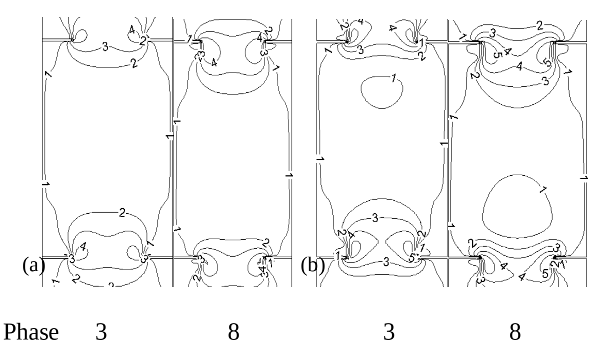

Fig. 4 Velocity vector map for Realizable *k*-*ε* model at different time step size (a) 0.01 (b) 0.001.

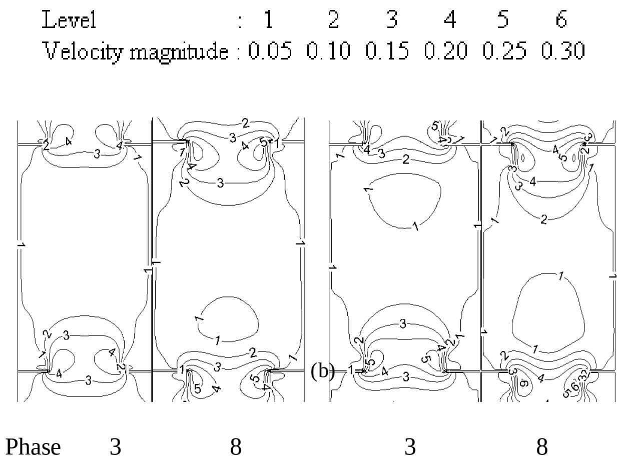

Fig. 5 Velocity vector map for RNG *k*-*ε* model at different time step size (a) 0.01 (b) 0.001

In chemical engineering, the axial dispersion coefficient is the universal index used to describe the characteristics of mixing in both continuous and batch vessels [14]. Fig.s 6 and 7 showed the effect of the turbulent model with different time step size to axial velocity distributions. RNG *k*-*ε* model gives high axial velocity values for both time step size while the SST model produces the lowest value. Axial velocity profile is the same for all models used at different time step, but the small-time step size produced the higher axial velocity. Axial velocity at point 1 and 4 are higher than those at point 2 and 3. This condition is caused by the displacement of fluid by the piston from large to the small-diameter area (free baffle area) produces a higher velocity. This decision coincides with the velocity vector maps obtained as in Fig.s 3-5 where the maximum velocity occurs in the baffle opening and surrounding areas only.

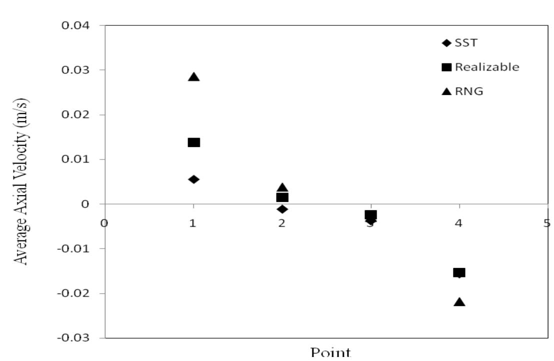

Fig. 6 Average axial velocity with points for Δt = 0.01 s

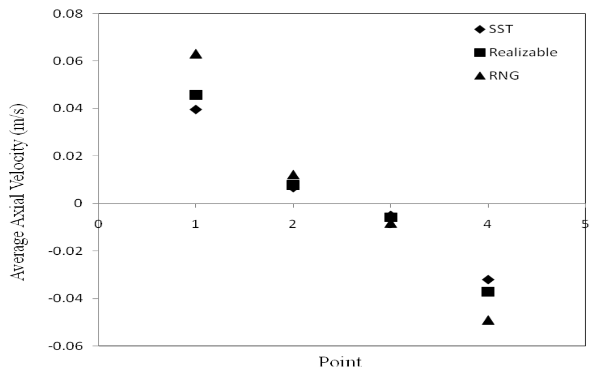

Fig. 7 Average axial velocity with points for Δt = 0.001 s

Fig.s 8 and 9 show simulation results of 0.01 and 0.001 s time step size for SST, Realizable and RNG turbulent models in terms of average radial velocity against four points at different position (Fig. 3b) in OBC respectively. It is obvious from Fig. 8 that 0.01 s time step size are not applicable for RNG k–ε type models in terms of average radial velocity estimation. The radial velocity profile for all three models is the same for time step size (0.001 s). This situation shows that the RNG k–ε model is very sensitive about the time step size. RNG k–ε model produces the highest radial velocity estimation, while the SST k–ε produced the lowest radial velocity.

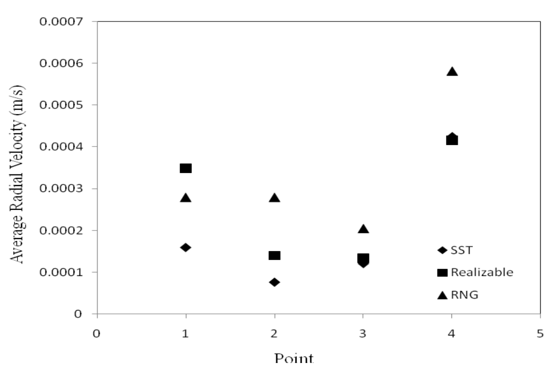

Fig. 8 Average radial velocity with points for Δt = 0.01 s

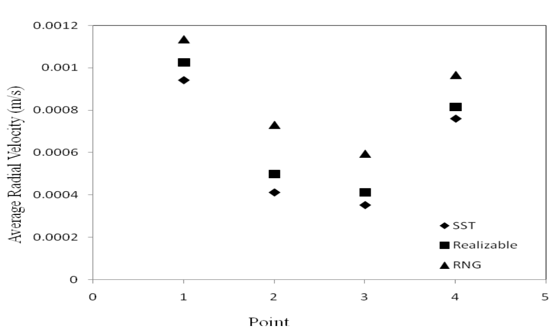

Fig. 9 Average radial velocity with points for Δt = 0.001 s

Fig.s 10 and 11 shows turbulent kinetic energy at various points for different turbulent models. For the time step 0.01 s (Fig. 10), the SST k–ε model produces the highest value while, RNG k–ε and Realizable k–ε models produce closely similar values. This situation is different when the time step (0.001 s) was used in which all turbulence models produce almost the same value at various points of TKE respectively (Fig. 11).

OBC privilege is by plug flow created, which can increase the rate of mixing than the stirred tank and bubble column. To achieve plug flow, it is necessary for the oscillatory flow to be dominant for the full effect of the vortex cycle which is formation and destruction of vortexes is maximum. For this criterion to be satisfied, the ratio of oscillatory Reynolds number to net Reynolds number, ψ should be, in practice, above 2 [15]. Stonestreet & Van Der Veeken [16] suggested values 2 < ψ < 6 to achieve plug flow.

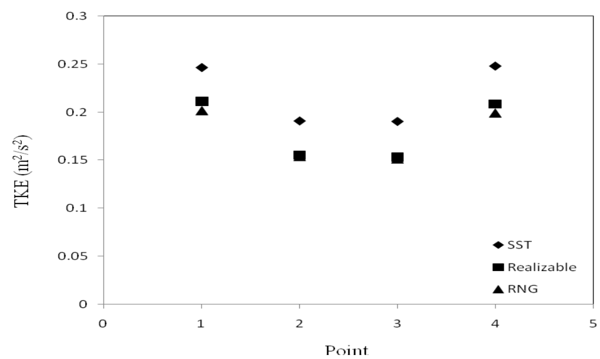

Fig. 10 Average turbulent kinetic energy with points for Δt = 0.01 s

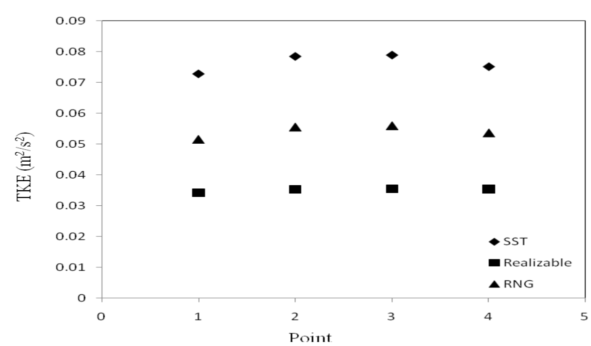

Fig. 11 Average turbulent kinetic energy with points for Δt = 0.001 s

OBC privilege is by plug flow created, which can increase the rate of mixing than the stirred tank and bubble column. To achieve plug flow, it is necessary for the oscillatory flow to be dominant for the full effect of the vortex cycle which is formation and destruction of vortexes is maximum. For this criterion to be satisfied, the ratio of oscillatory Reynolds number to net Reynolds number, ψ should be, in practice, above 2 [15]. Stonestreet & Van Der Veeken in1999 [16] suggested values $2 < \psi < 6$ to achieve plug flow.

Table 3 shows predicted value of ψ for various cases at different time steps size. Results shown both time step size indicates that not one case that reached a plug flow. Case 2 (Realizable k-ε) gave the lowest value for both time step size while case 1 (SST k-ε) and case 3 (RNG k-ε) slightly same for 0.001 s time step size and quite different for 0.01 s time step size.

Table 3 Mixing intensity for every case

Time step size	Mixing intensity		
	Case 1	Case 2	Case 3
0.01	1.29	1.21	1.43
0.001	1.09	1.01	1.08

4.0 CONCLUSION

Numerical study on the effect of turbulence models to oscillatory flow in baffled column is presented. The results demonstrate, RNG k-ε is most suitable for flow pattern predicted than Realizable k-ε and SST k-ε. Nevertheless, this model gave inaccurate prediction for radial velocity at 0.01 s. To note, RNG k-ε is very sensitive to the time step size which small time step size gave more accurate prediction. SST k-ε not give a good prediction for turbulent kinetic energy estimation but mostly good for radial and mixing intensity study. Realizable k-ε gives a fairly good result in the two other models which lay at the middle graphs for each parameter prediction.

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