Computational Fluid Dynamics Analysis for Wastewater Floc Breakage in Orifice Flow

by

Aaron Xavier Fernandes

A thesis submitted in conformity with the requirements for the degree of Masters of Applied Science in Chemical Engineering and Applied Chemistry
University of Toronto

© Copyright by Aaron Xavier Fernandes 2012
Computational Fluid Dynamics Analysis for
Wastewater Floc Breakage in Orifice Flow

Aaron Xavier Fernandes
Masters of Applied Science
Chemical Engineering and Applied Chemistry
University of Toronto
2012

Abstract

In the present work, the breakage of wastewater particles in orifice flow is investigated through numerical simulations. Using maximum strain rate along particle paths as the breakage criterion, breakage is predicted using computational fluid dynamics. The numerical simulations confirm that nominal orifice strain rate cannot explain the higher particle breakage in single-orifice systems compared to that of multi-orifice systems, instead particle breakage was found to correlate well with the maximum strain rates in the system. On the issue of effect of initial particle location on breakage, numerical modeling shows that particles travelling along the centerline are suspected to break less than those travelling near the wall. However, experiments designed to study the breakage of particles injected at various radial locations proved inconclusive. Finally, results suggest that while single orifice systems are ideal for strong particles, multi-orifice systems may be more effective in breaking weak particles.
Acknowledgements

Thanks to my parents, Simon and Perpetua,

and sister, Tresanne

for their patience and support along this journey

---

Thanks to my friends for the laughs and many intellectual discussions

---

This project would not have been possible without generous funding from

The Canadian Water Network and Ontario Graduate Scholarship

---

Special thanks to the staff at the Environment Canada Water Technology Centre

for space, equipment and technical support

---

A huge thank you to Professor Ramin Farnood and Professor Yuri Lawryshyn

for the help, support and confidence you offered

---

And to God, for abundant Blessings
# Table of Contents

Acknowledgements ........................................................................................................ iii

Table of Contents ........................................................................................................ iv

Nomenclature .............................................................................................................. vii

List of Tables .............................................................................................................. ix

List of Figures ............................................................................................................. x

List of Appendices .................................................................................................... xii

Chapter 1 ..................................................................................................................... 1

1 Introduction .............................................................................................................. 1

   1.1 An Opportunity to Optimize Wastewater Treatment ........................................ 1

   1.2 Hypothesis and Objective ............................................................................. 2

   1.3 Document Structure ..................................................................................... 3

Chapter 2 ..................................................................................................................... 4

2 Literature Review .................................................................................................. 4

   2.1 The Study of Orifice Flow .......................................................................... 4

   2.2 Breakage of Particles Suspended in Liquid ............................................... 5

      2.2.1 Breakage of Suspended Particles by Turbulent Flow ..................... 5

      2.2.2 Breakage of Suspended Particles by Extensional Flow ............... 5

   2.3 Characterizing particle breakage ................................................................ 7

   2.4 Studies of Particle Breakage in Orifice Flow ............................................. 8

      2.4.1 Particle Breakage in Single-orifice Systems .................................. 8

      2.4.2 Particle Breakage in Multi-orifice Systems ................................... 11

   2.5 Summary of the Existing Literature .......................................................... 11

Chapter 3 ..................................................................................................................... 13

3 Methodology .......................................................................................................... 13
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1</td>
<td>CFD Simulations</td>
<td>13</td>
</tr>
<tr>
<td>3.1.1</td>
<td>Geometry and Meshing</td>
<td>13</td>
</tr>
<tr>
<td>3.1.2</td>
<td>CFD Flow Simulations</td>
<td>15</td>
</tr>
<tr>
<td>3.1.3</td>
<td>Particle Breakage Criteria</td>
<td>16</td>
</tr>
<tr>
<td>3.2</td>
<td>Estimating Particle Breakage</td>
<td>18</td>
</tr>
<tr>
<td>3.2.1</td>
<td>Critical Value of Particle Breakage Indicators</td>
<td>18</td>
</tr>
<tr>
<td>3.2.2</td>
<td>Experimental Breakage Data</td>
<td>21</td>
</tr>
<tr>
<td>3.3</td>
<td>Injection Experiments</td>
<td>23</td>
</tr>
<tr>
<td>4</td>
<td>Results and Discussion</td>
<td>26</td>
</tr>
<tr>
<td>4.1</td>
<td>Details of CFD Simulations</td>
<td>26</td>
</tr>
<tr>
<td>4.1.1</td>
<td>Simulated Cases</td>
<td>26</td>
</tr>
<tr>
<td>4.1.2</td>
<td>CFD Model Validation</td>
<td>27</td>
</tr>
<tr>
<td>4.2</td>
<td>Simulation Results</td>
<td>29</td>
</tr>
<tr>
<td>4.2.1</td>
<td>Hydrodynamic Effects Along Particle Tracks</td>
<td>29</td>
</tr>
<tr>
<td>4.2.2</td>
<td>Distribution Functions for Critical Breakage Indicators</td>
<td>31</td>
</tr>
<tr>
<td>4.2.3</td>
<td>Selection of Breakage Indicator</td>
<td>35</td>
</tr>
<tr>
<td>4.3</td>
<td>Comparison with Experimental data</td>
<td>37</td>
</tr>
<tr>
<td>4.3.1</td>
<td>Effect of Orifice Length</td>
<td>37</td>
</tr>
<tr>
<td>4.3.2</td>
<td>Breakage-Strain Relationship for Single-orifice Systems</td>
<td>38</td>
</tr>
<tr>
<td>4.3.3</td>
<td>Breakage-Strain Relationship for Multi-orifice Systems</td>
<td>39</td>
</tr>
<tr>
<td>4.4</td>
<td>The Role of Initial Position in Breakage</td>
<td>42</td>
</tr>
<tr>
<td>4.4.1</td>
<td>Particle Injection Experiments</td>
<td>43</td>
</tr>
<tr>
<td>5</td>
<td>Conclusions</td>
<td>45</td>
</tr>
<tr>
<td>5.1</td>
<td>Potential Improvements and Opportunities for Future Work</td>
<td>46</td>
</tr>
</tbody>
</table>
Nomenclature

A fitting parameter
D pipe diameter (m)
E nominal orifice strain rate (s$^{-1}$)
F function
G velocity gradient (s$^{-1}$)
$K_L$ loss coefficient
S strain rate (s$^{-1}$)
a lower end of uniform distribution
b upper end of uniform distribution
b fitting parameter
g fitting parameter
g $g$ gravitational acceleration (m/s$^2$)
h fitting parameter
$h_L$ head loss (kPa)
i index variable
k index variable for path
m number of intervals over which distributions are evaluated
n index variable for particle travelling along path
\( u \)  
\( x \)-component of velocity \\
\( v \)  
\( y \)-component of velocity \\
\( v_{\text{orif}} \)  
average velocity through orifice (m/s) \\
\( w \)  
\( z \)-component of velocity \\
\( \Omega \)  
critical value of breakage indicator \\
\( \alpha \)  
parameter of impulse distribution \\
\( \varepsilon_{ij} \)  
component of velocity tensor \\
\( \mu \)  
parameter of log-normal distribution \\
\( \sigma \)  
parameter of log-normal distribution
List of Tables

Table 1 - Experimental Parameters used by Gibson (2011) ................................................................. 14

Table 2 - Distribution functions for critical value of particle breakage indicators, $\Omega$ .............. 20

Table 3 - Fitting Parameters for equations representing Experimental Breakage ......................... 22

Table 4 - Details of orifice geometry and flow conditions used in CFD simulations. The calculated nominal orifice strain rate and pressure drop data are also provided. ...................... 27

Table 5 - Increment size and maximum ranges used for strain rate and velocity gradient distributions........................................................................................................................................ 31

Table 6 - Simulation breakage predictions using various distribution functions ...................... 32

Table 7 - Average Relative Error for Predicted vs Experimental breakage and parameters used in selection of distribution function ................................................................................................................. 32

Table 8 - Predicted % Breakage of particles using various breakage indicators ....................... 35

Table 9 - Average Relative Error for predicted vs experimental breakage and parameters used in selection of Breakage Indicator ................................................................................................................. 36
List of Figures

Figure 1 - Schematic diagram of a 4-roll mill (Blaser, 2000) Reproduced with permission from Elsevier ................................................................. 6

Figure 2 - Schematic diagram of a cross slot device (Hsieh et al., 2005) Reproduced with permission from Elsevier ............................................................................. 6

Figure 3 - Breakage of ferric hydroxide flocs approaching the stagnation point (flow from left to right) in two-dimensional extensional flow, as per CCD (Charged Couple device) camera (Blaser, 2000) Reproduced with permission from Elsevier .......................................................... 7

Figure 4 - Energy dissipation rate through orifice flow (Zumaeta et al., 2008) ........................................ 9

Figure 5 - Inactivation curves before and after particle breakage (Gibson, 2011) ......................... 10

Figure 6 - Comparison of wastewater particle breakage in the single-orifice versus the multi-orifice system (Gibson 2011) Reproduced with permission from the author .................................. 11

Figure 7 - Basic orifice system geometry ......................................................................................... 13

Figure 8 - Configurations of orifices on each of the single-orifice and multi-orifice system (Not to scale) ............................................................................................................. 14

Figure 9 - Mesh used in CFD simulations ....................................................................................... 15

Figure 10 - Region of consideration for hydrodynamic effects ......................................................... 18

Figure 11 - Particle Breakage Results of Gibson (2011) and Gibson et al. (2012) ................. 21

Figure 12 - Flow chart of the procedure used for particle breakage prediction ............................ 23

Figure 13 - Schematic diagram of injection apparatus ..................................................................... 24

Figure 14 - Vector Plot of Cross section of orifice flow (Case S2) ............................................... 28

Figure 15 - Validation of orifice flow simulations via experimental and predicted pressure drop data. Orifice diameter: 1.6mm ................................................................. 29
Figure 16 - Strain rate along particle paths. Image represents an area of 35 mm (L) × 9.5 mm (The color scale represents strain rate in (s\(^{-1}\))).

Figure 17 - Comparing strain rate experienced along two center-line and near-wall particle paths as per Figure 16. The x-axis is the distance from the centre of the orifice. Pipe Velocity=0.05m/s, Orifice Velocity=7.2m/s, ΔP =170kPa (25psi).

Figure 18 - Parity Plots of Predicted vs Experimental Breakage for various distribution functions

Figure 19 - Distributions of critical strain rate, \(S_{crit}\), for Samples A and B

Figure 20 - Parity Plots of Predicted vs Experimental Breakage for various Breakage Criteria

Figure 21 - Effect of orifice length on particle breakage (Cases S1-S3, S14-S16)

Figure 22 - Experimental and predicted breakage data for Sample A using the strain rate as breakage criterion (Cases S1-S9)

Figure 23 - Particle Breakage for Sample B in Single- and Multi-orifice Systems (Cases S1, S4, S6-S9 and S11-S13)

Figure 24 - Maximum strain rates in single-orifice system

Figure 25 - Maximum strain rate against initial particle position for multitude of paths (Case S2)

Figure 26 - Dye test illustrating injection

Figure 27 - Particles entrained upon injection

Figure 28 - Particle size distributions before (control) and after orifice flow treatment for centre-line and near-wall particles. Pipe velocity: 10mm/s, Orifice Velocity: 23m/s, ΔP: 450kPa (65psi).
List of Appendices

Appendix A - Matlab Code for Post-Processing................................................................. 52

Appendix B - Experimental Standard Operating Procedure.......................................... 59
Chapter 1

1 Introduction

1.1 An Opportunity to Optimize Wastewater Treatment

Water is an essential element of life on earth. To ensure that it is fit for human consumption, a multitude of processes can be employed. Typical North American processes involve settling, biological treatment, further settling and disinfection. Ultraviolet (UV) disinfection is becoming popular in many wastewater treatment plants (Yong et al., 2009). Unlike other processes, UV treatment uses only light to inactivate pathogens, and so does not introduce any harmful chemicals into the water. While it is an effective technique, it also consumes large amounts of electricity. This energy requirement can be lowered, however, by the breakage of suspended flocs (i.e. aggregates of microorganisms) into smaller pieces. Breakage of these flocs helps to expose contained microbes for more effective disinfection (Yong et al., 2009; Gibson et al., 2009). While Yong et al. (2009) and Gibson et al. (2009) used ultrasound to disrupt and break up particles, other techniques are also possible. In the present study, orifice flow for breakage of suspended particles is investigated.

Orifice flow seems a simple process, but the fluid mechanics associated with it are known to be relatively complex. Orifice flow involves forcing a liquid through a small constriction. In order to pass through the constriction, the liquid undergoes a sharp increase in velocity. The associated fluid dynamics produce extensional flow, which can disrupt and break up particles (Sonntag and Russel, 1987). Efforts to understand the flow fields have included investigations using experiments (Sonntag and Russel, 1987; Kobayashi, 2004), analytical analyses (Nguyen and Kausch. 1988; Higashitani et al., 1991) and computational fluid dynamics (CFD) modeling (Zumaeta et al., 2006), but the exact mechanism of particle breakage and where in the system it occurs remain uncertain. Furthermore, while experimental results of particle breakage in single orifice flow correlate well with the average strain rate in the orifice (Gibson et al., 2012), this parameter fails to predict the observed behavior in multi orifice systems.
1.2 Hypothesis and Objective

It is our hypothesis that:

The maximum strain rate along a particle path can be used to explain experimentally observed trends in the breakage of wastewater particles in orifice flow.

Accordingly, the objective of this thesis is to explore the phenomenon of suspended particle breakage in orifice flow and establish an effective indicator parameter which can predict the extent of this breakage using computational fluid dynamics (CFD) that is applicable in both single and multi-orifice flow.

Our results show that a combination of strain rate and shear stress (as estimated by FLUENT™ software) had a strong correlation with experimental breakage data. In addition, the use of a distribution function to represent breakage resistance was found to be an important factor in predicting the breakage of particles in both single and multi-orifice systems. Results indicate that experimentally observed higher breakage in single-orifice flow than multi-orifice flow is due to higher maximum strain rates in the single-orifice system. Furthermore, results suggest that while single orifice systems are ideal for strong particles, multi-orifice systems may be more effective in breaking weak particles.

The comparison of breakage for centerline and near-wall particles flowing through the system was also investigated, as the literature illustrates uncertainty as to which path results in greater breakage (Hsieh et al., 2005). An experimental technique was developed to evaluate the difference between breakage along each of the centreline and near-wall paths. While our preliminary experiments proved inconclusive, CFD results implied that near-wall particles are more likely to break.

Ultimately the technique developed here provides a framework for optimizing the orifice geometry to achieve maximum particle breakage with minimum energy input in orifice flow.
1.3 Document Structure

This thesis is divided into five chapters. This chapter introduces and motivates the work as well as provides an overview of the thesis. Chapter 2 provides a review of the relevant literature, including a brief overview of existing knowledge on orifice flow, particle breakage, particle breakage in extensional flow and particle breakage specifically in orifice flow. Chapter 3 describes the approaches taken in CFD modeling, analyzing models and predicting breakage. It goes on to describe the methods used in experimental work to determine the role of particle position in breakage. Chapter 4 presents the results of simulation and experimental analyses, and discussion on interpretation and implications of the findings. Chapter 5 summarizes key conclusions of the thesis and provides a discussion regarding future work.
Chapter 2

2 Literature Review

Converging orifice flow is a unique form of extensional flow. It has been studied for many years for a variety of reasons and using a number of different techniques (Section 2.1). As an extensional flow (one which elongates fluid elements), orifice flow has the capacity to break up suspended particles. Section 2.2 explains that particles suspended in liquids can be broken in different ways, including by turbulence (Section 2.2.1) and in extensional flow (Section 2.2.2). Section 2.3 discusses means of characterizing particle breakage and Section 2.4 expands on particle breakage in orifice flow.

2.1 The Study of Orifice Flow

Orifice flow involves the forcing of a fluid through a constriction or hole. One of its commonly known uses is in pressure measurement, as the pressure drop it introduces into a flowing system is closely tied to the flow rate (Munson et al., 2006). Aside from pressure, however, flow fields associated with orifices have a number of unique characteristics. For one, jets with high velocity are formed at orifice exits. Jets produced by orifices and associated velocities, shapes and separation extents were examined using particle image velocimetry (PIV) by both Ramesh et al. (2006) and Mi et al. (2010) and direct photography by Ramamurthi and Nandakumar (1999). Recirculation zones are expected in the region after the orifice unless the jet releases into air. A final key characteristic is that orifice flow fields include zones of extensional flow (Hunkeler et al., 1996), as detailed in Section 2.4.

Orifice flow has been studied via various means at least since the 1930s. Correlations relating head loss to velocity squared in orifice flow were developed by Kunz in 1935. By the 1990s, such correlations were still in use but began to factor in orifice edge shape (Walker, 1999). Correlations explored by Borutzky et al. (2002) also relate flow rate and pressure.

Beyond correlations, analytical models of orifice flow can help to analyze entire flow fields. Shammaa et al. (2005) approached the analysis using point-and-sink potential flow solution. Multiple sinks were placed in the orifice opening, and analytical manipulation was used to develop equations which govern the near-orifice flow field. These equations, validated by
comparing isovel profiles with experimental data, allow for analysis of the orifice flow system. Isovels were observed to be shaped as semi-ellipsoids near the orifice and hemispheres further from the orifice. Shammaa et al. (2005) also studied the effects of orifice shape and size on the flow field using their equations. The potential flow solutions of Shammaa et al. (2005) were improved in the work of Bryant et al. (2008). The new models better predicted velocities in orifice flow. The effectiveness of the models created by Bryant et al (2008) were confirmed by comparison with experimental results obtained by microacoustic Doppler velocimetry (ADV). The velocity fields associated with multi-orifice flow were also investigated analytically by Bryant et al. (2008).

CFD software packages are also able to accurately predict flow fields in this unique flow system. Both Zumaeta et al. (2007) and El Drainy et al. (2009) were able to support CFD simulations with experimental results.

2.2 Breakage of Particles Suspended in Liquid

2.2.1 Breakage of Suspended Particles by Turbulent Flow

Turbulent flow can often lead to the breakage of suspended particles. Shear effects often play a large part in this observed breakage effect (Kao and Mason, 1975). Experimental work by Kao and Mason (1975) as well as Yuan and Farnood (2010); among others, demonstrate the capacity of turbulent flow conditions to break up particles. Yuan and Farnood (2010) were able to develop a relationship between turbulent shear rate and extent of particle breakage for wastewater particles. Turbulent flow can also result in particle breakage by other means. Turbulent eddies were thought to pull particles apart in an analysis done by Parker et al. (1972).

2.2.2 Breakage of Suspended Particles by Extensional Flow

In orifice flow, the primary mechanism of particle breakage is thought to be extensional flow. Extensional flow is characterized by elongation of fluid elements. Many different systems have been used in the past to generate and analyze extensional flow in its purest forms, as illustrated in Figure 1 and Figure 2. While in some cases extensional flow is studied for its effect on liquids alone (Mackay et al., 1995; McGlashan et al., 1998), in many cases it has been investigated for its effects on suspended particles (Blaser, 2000). These particles are often larger than nearby fluid elements and thus are subjected to disruptive forces acting along their bodies. For example,
in the work of Blaser (2000), extensional flow of the surrounding fluid caused the breakage of mineral aggregates in a four roll mill, via fragmenting as opposed to eroding (Figure 3). In another study by Perkins et al. (1997), stretched DNA molecules were directly visualized by fluorescence microscopy in a planar elongational flow, created by a cross slot apparatus. Polymer chains in cross slotted devices have also been shown to elongate and even break (Hsieh et al., 2005). Such experimental results were matched by analytical models. All such models begin with some model of the particles themselves. Particles can be considered deformable spheres (Sonntag and Russel, 1987) or even ellipsoids (Blaser, 2000). Many researchers expanded to considering multi-body models. Two-bead particles were adopted by Parker et al. (1972) and Neumann (1999) and Rouse chains by Bird et al. (1993). Higashitani et al. (2001) went further, to clusters of combined spherical particles adhered together by van der Waals forces to better simulate aggregates. However, detailed discussion of these models is beyond the scope of our study.

![Figure 1 - Schematic diagram of a 4-roll mill (Blaser, 2000) Reproduced with permission from Elsevier](image1)

![Figure 2 - Schematic diagram of a cross slot device (Hsieh et al., 2005) Reproduced with permission from Elsevier](image2)
2.3 Characterizing particle breakage

Experimentally, particle breakage can be achieved by numerous methods including micromechanical stretching (Yeung and Pelton, 1996), ultrasound (Gibson et al., 2009) and hydrodynamic methods (Gibson et al., 2012), to name a few. The mechanism of breakage of interest in this study is large scale fragmentation due to hydrodynamic forces, as it is common in tensile breakage (Jarvis et al., 2005). Large scale fragmentation involves a floc breaking into particles of similar mass or size. To break a particle, a critical threshold must be achieved beyond which particle integrity is compromised. This threshold could be the degree of deformation required to break the particle or the force needed to overcome internal bonding forces of the particle.

Previous work shows that particle strength, or the resistance of a given particle to being broken, exhibits a high degree of variability. Large particles are often found to break more easily than small ones. (Higashitani et al., 1991; Yeung and Pelton, 1996; Gibson et al., 2012). In some cases, rupture strength can vary up to 10-fold (Yeung and Pelton, 1996). Sometimes, the presence of weak spots within flocs dictates strength (Yeung and Pelton, 1996). These variations
in strength are often taken into account using ranges of particle strengths to represent given samples (Yeung and Pelton, 1996; Blaser, 2000; Yuan and Farnood, 2010).

2.4 Studies of Particle Breakage in Orifice Flow

2.4.1 Particle Breakage in Single-orifice Systems

Particle breakage is known to occur in orifice flow as deduced by Sonntag and Russel (1987), Nguyen and Kausch (1988), Higashitani et al. (1991) and Zumaeta et al. (2008). Breakage has been observed in the forcing of suspensions through pumps, elbows and other disruptive flow fields, thus becoming the centre of numerous investigations (Kobayashi, 2004; Zumaeta et al., 2008). Controlled experiments on proteins (Zumaeta et al., 2008), polymers (Hunkeler et al., 1996) and wastewater aggregates (Gibson et al., 2012) have decisively demonstrated effective breakage. Polymeric substances were shown to exhibit permanent deformation in orifice flow by Sonntag and Russel (1987) and Higashitani et al. (2001). A comprehensive and universally accepted understanding of the mechanisms at work, however, has yet to be achieved.

Studies of orifice breakage have used many different theories to help correlate models to experimental observations. Zumaeta et al. (2008) observed orifice breakage effect in the flow of suspended proteins, and also attempted to quantify the breakage using CFD. Breakage criteria involved flow field intensity, which is a measure of fluid strain and shear, shown to get strong within orifice systems (Figure 4). Straining over a distance was suggested by Galinat et al. (2007), who presented evidence by demonstrating the elongation of droplets in orifice flow. Analytical equations calculating velocity gradient with distance were used by Higashitani et al. (1991). While general studies in turbulent flow point to eddies stretching and breaking particles (Parker et al., 1972), a study by Kobayashi (2004) demonstrated orifice breakage in laminar conditions.
While the “vicinity of the orifice” is known to be the region of interest in the particle breakage phenomenon, the exact location within the system where breakage occurs is a point of contention. In the direction of flow, orifice flow used to break liquid droplets demonstrated breakage “right after” the orifice (Galinat et al. 2007), while Zumaeta et al. (2008) predicted particle breakage before, inside and past the orifice. Both Sonntag and Russel (1987) and Higashitani et al. (1991) examined the significance of the entrance to the orifice in particle breakage. Higashitani et al. (1991) found approach effects significant, while Sonntag et al. (1987) discounted approach effects as “weak”.

Earlier models generally ignore the effect of radial position of particles on their breakage and only consider average effects over cross sections of the system (Zumaeta et al., 2008). It is reasonable to suppose that averaging over the cross section may skew CFD predictions by masking localized effects. In contrast, equations by Higashitani et al. (1991) examined a line of flow, but only along the centreline. The centreline of flow was also the focus of analytical equations developed by Nguyen and Kausch (1988), while other pathlines were proposed to achieve only a fraction of the centreline breakage. These equations suggested particles travelling along the centreline of flow would experience the most elongation and thus the most breakage. Simulation work for extensional flow using a cross-slot system, on the other hand, found that “cornering” has a dramatic stretching effect on polymer deformation (Hsieh et al., 2005). A study on particle breakage in orifice flow by Sontag and Russel (1987) used an analytical approach but suggested that particles which began further from the centreline would experience a
higher breakage rate. They suggested that the breakage of particles in the orifice flow is a function of the nominal orifice strain rate, E, defined as:

$$E = \frac{Q}{\pi r^3}$$  \hspace{1cm} (1)

where $Q$ is the flow rate and $r$ is orifice radius. A more recent study by Gibson et al. (2012) shows that the above parameter correlates well with breakage of wastewater particles as well. To quantify this breakage, Gibson (2011) and Gibson et al. (2012) employ the following equation:

$$\% \text{ Breakage} = 100 \times \frac{N_0 - N_T}{N_0}$$  \hspace{1cm} (2)

where $N_0$ and $N_T$ are the number of flocs larger than the mode floc size ($d>d_{\text{mode}}$) before and after hydrodynamic treatment, respectively, for a certain size fraction. The same approach has been used to quantify the breakage of flocs in hydrodynamic shear (Yuan and Farnood, 2010) and after sonication (Yong et al., 2009). The use of the mode negates the effects of birthing for flocs in a given size fraction (Yuan, 2007).

Particle breakage is of interest because it has been shown that particle breakage by orifice flow reduced the UV dose required to achieve certain levels of disinfection (Gibson, 2011), as shown in Figure 5.

![Figure 5 - Inactivation curves before and after particle breakage (Gibson, 2011)](image-url)
2.4.2 Particle Breakage in Multi-orifice Systems

Multi-orifice flow for particle breakage was developed by Gibson (2011) as part of scale-up efforts of a wastewater particle breakage system. It was designed to match nominal orifice strain rates of similar single-orifice systems. Despite reaching substantial nominal orifice strain rate, the multi-orifice system was found to produce lower breakage than the associated single-orifice system, as demonstrated in Figure 6. The reason for this difference was not apparent, but proved to be consistent over a series of multiple experiments. Without any analytical or numerical studies to examine hydrodynamic forces in multi-orifice flow, this discrepancy is difficult to explain.

![Figure 6 - Comparison of wastewater particle breakage in the single-orifice versus the multi-orifice system (Gibson 2011) Reproduced with permission from the author](image)

2.5 Summary of the Existing Literature

The breakage of particles in orifice flow is a unique phenomenon which has been demonstrated with a variety of particles. It is a form of extensional flow, and thus involves stretching of suspended particles to the point of breakage. Multiple models exist to represent these particles, including those which consist of single bodies and those which consist of multiple bodies with some volume. In orifice flow, it is believed that different degrees of particle breakage are achieved along the centerline compared with near wall paths, though the extent in each case remains uncertain. While single-orifice flow has been well explored and is known to produce
substantial breakage, multi-orifice flow is far less studied and has been found to be relatively inferior to single orifice systems for unknown reasons. As multi-orifice flow for particle breakage has not been examined analytically or numerically, it remains a topic worthy of investigation.
Chapter 3

3 Methodology

The present study is based primarily on CFD simulations, but also on some experiments. To perform simulations, a structure was modeled as described in Section 3.1.1, and then flow was simulated within the structure as outlined in Section 3.1.2. Section 3.1.3 describes the techniques used to analyze simulation results and Section 3.2 explains the extension to predict particle breakage. Predictions require the use of distribution functions, as outlined in Section 3.2.1. Finally, experimental work designed to address the relationship between particle path and likelihood of breakage is documented in Section 3.3.

3.1 CFD Simulations

3.1.1 Geometry and Meshing

CFD model geometries are created using ANSYS ICEM software (ANSYS Inc., Canonsburg, PA). All models are 3-dimensional and consist of a length of pipe, followed by an orifice and another length of pipe. Geometries are to-scale replications of the systems used by Gibson (2011) as his breakage results are used in calibrating and validating simulation breakage predictions. The most basic geometry is illustrated in Figure 7.

![Basic orifice system geometry](image)

**Figure 7 - Basic orifice system geometry**

The single-orifice system consists of a 159mm length of 19mm diameter pipe feeding a single orifice hole (diameters of 1.6, 2.4 and 3.2mm) at the centre of the pipe. The orifice is a 1.6mm long circular conduit with sharp edges that opens up to another length of 19mm diameter circular pipe. In the multi-orifice system a 51mm diameter pipe feeds into a series of 8 orifices each having a diameter of 1.6mm. The orifices are placed in two columns of four. Columns are 6.4mm apart and orifice centres are spaced 3.2mm apart with each column, as illustrated by Figure 8.
Simulated pipe-and-orifice models are designed primarily based on the experimental work of Gibson (2011) and Gibson et al. (2012) who used system parameters as illustrated in Table 1.

**Table 1 - Experimental Parameters used by Gibson (2011)**

<table>
<thead>
<tr>
<th>Experiment ID</th>
<th>Number of Orifices</th>
<th>Orifice Diameter (mm)</th>
<th>Pipe Diameter (mm)</th>
<th>Orifice Length (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>E1</td>
<td>1</td>
<td>1.6</td>
<td>19</td>
<td>1.6</td>
</tr>
<tr>
<td>E2</td>
<td>1</td>
<td>1.6</td>
<td>19</td>
<td>3.2</td>
</tr>
<tr>
<td>E3</td>
<td>1</td>
<td>2.4</td>
<td>19</td>
<td>3.2</td>
</tr>
<tr>
<td>E4</td>
<td>1</td>
<td>3.2</td>
<td>19</td>
<td>3.2</td>
</tr>
<tr>
<td>E5</td>
<td>8</td>
<td>1.6</td>
<td>51</td>
<td>1.6</td>
</tr>
</tbody>
</table>

ICEM software is used to discretize the space into a tetrahedral mesh, with each mesh consisting of $10^6$-$10^7$ elements. The majority of these elements are concentrated in the orifice region, as shown in Figure 9, to help capture the intricacies of the flow. All cells in the orifice are less than 0.002D (where D is pipe diameter), which Erdal and Andersson (1997) showed can make orifice simulations effectively grid-independent with respect to pressure measurements. Just outside the concentrated area, elements grow successively larger, as can be seen in Figure 9. El Drainy et al. (2009) and Erdal and Andersson (1997) recommend the incremental size increase be governed by expansion ratios of 1.1 and 1.2 respectively, so 1.15 is selected for the present work.
Once built, meshes are checked for holes or inconsistencies. When it is confirmed that cells have been constructed correctly, meshes are transferred to ANSYS FLUENT for flow simulations.

3.1.2 CFD Flow Simulations

All flow simulations are completed using ANSYS FLUENT Version 12.1 and a steady state, realizable $\kappa$-$\varepsilon$ turbulence model. The selection of this model is based on other researchers’ evaluations of the available turbulence models. The $\kappa$-$\varepsilon$ model best predicted macro flow variables for orifice flow simulations when compared with the Reynolds stress model (RSM) and shear stress transport (SST) model, according to a study done by Zumaeta et al. (2007). Second order spatial discretization is used for momentum, turbulent kinetic energy and turbulent dissipation rate as it provides higher order accuracy at cell faces (Ansys, Fluent Theory Guide, 2009).

The flow, itself, is simulated as water alone in a manner similar to Zumaeta et al. (2006, 2007) and El Drainy et al. (2009). The water is introduced from an inlet surface perpendicular to the
pipe using a “velocity inlet”, which allows for a uniform inlet velocity into the system. At the walls and system exit, no-slip boundary conditions and an “outflow” surface, respectively, are used to direct the simulated water as required.

Once each flowing system simulation has converged, massless particles are injected into the system, tracked and used for analysis. For each simulation, over 400 massless particles are introduced at random locations on the inlet surface and carried along with flow. Once injection locations are randomly selected, these locations and the resulting paths are held consistent for each simulation analysis. The use of these paths assumes that, within physical systems, wastewater particles do not have their own inertia but follow pathlines. This assumption is justified by the fact that wastewater particles consist primarily of water and thus have a specific gravity of close to 1.0. Data for each of the massless particles is output in basic data files. Data in the files include position, velocity components (u, v and w) and velocity gradient components \( \frac{\partial u}{\partial x}, \frac{\partial v}{\partial y}, \frac{\partial w}{\partial z}, \frac{\partial u}{\partial y}, \frac{\partial v}{\partial z}, \frac{\partial w}{\partial x} \), for each time step of each particle as it travels through the system. Up to 12,000 time steps are tracked per particle, though typically particles exit within 2000-3000 steps. Simulations are done for three different orifice sizes and various flow rates. The value of particle tracking is demonstrated in Section 4.2.1.

The meshes and simulations used in this thesis are not the product of exhaustive evaluations of modeling techniques, instead the mesh designs often represent the maximum available computational capacity, and model assumptions are usually based on literature or Fluent default values. Validation studies (Section 4.1.2), however, support the validity of the meshes and simulations developed, and thus they are considered to be sufficient for the current study. Further confidence in the models is obtained from the ability of the models to match experimental breakage trends (Section 4.2.3).

### 3.1.3 Particle Breakage Criteria

The breakage of particles in this study is considered to be based on maximum strain criterion; i.e. breakage occurs once the particle strain exceeds a critical value. To identify the most relevant indicator for particle breakage, two hydrodynamic parameters are evaluated. These are the strain rate and velocity gradient along the particle path. The strain rate, \( S \), that combines normal strain and shear effects is defined by the Fluent User’s Guide (Ansys, 2009) (and is also used in aerodynamics applications by Dacles-Mariani et al. (1995) and Shur et al. (2000)):
\[ S^2 = 2 \times (\varepsilon_{xx}^2 + \varepsilon_{xy}^2 + \varepsilon_{yx}^2 + \varepsilon_{yy}^2 + \varepsilon_{yz}^2 + \varepsilon_{zx}^2 + \varepsilon_{zy}^2 + \varepsilon_{zz}^2 + \varepsilon_{xz}^2 + \varepsilon_{yz}^2) \]  

Where \( \varepsilon_{ij} \) is the components of the strain tensor defined as:

\[ \varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]  

In the above equation, \((u_1, u_2, u_3)\) correspond to the components of velocity vectors or \((u, v, w)\) and \((x_1, x_2, x_3)\) represent the three dimensional coordinates \((x, y, z)\). Hence, it can be shown that:

\[ S^2 = \left[ \frac{\partial u}{\partial x} \left( \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \right) + \frac{\partial u}{\partial y} \left( \frac{\partial v}{\partial x} + \frac{\partial w}{\partial z} \right) + \frac{\partial u}{\partial z} \left( \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] + \]

\[ \left[ \frac{\partial v}{\partial x} \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial y} \right) + \frac{\partial v}{\partial y} \left( \frac{\partial w}{\partial y} + \frac{\partial u}{\partial z} \right) + \frac{\partial v}{\partial z} \left( \frac{\partial w}{\partial y} + \frac{\partial u}{\partial x} \right) \right] + \]

\[ \left[ \frac{\partial w}{\partial x} \left( \frac{\partial v}{\partial x} + \frac{\partial w}{\partial z} \right) + \frac{\partial w}{\partial y} \left( \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + \frac{\partial w}{\partial z} \left( \frac{\partial v}{\partial y} + \frac{\partial w}{\partial x} \right) \right] \]  

The second parameter used in this study is the velocity gradient along the particle path, \(G\), that is calculated as:

\[ G = \frac{\Delta vel_{1\rightarrow2}}{\Delta dist_{1\rightarrow2}} \]  

The distance between positions 1 and 2, \(\Delta dist_{1\rightarrow2}\), is distance between positions 1 and 2 that is calculated from:

\[ \Delta dist_{1\rightarrow2} = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2} \]  

where \((x_i, y_i, z_i)\) are the coordinates of position \(i = 1, 2\). In this study, \(\Delta dist_{1\rightarrow2}\) is kept constant at 50\(\mu m\), that is approximately equal to the average diameter of wastewater particles. Similarly, the velocity difference between locations 1 and 2, \(\Delta vel_{1\rightarrow2}\), is determined from the calculated velocity data obtained from the CFD simulations:

\[ \Delta vel_{1\rightarrow2} = \sqrt{(u_2 - u_1)^2 + (v_2 - v_1)^2 + (w_2 - w_1)^2} \]
3.2 Estimating Particle Breakage

Once obtained from CFD simulations, the particle data files are analyzed using a custom code written in Matlab (see Appendix A). Particle paths are processed one by one to extract data in the region of interest. The region of interest includes the orifice approach region (3 orifice diameters upstream of the orifice entrance) and the region inside the orifice, as illustrated in Figure 10. Moreover, to reduce the noise in the data, every fifth time step is considered for calculations. It should be emphasized that excluding the region downstream of the orifice is justifiable since CFD modeling shows less than 2% change in the predicted % breakage due to this assumption.

Figure 10 - Region of consideration for hydrodynamic effects

Using the particle data, values of breakage indicators, S and G, are calculated at time-step, \( t \), within the region of interest for all particle paths. Subsequently, maximum values of these indicators are determined and used to predict particle breakage according to the procedure described in the following sections.

3.2.1 Critical Value of Particle Breakage Indicators

The breakage model is based on the assumption that breakage of a particle occurs if maximum value of breakage indicators along the particle path; \( S_{max} \) or \( G_{max} \), exceeds a critical value, \( S_{crit} \) or \( G_{crit} \). Here, for simplicity these critical values are denoted by \( \Omega \).

Due to the natural variability in the composition and structure of wastewater particles, \( \Omega \) is particle-dependent and could exhibit a wide distribution for any given wastewater particle sample. In this study, three types of distribution functions are considered for further analysis: the
impulse distribution, the uniform distribution and the log-normal distribution. Mathematical expressions for these distributions are provided in Table 2. The impulse distribution function assumes that $\Omega$ is equal to a constant (denoted by $\alpha$) for all individual particles while for the uniform distribution $\Omega$ varies from particle to particle and is uniformly distributed between ‘a’ and ‘b’. The log-normal distribution also assumes that $\Omega$ is particle-dependent; however, in this case the distribution is positively skewed; i.e. there are fewer “stronger” particles than the “weaker” ones in a given sample. This distribution is characterized by parameters $\mu$ and $\sigma$ that are related to the mean and standard deviation of $\Omega$. The log-normal distribution function conventionally covers a semi-infinite domain; i.e. $(0,+\infty)$. However, this function was truncated to avoid the introduction of “super-strong” particles in the calculations that can skew the predicted % breakage values. Furthermore, given that the log-normal distribution is highly non-linear, to simplify the numerical calculations in breakage modeling, it is discretized into “$m$” equal intervals of width $\Delta\Omega$. The value of $m$ was typically set at 4000 in our calculations. Accordingly, the probability distribution function of $\Omega$ for interval ‘$i$’, $P(\Omega_i)$, can be written as:

$$P(\Omega_i) = \frac{f(\Omega_i)}{\sum_{i=1}^{m} f(\Omega_i) \Delta\Omega}$$

where $f$ is the standard log-normal probability function and $\Omega_i$ ($i = 1, 2, \ldots, m$) is the critical value of breakage indicator for interval ‘$i$’.

The upper limits of the uniform and log-normal distribution functions; i.e. ‘b’ and ‘$\Omega_{\text{max}}$’, respectively, are determined based on the maximum value of breakage indicators within the region of interest, as estimated by the CFD models.

The parameters of the above distributions are obtained using an exhaustive optimization procedure to match the experimental breakage data. The $fminsearch$ function in Matlab is used to minimize the sum of square error (SSE) between experiment-based % breakage, $Break_{\text{ExpEqm}}$, and the predicted % breakage values generated using the appropriate distribution functions $Break_{\text{SimPredic}}$:

$$SSE = \sum_{q=1}^{q_{\text{max}}} (Break_{\text{ExpEqm}} - Break_{\text{SimPredic}})^2$$
Table 2 - Distribution functions for critical value of particle breakage indicators, $\Omega$

<table>
<thead>
<tr>
<th>Distribution</th>
<th>Expression</th>
<th>Range</th>
<th>Eqn.</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Impulse</td>
<td>$P(\Omega) = 1 \text{ for } \Omega = \alpha$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$= 0 \text{ for } \Omega \neq \alpha$</td>
<td>$\Omega = \alpha$</td>
<td>(11)</td>
<td>$\alpha$</td>
</tr>
<tr>
<td>Uniform</td>
<td>$P(\Omega) = \frac{1}{b - a}$</td>
<td>$\Omega \in (a, b)$</td>
<td>(12)</td>
<td>$a, b$</td>
</tr>
<tr>
<td>Truncated Log-Normal</td>
<td>$P(\Omega_i) = \frac{f(\Omega_i)}{\sum_{i=1}^{m} f(\Omega_i)\Delta\Omega}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$f(\Omega) = \frac{1}{\Omega \sigma \sqrt{2\pi}} e^{-\frac{(\ln(\Omega) - \mu)^2}{2\sigma^2}}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\Omega \in (0, \Omega_{\text{max}})$</td>
<td>(13)</td>
<td>$\mu, \sigma$</td>
<td></td>
</tr>
</tbody>
</table>

Accordingly, the % breakage of particles along path ‘k’ is calculated by:

$$\text{(% Breakage)}_k = \frac{\text{(# of Particles Broken)}_k}{n_{\text{max}}}$$  \hspace{1cm} (14)

Where $n_{\text{max}}$ is the total number of particles which travel along path ‘k’. Assuming a uniform concentration of particles and a uniform velocity field at the inlet face of the orifice flow system, $n_{\text{max}}$ is the same for all particle paths.

As discussed before, if strain rate is used as the breakage criterion, the condition for the breakage of a particle is that the maximum strain rate along the particle path is greater than the critical value of strain rate for that particle; i.e. $S_{\text{max}} > S_{\text{crit}}$. Similarly, if velocity gradient is the basis for particle breakage calculations, the condition for breakage can be presented as $G_{\text{max}} > G_{\text{crit}}$. Hence, the number of particles broken along path ‘k’ can be calculated by:

$$\text{(# of Particles Broken)}_k = \sum_{n=1}^{n_{\text{max}}} F \times P(\Omega_n) \Delta\Omega \times n_{\text{max}}$$  \hspace{1cm} (15)

Where $P(\Omega_n) \Delta\Omega$ is the probability that the $\Omega$ for particle ‘n’ is between $\Omega_n$ and $\Omega_n + \Delta\Omega$, and $F$ is defined as:

$$F = 1; \text{ if } \Omega_{\text{max,k}} > \Omega_n$$

$$= 0; \text{ otherwise}$$
Here, $\Omega_{max,k}$ is either $S_{max,k}$ or $G_{max,k}$; i.e. the maximum value of strain rate and velocity gradient for path ‘k’, respectively, depending on whether strain rate or velocity gradient are used as breakage criterion. Accordingly, the overall % breakage is determined as follows:

$$\text{Overall \% Breakage} = \text{Break}_{\text{SimPred}} = \frac{\text{Total \# of Particles Broken}}{\text{Total \# of Particles Analyzed}}$$  \hspace{1cm} (16)

### 3.2.2 Experimental Breakage Data

In this study, experimental breakage data from Gibson (2011) and Gibson et al. (2012) is used for CFD model development. Results provided in Figure 11 show orifice flow measurements for two samples collected from two different sources with significantly different breakage resistances: Sample A that exhibits greater than 80% breakage at high nominal orifice strain rates (>10,000 s$^{-1}$) and appears to consist of mostly weak particles, and Sample B that had considerably less breakage under similar nominal strain rates. Moreover, a notable difference in terms of particle breakage is evident between the single-orifice and multi-orifice systems for Sample B.

![Figure 11 - Particle Breakage Results of Gibson (2011) and Gibson et al. (2012)]
In order to simplify the CFD model development, the above experimental data were fit to simple
equations that relate % breakage as a function of nominal orifice strain rate, $E$. For Sample A,
particle breakage appears to be a hyperbolic function of $E$ and can be represented by:

$$ \text{Break}_{ExpEqn} = \% \text{Breakage} = \frac{AE}{E + b} $$

(17)

where $A$ and $b$ are fitting parameters.

The breakage data for Sample B is best expressed using a linear equation, as follows:

$$ \text{Break}_{ExpEqm} = \% \text{Breakage} = gE + h $$

(18)

where $g$ and $h$ are constants.

The fitting parameters in the above equations; $A$, $b$, $g$ and $h$, (shown in Table 3) are determined
by minimizing the sum of squares of error between experimental and calculated % breakage
values:

$$ SSE = \sum_{q=1}^{q_{\text{max}}} (\text{Break}_{ExpEqm} - \text{Break}_{ExpObs})^2 $$

(19)

where $\text{Break}_{ExpObs}$ is experimental breakage data from Gibson (2011) and Gibson et al. (2012).

**Table 3 - Fitting Parameters for equations representing Experimental Breakage**

<table>
<thead>
<tr>
<th>Sample</th>
<th>Arrangement</th>
<th>Parameters</th>
<th>Relative Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Single-Orifice</td>
<td>$A=1.142; b=6608$</td>
<td>7.8</td>
</tr>
<tr>
<td>B</td>
<td>Single-Orifice</td>
<td>$g=3.45 \times 10^{-3}; h=-0.111$</td>
<td>6.7</td>
</tr>
<tr>
<td>B</td>
<td>Multi-Orifice</td>
<td>$g=2.42 \times 10^{-3}; h=-0.258$</td>
<td>11.0</td>
</tr>
</tbody>
</table>

For each case from S1 to S13 (see Table 4), % breakage is predicted according to the
methodology described earlier and results are compared to the experimental breakage values
using the above equation. Figure 12 illustrates a simplified flow chart of this procedure.
3.3 Injection Experiments

To examine the role of initial position of particles on breakage rate, an experimental system is designed to inject wastewater particles at various radial locations upstream of the orifice plate. A vertical pipe with an injector tube is the backbone of the setup, as shown in Figure 13. The vertical orientation of this setup is necessary because horizontal orientation could result in particle settling and hence introduce error in the estimated particle breakage. A 1.8m length of 75mm clear PVC pipe is flanged to an orifice plate, with a further 1.2m of pipe downstream of the orifice. Pipe length before the orifice is selected such that fully developed flow is achieved. The orifice plate itself is a 1.6mm thick stainless steel plate with a 1.6mm drilled hole. The plate is placed so that the orifice is centered in the pipe for the current experiments. A stainless steel injection tube, 3.2mm in diameter, is introduced through the pipe wall 0.2m above the plate, bending 90 degrees so it is directed toward the orifice plate. CFD simulations are used to confirm that, with the selected system dimensions, the flow recovers well from the interference of the injection tube before orifice entry.

A separate vessel, used to hold wastewater particles before injection, consists of a vertical clear PVC pipe, 0.3m long and 50mm in diameter, capped at the bottom. Valves at the top allow for the vessel to be sealed to the atmosphere and for compressed air to be introduced. A magnetic stir bar is used to keep particles well mixed in the vessel, and a hole tapped into the bottom of the pipe wall connects the vessel to the injection tube via 3.2mm flexible PVC tubing.
Particle samples are prepared by sieving one liter of mixed liquor from a pilot-scale sequencing batch reactor. The 53-75μm fraction is used in this study to ensure that particle size is less than 20x orifice diameter. Sieved particles are diluted to a total volume of 500mL and the mixture is poured into the injection vessel. Water is pumped from a 250 L tank via a progressive cavity pump into the top of the main pipe and flows down through the orifice. To remove air bubbles introduced during filling of the system a vent is placed at the top of the setup that allows air to exit the system through a hose to the drain. Once steady flow is established in the main pipe, the particles are introduced via the injection tube, where they are entrained in the water flow and carried through the orifice. The injection flow rate, targeted at approximately one mL/s, is measured by the change in height of the suspension in the particle concentrate vessel over time. Digital pressure gauges are used to better monitor and control pressure in the vessel, but injections are controlled by plant air that could introduce variability in the experimental results. For example, at pressures exceeding 420 kPa (60psi) in the vessel, fluctuations of less than 7 kPa (1.0 psi) in the air pressure could change the injection flow rate by a factor of two. Changes in
the injection flow rate results in fluctuations in the particle concentration in the orifice flow system and hence introduces uncertainty in the particle breakage measurement. In addition, excessive reduction of the injection flow rate may cause particles to settle and form agglomerates in the injection tubing which are sporadically released into pipe.

To evaluate breakage, outflow from the orifice is collected and particle size is analyzed using a Rapid VUE (Beckman Coulter, Miami, USA), which measures particles in the range of 10 to 1000 \( \mu m \) equivalent area diameter (EAD). Size distributions of particles from the orifice are compared with those from an untreated control sample taken directly from the injection vessel. The untreated sample is diluted according to the relative flow rates of water and particle injection in the main system.
Chapter 4

4 Results and Discussion

Simulation and experimental results are disseminated and discussed in this Chapter. Details of orifice geometry and flow conditions and validation of CFD model are presented in Section 4.1. Section 4.2 includes the distribution functions used in this study and the predicted particle breakage for various conditions. Section 4.4 discusses the role of radial position of particles in breakage, and experimental and simulation work designed to correlate position and breakage.

4.1 Details of CFD Simulations

As outlined in Chapter 2, many approaches to CFD analysis of orifice systems have been reported in the past, with a few extended to predict breakage of suspended particles. Some of these approaches involved an averaging or a generalized equation to predict breakage, and many were based on analytical analyses which cannot be extended to multi-orifice systems. Therefore, a more fundamental approach is developed here for the prediction of particle breakage using CFD and is verified against experimental particle breakage data when possible.

4.1.1 Simulated Cases

The operating parameters used for each CFD simulation are given in Table 4. Simulation parameters include three different orifice sizes and various flow rates from 14 to more than 300 mL/s. These flow rates coupled with the pipe diameters of 19mm and 51mm result in Reynold’s numbers generally greater than 2500, so in the turbulent regime. Single and multi-orifice scenarios are both investigated. These parameters were selected to encompass a wide range of nominal orifice strain rates and orifice geometries.
Table 4 - Details of orifice geometry and flow conditions used in CFD simulations. The calculated nominal orifice strain rate and pressure drop data are also provided.

<table>
<thead>
<tr>
<th>Simulation/Case ID</th>
<th>Number of Orifices</th>
<th>Orifice Diameter (mm)</th>
<th>Pipe Diameter (mm)</th>
<th>Orifice Length (mm)</th>
<th>Inlet Velocity (m/s)</th>
<th>Flow Rate (mL/s)</th>
<th>Nominal Orifice Strain Rate (s⁻¹)</th>
<th>Pressure Drop (kPa)</th>
<th>Pipe Reynolds Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td>1</td>
<td>1.6</td>
<td>19</td>
<td>1.6</td>
<td>0.05</td>
<td>14</td>
<td>8,860</td>
<td>41</td>
<td>950</td>
</tr>
<tr>
<td>S2</td>
<td>1</td>
<td>1.6</td>
<td>19</td>
<td>1.6</td>
<td>0.15</td>
<td>43</td>
<td>26,590</td>
<td>393</td>
<td>2,850</td>
</tr>
<tr>
<td>S3</td>
<td>1</td>
<td>1.6</td>
<td>19</td>
<td>1.6</td>
<td>0.2</td>
<td>57</td>
<td>35,460</td>
<td>690</td>
<td>3,800</td>
</tr>
<tr>
<td>S4</td>
<td>1</td>
<td>2.4</td>
<td>19</td>
<td>1.6</td>
<td>0.2</td>
<td>57</td>
<td>10,500</td>
<td>152</td>
<td>3,800</td>
</tr>
<tr>
<td>S5</td>
<td>1</td>
<td>2.4</td>
<td>19</td>
<td>1.6</td>
<td>0.45</td>
<td>128</td>
<td>23,640</td>
<td>648</td>
<td>8,550</td>
</tr>
<tr>
<td>S6</td>
<td>1</td>
<td>3.2</td>
<td>19</td>
<td>1.6</td>
<td>0.1</td>
<td>29</td>
<td>2,220</td>
<td>14</td>
<td>1,900</td>
</tr>
<tr>
<td>S7</td>
<td>1</td>
<td>3.2</td>
<td>19</td>
<td>1.6</td>
<td>0.2</td>
<td>57</td>
<td>4,430</td>
<td>69</td>
<td>3,800</td>
</tr>
<tr>
<td>S8</td>
<td>1</td>
<td>3.2</td>
<td>19</td>
<td>1.6</td>
<td>0.4</td>
<td>114</td>
<td>8,860</td>
<td>235</td>
<td>7,600</td>
</tr>
<tr>
<td>S9</td>
<td>1</td>
<td>3.2</td>
<td>19</td>
<td>1.6</td>
<td>0.7</td>
<td>200</td>
<td>15,510</td>
<td>759</td>
<td>13,300</td>
</tr>
<tr>
<td>S10</td>
<td>1</td>
<td>3.2</td>
<td>19</td>
<td>1.6</td>
<td>1</td>
<td>285</td>
<td>22,160</td>
<td>1552</td>
<td>19,000</td>
</tr>
<tr>
<td>S11</td>
<td>8</td>
<td>1.6</td>
<td>51</td>
<td>1.6</td>
<td>0.05</td>
<td>101</td>
<td>7,880</td>
<td>138</td>
<td>2,550</td>
</tr>
<tr>
<td>S12</td>
<td>8</td>
<td>1.6</td>
<td>51</td>
<td>1.6</td>
<td>0.13</td>
<td>263</td>
<td>20,490</td>
<td>241</td>
<td>6,630</td>
</tr>
<tr>
<td>S13</td>
<td>8</td>
<td>1.6</td>
<td>51</td>
<td>1.6</td>
<td>0.15</td>
<td>304</td>
<td>23,640</td>
<td>345</td>
<td>7,650</td>
</tr>
<tr>
<td>S14</td>
<td>1</td>
<td>1.6</td>
<td>19</td>
<td>6.4</td>
<td>0.05</td>
<td>14</td>
<td>8,860</td>
<td>41</td>
<td>950</td>
</tr>
<tr>
<td>S15</td>
<td>1</td>
<td>1.6</td>
<td>19</td>
<td>6.4</td>
<td>0.095</td>
<td>27</td>
<td>16,840</td>
<td>345</td>
<td>1,805</td>
</tr>
<tr>
<td>S16</td>
<td>1</td>
<td>1.6</td>
<td>19</td>
<td>6.4</td>
<td>0.15</td>
<td>43</td>
<td>26,590</td>
<td>359</td>
<td>2,850</td>
</tr>
</tbody>
</table>

4.1.2 CFD Model Validation

Simulations are confirmed to be consistent with the continuity principle and achieved accurate flow rates for each given inlet velocity. Qualitatively, flow fields seen in simulations have the characteristic dissipating jet observed by Ramamurthi and Nandakumar (1999) and “deadwater” recirculation zones after the orifice as described by White (1994). These can be seen in the vector field shown in Figure 14. Also present in simulations are the separation zone in the orifice entrance (also noted by Ramamurthi and Nandakumar (1999)). Finally, isovels in the orifice approach exhibit the same semiellipsoid shape which Shammaa et al. (2005) recorded.
Further validation includes comparison with established theory and experimental work, namely in terms of pressure drop. While pressure can be difficult to accurately predict with CFD (El Drainy et al., 2009; Erdal and Andersson, 1997), such comparisons are commonly used to gain confidence in the CFD model predictions.

Pressure drop data reported by Gibson (2010) are used for validation studies in this work. In addition, theoretical pressure drop values are calculated and compared to the CFD predictions according to:

\[ h_L = K_L \frac{v^2_{orif}}{2g} \]  \hspace{1cm} (20)

where \( g \) is the gravitational acceleration, \( v \) is average velocity through the orifice and \( K_L \) is the loss coefficient. The value of \( K_L \) is estimated based on area ratios of the orifice and pipe, as per Munson et al. (2006). The total theoretical pressure loss is the sum of losses calculated at the entrance and exit from the orifice for the required flow rates.

Figure 15 is a graph of experimental and predicted pressure drop values against nominal orifice strain rate. CFD models generally converged to residuals below of \( 10^{-3} \) for each of the continuity equation, the velocity components, \( \kappa \) and \( \varepsilon \). While some fluctuation is visible at high nominal
orifice strain rate, the graph demonstrates a good correlation between CFD simulation results and experimental data as well as theoretical predictions.

Figure 15 - Validation of orifice flow simulations via experimental and predicted pressure drop data. Orifice diameter: 1.6mm

4.2 Simulation Results

4.2.1 Hydrodynamic Effects Along Particle Tracks

Individual particles are tracked in the single orifice system. Tracking of each individual particle reveals a unique set of hydrodynamic conditions for each path. For example, strain rate, as defined in Section 3.1.3, is used to illustrate the extent of variability for particle paths in Figure 16 and Figure 17.
Figure 16 - Strain rate along particle paths. Image represents an area of 35 mm (L) × 9.5 mm (The color scale represents strain rate in (s\(^{-1}\)).

Figure 17 - Comparing strain rate experienced along two centre-line and near-wall particle paths as per Figure 16. The x-axis is the distance from the centre of the orifice. Pipe Velocity=0.05m/s, Orifice Velocity=7.2m/s, ΔP =170kPa (25psi).
Comparing the near-wall and the centre-line paths (Figure 17), each path has a distinctly different maximum strain rate, observable in the orifice area. Particles originated near the pipe wall, and travel radially as well as axially to enter the orifice are exposed to higher maximum strain rates than those which travel close to the pipe centreline. A similar result is obtained for the velocity gradient along particle paths. Hence, the initial position of the particle in terms of its proximity to the pipe wall affects the magnitude of the maximum strain rate experienced by that particle. This finding emphasizes the significance of tracking of particle paths for analyzing particle breakage in orifice flow. This issue becomes even more important when analyzing the multi-orifice system in which orifice holes are positioned at varying distances from the pipe wall.

### 4.2.2 Distribution Functions for Critical Breakage Indicators

As much as it is important to recognize the uniqueness of individual particle paths, it is equally important to consider the natural variability in particle strength for predicting the particle breakage rates. According to the experimental data in Figure 11, two sets of particles with distinctly different breakage characteristics; namely Sample A and Sample B, are studied in the present work.

To find a suitable distribution function to represent these samples, impulse, uniform and truncated log-normal distributions are analyzed using the procedure outlined in Section 3.2. The maximum values and the increment sizes for critical values of strain rate and velocity gradient distributions are given in Table 5. Using \( m = 4000 \) increments, changing the number of increments, \( m \), by +/- 50% caused less than one percent change in SSE of breakage predictions.

<table>
<thead>
<tr>
<th></th>
<th>( \Delta \Omega ) (s(^{-1}))</th>
<th>( \Omega_{\text{max}} ) (s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strain Rate</td>
<td>250</td>
<td>1,000,000</td>
</tr>
<tr>
<td>Velocity Gradient</td>
<td>400</td>
<td>1,600,000</td>
</tr>
</tbody>
</table>

To illustrate the procedure used for selecting a suitable distribution function, the critical value of strain rate is used here. Table 6 provides the calculated breakage after parameter optimization for various distribution functions for simulation cases S1-S13. All three distribution functions provide breakage predictions with a relative error of better than 50% compared to the
experimental values; and the relative error of most predictions is better than 20%. The log-normal distribution slightly outperforms the other two distributions, however, and has a smaller average relative error. The average relative error for each is presented in Table 7, along with the parameters of the distributions.

Table 6 - Simulation breakage predictions using various distribution functions

<table>
<thead>
<tr>
<th>Case</th>
<th>Sample A</th>
<th>Sample B</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Calculated Particle Breakage (%)</td>
<td>Calculated Particle Breakage (%)</td>
</tr>
<tr>
<td></td>
<td>Experimental*</td>
<td>Impulse</td>
</tr>
<tr>
<td>S1</td>
<td>65.4</td>
<td>69.0</td>
</tr>
<tr>
<td>S2</td>
<td>91.5</td>
<td>99.8</td>
</tr>
<tr>
<td>S3</td>
<td>96.3</td>
<td>100.0</td>
</tr>
<tr>
<td>S4</td>
<td>70.1</td>
<td>71.0</td>
</tr>
<tr>
<td>S5</td>
<td>89.3</td>
<td>100.0</td>
</tr>
<tr>
<td>S6</td>
<td>28.7</td>
<td>21.5</td>
</tr>
<tr>
<td>S7</td>
<td>45.8</td>
<td>30.2</td>
</tr>
<tr>
<td>S8</td>
<td>65.4</td>
<td>73.8</td>
</tr>
<tr>
<td>S9</td>
<td>80.1</td>
<td>100.0</td>
</tr>
<tr>
<td>S11</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>S12</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>S13</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

*Calculated using Equations (17) or (18).

Table 7 - Average Relative Error for Predicted vs Experimental breakage and parameters used in selection of distribution function

<table>
<thead>
<tr>
<th></th>
<th>Sample A</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Impulse</td>
<td>Uniform</td>
<td>Log-Normal</td>
<td>Impulse</td>
<td>Uniform</td>
<td>Log-Normal</td>
<td></td>
</tr>
<tr>
<td>% Average Error</td>
<td>14</td>
<td>8</td>
<td>4</td>
<td>28</td>
<td>23</td>
<td>24</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Parameters of Distribution Function</td>
<td>α=22,750</td>
<td>a=0</td>
<td>μ=10.0</td>
<td>σ=1.1</td>
<td>α=95,550</td>
<td>a=67,250</td>
<td>μ=11.5</td>
<td>σ=0.2</td>
</tr>
</tbody>
</table>

To better compare the above distribution functions, the parity plots comparing predicted breakage with experimental are provided in Figure 18. The results generated using the log-normal distribution demonstrate a quality fit between the sets of predicted breakage data, with $R^2$ values of 0.98 and 0.77 for Samples A and B respectively.
Sample A
Strain Rate
Impulse Distribution
$R^2=0.75$

Sample B
Strain Rate
Impulse Distribution
$R^2=0.72$

Sample A
Strain Rate
Uniform Distribution
$R^2=0.94$

Sample B
Strain Rate
Uniform Distribution
$R^2=0.77$
Figure 18 - Parity Plots of Predicted vs Experimental Breakage for various distribution functions

Using the above parameters, the log-normal distribution functions for Samples A and B are plotted in Figure 19. The difference between the distributions is expected since these samples are from different origins and exhibit different resistance to breakage (see Figure 11). The discrepancy could also result from sample handling. Sample B was pumped several times before introduction to the orifice system. This could have disintegrated weak particles within the sample, leaving only strong particles behind and hence shifting the distribution to larger values along the x-axis.
Using a similar approach, the lognormal distribution is found to be also suitable for velocity gradients as well and is hence used in the remainder of this study.

### 4.2.3 Selection of Breakage Indicator

The predicted breakage results using strain rate and the velocity gradient over a particle are provided in Table 8. These breakage indicators were able to match the experimental values with an average relative error of less than 50%, but the effectiveness of the strain rate was much higher than that of the velocity gradient, as illustrated by the average errors reported in Table 9.

<table>
<thead>
<tr>
<th>Case</th>
<th>% Breakage for Sample A</th>
<th>% Breakage for Sample B</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Experimental*</td>
<td>Strain Rate (s^{-1})</td>
</tr>
<tr>
<td>S1</td>
<td>65.4</td>
<td>68.3</td>
</tr>
<tr>
<td>S2</td>
<td>91.5</td>
<td>90.2</td>
</tr>
<tr>
<td>S3</td>
<td>96.3</td>
<td>93.5</td>
</tr>
<tr>
<td>S4</td>
<td>70.1</td>
<td>66.6</td>
</tr>
<tr>
<td>S5</td>
<td>89.3</td>
<td>87.1</td>
</tr>
<tr>
<td>S6</td>
<td>28.7</td>
<td>29.7</td>
</tr>
<tr>
<td>S7</td>
<td>45.8</td>
<td>40.5</td>
</tr>
<tr>
<td>S8</td>
<td>65.4</td>
<td>70.1</td>
</tr>
<tr>
<td>S9</td>
<td>80.1</td>
<td>80.9</td>
</tr>
<tr>
<td>S11</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>S12</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>S13</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

*Calculated using Equations (17) or (18)
Table 9 - Average Relative Error for predicted vs experimental breakage and parameters used in selection of Breakage Indicator

<table>
<thead>
<tr>
<th></th>
<th>Sample A</th>
<th>Sample B</th>
</tr>
</thead>
<tbody>
<tr>
<td>% Average Error</td>
<td>4</td>
<td>24</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>46</td>
</tr>
<tr>
<td>Parameters of</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Log Normal Distribution</td>
<td>μ=10.0, σ=1.1</td>
<td>μ=11.5, σ=0.2, μ=19.6, σ=4.5</td>
</tr>
<tr>
<td>Log-Normal Distribution</td>
<td>R²=0.98</td>
<td>R²=0.77</td>
</tr>
</tbody>
</table>

Parity plots for the predicted particle breakage using various breakage indicators are given in Figure 20, with the corresponding $R^2$ values. The log-normal distribution parameters for these indicators are also provided in Table 9. Based on these results, the strain rate is a better indicator of the particle breakage than the velocity gradient and hence is used in the remainder of this document. Velocity gradient was effective for the single-orifice system but predicted higher breakage in multi-orifice than single orifice, further challenging its effectiveness as a breakage indicator.

[Parity plots for Sample A and Sample B showing predicted vs experimental breakage for strain rate and velocity gradient.]
4.3 Comparison with Experimental data

4.3.1 Effect of Orifice Length

Gibson (2010) have reported that increasing the orifice length by a factor of 3 had little effect (<5%) on the particle breakage. Accordingly, simulations S14-S16 involved longer orifices (6.4 mm) compared to S1-S3 (1.6mm). Figure 21 shows that consistent with the experimental observation, there is little difference between long and short orifices under the same flow conditions.
4.3.2 Breakage-Strain Relationship for Single-orifice Systems

Figure 22 demonstrates the agreement between the experimental breakage data of Gibson et al. (2012) for single orifice systems and the predicted values in this work. Breakage criterion is based on the critical strain rate with a log-normal distribution function and using the parameters provided in Table 9. The simulation cases include three different orifice diameters and a wide range of flow rates from 14 to 200 mL/s. Predicted breakage results closely follow the “master curve” experimentally observed by Gibson et al. (2012).
4.3.3 Breakage-Strain Relationship for Multi-orifice Systems

Figure 23 illustrates the experimental breakage results of Gibson (2011) as well as the simulation breakage predictions for Sample B. The single-orifice system consistently outperforms the multi-orifice system. The experimental results indicate that to achieve 20% breakage, for example, the single orifice system requires an energy density of 1.4 J/mL, while the multi-orifice system requires 3.5 J/mL. Furthermore, experimental data in Figure 23 show that at the same nominal orifice strain rate, single orifice system produces a higher breakage than multi-orifice system. Simulation results also correctly predict a lower breakage for multi-orifice flow than the single-orifice geometry at a given nominal orifice strain rate; however, the predicted values for single orifice geometry are generally lower than the experimental values. Despite this discrepancy, the ability of the simulation breakage model to predict the differences between the performance of single-orifice and multi-orifice systems is a notable advantage of this model.
Figure 23 - Particle Breakage for Sample B in Single- and Multi-orifice Systems (Cases S1, S4, S6-S9 and S11-S13)

To better understand the superior performance of the single-orifice system, the distribution function for the maximum strain rate experiences by particles (calculated by the simulation program) is plotted in Figure 24. Based on the model simulations, it can be seen that in the single-orifice system particles could experience much higher maximum strain rates, and hence are more likely to break. For example, maximum strain rates of up to 500,000 s\(^{-1}\) are imposed on certain particles while in the multi-orifice case the maximum strain never exceeds 150,000 s\(^{-1}\). Particles with a critical strain rate higher than 150,000 s\(^{-1}\), thus, would not be broken in the multi-orifice system, while 30% of them would be broken in the single orifice system. It is worth noting, however, that the cumulative distribution plots in Figure 24 intersect. At critical strain rate of less than 90,000 s\(^{-1}\), the curve for the multi-orifice system is below that for the single-orifice system, suggesting that the multi-orifice system could produce higher breakage for weaker particles. Given that multi-orifice systems are capable of handling higher flow rates at lower pressure drops, they may seem to be suitable for the breakage of wastewater particles. However, the relatively poor performance of these systems compared to the single orifice systems in terms of particle breakage needs to be taken into consideration in such applications.
Figure 24 - Maximum strain rates in single-orifice system compared with multi-orifice system. Nominal Orifice Strain Rate = 23,600s\(^{-1}\) (Cases S5 and S13).
4.4 The Role of Initial Position in Breakage

As described in Section 2.4, it is generally agreed that particles travelling along the pipe centreline experience different breakage conditions than those originating near the pipe wall. However, the exact effect of initial particle position on breakage remains unclear. Nguyen and Kausch (1988) suggested that maximum breakage occurs for particles located at the centreline while Sontag and Russel (1987) and Hsieh et al. (2005) suggested that particles originating farther from the centreline are more likely to break.

Figure 25 illustrates the relationship between the predicted maximum strain rate experiences by particles versus the initial particle position based on the simulation. Despite scatter in the data, the near wall particles are more likely to experience a higher maximum strain rate.

![Figure 25 - Maximum strain rate against initial particle position for multitude of paths (Case S2)](image)
To clarify this issue, an experimental set up is developed to inject particles at various radial locations upstream of an orifice in a flow through system. Despite many attempts at optimizing the system, no concrete results were achieved. Simulation work, on the other hand, clearly suggested that near-wall paths produce elevated breakage.

4.4.1 Particle Injection Experiments

To further examine the role of initial particle location on the breakage, wastewater particles were injected into an orifice flow system at various radial positions using the setup described in Section 3.3. Particle entrainment was monitored visually as illustrated in Figure 26 and Figure 27.

The particle size distributions before and after orifice treatment for centerline and near-wall injections are given in Figure 28. As expected, the particle size distributions show a shift to smaller sizes after orifice treatment. However, there is no significant difference between particle size distribution of centerline and near-wall particles after orifice flow treatment.
This could be caused by poor control of the injection flow rate that, as discussed earlier, could have a significant effect on the measured breakage data. Additional work is required to improve design of the injection flow system to ensure a stable injection flow rate.
Chapter 5

5 Conclusions

Orifice flow is known to break particles contained in suspensions. CFD simulations were used to track massless particle paths through the orifice system in order to identify an indicator which can be used to predict breakage of wastewater particles. Only the region before and inside the orifice was considered, and strain rate, as calculated by Ansys Fluent, was identified as effective to indicate breakage. Distribution functions were also used in breakage predictions, and were shown to vary; with particles which have been pumped or otherwise disrupted being more resistant to breakage. The difference in strength was traced back to handling, as weak particles are broken upon disruption leaving only the strong particles behind. The combination of following paths, monitoring strain rate and implementing distribution functions allowed for effective prediction of breakage when compared with experimental results. The prediction technique was successful for both single orifice and multi-orifice systems. Observation of the elevated breakage potential of the single-orifice over the multi-orifice system, despite the same flow rates through the same sized orifices, is explained by the current model. Previously thought to be an experimental anomaly, the phenomenon is explained by the observation that the single-orifice system reaches higher maximum strain rates than the multi-orifice system. Ultimately, this work provides a tool which can effectively indicate particle breakage trends in various orifice systems, and can be used to optimize these systems to break the most particles with the least energy input.

Equipment was developed to verify the simulation conclusion that near wall particles are more likely to break than those which travel along the centerline of flow. While issues with controlling the rate of injection limited the value of the results, improvements can likely bring the apparatus to a point where it can perform effectively and provide meaningful data. This could support what simulations have suggested, that particles which travel near the wall and must change direction to enter the orifice are more likely to break than those travelling along the centerline.
5.1 Potential Improvements and Opportunities for Future Work

The CFD based breakage prediction techniques developed in this thesis can be used in optimization of the orifice breakage system. Gibson (2010) showed knife-edged orifices to be more effective than square-edged ones, so orifice shape can likely be optimized to use minimal energy while still achieving substantial breakage. Optimization efforts, therefore, ought to include evaluation of a variety of new orifice geometries. Slots to increase orifice wall surface area, square orifices to further emphasize the cornering effect and different orifice positioning to maximize changes in direction can all be explored using simulations. These new geometries can be evaluated using the breakage prediction tools developed here. Those geometries which are deemed ineffective can be discarded, while those which are shown to be most effective can be built for experimental testing.

While experimental trends were matched by simulation predictions using the analysis detailed here, this simulation based breakage prediction technique is not all-encompassing. It neglects consideration of particle elasticity and time dependent effects. Studies on biofilms by Towler et al. (2007) illustrate that biological entities have elastic tendencies. Elastic behavior and yield stress could even be determined directly using micromechanical stretching or another mechanical means to stretch individual particles. In order to address elasticity in simulations, the Burger model could be used. This model involves springs and dashpots and is represented by the following equation (Towler et al., 2007):

\[
\sigma + A \frac{\partial \sigma}{\partial t} + B \frac{\partial^2 \sigma}{\partial t^2} = C \frac{\partial \varepsilon}{\partial t} + D \frac{\partial^2 \varepsilon}{\partial t^2}
\] (21)

Time dependent effects would allow for strain to be evaluated over a particle path, not simply at one location. Stresses can be predicted using the filament model of Parker et al (1972), which proposes that particles be considered as two spheres connected by a filament. A force balance on the system allows stress to be related to velocity. Velocity and acceleration data is available from the Fluent CFD simulations. More detailed analysis would involve writing user defined functions within Fluent to model particle bodies within the flow.

The particle injection system developed in this work has the capacity to determine, ultimately, the role of position in breakage. While simulations indicate that centerline particles are less
likely to break than near-wall particles, the discussion around the uncertainty would be conclusively ended with decisive results from the injection experiments. Future experiments require controlled injection in order to demonstrate a difference between centreline and near-wall injection breakage. Higher flow to produce higher breakage will help to magnify differences between centerline and near-wall injection breakage results. To eliminate the issues associated with variable wastewater particle size and low concentration, injection of a concentrated suspension of uniform synthetic particles could be used. Using uniform, synthetic particles would isolate particle position as the only variable and allow for identification of the path producing the highest breakage. Further tests with these modifications would be necessary to properly investigate the difference between centerline and near-wall particle breakage.

If particle breakage in orifice flow is to have any industrial application in the wastewater industry, a detailed cost analysis must be completed. Orifice flow remains highly energy intensive as the particle suspension must be pumped through the orifice. A detailed analysis could confirm that the savings in UV energy would outweigh the added pumping cost to operate orifice flow. Economic uncertainties aside, this work has made an academic contribution to the discussion surrounding particle breakage in orifice flow.
Bibliography


Appendices

Appendix A - Matlab Code for Post-Processing

A-1 Data Reading and Filtering

% tic

Code='16thPl_16th1H_100psi'; %This is where file Code is entered
PDiam=50/1000000; %Enter Diam of particles, in microns
Highest=1000000; %Set maximum value of total stretch
Div=4000; %Set incremental size of bins
ThreshDiv=6000; %Set Incremental size of Threshold Distribution
PathCount=442;%814;
pipesize=1;%2.6667; %Set up option for Large scale 8 hole

% Matrix to hold strength distributions Row 1 = Strengths
Distrib=zeros(2,20);
%
% Row 2 = #of particles in there
for i=1:1:20
    Distrib(1,i)=i*ThreshDiv;
end
Distrib(2,:)=[0 15 14 13 11 9 8 7 6 5 5 0 0 0 0 0 0 0 0 0]; %TruncatedLogNormalDistrib
Distrib(2,:)= [0 12 11 10 8 7 6 6 5 5 4 4 3 3 3 3 2 2 2 2]; %LogNormalDistrib
Distrib(2,:)=5; %Uniform Distrib
Distrib(2,:)= [0 0 1 2 3 5 7 9 11 12 12 11 9 7 5 3 2 1 0 0]; %NormalDistrib
Distrib(2,:)= [0 0 0 0 0 1 4 15 30 30 15 4 1 0 0 0 0 0]; %NarrowNormalDistrib
Distrib(2,:) = [0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0]; %ReverseTruncatedLogNormalDistrib

%Naming for files, must have same length
Names=cellstr(['Xpos';'Ypos';'Zpos';'Vmag';'StRt';
    'dUdx';'dVdx';'dWdx';'dUdy';'dVdy';'dWdy';'dUdz';'dVdz';'dWdz';'Xvel';'Yvel';
    'Zvel']);
DataMtx=cell(17,900); %Each Particle has own array, rows for params
for ftype=1:17
    %For loop to extract each param
    str=sprintf('%s_%s',Code,Names(ftype)); %Combine parts of name
    fid=fopen(str); %Open file with combined name

    %Read data in, skip between text
    DataMtx{ftype,1}=textscan(fid,'%f %f','headerLines',4);
    for i=2:900;
        %Read data for every step of up to 1000 particles
        DataMtx{ftype,i}=textscan(fid,'%f %f','headerLines',3);
    end
    fclose(fid);
end
Create Mtx to record Stretch Measure of each particle

AccumStretches=zeros(3,900);

PAccStretch=0;
BrokeCount=0;  %Brokecount for all particles

for j=1:PathCount    %Assign j to look at each particle one at a time

    %For Every Step along Particle j's path
    for k=5:1:numel(DataMtx{1,j}{1,1})
        if round(k/5)==k/5    %Only looks at every 5th step

            %Shift coords so orif entr is 0,0,0
            if z>=0.0015875  %Is particle before end of orifice?
                x=DataMtx{1,j}{1,2}(k);
                y=DataMtx{2,j}{1,2}(k);

            %Set region of stretch interest to 6 OrifDiamCirc
            if sqrt(x^2+y^2+z^2)<(0.005*pipesize)

                dx=DataMtx{1,j}{1,2}(k)-DataMtx{1,j}{1,2}(k-5);
                dy=DataMtx{2,j}{1,2}(k)-DataMtx{2,j}{1,2}(k-5);
                dz=DataMtx{3,j}{1,2}(k)-DataMtx{3,j}{1,2}(k-5);
                S=DataMtx{5,j}{1,2}(k);
                du=DataMtx{15,j}{1,2}(k)-DataMtx{15,j}{1,2}(k-5);
                dv=DataMtx{16,j}{1,2}(k)-DataMtx{16,j}{1,2}(k-5);
                dw=DataMtx{17,j}{1,2}(k)-DataMtx{17,j}{1,2}(k-5);
                dDist=sqrt(dx^2+dy^2+dz^2);  %dDist=distance between steps
                dVeloc=sqrt(du^2+dv^2+dw^2);

                Strn=abs(DataMtx{6,j}{1,2}(k))+abs(DataMtx{10,j}{1,2}(k))+abs(DataMtx{14,j}{1,2}(k));

                if Strn>PAccStretch
                    PAccStretch=Strn;  %one of >> S or Shr or Strn
                end
                kp=k-5;
        end

    end

    %If step size>PDiam, gradient along step applies to particle also
    while dDist<PDiam
        dxp=DataMtx{1,j}{1,2}(kp)-DataMtx{1,j}{1,2}(k);
        dyp=DataMtx{2,j}{1,2}(kp)-DataMtx{2,j}{1,2}(k);
        dzp=DataMtx{3,j}{1,2}(kp)-DataMtx{3,j}{1,2}(k);

        %Add distance of step before
        dDist=dDist+sqrt(dxp^2+dyp^2+dzp^2);

        dup=DataMtx{15,j}{1,2}(kp)-DataMtx{15,j}{1,2}(k);
        dvp=DataMtx{16,j}{1,2}(kp)-DataMtx{16,j}{1,2}(k);
        dwp=DataMtx{17,j}{1,2}(kp)-DataMtx{17,j}{1,2}(k);

        %If step size<PDiam, must find veloc @ back end
    end

end

%Create Mtx to record Stretch Measure of each particle
 AccumStretches=zeros(3,900);

PAccStretch=0;
BrokeCount=0;  %Brokecount for all particles

for j=1:PathCount    %Assign j to look at each particle one at a time

    %For Every Step along Particle j's path
    for k=5:1:numel(DataMtx{1,j}{1,1})
        if round(k/5)==k/5    %Only looks at every 5th step

            %Shift coords so orif entr is 0,0,0
            if z>=0.0015875  %Is particle before end of orifice?
                x=DataMtx{1,j}{1,2}(k);
                y=DataMtx{2,j}{1,2}(k);

            %Set region of stretch interest to 6 OrifDiamCirc
            if sqrt(x^2+y^2+z^2)<(0.005*pipesize)

                dx=DataMtx{1,j}{1,2}(k)-DataMtx{1,j}{1,2}(k-5);
                dy=DataMtx{2,j}{1,2}(k)-DataMtx{2,j}{1,2}(k-5);
                dz=DataMtx{3,j}{1,2}(k)-DataMtx{3,j}{1,2}(k-5);
                S=DataMtx{5,j}{1,2}(k);
                du=DataMtx{15,j}{1,2}(k)-DataMtx{15,j}{1,2}(k-5);
                dv=DataMtx{16,j}{1,2}(k)-DataMtx{16,j}{1,2}(k-5);
                dw=DataMtx{17,j}{1,2}(k)-DataMtx{17,j}{1,2}(k-5);
                dDist=sqrt(dx^2+dy^2+dz^2);  %dDist=distance between steps
                dVeloc=sqrt(du^2+dv^2+dw^2);

                Strn=abs(DataMtx{6,j}{1,2}(k))+abs(DataMtx{10,j}{1,2}(k))+abs(DataMtx{14,j}{1,2}(k));

                if Strn>PAccStretch
                    PAccStretch=Strn;  %one of >> S or Shr or Strn
                end
                kp=k-5;
        end

    end

    %If step size>PDiam, gradient along step applies to particle also
    while dDist<PDiam
        dxp=DataMtx{1,j}{1,2}(kp)-DataMtx{1,j}{1,2}(k);
        dyp=DataMtx{2,j}{1,2}(kp)-DataMtx{2,j}{1,2}(k);
        dzp=DataMtx{3,j}{1,2}(kp)-DataMtx{3,j}{1,2}(k);

        %Add distance of step before
        dDist=dDist+sqrt(dxp^2+dyp^2+dzp^2);

        dup=DataMtx{15,j}{1,2}(kp)-DataMtx{15,j}{1,2}(k);
        dvp=DataMtx{16,j}{1,2}(kp)-DataMtx{16,j}{1,2}(k);
        dwp=DataMtx{17,j}{1,2}(kp)-DataMtx{17,j}{1,2}(k);

        %If step size<PDiam, must find veloc @ back end
    end

end
dwp=DataMtx{17,j}{1,2}(kp)−DataMtx{17,j}{1,2}(k);

% Gradient from kp up to k, whole PDiam
dVeloc=dVeloc+sqrt(dup^2+dvp^2+dwp^2);

% Keep kp moving back in case dDist still too small
kp=kp−5;

end

% Find the highest veloc gradient across particle
if (dVeloc/dDist*PDiam)>PAccStretch
% Assign that highest gradient to PAccStretch
PAccStretch=dVeloc/dDist*PDiam;
end
end
end

AccumStretches(1,j)=j; % Particle Number in first row, Init

AccumStretches(2,j)=1000*sqrt(DataMtx{1,j}{1,2}(1)^2+DataMtx{2,j}{1,2}(1)^2);
AccumStretches(3,j)=PAccStretch; % Theoretical Stretch in 3rd row

end
end
ThruDistrib=1;

% This while loop applies the strength distribution
while PAccStretch>Distrib(1,1)

% Adds number of particles for that strength
BrokeCount=BrokeCount+Distrib(2,1);
ThruDistrib=ThruDistrib+1;
% Exit loop if you’ve counted all the particles
if ThruDistrib==20
    if PAccStretch>Distrib(1,20)
% Adds number of particles for that last portion
        BrokeCount=BrokeCount+Distrib(2,20);
    end
    PAccStretch=0.000001;
end
end

PAccStretch=0;
end
remv=1;
% Eliminate zeroes, (P’s that didn’t get thru orif), check all P’s
while (remv-1)<numel(AccumStretches(1,:))
% As long as there’s some stretch value, carry on to next P
    if AccumStretches(3,remv)>0
        remv=remv+1;
    % If the stretch is zero, remove that column, don’t update remv
end

end
elseif AccumStretches(3,remv)==0
  %cause next column will have taken that index, needs checking
  AccumStretches(:,remv)=[];

end
end

Tot=(remv-1)*100; %Total number of particles in consideration

fprintf('%s %4f %2d
', Code, BrokeCount/Tot, ThreshDiv);

%fprintf('%s %d/%d = %4f for %2d %2d
', Code, BrokeCount, Tot, BrokeCount/Tot, PDiam*1000000, ThreshDiv);

edges=0:Div:Highest;
Sections=histc(AccumStretches(3,:),edges); %Sort total stretches into bins (cell 'Sections')

Breakdown=zeros(3,Highest/Div+1); %Place into Mtx 'Breakdown' the following:

Breakdown(1,1)=edges(1); %Deal with First Bin
Breakdown(2,1)=Sections(1);
Breakdown(3,1)=Sections(1)/Tot;
for i=2:1:Highest/Div+1
  Breakdown(1,i)=edges(i); %Row 1: Bin Name
  %Row 2: Number of Particles Belonging to Bin
  Breakdown(2,i)=Sections(i)+Breakdown(2,i-1);
  %Row 3: Percentage of total particles in Bin
  Breakdown(3,i)=Sections(i)/Tot+Breakdown(3,i-1);
end

%scatter(Breakdown(1,:),Breakdown(3,:),75,'filled')
%scatter(AccumStretches(2,:),AccumStretches(3,:),8,'filled')
%toc

A2 – Breakage Calculation

%tic
str=sprintf('RawVoerP.txt'); %File name

fid=fopen(str);
DataMtx2=cell(6, 15);
for a=1:12
  DataMtx2{1,a}=textscan(fid, '%35c 
'); %Scan Case Name
  DataMtx2{2,a}=textscan(fid, '%f'); %Scan Data
end
fclose(fid);

for a=1:12
  count=1;
  ...
TotPcount=442;
if a>9; TotPcount=814; end
while DataMtx2(2,a){1,1}(count)~=TotPcount %Loop to count # of particles not removed
    count=count+1;
end
Start=count*2+1;
End=Start+count-1;
for r=Start:End
    jumpback=r-(count*2);
    DataMtx2{3,a}{1,1}(jumpback)=DataMtx2{2,a}{1,1}(r);
end
end
PI=3.14159;
ThreshDiv=.02;
%Case=1;%Weak
Case=2; %Firm
if Case==2; amax=12; elseif Case==1; amax=9; end
Distrib=zeros(3,4010);
DataMt=zeros(9,amax);
DataMt(1,:)=1:amax;
if Case==1
    DataMt(2,:)= [8864 26593 35458 10506 23638 2216 4432 8864 15513];
    A=1.142; b=6608;
    DataMt(5,:)= A .* DataMt(2,:) ./ (b + DataMt(2,:));
    DataMt(6,:)= A .* DataMt(2,:) ./ (b + DataMt(2,:));
elseif Case==2
    DataMt(2,:)= [8864 26593 35458 10506 23638 2216 4432 8864 15513 7879 20487 23638];
    %DataMt(6,:)= 0.000034565 .* DataMt(2,:) - 0.11100;   %Single-Orifice Eq'n
    DataMt(5,:)= 0.000034565 .* DataMt(2,:) - 0.11100;   %Single-Orifice Eq'n
    DataMt(6,:)= 0.0000241757 .* DataMt(2,:) - 0.25834;   %Multi-Orifice Eq'n
end
mew=22;%515;
sigma=7;%36500;
% %mew=11.4;%11.45;%10;%9.6;% 11.2;%10;%11.5;
%sigma=.2;%0.15;%1.2;%1.1;% .1;%0.2;
IdealSSE=101;
%mew=5.9;
%sigma=3.3;
%mew=0.5;
%sigma=.4;
for mew=7:.10000:10.000;
for sigma=3.000:.2000:6.000;
    for s=1:4000;
        Distrib(1,s+1)=s*ThreshDiv;
        if (s*ThreshDiv)<=mew; if mew<((s+1)*ThreshDiv);
            Distrib(3,s+1)=1; end; end
        if (s*ThreshDiv)>mew;
            Distrib(3,s+1)=1/(sqrt(2*PI)*sigma)*exp((-1*((s*ThreshDiv)-mew)^2)/2/sigma^2);
        end
    end
    AreaUnd=sum(Distrib(3,:));
    for j=0:4000;
        Distrib(2,j+1)=(Distrib(3,j+1)/AreaUnd);
    end
end
for a=1:amax
    %BrokeCount=0;
    for m=1:numel(DataMtx2{3,a}{1,1}) %Loop through each of the hundreds of paths
        PAccStretch=DataMtx2{3,a}{1,1}(m);
        %BrokeCount=BrokeCount+(Distrib(2,1));
        BK=0;
        for ThruDistrib=2:3999
            if PAccStretch>Distrib(1,ThruDistrib) %This while loop applies the strength distribution
                BK=BK+(Distrib(2,ThruDistrib));
            end
        end
        DataMtx2{5,a}{1,1}(m)=BK;
    end
end
DataMt(8,a)=mean(DataMtx2{5,a}{1,1}(:));
%DataMt(4,a)=BrokeCount/numel(DataMtx2{3,a}{1,1})/sum(Distrib(2,:));
end
for a=1:amax
    for b=5:9
        if DataMt(b,a)<0
            DataMt(b,a)=0;
        elseif DataMt(b,a)>1
            DataMt(b,a)=1;
        end
    end
end
ErrorVector=zeros(1,12);
ErrorVector2=zeros(1,12);

for a=1:9; ErrorVector(1,a) = (DataMt(8,a) - DataMt(5,a)); end;
if Case==2; for a=10:12; ErrorVector2(1,a)=(DataMt(8,a)- DataMt(6,a)); end; end;
sse = sum(ErrorVector .^ 2 + 3*(ErrorVector2 .^ 2));

if sse<IdealSSE
    IdealSSE=sse;
    IdealMEW=mew;
    IdealSIG=sigma;

    DataMt(7,:)=DataMt(8,:);
end

end
end
Appendix B - Experimental Standard Operating Procedure

Preparation of test:
- Insert appropriate orifice plate, wrench into place
- Close Valve 5 on air inlet
- Open Main air, adjust Regulator as required
- Fill 260 L tank with water
- Open Valves 2, 3, 4
- Close Valve 7
- Place dirty bucket under Pipe bottom

- Start pump, allowing top portion to fill with water
- Close/Adjust Valve 1 as required
- When top portion is half full,
  - Open Valves 6, 7
  - Allow water into Particle Concentrate Vessel
  - Close Valve 7 when water Particle Concentrate Vessel has filled to 1/3
- When system full, Vent air bubbles through Valve 2,
  - Close Valve 2
- Close Valve 6
- Open Valve 7
- Adjust Regulator to achieve desired injection pressure
- Close Valves 7, 5
- Turn off pump

- Empty dirty bucket, place under Pipe bottom
- Collect mixed liquor at wastewater treatment plant
- Sieve
  - Sieve through appropriate screens
  - Wash thoroughly
  - Collect off desired size fraction
  - Check particle size with multisizer
  - Check number of particles per millilitre from multisizer
  - Establish volume of particles per millilitre of water from multisizer
  - Dilute to final injection concentration (50,000 particles/mL, [300mL, 4 min injection])
- Open Valve 6
- Put mixture in place for injection
- Close Valve 6
- Turn on stirring of Particle Concentrate Vessel
- Open Valve 5 to pressurize

**Actual Run**
- Turn on Pump
- Adjust Valve 1 to achieve desired pressure drop
- Measure flow rate at Pipe Bottom with stopwatch and graduated cylinder
- Once steady flow established
  - Open Valve 7 to inject particle solution
  - Adjust Regulator as required to ensure air flow is correct
- Wait for particles to enter pipe system and reach steady state
- Collect samples in 250 mL bottles

**Clean System**
- Flush with water with no injection
- Turn off Main Air
- Flush Injector
  - Open Valve 6
  - Fill Injector with water
  - Close Valve 6
  - Open Valve 7 to flush
  - Repeat 2-3 times as required
- Close Valve 7
- Turn off pump
- Open Valve 2
- Remove Tube from Injector bottom
- Wait for Pipe to drain
- Empty buckets of unwanted water
- Remove orifice and wash components

**Analysis**
- Measure breakage with multisizer (Volume fraction of particles within 53-75 micron range vs number at start)