Simulation investigation of the baffle overlapping rate on three-phase separation efficiency in a typical UASB reactor

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Abstract. In searching for a clearer vision and better understanding of the mechanism of the gas-liquid-solid separator in a UASB reactor, a 3-D CFD simulation code based on the Eulerian multiphase model with Shear Stress Transport turbulence model was adopted to evaluate the effects of overlapping rate of baffle plates on the separation of the three phases. In this approach, five (5) typical overlapping rate scenarios were investigated for a typical UASB reactor, and the flow pattern inside were visualised and analysed meanwhile. The results show that the averaged flow speed of three phases was doubled when they flew through the three-phase separator (TS) region, while obvious symmetrical vortexes and twisting flow patterns dominated in the TS region. The simulated characteristic circling flow pattern in the angled plate regions reveals a different separation mechanism of the TS, comparing the traditional theory accepted widely. Simulation investigation indicates that the baffle plate’s overlapping rate of the typical TS was not the most important configuration and had insignificant influences on the gas-liquid-solid phases’ averaged flow speed and separation efficiency among the five situations concerned in this article. This meant a more efficient arrangement of baffle’s overlapping scheme could apply: a baffle’s overlapping rate of 10% could achieve a separation rate as high as 99.1% for the gas-liquid-solid phases, while a reduction of 23.6% in the height occupation and a more 21.1% width of the TS could be optimized in this article case. On the other hand, the separation function of each layer of the typical TS was simulated and analysis could bring about some innovations for the widely used TS.

1. Introduction
In the field of environmental engineering, a variety of three-phase separator(TS) was equipped for most of the anaerobic reactors, as in UASB and EGSB anaerobic reactors, it typically embodied as a set of inclined, angled baffles and collected the gas bubbles, baffled the solid particles(sludge) to return to the reactor region while the gas-liquid-solid mixed liquor flowing up. For this reason, the TS plays a key role for the reactor and most was patented equipment [1-6], the efficiency and function of the anaerobic reactor are mostly depended on the TS’s special designation. Recently, with the continuous development of anaerobic reactor technology and people's attention to sustainable development, the application of anaerobic reactors in the field of environmental engineering is greatly increasing [7,8,18]. On the other hand, rarely theoretical studies about its design method, structure parameters are reported because of the flow relating to the interaction of gas, liquid and solid in TS, most of the research was focused on the TS’s imitation, structure improvement or analysis and
performance test, while not on the related fundamental theory of flow field and pattern formation of each phase, widely used TS in China were either imported aboard or engineered by more related with experiences, and the design theory obtained was the two-phase’s law of liquid-solid and gas-liquid[1-6].

A typical prototype of TS is a group of herringbone (angular) baffles configured in multi-layers, the upper and lower baffles overlapped in the vertical projection plane (from top view), to capture and stop the up-flowing gas bubbles as much as possible, from this point of view, the higher the overlap rate between the upper and the lower baffles, the more gas bubbles will be captured, but in the engineering, this will increase the number of baffles used and the height of the anaerobic reactor, the higher the expenses in the baffles and anaerobic reactor. So, the overlap rate of baffles is a key factor in TS design (another is the width in horizontal projection plane between baffles known as sludge return gap), at present in China, the design of the overlap rate of TS baffles is often from experience or experiment results, and the relevant theoretical basis is rarely reported.

In this paper, a widely used TS in China, which is developed from the European Patented structure, was investigated, using CFD technology [9-16], for five (5) baffle overlap rate settings, a 3D simulation is made to explore the three phases’ flow pattern inside and the influence of baffles’ overlap rate on the separation performance of solid particles, liquid and gas phase through the TS, this would be part of the theory for analysis and design of TS.

2. Theory

The mixed waste water flowing in the anaerobic reactor and TS is consist of three phases: gas, liquid and solid, the governing equation could be described as continuous based Eulerian-Eulerian multiphase model, or as Particle Transport model, where particulates are tracked through the flow in a Lagrangian way, rather than being modeled as an extra Eulerian phase. In Eulerian-Eulerian multiphase flow, two different sub-models are available: the homogeneous model and the inter-fluid transfer (Inhomogeneous) model [17]. In the anaerobic reactor case, the mass of most of the gas bubbles and sludge particles is very small and could be easily driven by the liquid current, the Eulerian-Eulerian Multiphase Model is suitable for this situation while the Inhomogeneous sub-model is chosen for describing the slight differences in the motion of gas bubbles and sludge particles. In the inhomogeneous multiphase model, each fluid possesses its own flow field and the fluids interact via interphase transfer terms, there is one solution field for each separate phase. Transported quantities interact via interphase transfer terms, and there will be a tendency for these to come to equilibrium through interphase drag and heat transfer terms, the theory of simulation is a set of governing equation consisting of a continuity equation, a momentum equation, a volume conservation, a pressure constraint and a total energy equation [17]:

Momentum equations (others were omitted for limited space):

\[ \frac{\partial}{\partial t} (r_{\alpha} \rho_{\alpha} U_{\alpha}) + \nabla \cdot \left( r_{\alpha} (\rho_{\alpha} U_{\alpha} \otimes U_{\alpha}) \right) = -r_{\alpha} \nabla p_{\alpha} + \nabla \left( r_{\alpha} \mu_{\alpha} \left( \nabla U_{\alpha} + (\nabla U_{\alpha})^T \right) \right) + \sum_{\beta \not= \alpha} \left( \Gamma_{\alpha \beta} U_{\beta} - \Gamma_{\beta \alpha} U_{\alpha} \right) + S_{\alpha} + M_{\alpha} \]  

(1)

Where: \( a, \beta \)—describes the different phases of fluids in lowercase; \( r_{\alpha} \)—the volume fraction of phase \( \alpha \); \( \rho_{\alpha} \)—the density of phase \( \alpha \), kg/m³; \( U_{\alpha} \)—the velocity vector of phase \( \alpha \), m/s; \( U_{\beta} \)—the velocity vector of phase \( \beta \), m/s; \( \nabla \) — the Hamilton operator; \( \otimes \) — the vector production operation; \( p_{\alpha} \)—the static pressure of phase \( \alpha \), Pa; \( \mu_{\alpha} \)—the molecular (dynamic) viscosity of phase \( \alpha \), Pa•s; \( Np \)—the number of phases; \( S_{\alpha} \)—momentum sources due to external body forces, and user-defined momentum sources; \( M_{\alpha} \)—the interfacial forces acting on phase \( \alpha \) due to the presence of other phases.

Gas bubbles and sludge particles are dispersed in the continuous fluid, assuming them all spherical particles (denoted in subscribe \( \beta \)), and are driven by continuous fluid (denoted in subscribe \( \alpha \)) for being subjected to various forces:

\[ M_{\text{eff}} = M_{\text{D}}^\alpha + M_{\text{T}}^\alpha + M_{\text{LD}}^\alpha + M_{\text{VM}}^\alpha + M_{\text{TG}}^\alpha + M_{\text{S}} + L \]  

(2)

The speed of mixed flow in the anaerobic reactor is designed very low relative to many air flow simulation cases, and a low Reynolds number is supposed, but in the TS’ region, the layered baffles complicated the flow field, disturbance would occur, a Shear Stress Transport turbulence model (SST)
is adopted for the continuous fluid simulation for its better performance than k-epsilon model for low-speed flow [17], the k-Omega based SST model accounts for the transport of the turbulent shear stress and gives highly accurate predictions of the onset and the amount of flow separation under adverse pressure gradients. For the turbulence of gas and sludge, a Dispersed Phase Zero Equation is adopted [17].

The wastewater flows into the anaerobic reactor, in which gas and sludge contained, but most of the gas(biogas) and sludge(microorganism) are generated and pre-inoculated in the reactors lower part, which could be approximately simulated with the following equation assuming no sludge wasting [18]:

$$P_{x,vss} = \frac{QY(S_b - S)}{1 + k_y \cdot T_{srt}} + f_y k_y Q(S_b - S) T_{srt} + Q_{avvss}$$

The related assumption is all the biogas produced is methane gas, and a production rate of 0.35 L/g COD$_{Cr}$ is set for this simulation, the gas produced where the sludge is distributed in the anaerobic reactor.

3. Simulation and geometry

For the anaerobic reactor in China, the most widely used in environmental engineering are the up flow anaerobic sludge blanket reactor(UASB) and the expanded granular sludge blanket reactor(EGSB), and the structure of TS constructed in the above reactors is mainly based on the European patent structure, or transformed from the structure of Paques® cooperation, characterized by three layers of staggered angled plates (as shown in Figure 1). Figure 1 shows a typical UASB reactor unit, the influent distribution system is at the bottom, the lower part of the reactor is the main body of biochemical reaction and TS is installed at the upper part of the reactor. Assuming the influent flows evenly into the reactor from the bottom and leaves the reactor from the top, the TS system is supposed to capture the gas bubbles in the top regions of the angled plates and settle and return the sludge particles from its two inclined plate’s surfaces. The dimension of the UASB unit in this simulation is 1.2 m(Length)x1.0 m(Width)x5.0 m(Height), the actual structure and dimension in UASB engineering is the same structure, extending by repeating in length and width.

![Figure 1. Schematic view of UASB unit simulation.](image)

Five overlapping rates of baffles are selected according to the engineering practice of TS design and installation for UASB reactor in China, i.e. 10%, 20%, 30%, 40%, and 50%. For the arrangement of TS’ baffles, Keeps the sludge return gap constant with 95mm when the overlapping rate changing.

The CFD simulation is carried out with the commercial software package Ansys CFX®14.0, the up flow speed is set as 1.0 m/h, some other settings and initial parameters of simulation are listed in Table 1.
Table 1. Some initial condition, parameters and settings of simulation.

| Item                          | Setting and Values                                                                                                                                   |
|-------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|
| UASB reactor                  | Influent: 4000 mg/L sCOD; Effluent: 1200 mg/L sCOD (70%)                                                                                               |
| Sludge particle               | 0.25~5mm[18], 1050 kg/m³                                                                                                                                |
| Gas bubble                    | 0100~300μm, Air, 25℃[18]                                                                                                                                  |
| Pre-inoculated                | 100 kg/m³(dry), evenly distributed                                                                                                                      |
| TS material                   | Plastic, PP                                                                                                                                               |
| Environment                   | 25℃, 101325Pa                                                                                                                                              |
| LIquid/gas pair coupling model | Interphase transfer: Particle Model; Drag force: Ishii Zuber Model; Lift force: Legenfre Magnaudent Model; Virtual mass force: Coefficient 0.5; Wall lubrication: Frank Model; Turbulent dispersion force: Favre Averaged; Turbulent transfer: Satio Enhanced Eddy Viscosity Model |
| Liquid/solid pair coupling model | Interphase transfer: Particle Model; Drag force: Ishii Gidaspow Model; Lift force: Saffman Mei Model; Virtual mass force: Coefficient 0.5; Wall lubrication: Antal Model; Turbulent dispersion force: Favre Averaged; Turbulent transfer: Satio Enhanced Eddy Viscosity Model |
| Buoyancy model                | Density Difference Model                                                                                                                                  |
| Turbulence model              | Gas phase: Dispersed Phase Zero Equation Model; Solid phase: Dispersed Phase Zero Equation Model; Solid pressure model: Gidaspow Model; Liquid phase: SST |
| Wall model                    | Liquid: No-slip; Gas/solid: Free-slip Model                                                                                                               |
| Solving method                | Finite volume method, fully implicit multi-grid coupled solution                                                                                         |
| Solving scheme                | High resolution, double precision                                                                                                                       |
| Convergence criterion         | RMS, 0.0001                                                                                                                                             |
| Convergence iteration         | step: 2s/10s, number of step: 300–420                                                                                                                   |

4. Results and discussion

The simulation is run on the workstation, and the main results are shown in Table 2, Figure 2, 3 and 4. The comparison and verification of theoretical simulation results with laboratory test are shown in another article [9]. Table 2 shows the overall averaged flow characteristics and separation rates of three phases in the UASB reactor (including the upper TS part and the lower UASB reactor part) for five settings of baffles’ overlapping. As can be seen from the table, the average velocity of each phase is far greater than the up-flow velocity designed for the UASB reactor (1m/h), while in the lower part of the reactor, the gas, liquid and solid phases exhibit a well-mixed flow corresponding to the homogenous simulation multiphase model, characterized by relative lower average velocity and small inter-phase velocity variations. The difference is that, due to the buoyancy and gravity, the average velocity of gas phase is slightly higher and the average solid velocity is slightly lower than the liquid phase (for solid phase, only up-flow velocity is counted, other direction components such as settlement and collision caused movement is eliminated for it’s too large and prone to misunderstanding). When the mixed fluid flows up into the TS region, because the baffles sharply narrowed the flow passage, the average velocity of gas, liquid and solid phase increase twice that in the lower part of the UASB reactor, but the velocity variations between phases decrease as that for the lower part of the UASB reactor. This may be due to the increase of the flow rate and occurrence of eddy flow, the effect of gravity and buoyancy to gas and solid phases weakened. The TS region still shows a homogenous mixed multiphase flow in velocity statistics, a homogenous flow runs from the lower part of the UASB reactor, increases its average velocity by twice while passing through the area between 1 and 2 layers of baffles, the turbulence is generated simultaneously and still keeps a homogenous multiphase flow (in average velocity statistics), then increases by 15% while passing through the area between 2 and 3 layers of baffles. In the last, into 2 to 3 layers of baffle area, velocity continues to improve, with 1-2 layers between the mean velocity increased about 15%, as a sudden release from a closed and suppressed channel.
**Table 2.** Averaged internal characteristic results of the TS simulation.

| Statistics items            | Location | The overlapping rate of layers of baffles /% |
|-----------------------------|----------|---------------------------------------------|
|                             |          | 10   | 20   | 30   | 40   | 50   |
| Average velocity of gas /m/s| Lower part | 0.031 | 0.031 | 0.031 | 0.032 | 0.027 |
|                             | 1–2      | 0.062 | 0.059 | 0.059 | 0.058 | 0.056 |
|                             | 2–3      | 0.075 | 0.071 | 0.070 | 0.066 | 0.061 |
| Average velocity of liquid /m/s | Lower part | 0.030 | 0.030 | 0.030 | 0.031 | 0.026 |
|                             | 1–2      | 0.062 | 0.059 | 0.059 | 0.058 | 0.056 |
|                             | 2–3      | 0.075 | 0.071 | 0.070 | 0.066 | 0.061 |
| Average velocity of solid /m/s | Lower part | 0.028 | 0.029 | 0.029 | 0.030 | 0.026 |
|                             | 1–2      | 0.062 | 0.059 | 0.059 | 0.058 | 0.056 |
|                             | 2–3      | 0.075 | 0.071 | 0.070 | 0.066 | 0.061 |
| Separation rate of solid /%  | 1        | 94.60 | 95.10 | 95.60 | 94.84 | 94.16 |
|                             | 2        | 95.96 | 95.76 | 95.70 | 95.80 | 95.70 |
|                             | Overall  | 99.90 | 99.90 | 99.90 | 99.90 | 99.90 |
| Separation rate of gas /%    | 1        | 77.15 | 77.65 | 77.84 | 78.20 | 78.35 |
|                             | 2        | 98.10 | 98.40 | 98.50 | 98.70 | 98.70 |
|                             | Overall  | 99.10 | 99.40 | 99.50 | 99.70 | 99.90 |

Note: 1. The 1–2 and 2–3 in Location column refer to the area between 1 and 2, 2 and 3 layers of baffles of TS; 2. The 1, 2 in Location column refer to the mixed flow passing through the 1st and 2nd layer of TS baffles; 3. The separation rate of gas and liquid phases refer to the mass decreasing ratio between the flow entering and leaving the area.

**Figure 2.** Liquid velocity streamline simulation of TS (a) Front view (b) Side view.

**Figure 3.** Gas velocity streamline simulation of TS (10%) (a) Front view (b) Side view.

**Figure 4.** Solid velocity streamline simulation of TS (10%) (a) Front view (b) Side view.

When maintaining the sludge return gap width between fixed angle baffles, and changing the overlapping rate of angled baffles from 10% to 50% (hexagonal plates’ single edge vertical projection overlap ratio), the simulation results show that the average flow velocity of each phase decreases due to the increase of the narrow path length of flow, especially when the mixed flow passing through the area of 1 and 2 layers of baffles, with a drop of 18.6% of average velocity for all three phases, contrast
to a 9.6% drop in the area of 2 and 3 layers of baffles. Which means that increasing the overlap rate of the upper and lower layers of baffles can lead to a decrease in the average flow rate in the TS region, that is, the larger the upper and lower baffles overlapped, the lower the average flow velocity is, due to the greater blocking effect, for all three phases, the above variation trend is consistent.

The phase separation ratio varies when either changing the sludge return gap width of layers of TS baffles, or changing the overlapping ratio of upper and lower layers of baffles. Tab. 2, it can be seen that the three layers set of TS exhibits a high separation efficiency of 99.9% for all the five overlapping rates cases. With the increase of the overlapping rate, the solid phase’s separation ratio decreases slightly with a variation of less than 1% (absolute value), but for all three layers, the 1st layer of TS baffles separates more than 94.16% of all solid phase in the mixed flow while it increases to 95.17% when passing through the 2nd layer. Which suggests that for solid separation, a baffles overlapping rate of 10% could satisfy the engineering case, and meanwhile could reduce the height occupied by the TS, the number of angled plates used and the civil work for building the UASB reactor. For three layers set TS system, each layer should not be designed and fabricates as the same for their solid separation load varies significantly, more attention should be paid on the 1st layer of the TS baffles.

For the gas phase’s case, a relatively lower overall separation rate is presented, varying from 99.10% to 99.90% for all five cases. With increasing the overlapping rate of TS baffles from 10% to 50%, more gas bubbles are captured by the angled plates, and only a 0.8%(absolute value) increase of gas phase separate rate is obtained. This could be caused by the strong vortex of flow pattern which counteracts the gas capture function by the angled plates. Thus, from the point view of separation rate simulated in Figure 2, it is not the most effective way to increase the overlapping rate of TS baffles for a better gas phase separation or capture, more consideration should be paid on construction and economic requirements; compared with Figure 3 the effect of baffle on solid phase separation layer, second layer baffle on the separation of the gas phase has a greater contribution, more than 20%. From one side, it is indicated that the number of layers of the baffle is very important for the separation of gas and the number of layers of the baffle is also important for the separation of the gas phase in addition to the solid and gas separation.

Comparing to the significant difference of three layers of TS angled plates in solid separation rate, more layers needed to capture the gas bubbles for TS system, as for this case, more than 20% of gas separation is conducted in the 2nd layer of TS angled plate.

From the above analysis and data in Table 2, it is indicated that the number of layers of the TS baffles is another target to be re-investigated and re-optimized in addition to the widely accepted two main factors of TS.

Figure 2 shows the velocity streamline of selected liquid point in TS region with a 10% overlapping rate of TS baffles, it is a horizontal view from one side of the UASB reactor, so all the streamlines of the reactor space project to one plane. Each line starts from a pre-selected point and more points are selected in the TS region than in the lower part of UASB reactor. From the top side of Figure 2 the treated fluid flows out the reactor, and the bottom side is a part of the lower part of UASB reactor, the area with layers of angled plates in the middle part is the TS region of UASB reactor. Figure 2(a) is a front view of the TS region of UASB reactor, a regular and symmetric flow pattern could be found, characterized by symmetric vortex. The liquid phase uniformly flows up from the lower part of UASB reactor, crowds into the 1st layer of TS with a small increase of flow velocity, obvious and symmetric vortex formed for the most part of the flow, few disturbance and messy flow can be seen in the top angle area of 2nd layers of TS. For the 2nd layer of the TS, the liquid flow is pressed by the sludge return gap, with a velocity increased by about 3 times, and turns into a significant and intensive vortex. Then re-pressed by the 3rd layer of TS, the liquid flow accelerates and suddenly turns upward, flows out of the UASB reactor with huge and obvious vortex formed near the top plates. The general flow pattern in TS region is characterized by a winding up-flow mainstream with obvious, symmetric and regular vortex, this is significant deviation from the design philosophy of TS, where layers of angled plates formed layers of sedimentation hoppers return the
sludge to the lower part. But in this simulation, the liquid flow forms layers of vortex near the sludge return gap, this would disturb and block the supposed sedimentation process. The most likely reason for solid separation may arise from the rotation direction of the vortex, it rotates upward in the area far from the inclined plates and rotates downward near the inclined plates, which will bring the solid particles downward and back to the lower part of UASB reactor with high velocity. Although this flow pattern could bring sludge back to the reactor and act as a separation function, but the above discussion is only preliminary exploration and need more test and further investigation. Figure 2(b) is a horizontal view from the reactor’s side, an overall regular, parallel and up-strait flow pattern could be seen, with few intersection of streamline and few disturbances near the area of sludge return gap. This indicates that the up-flow design velocity is suitable for maintaining a steady flow pattern in the whole reactor.

Figure 2(b) is a horizontal view from the reactor’s side, an overall regular, parallel and up-strait flow pattern could be seen, with few intersection of streamline and few disturbances near the area of sludge return gap. This indicates that the up-flow design velocity is suitable for maintaining a steady flow pattern in the whole reactor.

Figure 3 is the side views of velocity streamline of gas phase in TS space, in which each streamline stands for a gas bubble’s moving track start from a selected point in the reactor, representative points are selected in all the reactor field with more in the TS region (some points are selected in the top area of TS, so the streamline of these points flow out of the reactor). Figure 3(a) is the front view of TS part and is characterized by similar vortex pattern as the liquid phase. This could be explained that the gas phase is swept forward by the liquid phase due to its light weight, during its upward flowing and rotating, the bigger and faster gas bubbles move to outside area of the vortex and then strike to the surface of the upper layer of plates from the bottom sides, then leave from the liquid vortex and form many irregular messy vortex, which moving along with the bottom sides of the angled plates to the top angle area for further collection; as for the smaller and slowly rotation gas bubbles, they will support by the liquid phase and pass through the sludge return gap to the upper layer of TS, and are not captured by the angled plates. The existence of the vortex is against the separation or capture of gas bubbles, for the gas phase separation philosophy assumed of TS is capturing the up-strait moving gas bubbles via angled plates, while the existence of vortex breaks the path line of gas bubbles, so a multilayer capturing plates system is needed, with suitable sludge return gap width simultaneously. Figure 3(b) shows the side view of the TS part of the UASB reactor, similar to Figure 2(b) of the liquid phase, significant disturbances occur in the angled plate’s area, which indicates a slower up flow velocity is needed for better gas separation.

Figure 4 shows the side views of velocity streamline of solid particle, similar flow pattern with symmetric and regular vortex dominates the TS area, the solid particles are captured by the liquid phase, moving upward, rotating between the layers of TS plates and then strike to the top surface of the angled plates, moving downward back to the reaction area. For its relatively heavy weight, the collision with plates and between particles lead to the most turbulence for solid moving (Figure 2(b)) as for liquid and gas phases.

5. Conclusions

From the simulation, the averaged velocity of three phases is much higher than that the pre-designed up-flow velocity of the UASB reactor, the velocity difference between gas, liquid and solid is very close and homogeneous mixed flow could be the typical flow pattern for the whole UASB reactor in the view of velocity statistics. The mixed flow runs up evenly from the bottom part of UASB reactor and increases its velocity by about twice for the TS baffles narrowing its passage. Where significant regular and symmetry vortexes are observed other than the plug flow as supposed for the reactor in the first design stage, the flow pattern in the TS region is characterized by winding, reflecting, suppressing and symmetry vortexes, a winding up-flow with rotating swirls flow pattern is more different from that the separation flow pattern philosophy designed from the beginning, which need further investigation.

The existence of TS baffles consumes the energy of flow passing through, a typical 10% decrease of velocity for three phases are found for each layer of the TS baffles in this simulation.

The TS’s structure of layers of angled plates shows outstanding separation performance for both solid phase and gas phase, for all cases in this study, an average 99% or above separation rate for both phases is found. The overlapping rate of layers of TS baffles has influence on the separation rate, with
increasing the overlapping rate among five cases in this study, the separation rate of solid phase fluctuates down with a variation of 1% (absolute value), while fluctuate upward for gas phase, with a variation of 0.8% (absolute value). A conclusion could be drawn is that the more consideration could be paid in the economic needs for the UASB reactor in the design period, other than the increase of overlapping rate for higher separation rate.

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