



## Experimental and CFD studies of floc growth dependence on baffle width in square stirred-tank reactors for flocculation



Weipeng He<sup>a,\*</sup>, Lianpeng Xue<sup>a</sup>, Beata Gorczyca<sup>b</sup>, Jun Nan<sup>c</sup>, Zhou Shi<sup>a</sup>

<sup>a</sup> College of Civil Engineering, Hunan University, Changsha 410082, China

<sup>b</sup> Department of Civil Engineering, University of Manitoba, Winnipeg R3T 5V6, Canada

<sup>c</sup> School of Municipal and Environmental Engineering, Harbin Institute of Technology, Harbin 150090, China

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### ABSTRACT

This work mainly focuses on the effect of baffle width ( $B$ ) on floc growth within square stirred-tank reactors for flocculation. Firstly, a series of flocculation tests were carried out, using polyaluminum chloride (PACl) as coagulant, to evaluate flocculation performance in each tank at three typical shear rates of  $G_{ave} = 10, 30$  and  $70 \text{ s}^{-1}$ . Experimental results were reported in terms of kaolin-floc average size, size distributions and perimeter-based fractal dimension, derived from an in-situ recognition system for floc morphology. Then, the hydrodynamic environments (where the growth of floc took place) were characterized, by performing Computational Fluid Dynamics (CFD) simulations, with predicted results of area-weighted average turbulent kinetic energy and its dissipation rate in the plane containing the impeller, and circulation time (denoted as  $k_{0.33H}$ ,  $\epsilon_{0.33H}$  and  $t_c$ , respectively), followed by a detailed discussion based on experimental and numerical results. As expected, baffles with different widths caused distinct turbulent flow fields in corresponding stirred tanks at the same shear rates, thereby affecting the evolution of floc size and structure during flocculation.

According to CFD predictions, for a constant  $G_{ave}$ , the baffle width of  $B = 0.10D$  (where  $D$  is the bottom width of tank) gave rise to the highest values of  $k_{0.33H}$  and  $\epsilon_{0.33H}$ , as well as the shortest  $t_c$ , followed by  $B = 0.13D$ ,  $0$  (unbaffled) and  $0.07D$ , and for  $B = 0.20D$ , the lowest  $k_{0.33H}$  and  $\epsilon_{0.33H}$ , together with the longest  $t_c$ , were produced. It was found that the floc growth dependence on baffle width appeared to be greatly related to the predominant growth mechanism(s), i.e., at the shear rates of  $G_{ave} = 10$  and  $30 \text{ s}^{-1}$ , where the rate of breakage was approximately zero (because little or unimportant breakage was observed), a higher  $\epsilon_{0.33H}$  and a short  $t_c$  corresponded to an increased rate of floc growth resulting from higher particle collision frequency, thus forming larger flocs under the same shear-rate conditions, whereas at  $G_{ave} = 70 \text{ s}^{-1}$ , where breakage dominated over aggregation, larger flocs seemed to be produced by a lower  $\epsilon_{0.33H}$  and a longer  $t_c$ , likely as a result of a lower breakage rate and more sufficient opportunity for broken aggregates to reform or restructure during water flow circulation. Moreover, the effect on floc size and structure during flocculation was somewhat compressed when breakage became pronounced, and the same was true of the restructuring behavior. To enhance floc growth process, some baffles should be installed to break water flow co-rotation with the impeller (to increase axial flow rate), and however, larger-area dead zones might be simultaneously formed. Therefore, an appropriate width (e.g.,  $B = 0.10D$  or  $0.13D$ ) would be required to maintain a compromise. The present study may provide useful insights for optimizing the design and operation of baffled stirred-tank reactors for flocculation.

### 1. Introduction

Stirred tanks are commonly used as a flocculating reactor in drinking water treatment plants, and have been extensively selected to perform lab-scale studies on flocculation mechanisms, kinetics, and optimization [1–3]. Flocculation aims to encourage transport and attachment of destabilized particles via gentle mixing, forming larger and irregularly-shaped aggregates/flocs [4]. The performance of this

process in stirred-tank reactors is dependent upon not only physico-chemical conditions, including coagulant type and dosage, solution temperature and pH, and particle concentration; but also hydrodynamics, determined by tank geometry as well as impeller type and speed (mixing intensity) [5,6]. If properly controlled, the flocculation technology can be used to produce aggregates with desired size distribution, structure and settling rate [7]. Once the physicochemical conditions for flocculation are fixed, the growth of floc is mainly

\* Corresponding author at: Department of Water Engineering and Science, College of Civil Engineering, Hunan University, 2 Lushan South Road, Changsha 410082, China.  
E-mail address: [heweipengwater@163.com](mailto:heweipengwater@163.com) (W. He).

affected by hydrodynamic environments [8]. Therefore, it is essential to effectively describe the nature of flow generated by the interactions between the impeller, the tank wall, baffles and other internals in the impeller-based system.

For a stirred-tank reactor, the rotating impeller makes input energy dissipated in suspension by velocity gradients, and the mixing intensity is characterized by spatially averaged velocity gradient ( $G_{ave}$ ) throughout the reactor [9,10]:

$$G_{ave} = \left( \frac{\varepsilon_{ave}}{\nu} \right)^{1/2} = \left( \frac{N_p N^3 d^5}{V \nu} \right)^{1/2} \quad (1)$$

where  $\varepsilon_{ave}$  is the average rate of turbulent energy dissipation,  $\nu$  is the kinematic viscosity of water,  $V$  is the liquid volume,  $d$  is the impeller diameter,  $N$  is the rotational speed of impeller, and  $N_p$  is the impeller power number. Traditionally, the  $G_{ave}$  is used as a global hydraulic parameter that is important for the design of flocculating reactors and the prediction/study of flocculation kinetics [3]. At a given value of  $G_{ave}$ , the rate of floc growth is governed by a competition between aggregation and breakage, with flocs eventually reaching a steady-state size [11]. Investigations of flocculation behavior for velocity gradients above  $20 \text{ s}^{-1}$  demonstrated that the larger the value of  $G_{ave}$ , the smaller the average/median aggregate size under steady-state conditions [7,12]. On the contrary, Colomer et al. [13] found that the median aggregate size increased with increasing velocity gradients ranging from  $0.7$  to  $27.4 \text{ s}^{-1}$ . This discrepancy suggests that any flocculating device has a velocity gradient range within which there is a transition from aggregation dominated conditions to breakage dominated conditions [14]. The development of floc size during flocculation is generally accomplished by the change of floc structure, which can be made more compact by breakage and subsequent reformation [15]. Increased floc compaction is considered to improve floc strength due to an increase in the number of bonds holding the aggregate together. An empirical expression between the velocity gradient and the stable floc size ( $d_{ave} = C G_{ave}^{-\gamma}$ , where  $d_{ave}$  is the average floc size at steady state,  $C$  is the floc strength co-efficient, and  $\gamma$  is the stable floc size exponent) has been widely used to compare floc strength within specific experiment systems [11]. In addition, the shear history effect on floc size and structural evolution has been broadly investigated during cycled-shear, tapered-shear and even increased-shear flocculation in stirred-tank reactors [16–18].

Nevertheless, many researchers [3,12,19] have questioned the use of  $G_{ave}$  in Eq. (1) as a single parameter to represent flow behavior and thereby, flocculation performance within a stirred-tank reactor. As expected, experimental observations revealed that different floc size distributions were produced at the same velocity gradients when changing impeller type [4,10] or tank size [1], probably attributed to the dependence of aggregation and breakage kinetics on local turbulent characteristics of flow [9,20]. As flow conditions are heterogeneous in stirred tanks, with local power consumption varying as much as several orders of magnitude from impeller discharge zone to the rest of the tank, the  $G_{ave}$  value does not describe adequately the magnitude and fluctuations in local velocity gradient to which a floc is subjected [10]. Spicer et al. [4] suggested that higher mixing and circulation led to an increase in floc exposure to the impeller zone and consequently, more breakage, whereas Kilander et al. [21] argued that water surface seemed to be more important for floc breakage than the impeller zone. Anyway, much attention should be paid to the effect of velocity gradient distribution on the likelihood of floc aggregation and breakage during flocculation [22]. A similar point of view was proposed by Bridgeman et al. [19], who considered that comparisons of previous flocculation-test data with new ones needed to be made cautiously since those experiments might be carried out in lab-scale flocculating reactors with different geometrical configurations.

Up to now, the Computational Fluid Dynamics (CFD) simulation has proven to be a powerful approach to get a deep insight into complex

flow field within a stirred tank, by virtue of predicting detailed information on spatial variation of mean velocity and turbulent fields and then, discussing their effects on mixing time (or circulation time) and power dissipated [23,24]. The CFD predictions are considered favorable for identification of dead zones in the tank and evaluation of mixing efficiency [25,26]. Although numerous computational studies have been performed over the last decades to explore complexity of turbulent flow generated in stirred tanks [27–29], very few attempts have been made to establish the linkage between numerical results of local hydrodynamics and flocculation performance. With the help of CFD simulations, Prat and Ducoste [22] evaluated the impeller type effect on spatial heterogeneity for steady-state floc size and on transient spatial evolution of mean floc size, while Samaras et al. [2] simulated the operation of a full-scale stirred tank for flocculation in the presence of very low solids concentration. Jar-test simulation results in the work of Bridgeman et al. [19] exhibited that hydrodynamic environments generated by the same impeller at the same mixing speeds could be significantly different in cylindrical and square stirred tanks, thus affecting flocculation behavior. The research work just mentioned indicates that the CFD technology would have great potential in evaluating the floc growth dependence on the distribution of turbulent flow generated in stirred-tank reactors with different geometrical configurations.

Among stirred tanks for flocculation in the literature [6,10,30], some have been baffled, but others unbaffled. Existence of baffles may be beneficial for breaking flow co-rotation with the impeller and for increasing axial flow rate due to resultant impeller-baffle interactions, thus enhancing turbulent macro-mixing. On the other hand, baffled tanks give rise to more dead zones in the fluid than unbaffled ones, possibly worsening mixing efficiency [23,31]. Results of CFD simulations conducted by Vakili and Esfahany [27], who divided a fully baffled stirred tank into three mixing zones (impeller, baffle and circulation) and investigated the baffle width effect on turbulent flow field in these zones, showed that larger baffles decreased velocity magnitude and hence, turbulent kinetic energy in baffle and circulation zones, owing to an increase in the volume of dead zone, for example, between baffle base and tank wall. Vakili and Esfahany [27] also found that with increasing baffle widths, the volume density distribution of energy dissipation rate changed significantly. Considering the connection between energy dissipation rate and flocculation performance [3], it could be inferred that these different distributions of turbulent flow would have a significant effect on floc size and structural evolution during flocculation. Unfortunately, there is little reported research which has focused on this aspect.

The purpose of the present work was to explore the baffle width and velocity gradient effects on floc growth during flocculation in square stirred-tank reactors, by using experimental and simulation methods, in order to evaluate how a change in the baffle width of tank affected flocculation behavior in associated turbulent flow field. Firstly, lab-scale flocculation tests were carried out to determine morphological properties and settling performance of flocs formed in stirred tanks with different baffle widths. The morphology of flocs was characterized by average size and fractal dimension, derived from a non-intrusive optical sampling and digital image analysis technique. Then, a commercially-available CFD software, FLUENT v6.3.26, was applied to simulate turbulent flow field within each stirred-tank reactor, followed by a detailed discussion on experimental and numerical data for given velocity gradients.

Here, square stirred tanks, designed based on the standardized stirred-tank model (see Section 2.1), were used mainly because of the relevance of this tank shape with water treatment facilities and the fact that the square geometry has been poorly studied before [1]. This topic has important implications for increasing the understanding of floc aggregation and breakage mechanisms, as well as optimizing the design and operation of stirred-tank reactors for flocculation.

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