

Dashboard / ... / CFD Simulation

CFD Flocculation Tank 3D Simulation

Created by Wenqi Yi, last modified by Steven Christopher Southern on Dec 08, 2009

Computational Fluid Dynamics

Flocculation Tank Simulation

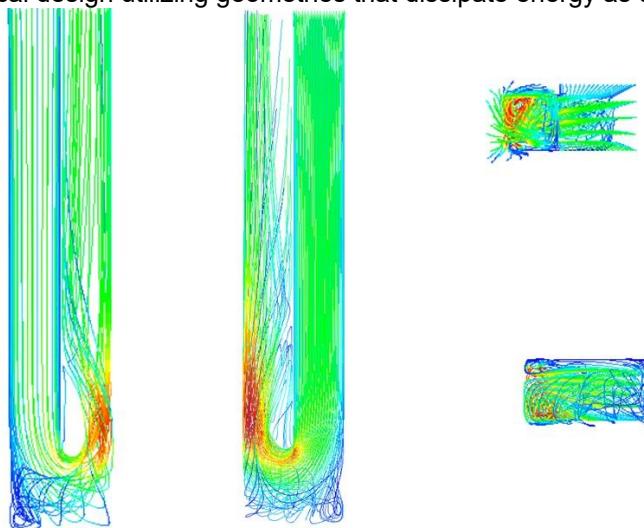
Overview

The flocculation tank simulation team works on building a stable and reliable numerical model to simulate the flow inside the hydraulic flocculation tank, and providing well-studied guidelines for design, construction and operation of the flocculation tank.

Gravity powered hydraulic flocculators are used by AguClara small-scale water treatment plants due to their low cost, inherent simplicity and robust operation. However, their inflexibility of energy input into the water relative to mechanical flocculators requires well studied design based on the understanding of the flow field and relevant performance parameters.

An appropriate CFD simulation can provide detailed numerical solutions for all the variables in the flow field, and by varying parameters such as tank geometry and flow conditions, we could obtain predictions of each of the flow variables and thus optimize the design towards lower cost and better performance.

Currently, our effort is focused on depicting an accurate energy dissipation map inside the flocculator, describing the size and the shape of the region where most of the energy is dissipated and the formation and collisions of flocs happen, thus providing basis for more efficient and economical design utilizing geometries that dissipate energy as uniformly as possible.



Pathlines of the fluid in a single baffle flocculator, viewed from left, right, top and bottom

Research

Performance parameters analysis in 2D

Characterized the performance of flocculation tanks of different geometry (different ratios of flocculation tank height/baffle spacing), using parameters derived from a semi-empirical flocculation mode, calculated from numerical values of each nodes in the CFD solution.

- **Parameter formulation:** derivation of performance parameters.([word file](#))
- **Preliminary simulation experiments:** exploratory experiments with encouraging observations and findings about set-up of boundary conditions.
- **Simulation experiments:** characterize performance parameters as a function of flocculation tank height/baffle spacing ratio.

- **Sensitivity analysis:** further investigate the sensitivity of the results to different boundary condition settings at water-air interface and to different convergence(residual) level.

Comparison of 2D model and 3D model with periodic boundary condition using k-epsilon realizable solver

Part of the preliminary effort to extend the 2D models into 3D settings, illustratively demonstrating the underlying simplification - no variation in z-direction - of simulating 3D flows with a 2D model

2D simulations with Reynolds Stress turbulence model

preliminary simulations in 2D settings

3D simulations with k-epsilon realizable turbulence model

Investigating 3D effects with finer mesh and thus better convergence level

Fall 2008

Preliminary 3D CFD simulations of a Hydraulic Flocculation Tank with a Single Baffle

- Fact-finding tests to determine the scope and approach of further research;
 - Investigate 3D model's difficulty in converging
 - Compare the assumption and validity of 2D and 3D models

Additional Resources

FLUENT quick start

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1 Comment



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performance parameter analysis in 2D - parameter formulation

Created by Wenqi Yi, last modified on Jun 02, 2009

Parameter Formulation – Characterize Collision Potential

Introduction

The formulation of parameters

$\theta_{\varepsilon}^{1/3}$, K_{baffle} , Π_{cell} and are described below, for characterizing flocculation potential using numerical solutions from CFD simulations. Note that this is a work in progress, so the notation of variables and interpretation of equations still need to be further clarified.

$\theta_{\varepsilon}^{1/3}$:

Calculating a flow weighted average of $\theta_{\varepsilon}^{1/3}$:

$$\theta_{baffle\varepsilon}^{1/3} = \frac{1}{Q} \sum_{fe} \theta_{fe} \varepsilon_{fe}^{1/3} Q_{fe}, \text{ where}$$

$$\theta_{fe} = \frac{\forall_{fe}}{Q_{fe}} = \frac{\Delta x \Delta y}{|v_x \Delta y| + |v_y \Delta x|},$$

$$\theta_{baffle\varepsilon}^{1/3} = \frac{1}{Q} \sum_{fe} \forall_{fe} \varepsilon_{fe}^{1/3}$$

Thus

K_{baffle} :

$$\varepsilon_{fe} = \frac{gh_l}{\theta_{fe}} h_e = K_{baffle} \frac{V^2}{2g} h_l = \frac{\varepsilon_{fe} \theta_{fe}}{g}$$

$$K_{baffle} = h_e \frac{2g}{V^2}$$

where

$$\theta_{fe} = \frac{\forall_{fe}}{Q_{fe}} = \frac{\Delta x \Delta y}{|v_x \Delta y| + |v_y \Delta x|}$$

$$K_{baffle} = \frac{1}{Q} \sum_{fe} \frac{\varepsilon_{fe} \theta_{fe}}{g} \frac{2g}{V^2} Q_{fe}$$

$$K_{baffle} = \frac{2}{QV^2} \sum_{fe} \varepsilon_{fe} \forall_{fe}$$

$$K_{baffle} = \frac{2}{bwV^3} \sum_{fe} \varepsilon_{fe} \forall_{fe}$$

where

$$Q = V bw$$

Π_{cell} :

$$\varepsilon_{cell} = \frac{K_{baffle} V^3}{2\Pi_{cell} b}, \text{ plug in } K_{baffle}$$

and simplify:

$$\Pi_{cell} = \frac{1}{b^2 w} \frac{\left(\sum_{fe} \forall_{fe} \varepsilon_{fe}^{1/3} \right)^{3/2}}{\left(\sum_{fe} \forall_{fe} \varepsilon_{fe} \right)^{1/2}}$$

$G\theta$:

$$G\theta_{baffle} = \frac{1}{Q} \sum_{fe} G_{fe} \theta_{fe} Q_{fe}$$

$$\theta_{fe} = \frac{\forall_{fe}}{Q_{fe}} = \frac{\Delta x \Delta y}{|v_x \Delta y| + |v_y \Delta x|}$$

$$G\theta_{baffle} = \frac{1}{Q} \sum_{fe} G_{fe} \forall_{fe}$$

$$G_{fe} \propto \sqrt{\frac{\varepsilon_{fe}}{\nu}}$$

$$G\theta_{baffle} = \frac{1}{Q} \sum_{fe} \sqrt{\frac{\varepsilon_{fe}}{\nu}} \forall_{fe}$$

$$G\theta_{baffle} = \frac{1}{Q\sqrt{\nu}} \sum_{fe} \varepsilon_{fe}^{1/2} \forall_{fe}$$

All parameters are calculated from summing over all nodes (finite element)

$\sum \forall_{fe} \varepsilon_{fe}^{1/3}, \sum \forall_{fe} \varepsilon_{fe}^{1/2}, \sum \forall_{fe} \varepsilon_{fe}$, which can be calculated using the following UDF script:[performance.c](#).

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performance parameters analysis in 2D - preliminary simulation experiments

Created by Wenqi Yi, last modified on May 04, 2009

Performance parameters analysis in 2D - preliminary simulation experiments

Objective

The effort began in Fall 2008 of trying to characterize flocculation tank performance using parameters calculated from numerical solutions from CFD simulations containing all values at each node of the mesh. The following sets of experiments are carried out to confirm the previous results and provide an exploratory basis for further investigation of the relationship between the performance parameters and geometry of the flocculation tank.

Methods and Procedures

h/b ratios of 5, 10 and 20 were tested with 5 baffles. The completed test are summarized in the following table:

Summary of completed tests

(Completed simulations are marked by "√")

material	top BC	convergence	h_over_b ration			note
			5	10	20	
water	symmetry top BC	converge to e-4	√	√	√	unable to converge to e-6 directly
		converge to e-5	√	unable to converged to e-5	√	
	wall top BC	converge to e-4		√		
		converge to e-5		√		
		performance parameters	√	√	√	

The series of geometries and meshes were created using the [journal file](#), by varying the flocculator height. The boundary conditions and all the other FLUENT settings can be found in the report summaries: [symmetry top boundary condition](#) and [wall top boundary condition](#)

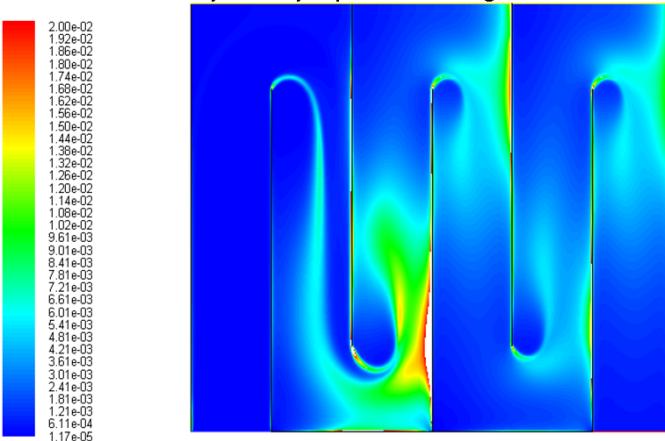
Results and Discussions

Click [here](#) for the results of the preliminary simulations, completely summarized in an Excel workbook. Only parts of the graphical results are given below.

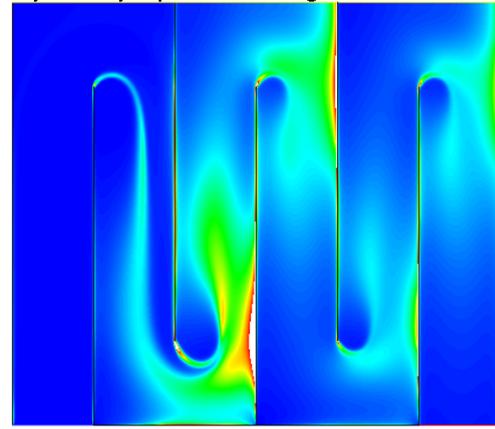
Shown below are contours of energy dissipation rate for h/b of 5 and 10, with symmetry boundary condition at the water air interface and one case with no slip(i.e. wall) boundary conditions.

Material: water

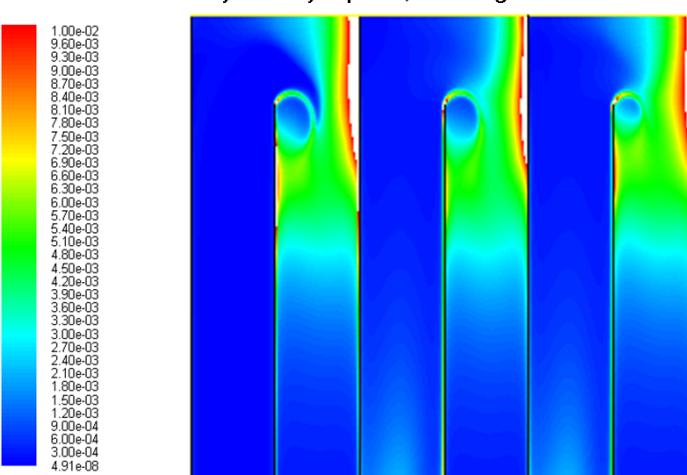
$h/b = 5$



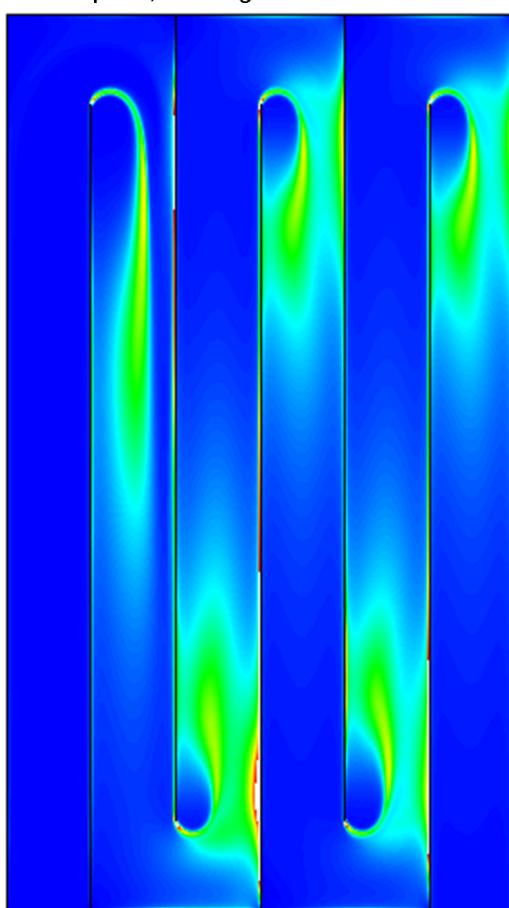
Symmetry top BC, converged to e-5



$h/b = 10$



Wall top BC, converged to e-4



As shown in the Excel workbook of graphical and quantitative results, the energy dissipation pattern is very sensitive to convergence level. One order of magnitude difference in residual results in completely different shapes of energy dissipation region at the top of flocculator. It is also noted that using symmetric boundary condition at the water-air interface at top of the flocculator makes it more difficult to converge to lower residual levels. The original purpose of using symmetric boundary condition is to mimic the frictionless condition at the water-air interface, but the energy dissipation contour of $h/b=20$ may also suggest whether using wall or symmetry boundary condition at water-air interface may not make a significant difference, and both cases could produce similar results at a better convergence level, which is consistent with our physical intuitions.

Conclusions

- Energy dissipation rate contour and quantitative analysis show dependence of performance parameters as a function of h/b ratio, which suggest it worth further investigation.
- Results are very sensitive to convergence levels.
- Symmetric boundary condition makes it difficult to converge.
- Symmetric boundary condition and wall boundary condition may have similar results at good convergence levels (residual below e-6). We can use wall boundary condition to replace symmetry boundary condition to ensure accuracy of the results.

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performance parameters analysis in 2D - sensitivity analysis

Created by Wenqi Yi, last modified on May 07, 2009

Performance parameters analysis in 2D - sensitivity analysis: convergence level and boundary condition at the water-air interface

Objective

The preliminary simulation experiments suggested that the results are sensitive to the residual levels the solutions converged to and the boundary conditions defined at the water-air interface. A more detailed sensitivity analysis is discussed in this section to exam the accuracy and validity of the results obtained in the [simulation experiments section](#), with respect to the above two conditions.

Methods and Procedures

An h/b ratio=5 was chosen for both the cases with symmetry(frictionless) and wall(no slip)boundary condition defined at the water-air interface. The solution data were saved for both simulations cases at the residual levels of e-4, e-5 and e-6 were saved and the respondent performance parameters were calculated. (Refer to *Method and Procedures* sections of either [simulation experiments section](#) or [preliminary simulation experiments section](#) for the creation of geometries and meshes, and the report summaries about all FLUENT settings).

The choices of h/b=5 and residual levels are decided based on the following:

1. The optimal h/b were shown to be 3~5.
2. Symmetry boundary condition cases had difficulty in converging to e-5, and e-4 in some cases.
3. The results change little from e-5 to e-6.

Results and Discussions

Click [here](#) for the results of the 2 series of cases, completely summarized in the last two worksheet of the Excel workbook.

Convergenc level

As shown in the workbook, the contour of energy dissipation rate changed little judging from eyeball examination between different convergence levels, but the calculated performance parameters still showed some variability as the convergence level changes. However, they stablized from e-5 to e-6.

Boundary conditions

A larger variability was shown in the parameters when compared between symmetry and wall boundary conditions, while little differences were observed in the energy dissipation contours with bare eyes. However, the variability are still within an acceptable ranging in terms of a varieity of other uncertainties in the practice of design and operation.

Convergence rate

The iteration steps needed for each cases at the three different convergence levels:

		needed iteration steps		
Convergence Level		e-4	e-5	e-6
Boundary Condition	symmetry (frictionless)	1970	2960	4480
	wall (no slip)	920	1740	2640

The above table suggests the case with wall boundary condition converges a lot faster

More comments

Also note that in all these cases the solutions were obtained by directly iterating towards e-6 with second order scheme, instead of the normal practice: iterating with first order to obtain a good initial guess and then with second order for more accurate values.

Conclusions

- e-6 is a residual level where the solutions are stabilized.
- Using wall boundary condition to replace the symmetry boundary condition is justifiable.
- Wall boundary condition makes iteration converge a lot faster.
- A residual of e-6 could be obtained by directly iterate toward e-6 with second order scheme.

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Comparison of 2D model and 3D model with periodic boundary condition

Created by Wenqi Yi, last modified on Mar 13, 2009

Comparison of 2D model and 3D model with periodic boundary condition using k-epsilon realizable solver

Hypothesis and Goals

Periodic boundary condition was applied to both side walls of the flocculation tank, imposing transitional repeating pattern of flow across the z direction in 3D model and zero pressure gradient. Thus all the results from 2D model are expected to be duplicated in the x-y plane in this 3D model with periodic boundary condition.

This is part of the preliminary simulation experiments extending the current 2D models into 3D, providing an intuitive illustration of the underlying simplifications of 2D models.

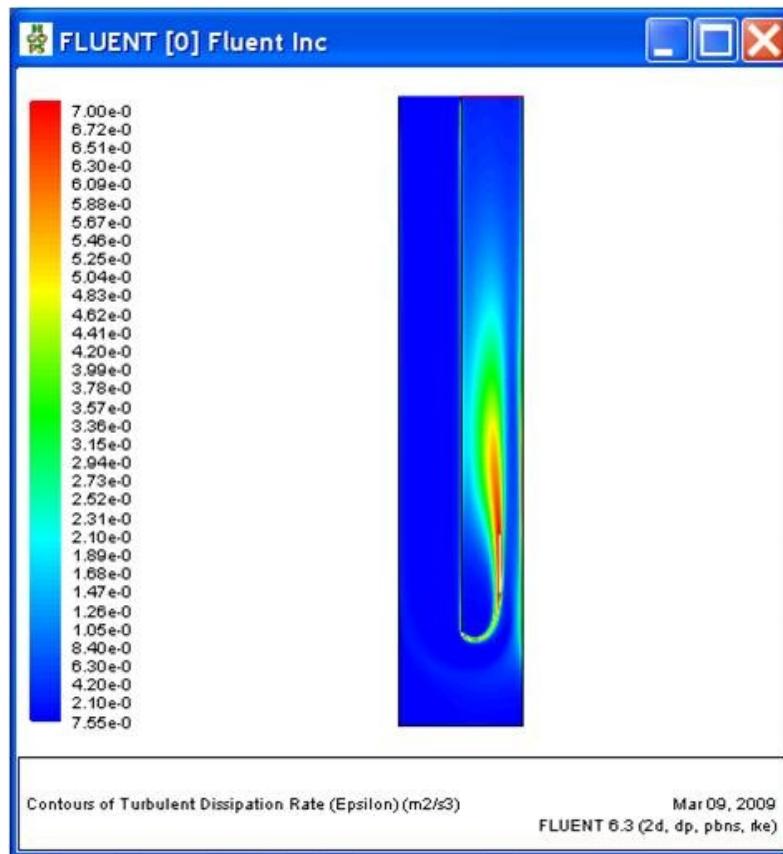
Methods and Procedures

Periodic boundary condition needs to be defined in text command interface as opposed to other common boundary conditions. Click [here](#) for a detailed description of each step, and [here](#) for the report summary containing all modeling parameters.

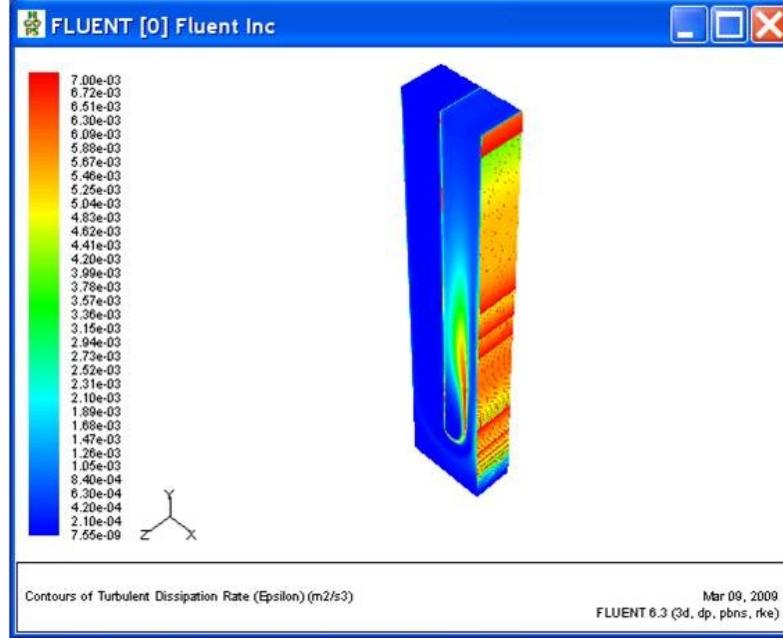
Results and Discussion

The results from 2D model was successfully duplicated in x-y plane of the 3D model with periodic boundary conditions. A comparison of the energy dissipation contours is shown below.

Energy dissipation contour of 2D model, k-epsilon realizable 1.5b



Energy dissipation contour of 3D model with periodic boundary condition, k-epsilon realizable



Since there is no variation in the z-direction in 3D model, the results from 2D is completely duplicated, which agrees with the underlying simplification of 2D simulation.

An important lesson

In FLUENT, the material property, in this case water liquid should be defined in the boundary conditions as well as in the material list. The default material in FLUENT is always air, which need to be checked and modified correctly before every simulation.

Report summary is a very good way to keep track of all the parameter settings. And more effective and efficient way of data management is necessary for carry out simulation experiments efficiently.

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2D simulations with Reynolds Stress turbulence model

Created by Wenqi Yi, last modified on May 07, 2009

2D simulations with Reynolds Stress turbulence model

Hypothesis and Goals

The Reynolds Stress model(RSM) is the most elaborate turbulence model that FLUENT provides. Abandoning the isotropic eddy-viscosity hypothesis, the RSM closes the Reynolds-averaged Navier-Stokes equations by solving transport equations for the Reynolds stresses, together with an equation for the dissipation rate. This means that five additional transport equations are required in 2D flows.

Since the RSM accounts for the effects of streamline curvature, swirl, rotation, and rapid changes in strain rate in a more rigorous manner than one-equation and two-equation models, it has greater potential to give accurate predictions for 180-degree-turning flow in the hydraulic flocculator.

Simulations using RSM was compared to results from the current k-epsilon realizable (rke) model.

Methods and Procedures

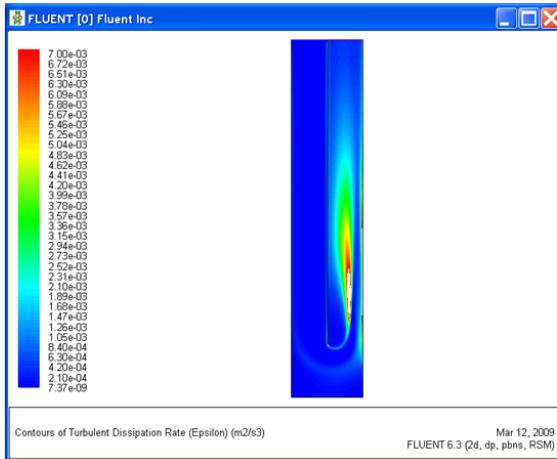
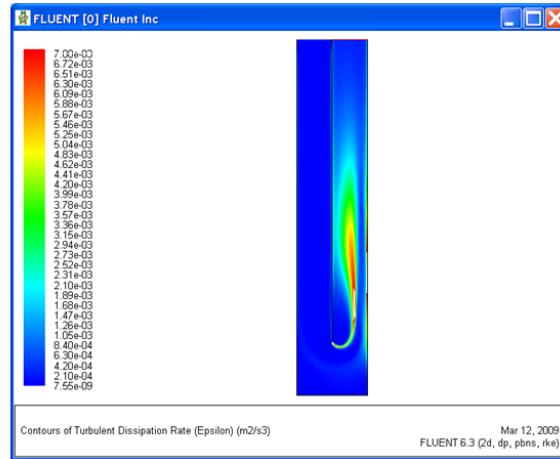
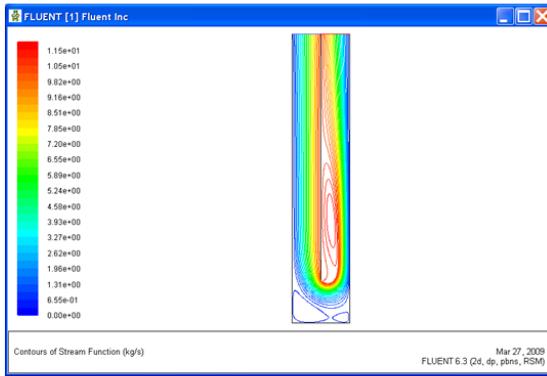
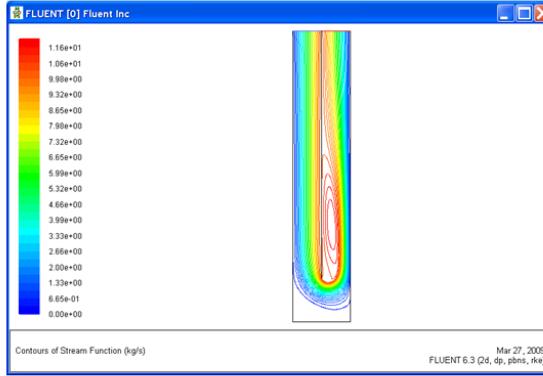
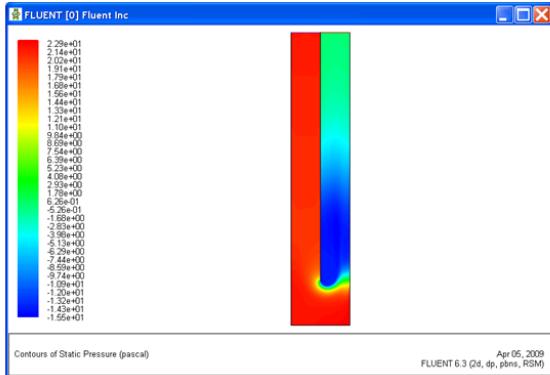
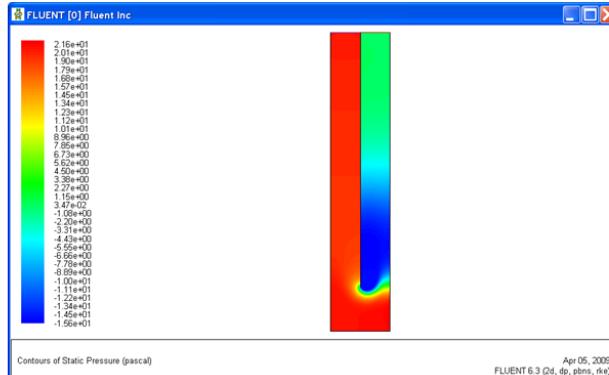
FLUENT settings can be found in the report summaries for [k-epsilon realizable model](#) and [Reynolds stress model](#)

Note that as opposed to k-epsilon realizable solver, RSM is quite sensitive to different specification methods of both inlet and outlet boundary conditions.

Results and Discussion

A comparison of the contours of energy dissipation rate, stream function and static pressure from RSM and rke are shown below.

Energy dissipation map from Reynolds Stress Model (2D)

Energy dissipation map from Reynolds Stress Model (2D)**Energy dissipation map from k-e realizable model (2D)****Stream function from Reynolds Stress Model (2D) (level=30)****Stream Function from k-e realizable model (2D) (level=30)****Contour of Static Pressure from Reynolds Stress Model (2D) (level=30)****Contour of Static Pressure from k-e realizable model (2D) (level=30)**

As shown above, results from the two turbulence models appear similar in terms of the lengths and shapes of the energy dissipation zone and the range of the energy dissipation value, while more detailed minor discrepancies indicates the differences of the two models in terms of their underlying assumptions and methodology.

Further Research

- RSM is quite sensitive to turbulence specification method of both inlet and out boundary conditions, thus more simulation experiments and research on the underlying methodology are needed to investigate about this parameter.
- The current comparison between RSM and RKE is quite preliminary. Comparisons of other pertinent parameters are necessary for better understanding of the models and how to choose between them for our specific flow.

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3D simulations with k-epsilon realizable turbulence model

Created by Wenqi Yi, last modified on May 07, 2009

3D simulations with k-epsilon realizable turbulence model

Simulations with finer mesh

Hypothesis and Goals

The preliminary 3D simulations using k-epsilon realizable (RKE) turbulence model failed to converge to a satisfactory level. Based on the results and discussion of previous models , a finer mesh in z-direction should the first attempt to resolve the convergence issue.

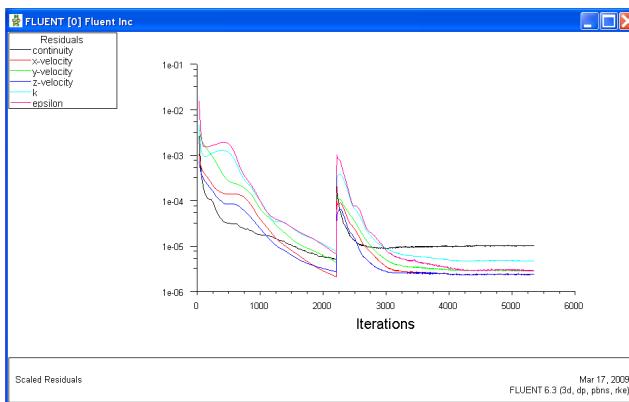
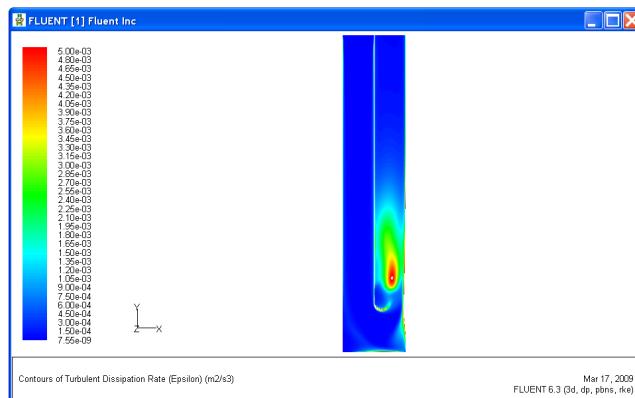
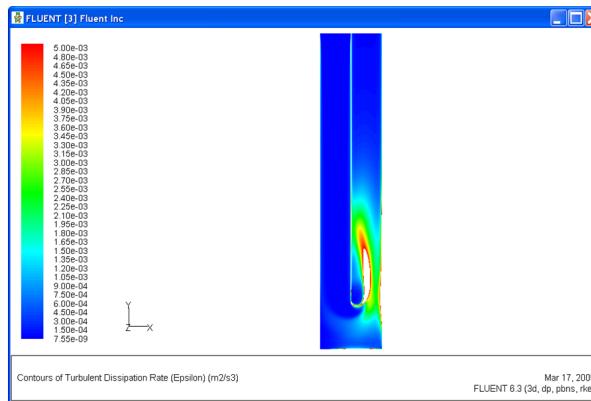
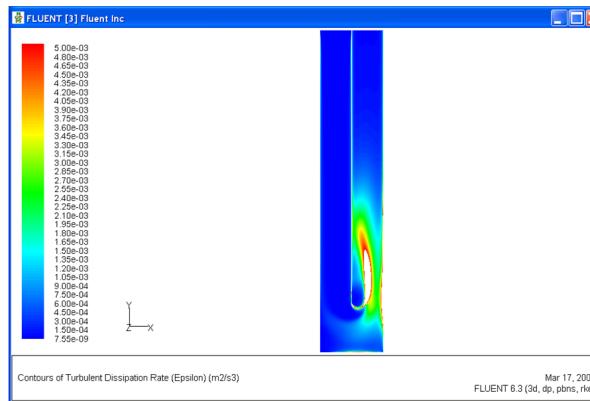
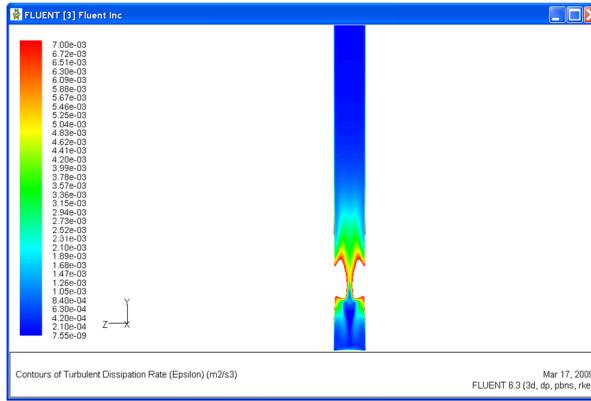
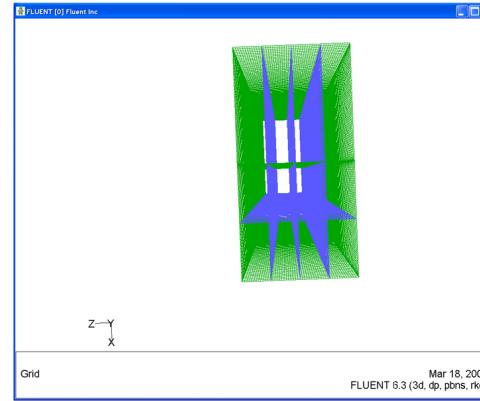
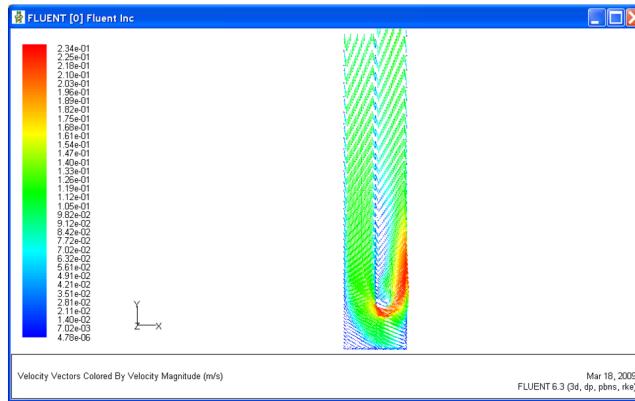
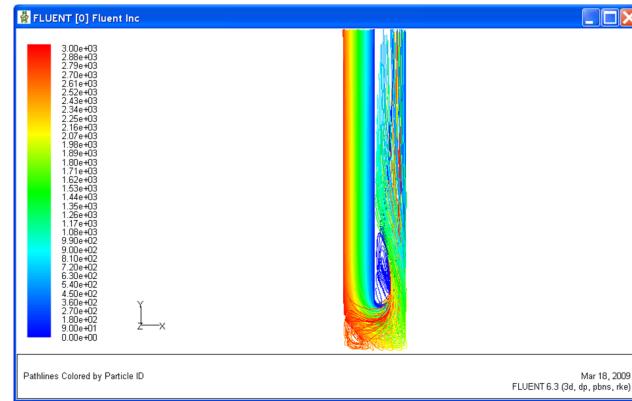
Methods and Procedures

The mesh of 2D models is swept in the z-direction with a width of 0.1m ($\text{length} \times \text{height} \times \text{width} = 0.2 \times 1 \times 0.1$), and a mesh interval size of 0.002m (#intervals=50), which is in the same order of magnitude as that of x and y directions.

Results and Discussion

Since the finer mesh contains 1,500,000 cells, which is 50 times as many as that of the 2D mesh and 70 times as big as the 2D mesh in terms of the file size, the iteration takes about 30 seconds per step. After about 3000 iterations for 30 hours, the residual plots started to oscillating with no further trend of convergence. The residual of continuity stays a little above e-5 and the others between e-6 and e-5.

Shown below are the residual plot, energy dissipation contour of various rendering surface and the pathline in mid-width plane and the whole domain.

Residual Plot**Energy dissipation contour of mid-width plane****Energy dissipation contour of quarter width plane z = 0.025****Energy dissipation contour of quarter width plane z = 0.075****quarterlength3 x = 0.15 look from +x(right)****rendering surfaces****velocity vector at mid-width plane****Pathlines**

The solution were not converged enough for the flow to be fully developed. As demonstrated in a simulation later this semester, the contour of energy dissipation rate is quite sensitive to the convergence rate, thus nothing conclusive could be drawn from the solution.

To improve convergence, we can try modifying the mesh to reduce the number of cells in stagnation region.

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Preliminary 3D CFD Simulations

Created by Wenqi Yi, last modified on Dec 22, 2008

Preliminary 3D CFD Simulations of a Hydraulic Flocculation Tank with a Single Baffle

Abstract

To extend the current 2D CFD models of flocculation tank in to 3D will greatly enhance our understanding of the fluid dynamics inside the flocculation tank. In this report, four sets of preliminary 3D computational simulations were presented and discussed: first on investigating the difficulty of 3D models in converging to satisfactory residual; and then on comparing the validity of 2D and 3D models by running 3D simulations with the model on which 2D assumptions were imposed.

Introduction

Compared with 2D models, CFD simulations in 3D provide closer numerical approximation to the real fluid flows in hydraulic flocculators, which enable better quantitatively investigation of performance parameters of flocculation and thus lead to well-studied guidelines for the design, construction and operation of hydraulic flocculators of AguAclara treatment plants.

To extend the current 2D model into 3D, preliminary simulations were essential for evaluate the scope of the project before more conclusive tests. The goals were: to get familiar with using Gambit and FLUENT in 3D settings; to come up with effective approaches for 3D simulations; and to evaluate the relative validity of 2D models vs 3D models. In this report, the 2D model was extended to 3D by minor modifications of its mesh and FLUENT parameters.

Procedures

Investigation of Convergence

Four simulations were attempted to investigate the effect of mesh and FLUENT parameters on the convergence of 3D models, aimed at smaller residual in the resultant numerical solution:

- Case 1: 1st order solver with convergence criteria of 10^{-3} ;
- Case 2: 1st order solver with convergence criteria of 10^{-6} , and to investigate the effect of inlet turbulence intensity and hydraulic radius:
 - turbulence intensity: 10%, hydraulic radius: 0.004;
 - turbulence intensity: 1%, hydraulic radius: 0.04;
- Case 3: Coarsened mesh in x, y and z directions, 1st order solver with convergence criteria of 10^{-9} and 2nd order solver with convergence criteria of (solution obtained from the 1st order solver was used as an initial guess for the 2nd order solver).

Comparison of 3D simulation results with 2D

2D models approximate the real 3D flows by assuming all variables of fluid flows are uniform along the 3rd dimension, i.e. the z direction. Thus it was expected that the results from 2D models could be duplicated if imposing this "uniform" condition on the 3D model. In Case 4, this imposition was incorporated in the 3D model by applying periodic boundary condition to the walls in the 2D plane, i.e. the x-y plane, assuming that periodic repetition along the z direction was equivalent to "uniform":

- Case 4: Periodic boundary condition was defined at the walls along the x-y plane, 1st order solver with convergence criteria of 10^{-6} 2nd order solver with convergence criteria of 10^{-6} (solution obtained from the 1st order solver was used as an initial guess for the 2nd order solver).

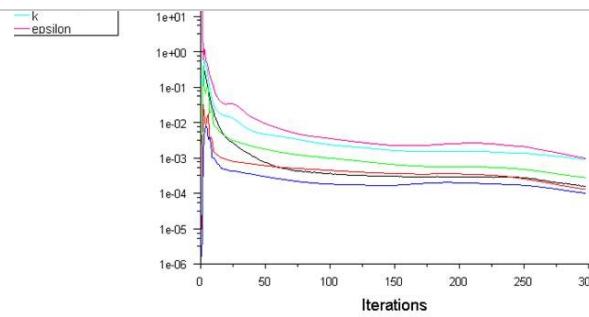
Click [here](#) for more detailed procedures of mesh generation in Gambit and problem definition in FLUENT.

Results and Discussion

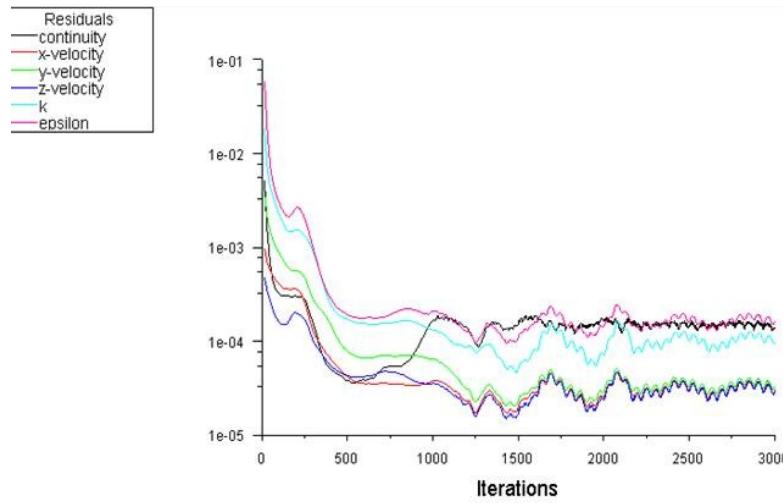
The solution data of FLUENT contains the numerical values of a complete set of fluid dynamics variables at all the nodes defined by the mesh. These values can be used to calculate all relevant characteristic parameters. Presented in the following discussions are the plots of residual as a function of iteration steps and contours of energy dissipation rate.

Investigation of Convergence

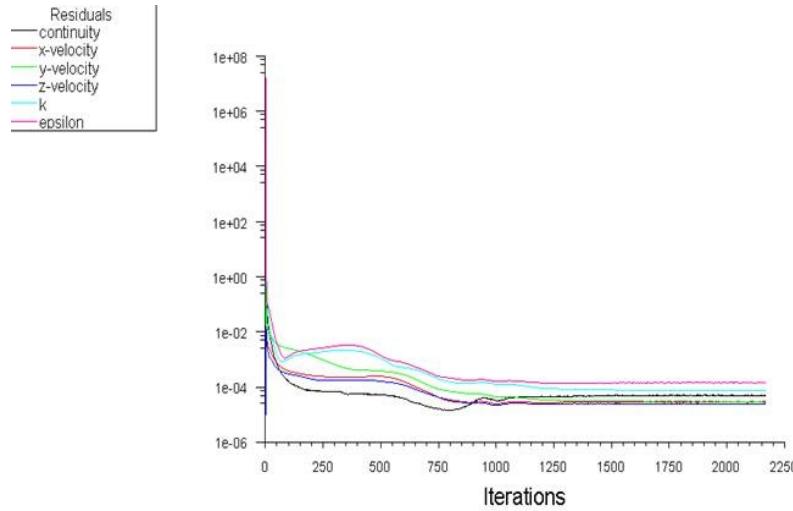
Results are shown in Figure 1 and Figure 2 below. Figure 3 indicates the plane where the contour in Figure 2 were drawn, in



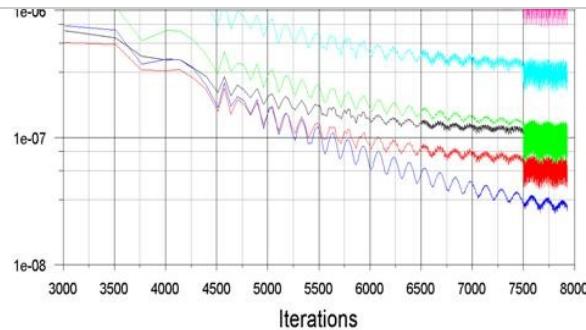
a. Case 1



b. Case 2a

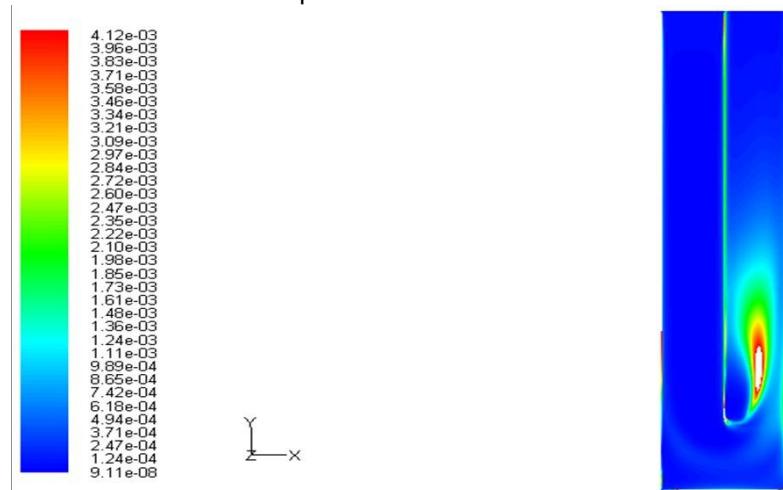


c. Case 2b

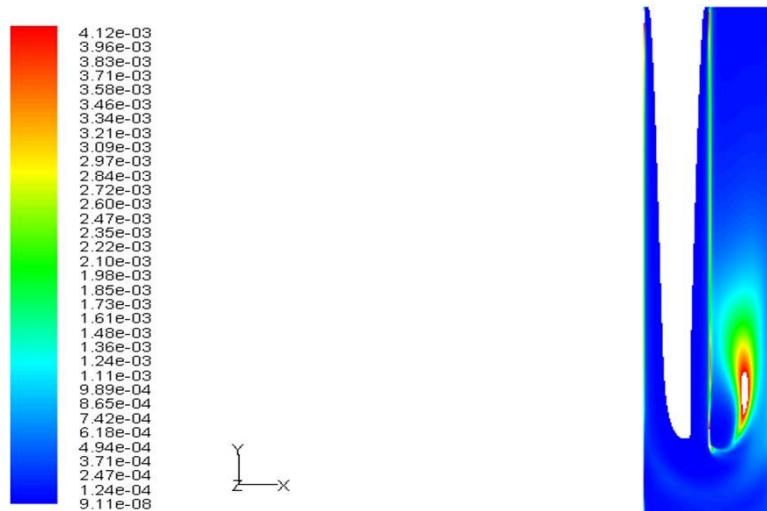


d. Case 3

Figure 1 Plots of residuals as a function of iteration steps



a. Case 2a



b. Case 2b

Figure 2 Contours of energy dissipation rate showing the effects of turbulence intensity and hydraulic diameters, drawn on the same scale

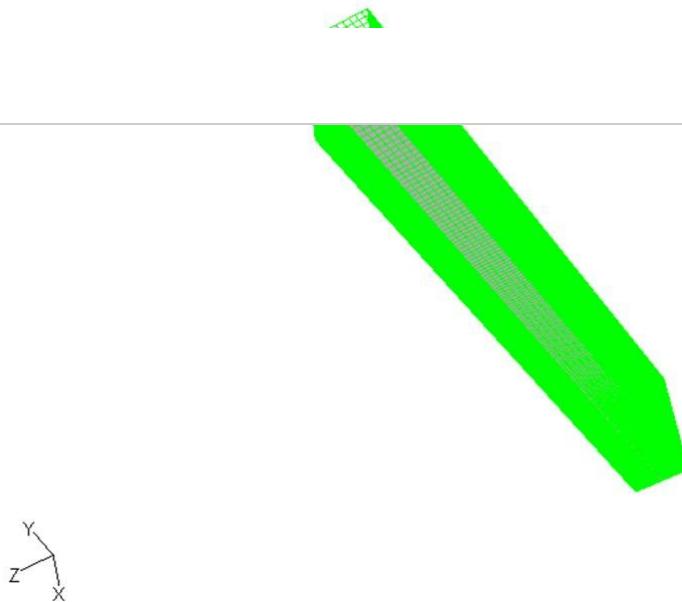


Figure 3 The plan where the contours were drawn, in grey

Observations:

- Case 1 converged to 10^{-3} within 300 iteration steps;
- Case 2a converged to 10^{-3} within 300 iteration steps, stopped converging after 500 steps and started fluctuating after 1000 steps;
- Case 2a converged to 10^{-3} within 200 iteration steps, stopped converging after 1000 steps and started fluctuating after 1000 steps;
- Case 3 converged to 10^{-9} with 1st order solver and then to 10^{-6} with second order solver within altogether 8000 iteration steps.
- There was no observable significance difference in the results between different turbulence intensity and hydraulic diameters at the inlet, except for less turbulent flow had lower minimum energy dissipation rate at the entrance region.

Discussion:

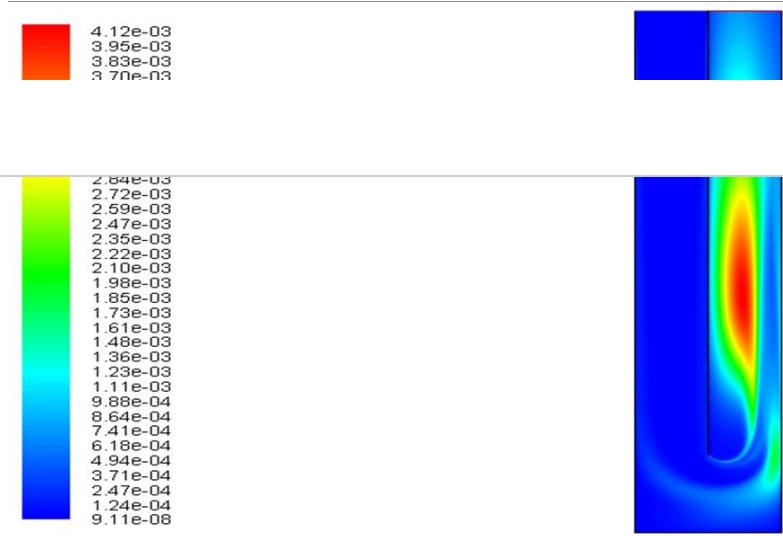
The failure of convergence was caused by ill-conditioning of the problem. In CFD simulations, numerical values are solved for from large systems of linear equations with the basic fluid variables at the mesh nodes as unknowns. In Case 1, 2a and 2b, the mesh density along the xy plane and the z direction differed by a factor of 2~5. This difference could make some numbers in the intermediate steps of iteration smaller/larger, and could be propagated through the process of matrix operations into several orders of magnitude in the 3D system of $\sim 10^5$ cells. The extremely small number thus appeared could be close to machine precision, and couldn't reduce to any smaller number through iteration, which led to the stagnation of residual plots observed in Figure 1. As was shown in Case 3 Figure 1c, after the mesh in xy plane was coarsened to the same order as the mesh in z direction, the residual converged to 10^{-9} with 1st order solver and then to 10^{-6} with second order solver after enough number of steps. The fluctuation in the tails of the residual plots could either be caused by fluctuation of extremely small numbers, or the fluctuation term defined in the turbulence model. Further experiments should be designed to verify the above hypothesis.

The results were not sensitive to different inlet turbulence intensity and hydraulic radius. And this minor difference were overwhelmed around the 180 degree turning.

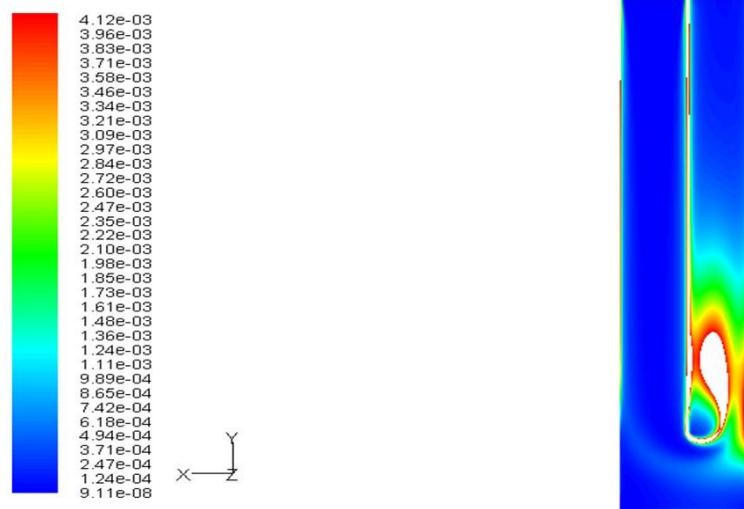
To create a more stable model that converge more accurate solution, the mesh in z direction must be refined along with proper boundary layers. And to explain the fluctuating tails in residual plots, more knowledge was needed about both the algorithms used by FLUENT numerical solvers and the turbulence model.

Comparison of 3D simulation results with 2D

The results from Case 4 are shown in the following Figures.

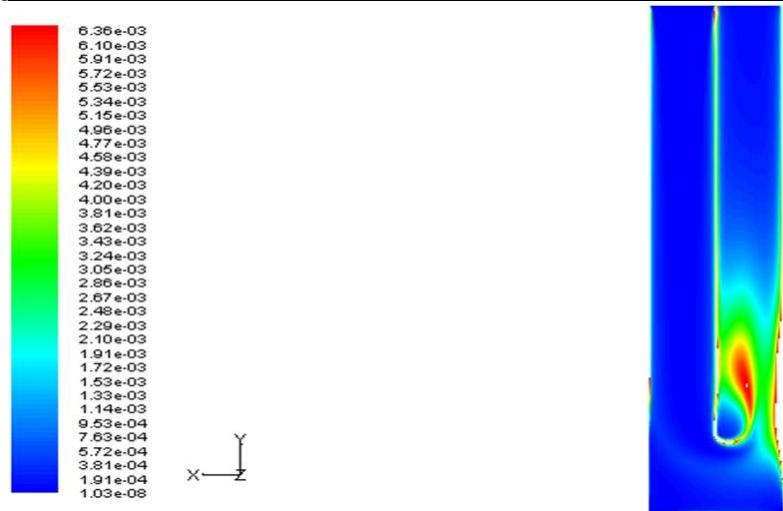


a. Contour of energy dissipation rate of the 2D model

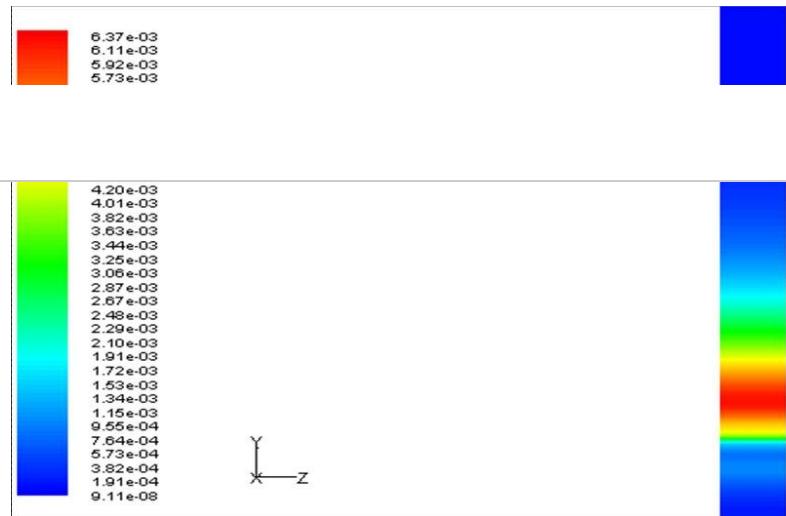


b. Contour of energy dissipation rate of the 3D model with periodic boundary condition

Figure 4 Comparison of energy dissipation maps of 2D and 3D models, drawn on the same scale

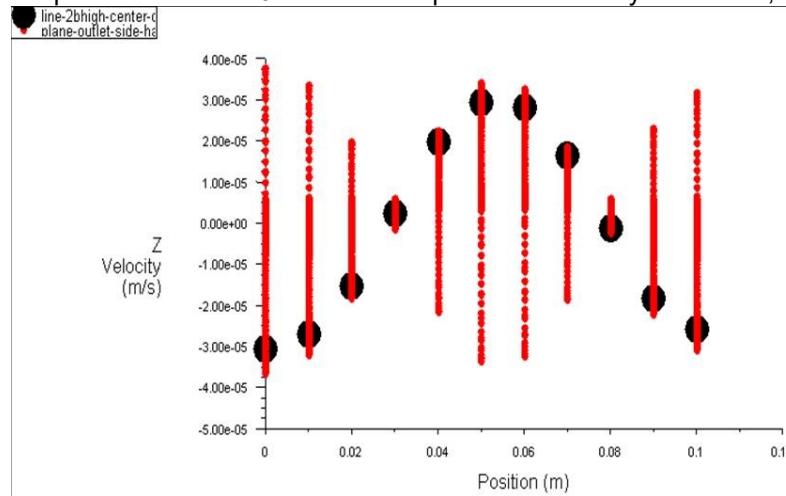


a. Contour of energy dissipation rate along the plane indicated in Figure 3

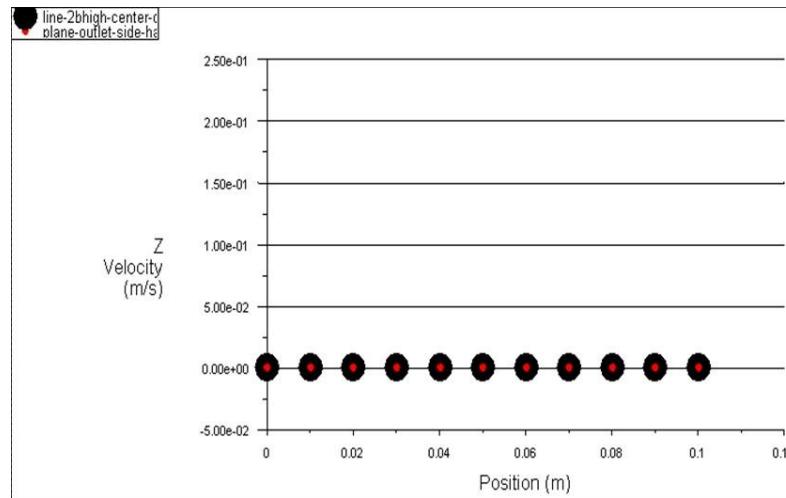


b. Contour of energy dissipation rate along the plan indicated in Figure 7

Figure 5 Contours of energy dissipation rate of the 3D model with periodic boundary conditions, drawn on its max/min scale



a. Velocity profile along the plane and line indicated in Figure 7, drawn on the max/min scale of the z velocity in the indicated line and plane



b. Velocity profile along the plane and line indicated in Figure 7, drawn on the max/min scale of the x,y,z velocity in the whole domain.

Figure 6 z velocity profile

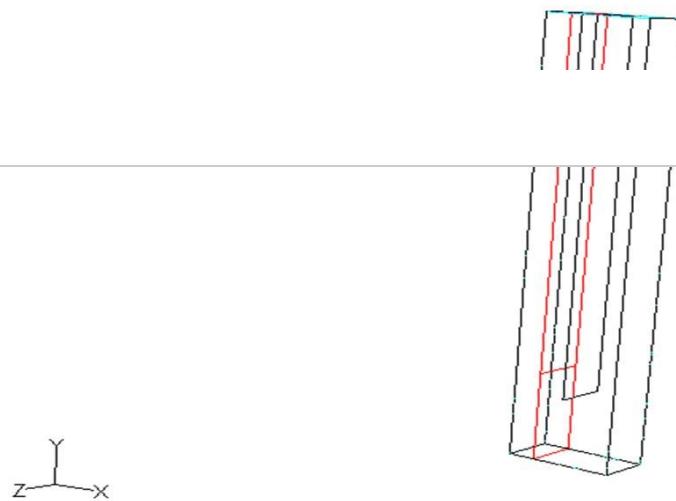


Figure 7 The plane and line referred to in Figure 5 and Figure 6, in red

Observations:

- 3D and 2D models resulted in different predictions of the shape and size of energy dissipation region after the baffle turning; (Figure 4)
- 3D model predicted a higher maximum energy dissipation rate and a smaller energy dissipation zone; (Figure 4)
- Energy dissipation rate was uniform along the z direction, as expected;(Figure 5)
- There were still non-zero components of velocity in z direction, though insignificant, and not uniform along the z direction.

Discussion:

The difference of the prediction from 3D and 2D models indicates the importance of z component in the flow field, which made the assumption of the equivalence of periodic 3D model and 2D model invalid. When we used 2D model to approximate 3D flows, other than only uniform condition, along z direction, we were actually assuming the all the fluid variables only have x,y components and no z components. When applying the periodic boundary conditions to the walls in xy plane, although the assumption that periodic repetition in z direction were equivalent to "uniform" could be valid, uniformity in z direction alone wasn't equivalent to "no components" in z direction. Thus these two models could not be good approximation to each other, and could generate significantly different predictions. As shown in Figure 6, there were still non-zero components of velocity in z direction, though insignificant in magnitude, and not uniform along the z direction.

Furthermore, the importance of z components could put the validity of 2D model as an approximation in question: in Case 4, even small components in z direction could make significant difference in results from 2D model, let alone in the real flow.

However, the above hypothesis must be further investigated, ruling out all other possible causes of differences. Particularly, the effect of the length of the period must be investigated by vary the width of the flocculator. Ideally, periodic repetition with infinitely small period length is equivalent to "uniform".

Conclusions

To build a well-conditioned model that converges to accurate numerical solution, the mesh density in all 3 dimensions must be in the same order of magnitude, and refined enough to resolve the region where fluid flows vary violently; "uniform" in z direction is not equivalent to no components in z direction, thus 3D model with periodic boundary condition may not be equivalent to 2D model, which also put the validity of 2D models in doubts.

Future Simulation Experiments

Possible future simulation experiments and research topics are:

- To create refined mesh with proper boundary layers, and run simulations on SGI server, check grid convergence;
- To investigate the fluctuating tail of residual plots;
 - Design numerical experiments to observe the fluctuation of extremely small numbers;
 - Use difference turbulence models and compare the shape of the tails;
- Simulation with periodic boundary conditions with various period length
- Use backstep experimental data to validate 3D models with periodic boundary conditions;
- Find and compare with experimental data of free/confine jets .

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performance parameters analysis in 2D - simulation experiments

Created by Wenqi Yi, last modified on May 04, 2009

Parameters analysis in 2D - simulation experiments

Objectives and Hypothesis

The preliminary simulations had encouraging outcomes about the dependence of performance parameters on h/b ratio. In further experiments described below, we simulated a series of cases with h/b ratio of 2, 3, 4, 5, 8, 10, 15, 20 and 40 and plotted each performance parameters as a function of h/b ratio. We would expect:

1. K_baffle is a measure of energy loss within each baffle spacing. It will converge as h/b ratio increases, and will also converge in a single baffle for successive turnings. Shultz and Okun has suggested its value is between 3 and 4.
2. Pi_cell will increase as h/b ratio increase, which measure the active volume of flocculation tank. $\Pi_{cell}/(h/b)$ can be a measure of the active fraction of flocculation tank, which is expected to decrease as h/b ratio increases.

Methods and Procedures

h/b ratios of 2, 3, 4, 5, 8, 10, 15, 20 and 40 were tested with 5 baffles. The completed test are summarized in the following table:

Summary of simulation experiments		(Completed simulation marked by "✓")									
		2	3	4	5	8	10	15	20	40	note
wall top BC	converge to e-5	✓	✓	✓	✓	✓	✓	✓	✓	✓	iterate directly to e-6 using 2nd order (using e-6 data)
	converge to e-6	✓	✓	✓	✓	✓	✓	✓	✓	✓	
	performance parameters	✓	✓	✓	✓	✓	✓	✓	✓	✓	

Some of the important parameters are summarized below:

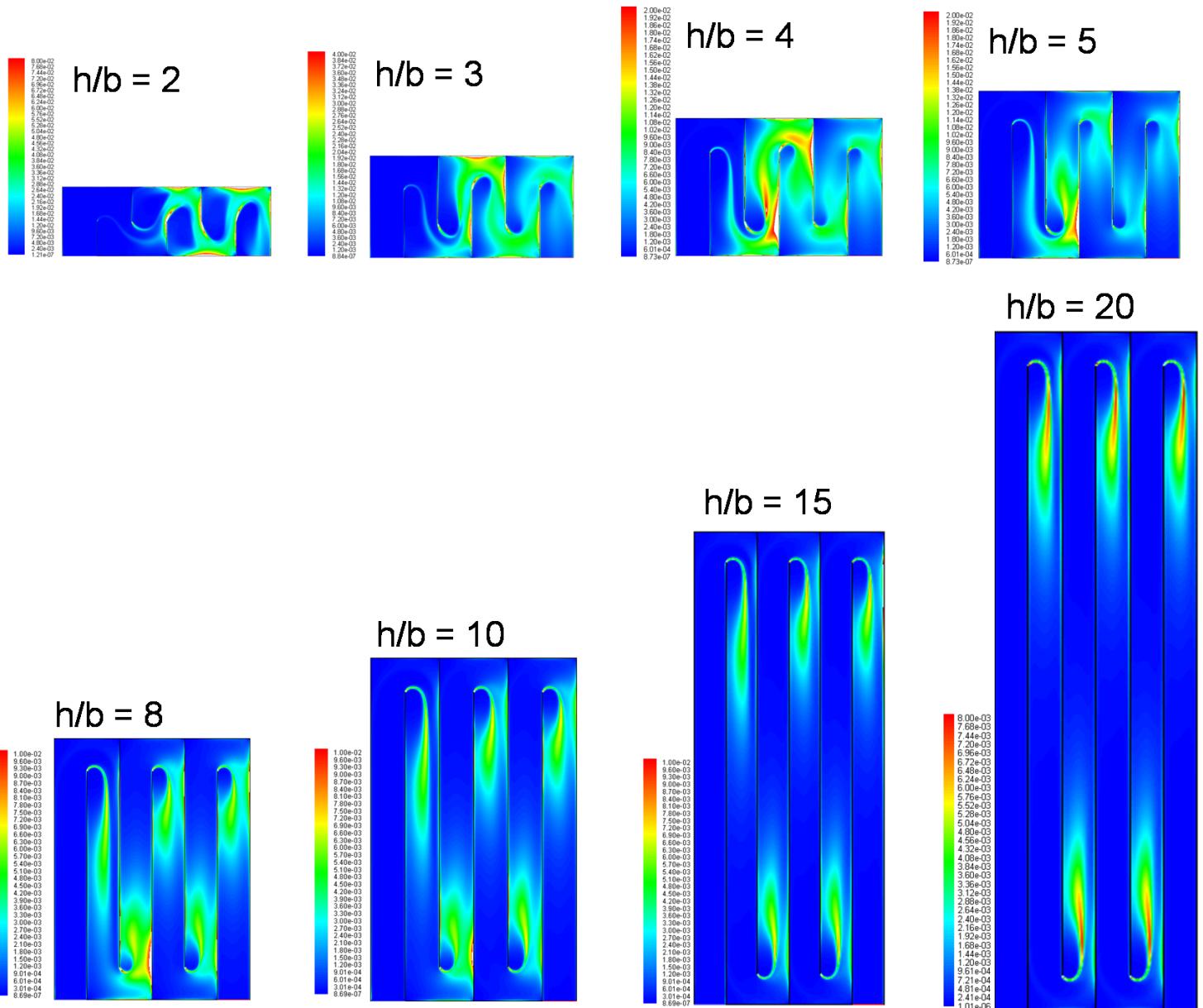
Important Boundary Conditions				
material	water-liquid	density =	1000kg/m ³	viscosity = 0.001003kg/(m*s)
inlet	v_y =	0.1m/s	turbulence intensity: 10%	turbulence length scale: 0.004
outlet	gauge pressure =	0	turbulence intensity: 10%	turbulence length scale: 0.004
top	wall	no slip		

Geometry and other parameters	
width w	0.1m
clearance b	0.1m
Reynolds number	9970.09

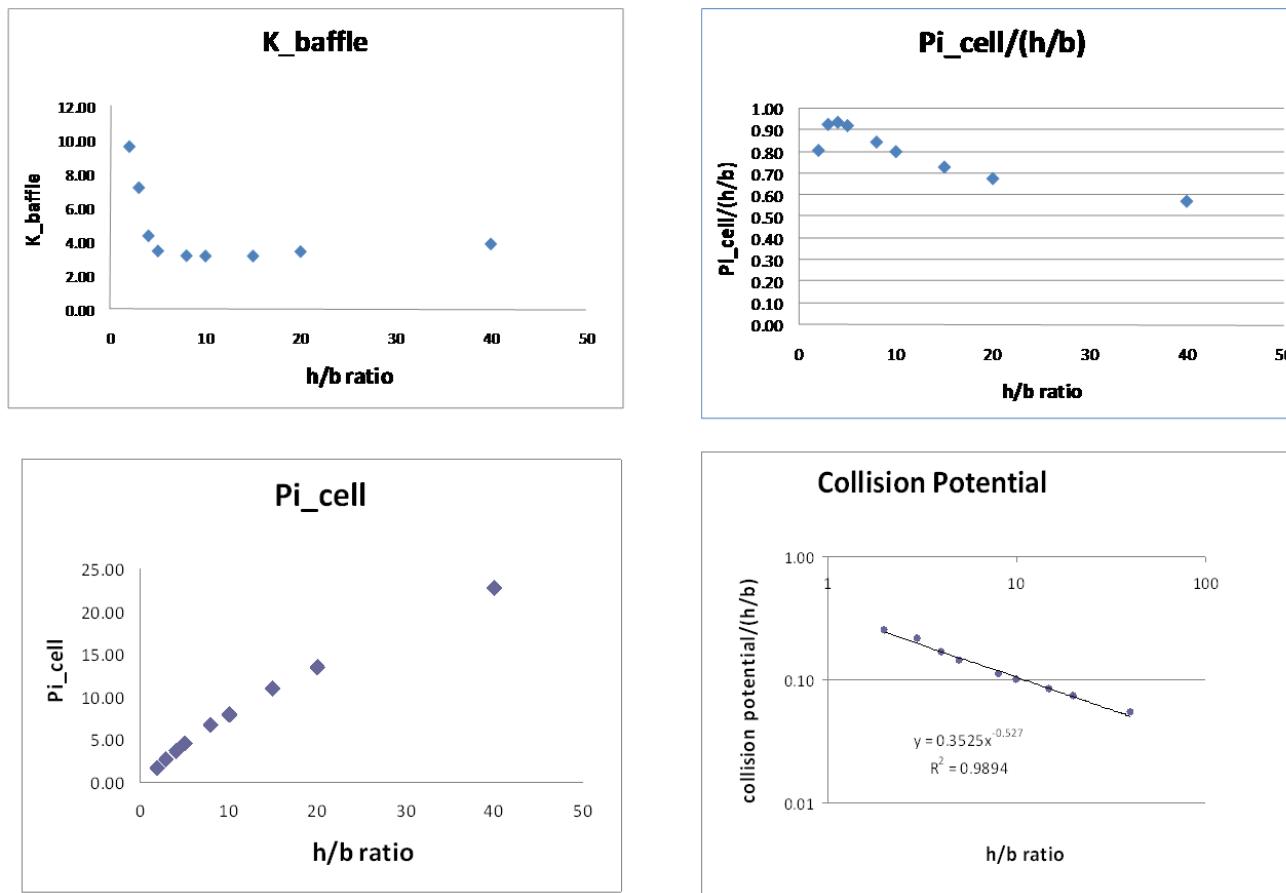
The various geometry and mesh are created from journal file, by varying the flocculation tank height. All the FLUENT settings including turbulence model, boundary conditions, solutions schemes etc. can be found in a sample of report summary for h/b=2 case.

Results and Discussion

Click [here](#) for the results of the series of simulation experiments and parameter analysis, completely summarized in an Excel workbook. Only parts of the results are given graphically below.



Take the values calculated from the 4th baffle, and plot each parameter as a function of h/b :



Number of baffles

Note that in the [Excel workbook](#), the performance parameters were calculated for both the 4th and 5th baffles. There are minor differences in numerical values while the general trend stays the same. Particularly, a more pronouncing difference is observed for $h/b=4$. Thus simulations with more baffles and a sensitivity analysis of the number of baffles could be included in the future work.

K_baffle

As shown in the plots above (and the [Excel workbook](#)), the trend of K_{baffle} values is consistent with the hypothesis. It decreases rapidly for $h/b = 2\sim 5$ and stabilizes around 3.2. An upward trend appear around the tail of the K_{baffle} vs h/b curve, which indicates the major loss in addition to minor losses is playing a more significant part in the total energy loss.

Pi_cell

Pi_{cell} was shown to increase continually as h/b ratio increases in preliminary experiments, which was also reported in [Fall 2008 research](#). This trend is further confirmed with a large h/b ratio of 40. As reported in [Fall 2008 research](#), Pi_{cell} value keeps increasing because energy is dissipated along the wall as well as around the 180 degree turning region.

Pi_cell/(h/b)

The plot of $Pi_{cell}/(h/b)$ as a function of h/b is also consistent with the hypothesis. As a measure of active fraction of the total volume of the flocculator, it reaches a maximum of 95% for $h/b=4$, and keeps decreasing as h/b increases. However, the curved flattens out at the tail. This also suggests although an optimal value exists for h/b , it wouldn't be the most critical constraint for design, since even for an un-practically tall flocculator of $h/b=20$, it still has an active volume fraction value around 70%.

Collision potential/(h/b)

The power function fit for collision potential ($\theta \cdot \epsilon^{(1/3)}/(h/b)$) was suggested by Dr Monroe Weber-Shirk. It shows a unexpectedly simple relationship with a power of about -0.5 and a coefficient of 0.33. Further investigation is needed to better interpret this relationship.

Conclusion

- The number of baffle used are not enough for the cases of $h/b= 2\sim 5$ to converge.
- The formulation of the K_{baffle} and Pi_{cell} are valid and consistent. They captures some of the characteristics of flocculator performance.
- Optimal values of $h/b=4$ is observed in terms of $Pi_{cell}/(h/b)$ value.
- Relationships between $(\theta \cdot \epsilon^{(1/3)})/(h/b)$ and h/b is unexpectedly simple and needs further investigation.

Future Work

- Simulations with more baffles and investigate the sensitivity to the number of baffles used, especially for $h/b=4$.
- More detailed comparison between symmetry boundary conditions and the wall boundary condition at the water-air interface.
- Simulations with different Reynolds numbers.
- Non-dimensionalize the results.

- Characterize the maximum energy dissipation rate to characterize floc break-up

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